



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 10:29 PM BST

PDB ID : 4V81
Title : The crystal structure of yeast CCT reveals intrinsic asymmetry of eukaryotic cytosolic chaperonins
Authors : Dekker, C.; Roe, S.M.; McCormack, E.A.; Beuron, F.; Pearl, L.H.; Willison, K.R.
Deposited on : 2010-10-17
Resolution : 3.80 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

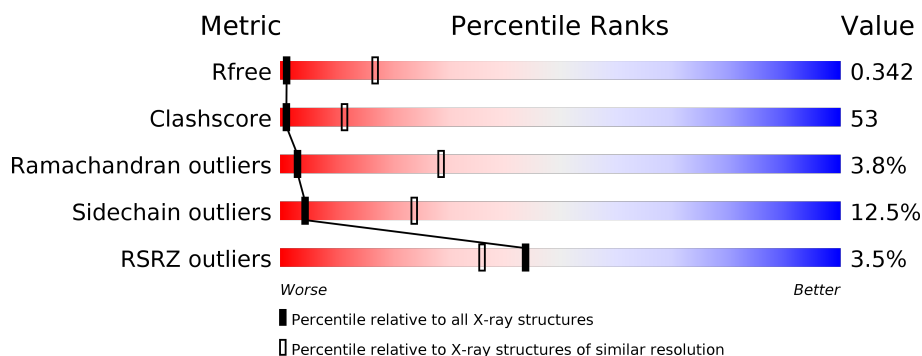
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 130704 | 1212 (4.00-3.60) |
| Clashscore | 141614 | 1288 (4.00-3.60) |
| Ramachandran outliers | 138981 | 1243 (4.00-3.60) |
| Sidechain outliers | 138945 | 1237 (4.00-3.60) |
| RSRZ outliers | 127900 | 1121 (4.00-3.60) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | A | 559 | <div> <div>2%</div> <div>52% 39% 6%</div> </div> |
| 1 | I | 559 | <div> <div>5%</div> <div>53% 38% 6%</div> </div> |
| 1 | a | 559 | <div> <div>3%</div> <div>89% 8%</div> </div> |
| 1 | i | 559 | <div> <div>3%</div> <div>89% 8%</div> </div> |
| 2 | B | 527 | <div> <div>%</div> <div>36% 49% 11%</div> </div> |
| 2 | J | 527 | <div> <div>3%</div> <div>34% 51% 12%</div> </div> |


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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2 | b | 527 | |
| 2 | j | 527 | |
| 3 | C | 590 | |
| 3 | K | 590 | |
| 3 | c | 590 | |
| 3 | k | 590 | |
| 4 | D | 528 | |
| 4 | L | 528 | |
| 4 | d | 528 | |
| 4 | l | 528 | |
| 5 | E | 562 | |
| 5 | M | 562 | |
| 5 | e | 562 | |
| 5 | m | 562 | |
| 6 | F | 546 | |
| 6 | N | 546 | |
| 6 | f | 546 | |
| 6 | n | 546 | |
| 7 | G | 550 | |
| 7 | O | 550 | |
| 7 | g | 550 | |
| 7 | o | 550 | |
| 8 | H | 568 | |
| 8 | P | 568 | |
| 8 | h | 568 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 8 | p | 568 |  |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 10 | BEF | C | 1102 | - | - | X | - |
| 10 | BEF | F | 602 | - | - | X | - |
| 10 | BEF | N | 602 | - | - | X | - |
| 9 | ADP | A | 601 | X | - | - | - |
| 9 | ADP | B | 601 | X | - | - | - |
| 9 | ADP | C | 1101 | X | - | - | - |
| 9 | ADP | D | 601 | X | - | - | - |
| 9 | ADP | E | 601 | X | - | - | - |
| 9 | ADP | G | 601 | X | - | - | - |
| 9 | ADP | H | 601 | X | - | - | - |
| 9 | ADP | J | 601 | X | - | - | - |
| 9 | ADP | M | 601 | X | - | - | - |
| 9 | ADP | N | 601 | X | - | - | - |
| 9 | ADP | P | 601 | X | - | - | - |
| 9 | ADP | a | 1601 | X | - | - | - |
| 9 | ADP | b | 1601 | X | - | - | - |
| 9 | ADP | e | 1601 | X | - | - | - |
| 9 | ADP | f | 1601 | X | - | - | - |
| 9 | ADP | g | 1601 | X | - | - | - |
| 9 | ADP | h | 1601 | X | - | - | - |
| 9 | ADP | k | 2101 | X | - | - | - |
| 9 | ADP | m | 1601 | X | - | - | - |
| 9 | ADP | n | 1601 | X | - | - | - |
| 9 | ADP | p | 1601 | X | - | - | - |

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 111235 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 T-complex protein 1 subunit alpha.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | A | 544 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3492 | 2146 | 600 | 732 | 14 | | | |
| 1 | I | 544 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3492 | 2146 | 600 | 732 | 14 | | | |
| 1 | a | 544 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3492 | 2146 | 600 | 732 | 14 | | | |
| 1 | i | 544 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3492 | 2146 | 600 | 732 | 14 | | | |

- Molecule 2 is a protein called T-complex protein 1 subunit beta.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2 | B | 513 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3459 | 2125 | 597 | 728 | 9 | | | |
| 2 | J | 513 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3459 | 2125 | 597 | 728 | 9 | | | |
| 2 | b | 513 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3460 | 2126 | 597 | 728 | 9 | | | |
| 2 | j | 513 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3457 | 2123 | 597 | 728 | 9 | | | |

- Molecule 3 is a protein called T-complex protein 1 subunit gamma.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 3 | C | 514 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3392 | 2104 | 590 | 685 | 13 | | | |
| 3 | K | 514 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3393 | 2104 | 590 | 685 | 14 | | | |
| 3 | c | 514 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3395 | 2106 | 590 | 685 | 14 | | | |
| 3 | k | 514 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3395 | 2106 | 590 | 685 | 14 | | | |

There are 224 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| C | 1001 | GLY | - | SEE REMARK 999 | UNP P39077 |
| C | 1002 | SER | - | SEE REMARK 999 | UNP P39077 |
| C | 1003 | GLY | - | SEE REMARK 999 | UNP P39077 |
| C | 1004 | SER | - | SEE REMARK 999 | UNP P39077 |
| C | 1005 | GLY | - | SEE REMARK 999 | UNP P39077 |
| C | 1006 | TRP | - | SEE REMARK 999 | UNP P39077 |
| C | 1007 | SER | - | SEE REMARK 999 | UNP P39077 |
| C | 1008 | HIS | - | SEE REMARK 999 | UNP P39077 |
| C | 1009 | PRO | - | SEE REMARK 999 | UNP P39077 |
| C | 1010 | GLN | - | SEE REMARK 999 | UNP P39077 |
| C | 1011 | PHE | - | SEE REMARK 999 | UNP P39077 |
| C | 1012 | GLU | - | SEE REMARK 999 | UNP P39077 |
| C | 1013 | LYS | - | SEE REMARK 999 | UNP P39077 |
| C | 1014 | GLY | - | SEE REMARK 999 | UNP P39077 |
| C | 1015 | SER | - | SEE REMARK 999 | UNP P39077 |
| C | 1016 | GLY | - | SEE REMARK 999 | UNP P39077 |
| C | 1017 | LYS | - | SEE REMARK 999 | UNP P39077 |
| C | 1018 | ARG | - | SEE REMARK 999 | UNP P39077 |
| C | 1019 | ARG | - | SEE REMARK 999 | UNP P39077 |
| C | 1020 | TRP | - | SEE REMARK 999 | UNP P39077 |
| C | 1021 | LYS | - | SEE REMARK 999 | UNP P39077 |
| C | 1022 | LYS | - | SEE REMARK 999 | UNP P39077 |
| C | 1023 | ASN | - | SEE REMARK 999 | UNP P39077 |
| C | 1024 | PHE | - | SEE REMARK 999 | UNP P39077 |
| C | 1025 | ILE | - | SEE REMARK 999 | UNP P39077 |
| C | 1026 | ALA | - | SEE REMARK 999 | UNP P39077 |
| C | 1027 | VAL | - | SEE REMARK 999 | UNP P39077 |
| C | 1028 | SER | - | SEE REMARK 999 | UNP P39077 |
| C | 1029 | ALA | - | SEE REMARK 999 | UNP P39077 |
| C | 1030 | ALA | - | SEE REMARK 999 | UNP P39077 |
| C | 1031 | ASN | - | SEE REMARK 999 | UNP P39077 |
| C | 1032 | ARG | - | SEE REMARK 999 | UNP P39077 |
| C | 1033 | PHE | - | SEE REMARK 999 | UNP P39077 |
| C | 1034 | LYS | - | SEE REMARK 999 | UNP P39077 |
| C | 1035 | LYS | - | SEE REMARK 999 | UNP P39077 |
| C | 1036 | ILE | - | SEE REMARK 999 | UNP P39077 |
| C | 1037 | SER | - | SEE REMARK 999 | UNP P39077 |
| C | 1038 | SER | - | SEE REMARK 999 | UNP P39077 |
| C | 1039 | SER | - | SEE REMARK 999 | UNP P39077 |
| C | 1040 | GLY | - | SEE REMARK 999 | UNP P39077 |
| C | 1041 | ALA | - | SEE REMARK 999 | UNP P39077 |
| C | 1042 | LEU | - | SEE REMARK 999 | UNP P39077 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| C | 1043 | GLY | - | SEE REMARK 999 | UNP P39077 |
| C | 1044 | SER | - | SEE REMARK 999 | UNP P39077 |
| C | 1045 | GLY | - | SEE REMARK 999 | UNP P39077 |
| C | 1046 | HIS | - | SEE REMARK 999 | UNP P39077 |
| C | 1047 | HIS | - | SEE REMARK 999 | UNP P39077 |
| C | 1048 | HIS | - | SEE REMARK 999 | UNP P39077 |
| C | 1049 | HIS | - | SEE REMARK 999 | UNP P39077 |
| C | 1050 | HIS | - | SEE REMARK 999 | UNP P39077 |
| C | 1051 | HIS | - | SEE REMARK 999 | UNP P39077 |
| C | 1052 | HIS | - | SEE REMARK 999 | UNP P39077 |
| C | 1053 | HIS | - | SEE REMARK 999 | UNP P39077 |
| C | 1054 | GLY | - | SEE REMARK 999 | UNP P39077 |
| C | 1055 | SER | - | SEE REMARK 999 | UNP P39077 |
| C | 1056 | GLY | - | SEE REMARK 999 | UNP P39077 |
| K | 1001 | GLY | - | SEE REMARK 999 | UNP P39077 |
| K | 1002 | SER | - | SEE REMARK 999 | UNP P39077 |
| K | 1003 | GLY | - | SEE REMARK 999 | UNP P39077 |
| K | 1004 | SER | - | SEE REMARK 999 | UNP P39077 |
| K | 1005 | GLY | - | SEE REMARK 999 | UNP P39077 |
| K | 1006 | TRP | - | SEE REMARK 999 | UNP P39077 |
| K | 1007 | SER | - | SEE REMARK 999 | UNP P39077 |
| K | 1008 | HIS | - | SEE REMARK 999 | UNP P39077 |
| K | 1009 | PRO | - | SEE REMARK 999 | UNP P39077 |
| K | 1010 | GLN | - | SEE REMARK 999 | UNP P39077 |
| K | 1011 | PHE | - | SEE REMARK 999 | UNP P39077 |
| K | 1012 | GLU | - | SEE REMARK 999 | UNP P39077 |
| K | 1013 | LYS | - | SEE REMARK 999 | UNP P39077 |
| K | 1014 | GLY | - | SEE REMARK 999 | UNP P39077 |
| K | 1015 | SER | - | SEE REMARK 999 | UNP P39077 |
| K | 1016 | GLY | - | SEE REMARK 999 | UNP P39077 |
| K | 1017 | LYS | - | SEE REMARK 999 | UNP P39077 |
| K | 1018 | ARG | - | SEE REMARK 999 | UNP P39077 |
| K | 1019 | ARG | - | SEE REMARK 999 | UNP P39077 |
| K | 1020 | TRP | - | SEE REMARK 999 | UNP P39077 |
| K | 1021 | LYS | - | SEE REMARK 999 | UNP P39077 |
| K | 1022 | LYS | - | SEE REMARK 999 | UNP P39077 |
| K | 1023 | ASN | - | SEE REMARK 999 | UNP P39077 |
| K | 1024 | PHE | - | SEE REMARK 999 | UNP P39077 |
| K | 1025 | ILE | - | SEE REMARK 999 | UNP P39077 |
| K | 1026 | ALA | - | SEE REMARK 999 | UNP P39077 |
| K | 1027 | VAL | - | SEE REMARK 999 | UNP P39077 |
| K | 1028 | SER | - | SEE REMARK 999 | UNP P39077 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| K | 1029 | ALA | - | SEE REMARK 999 | UNP P39077 |
| K | 1030 | ALA | - | SEE REMARK 999 | UNP P39077 |
| K | 1031 | ASN | - | SEE REMARK 999 | UNP P39077 |
| K | 1032 | ARG | - | SEE REMARK 999 | UNP P39077 |
| K | 1033 | PHE | - | SEE REMARK 999 | UNP P39077 |
| K | 1034 | LYS | - | SEE REMARK 999 | UNP P39077 |
| K | 1035 | LYS | - | SEE REMARK 999 | UNP P39077 |
| K | 1036 | ILE | - | SEE REMARK 999 | UNP P39077 |
| K | 1037 | SER | - | SEE REMARK 999 | UNP P39077 |
| K | 1038 | SER | - | SEE REMARK 999 | UNP P39077 |
| K | 1039 | SER | - | SEE REMARK 999 | UNP P39077 |
| K | 1040 | GLY | - | SEE REMARK 999 | UNP P39077 |
| K | 1041 | ALA | - | SEE REMARK 999 | UNP P39077 |
| K | 1042 | LEU | - | SEE REMARK 999 | UNP P39077 |
| K | 1043 | GLY | - | SEE REMARK 999 | UNP P39077 |
| K | 1044 | SER | - | SEE REMARK 999 | UNP P39077 |
| K | 1045 | GLY | - | SEE REMARK 999 | UNP P39077 |
| K | 1046 | HIS | - | SEE REMARK 999 | UNP P39077 |
| K | 1047 | HIS | - | SEE REMARK 999 | UNP P39077 |
| K | 1048 | HIS | - | SEE REMARK 999 | UNP P39077 |
| K | 1049 | HIS | - | SEE REMARK 999 | UNP P39077 |
| K | 1050 | HIS | - | SEE REMARK 999 | UNP P39077 |
| K | 1051 | HIS | - | SEE REMARK 999 | UNP P39077 |
| K | 1052 | HIS | - | SEE REMARK 999 | UNP P39077 |
| K | 1053 | HIS | - | SEE REMARK 999 | UNP P39077 |
| K | 1054 | GLY | - | SEE REMARK 999 | UNP P39077 |
| K | 1055 | SER | - | SEE REMARK 999 | UNP P39077 |
| K | 1056 | GLY | - | SEE REMARK 999 | UNP P39077 |
| c | 2001 | GLY | - | SEE REMARK 999 | UNP P39077 |
| c | 2002 | SER | - | SEE REMARK 999 | UNP P39077 |
| c | 2003 | GLY | - | SEE REMARK 999 | UNP P39077 |
| c | 2004 | SER | - | SEE REMARK 999 | UNP P39077 |
| c | 2005 | GLY | - | SEE REMARK 999 | UNP P39077 |
| c | 2006 | TRP | - | SEE REMARK 999 | UNP P39077 |
| c | 2007 | SER | - | SEE REMARK 999 | UNP P39077 |
| c | 2008 | HIS | - | SEE REMARK 999 | UNP P39077 |
| c | 2009 | PRO | - | SEE REMARK 999 | UNP P39077 |
| c | 2010 | GLN | - | SEE REMARK 999 | UNP P39077 |
| c | 2011 | PHE | - | SEE REMARK 999 | UNP P39077 |
| c | 2012 | GLU | - | SEE REMARK 999 | UNP P39077 |
| c | 2013 | LYS | - | SEE REMARK 999 | UNP P39077 |
| c | 2014 | GLY | - | SEE REMARK 999 | UNP P39077 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| c | 2015 | SER | - | SEE REMARK 999 | UNP P39077 |
| c | 2016 | GLY | - | SEE REMARK 999 | UNP P39077 |
| c | 2017 | LYS | - | SEE REMARK 999 | UNP P39077 |
| c | 2018 | ARG | - | SEE REMARK 999 | UNP P39077 |
| c | 2019 | ARG | - | SEE REMARK 999 | UNP P39077 |
| c | 2020 | TRP | - | SEE REMARK 999 | UNP P39077 |
| c | 2021 | LYS | - | SEE REMARK 999 | UNP P39077 |
| c | 2022 | LYS | - | SEE REMARK 999 | UNP P39077 |
| c | 2023 | ASN | - | SEE REMARK 999 | UNP P39077 |
| c | 2024 | PHE | - | SEE REMARK 999 | UNP P39077 |
| c | 2025 | ILE | - | SEE REMARK 999 | UNP P39077 |
| c | 2026 | ALA | - | SEE REMARK 999 | UNP P39077 |
| c | 2027 | VAL | - | SEE REMARK 999 | UNP P39077 |
| c | 2028 | SER | - | SEE REMARK 999 | UNP P39077 |
| c | 2029 | ALA | - | SEE REMARK 999 | UNP P39077 |
| c | 2030 | ALA | - | SEE REMARK 999 | UNP P39077 |
| c | 2031 | ASN | - | SEE REMARK 999 | UNP P39077 |
| c | 2032 | ARG | - | SEE REMARK 999 | UNP P39077 |
| c | 2033 | PHE | - | SEE REMARK 999 | UNP P39077 |
| c | 2034 | LYS | - | SEE REMARK 999 | UNP P39077 |
| c | 2035 | LYS | - | SEE REMARK 999 | UNP P39077 |
| c | 2036 | ILE | - | SEE REMARK 999 | UNP P39077 |
| c | 2037 | SER | - | SEE REMARK 999 | UNP P39077 |
| c | 2038 | SER | - | SEE REMARK 999 | UNP P39077 |
| c | 2039 | SER | - | SEE REMARK 999 | UNP P39077 |
| c | 2040 | GLY | - | SEE REMARK 999 | UNP P39077 |
| c | 2041 | ALA | - | SEE REMARK 999 | UNP P39077 |
| c | 2042 | LEU | - | SEE REMARK 999 | UNP P39077 |
| c | 2043 | GLY | - | SEE REMARK 999 | UNP P39077 |
| c | 2044 | SER | - | SEE REMARK 999 | UNP P39077 |
| c | 2045 | GLY | - | SEE REMARK 999 | UNP P39077 |
| c | 2046 | HIS | - | SEE REMARK 999 | UNP P39077 |
| c | 2047 | HIS | - | SEE REMARK 999 | UNP P39077 |
| c | 2048 | HIS | - | SEE REMARK 999 | UNP P39077 |
| c | 2049 | HIS | - | SEE REMARK 999 | UNP P39077 |
| c | 2050 | HIS | - | SEE REMARK 999 | UNP P39077 |
| c | 2051 | HIS | - | SEE REMARK 999 | UNP P39077 |
| c | 2052 | HIS | - | SEE REMARK 999 | UNP P39077 |
| c | 2053 | HIS | - | SEE REMARK 999 | UNP P39077 |
| c | 2054 | GLY | - | SEE REMARK 999 | UNP P39077 |
| c | 2055 | SER | - | SEE REMARK 999 | UNP P39077 |
| c | 2056 | GLY | - | SEE REMARK 999 | UNP P39077 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| k | 2001 | GLY | - | SEE REMARK 999 | UNP P39077 |
| k | 2002 | SER | - | SEE REMARK 999 | UNP P39077 |
| k | 2003 | GLY | - | SEE REMARK 999 | UNP P39077 |
| k | 2004 | SER | - | SEE REMARK 999 | UNP P39077 |
| k | 2005 | GLY | - | SEE REMARK 999 | UNP P39077 |
| k | 2006 | TRP | - | SEE REMARK 999 | UNP P39077 |
| k | 2007 | SER | - | SEE REMARK 999 | UNP P39077 |
| k | 2008 | HIS | - | SEE REMARK 999 | UNP P39077 |
| k | 2009 | PRO | - | SEE REMARK 999 | UNP P39077 |
| k | 2010 | GLN | - | SEE REMARK 999 | UNP P39077 |
| k | 2011 | PHE | - | SEE REMARK 999 | UNP P39077 |
| k | 2012 | GLU | - | SEE REMARK 999 | UNP P39077 |
| k | 2013 | LYS | - | SEE REMARK 999 | UNP P39077 |
| k | 2014 | GLY | - | SEE REMARK 999 | UNP P39077 |
| k | 2015 | SER | - | SEE REMARK 999 | UNP P39077 |
| k | 2016 | GLY | - | SEE REMARK 999 | UNP P39077 |
| k | 2017 | LYS | - | SEE REMARK 999 | UNP P39077 |
| k | 2018 | ARG | - | SEE REMARK 999 | UNP P39077 |
| k | 2019 | ARG | - | SEE REMARK 999 | UNP P39077 |
| k | 2020 | TRP | - | SEE REMARK 999 | UNP P39077 |
| k | 2021 | LYS | - | SEE REMARK 999 | UNP P39077 |
| k | 2022 | LYS | - | SEE REMARK 999 | UNP P39077 |
| k | 2023 | ASN | - | SEE REMARK 999 | UNP P39077 |
| k | 2024 | PHE | - | SEE REMARK 999 | UNP P39077 |
| k | 2025 | ILE | - | SEE REMARK 999 | UNP P39077 |
| k | 2026 | ALA | - | SEE REMARK 999 | UNP P39077 |
| k | 2027 | VAL | - | SEE REMARK 999 | UNP P39077 |
| k | 2028 | SER | - | SEE REMARK 999 | UNP P39077 |
| k | 2029 | ALA | - | SEE REMARK 999 | UNP P39077 |
| k | 2030 | ALA | - | SEE REMARK 999 | UNP P39077 |
| k | 2031 | ASN | - | SEE REMARK 999 | UNP P39077 |
| k | 2032 | ARG | - | SEE REMARK 999 | UNP P39077 |
| k | 2033 | PHE | - | SEE REMARK 999 | UNP P39077 |
| k | 2034 | LYS | - | SEE REMARK 999 | UNP P39077 |
| k | 2035 | LYS | - | SEE REMARK 999 | UNP P39077 |
| k | 2036 | ILE | - | SEE REMARK 999 | UNP P39077 |
| k | 2037 | SER | - | SEE REMARK 999 | UNP P39077 |
| k | 2038 | SER | - | SEE REMARK 999 | UNP P39077 |
| k | 2039 | SER | - | SEE REMARK 999 | UNP P39077 |
| k | 2040 | GLY | - | SEE REMARK 999 | UNP P39077 |
| k | 2041 | ALA | - | SEE REMARK 999 | UNP P39077 |
| k | 2042 | LEU | - | SEE REMARK 999 | UNP P39077 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| k | 2043 | GLY | - | SEE REMARK 999 | UNP P39077 |
| k | 2044 | SER | - | SEE REMARK 999 | UNP P39077 |
| k | 2045 | GLY | - | SEE REMARK 999 | UNP P39077 |
| k | 2046 | HIS | - | SEE REMARK 999 | UNP P39077 |
| k | 2047 | HIS | - | SEE REMARK 999 | UNP P39077 |
| k | 2048 | HIS | - | SEE REMARK 999 | UNP P39077 |
| k | 2049 | HIS | - | SEE REMARK 999 | UNP P39077 |
| k | 2050 | HIS | - | SEE REMARK 999 | UNP P39077 |
| k | 2051 | HIS | - | SEE REMARK 999 | UNP P39077 |
| k | 2052 | HIS | - | SEE REMARK 999 | UNP P39077 |
| k | 2053 | HIS | - | SEE REMARK 999 | UNP P39077 |
| k | 2054 | GLY | - | SEE REMARK 999 | UNP P39077 |
| k | 2055 | SER | - | SEE REMARK 999 | UNP P39077 |
| k | 2056 | GLY | - | SEE REMARK 999 | UNP P39077 |

- Molecule 4 is a protein called T-complex protein 1 subunit delta.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 4 | D | 522 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3398 | 2092 | 609 | 686 | 11 | | | |
| 4 | L | 522 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3398 | 2092 | 609 | 686 | 11 | | | |
| 4 | d | 522 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3398 | 2092 | 609 | 686 | 11 | | | |
| 4 | l | 522 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3398 | 2092 | 609 | 686 | 11 | | | |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------------------|------------|
| D | 345 | ASP | GLY | ENGINEERED MUTATION | UNP P39078 |
| L | 345 | ASP | GLY | ENGINEERED MUTATION | UNP P39078 |
| d | 1345 | ASP | GLY | ENGINEERED MUTATION | UNP P39078 |
| l | 1345 | ASP | GLY | ENGINEERED MUTATION | UNP P39078 |

- Molecule 5 is a protein called T-complex protein 1 subunit epsilon.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5 | E | 525 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3437 | 2110 | 599 | 720 | 8 | | | |
| 5 | M | 525 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3437 | 2110 | 599 | 720 | 8 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5 | e | 525 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3437 | 2110 | 599 | 720 | 8 | | | |
| 5 | m | 525 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3437 | 2110 | 599 | 720 | 8 | | | |

- Molecule 6 is a protein called T-complex protein 1 subunit zeta.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 6 | F | 533 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3631 | 2253 | 629 | 740 | 9 | | | |
| 6 | N | 533 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3628 | 2250 | 629 | 740 | 9 | | | |
| 6 | f | 533 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3633 | 2255 | 630 | 739 | 9 | | | |
| 6 | n | 533 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3629 | 2252 | 629 | 739 | 9 | | | |

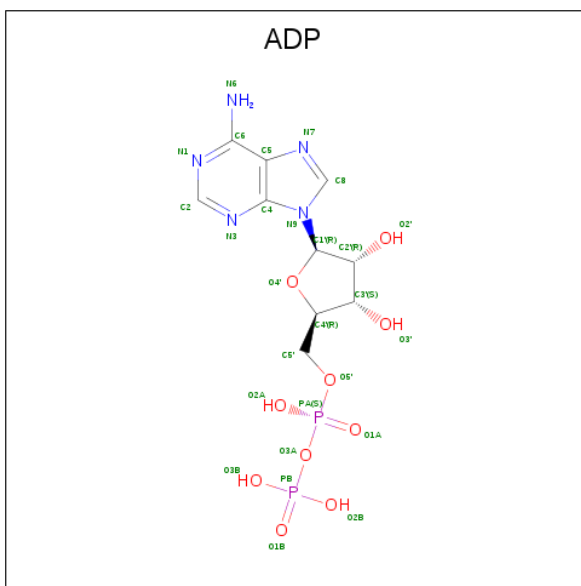
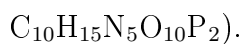
- Molecule 7 is a protein called T-complex protein 1 subunit eta.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 7 | G | 509 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3317 | 2055 | 583 | 669 | 10 | | | |
| 7 | O | 509 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3314 | 2052 | 583 | 669 | 10 | | | |
| 7 | g | 509 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3314 | 2052 | 583 | 669 | 10 | | | |
| 7 | o | 509 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3314 | 2052 | 583 | 669 | 10 | | | |

- Molecule 8 is a protein called T-complex protein 1 subunit theta.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 8 | H | 525 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3487 | 2161 | 608 | 705 | 13 | | | |
| 8 | P | 525 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3487 | 2161 | 608 | 705 | 13 | | | |
| 8 | h | 525 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3485 | 2159 | 608 | 705 | 13 | | | |
| 8 | p | 525 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3487 | 2161 | 608 | 705 | 13 | | | |

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:



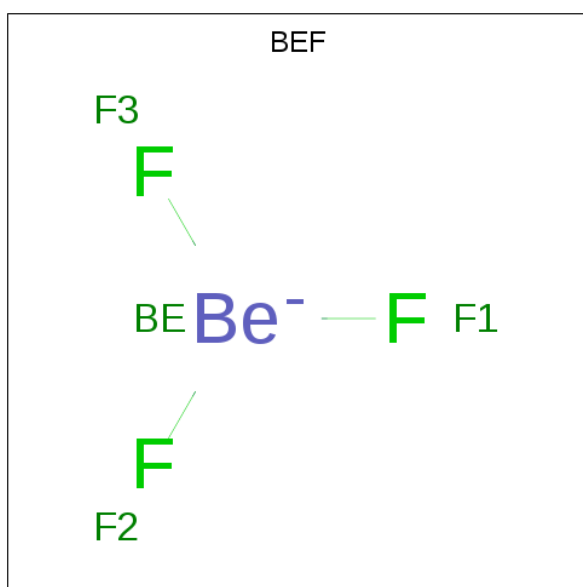
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|---------|
| 9 | A | 1 | Total 27 | C 10 | N 5 | O 10 | P 2 | 0 | 0 |
| 9 | B | 1 | Total 27 | C 10 | N 5 | O 10 | P 2 | 0 | 0 |
| 9 | C | 1 | Total 27 | C 10 | N 5 | O 10 | P 2 | 0 | 0 |
| 9 | D | 1 | Total 27 | C 10 | N 5 | O 10 | P 2 | 0 | 0 |
| 9 | E | 1 | Total 27 | C 10 | N 5 | O 10 | P 2 | 0 | 0 |
| 9 | F | 1 | Total 27 | C 10 | N 5 | O 10 | P 2 | 0 | 0 |
| 9 | G | 1 | Total 27 | C 10 | N 5 | O 10 | P 2 | 0 | 0 |
| 9 | H | 1 | Total 27 | C 10 | N 5 | O 10 | P 2 | 0 | 0 |
| 9 | J | 1 | Total 27 | C 10 | N 5 | O 10 | P 2 | 0 | 0 |
| 9 | L | 1 | Total 27 | C 10 | N 5 | O 10 | P 2 | 0 | 0 |
| 9 | M | 1 | Total 27 | C 10 | N 5 | O 10 | P 2 | 0 | 0 |
| 9 | N | 1 | Total 27 | C 10 | N 5 | O 10 | P 2 | 0 | 0 |
| 9 | P | 1 | Total 27 | C 10 | N 5 | O 10 | P 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 9 | a | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 9 | b | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 9 | e | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 9 | f | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 9 | g | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 9 | h | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 9 | k | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 9 | l | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 9 | m | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 9 | n | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 9 | p | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |

- Molecule 10 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF₃).



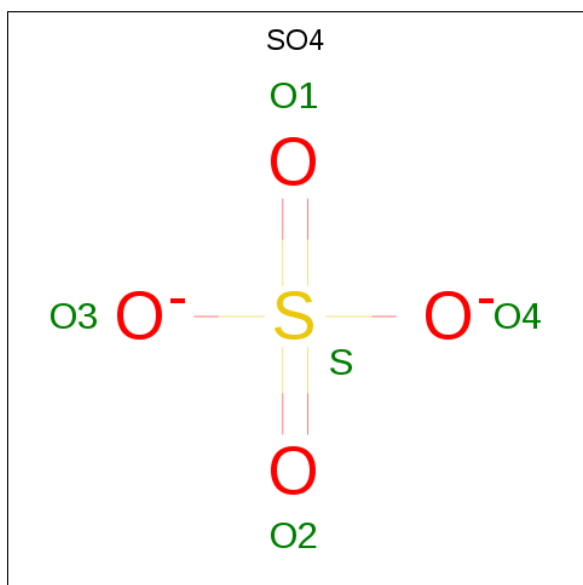
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|--------|---------|---------|
| 10 | A | 1 | Total 4 | Be 1 | F 3 | 0 | 0 |
| 10 | B | 1 | Total 4 | Be 1 | F 3 | 0 | 0 |
| 10 | C | 1 | Total 4 | Be 1 | F 3 | 0 | 0 |
| 10 | D | 1 | Total 4 | Be 1 | F 3 | 0 | 0 |
| 10 | E | 1 | Total 4 | Be 1 | F 3 | 0 | 0 |
| 10 | F | 1 | Total 4 | Be 1 | F 3 | 0 | 0 |
| 10 | G | 1 | Total 4 | Be 1 | F 3 | 0 | 0 |
| 10 | H | 1 | Total 4 | Be 1 | F 3 | 0 | 0 |
| 10 | J | 1 | Total 4 | Be 1 | F 3 | 0 | 0 |
| 10 | L | 1 | Total 4 | Be 1 | F 3 | 0 | 0 |
| 10 | M | 1 | Total 4 | Be 1 | F 3 | 0 | 0 |
| 10 | N | 1 | Total 4 | Be 1 | F 3 | 0 | 0 |
| 10 | P | 1 | Total 4 | Be 1 | F 3 | 0 | 0 |
| 10 | a | 1 | Total 4 | Be 1 | F 3 | 0 | 0 |
| 10 | b | 1 | Total 4 | Be 1 | F 3 | 0 | 0 |
| 10 | e | 1 | Total 4 | Be 1 | F 3 | 0 | 0 |
| 10 | f | 1 | Total 4 | Be 1 | F 3 | 0 | 0 |
| 10 | g | 1 | Total 4 | Be 1 | F 3 | 0 | 0 |
| 10 | h | 1 | Total 4 | Be 1 | F 3 | 0 | 0 |
| 10 | k | 1 | Total 4 | Be 1 | F 3 | 0 | 0 |
| 10 | l | 1 | Total 4 | Be 1 | F 3 | 0 | 0 |
| 10 | m | 1 | Total 4 | Be 1 | F 3 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 10 | n | 1 | Total | Be | F | 0 | 0 |
| | | | 4 | 1 | 3 | | |
| 10 | p | 1 | Total | Be | F | 0 | 0 |
| | | | 4 | 1 | 3 | | |

- Molecule 11 is SULFATE ION (three-letter code: SO4) (formula: O₄S).

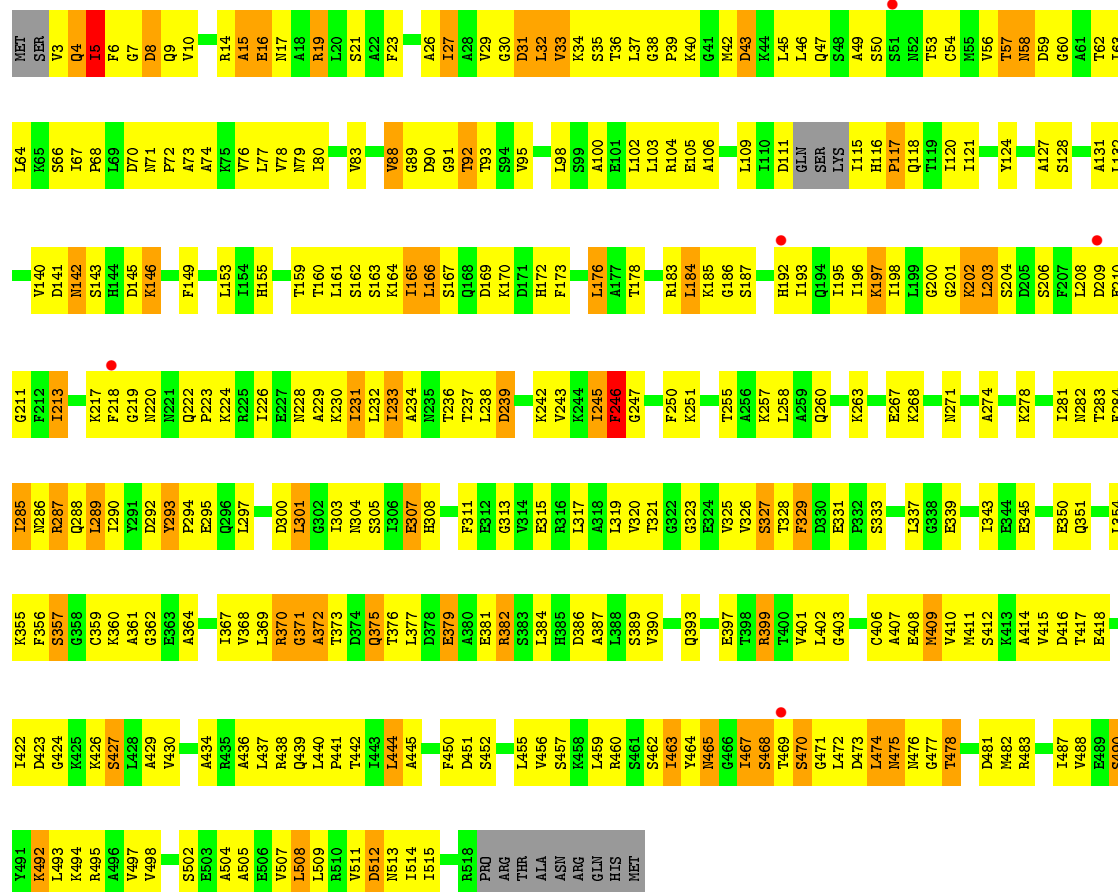
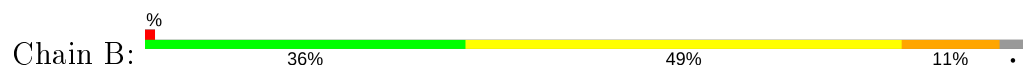


| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 11 | I | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 11 | K | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 11 | O | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 11 | c | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 11 | d | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 11 | i | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 11 | j | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 11 | o | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |

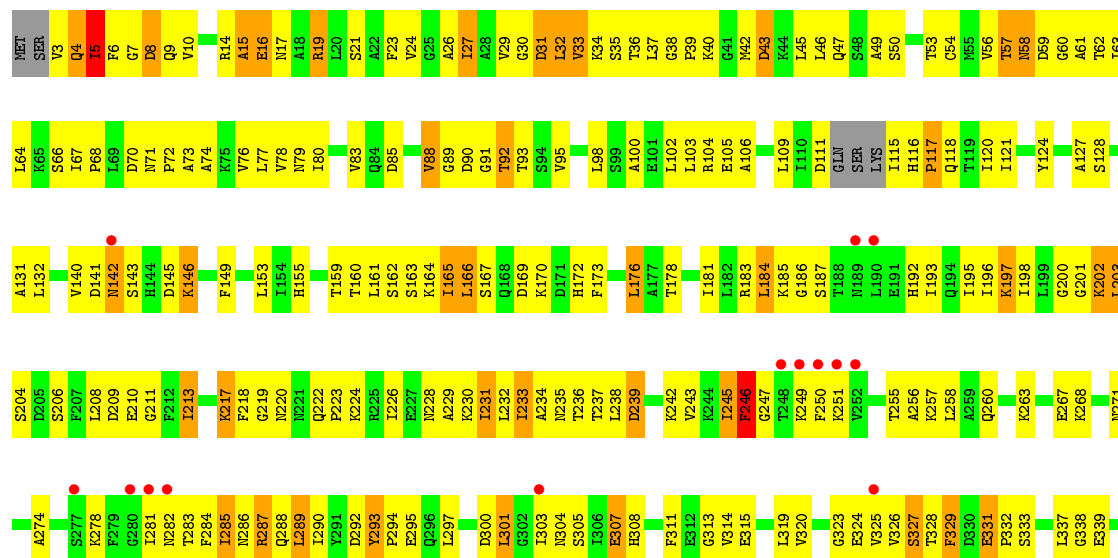
- Molecule 12 is water.

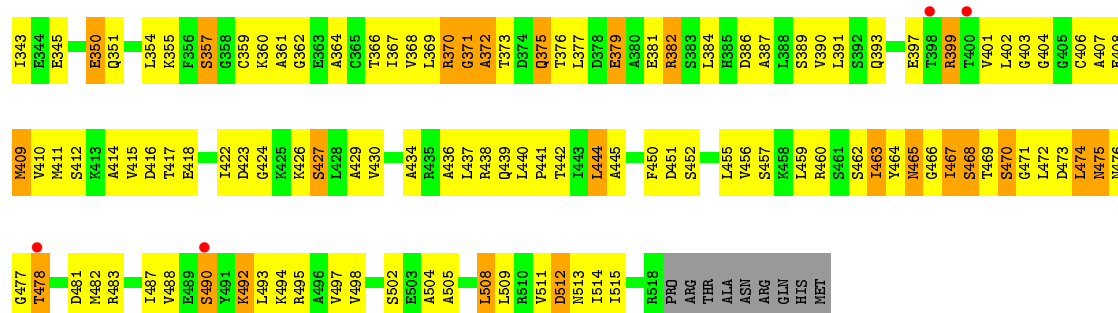
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|
| 12 | B | 1 | Total 1 | O 1 | 0 | 0 |
| 12 | E | 1 | Total 1 | O 1 | 0 | 0 |
| 12 | G | 1 | Total 1 | O 1 | 0 | 0 |
| 12 | M | 1 | Total 1 | O 1 | 0 | 0 |
| 12 | e | 1 | Total 1 | O 1 | 0 | 0 |
| 12 | g | 1 | Total 1 | O 1 | 0 | 0 |
| 12 | m | 1 | Total 1 | O 1 | 0 | 0 |



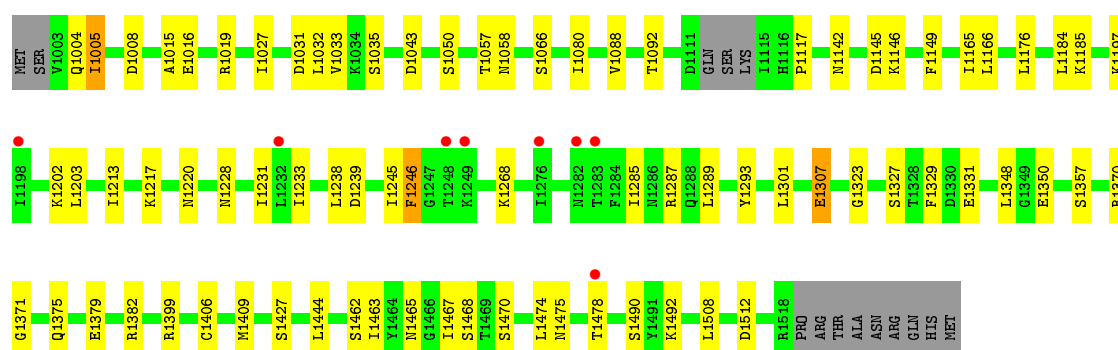
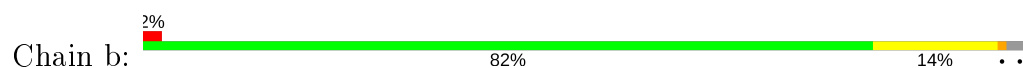


• Molecule 2: T-complex protein 1 subunit beta

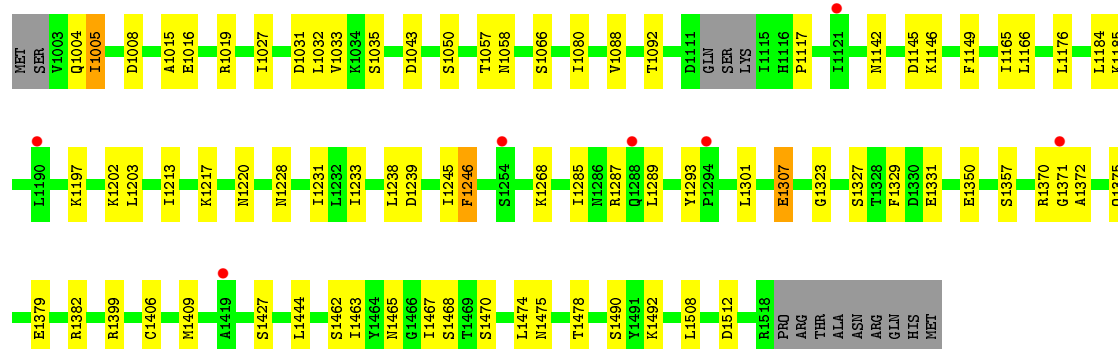
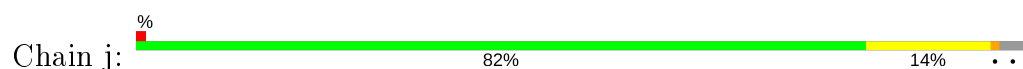




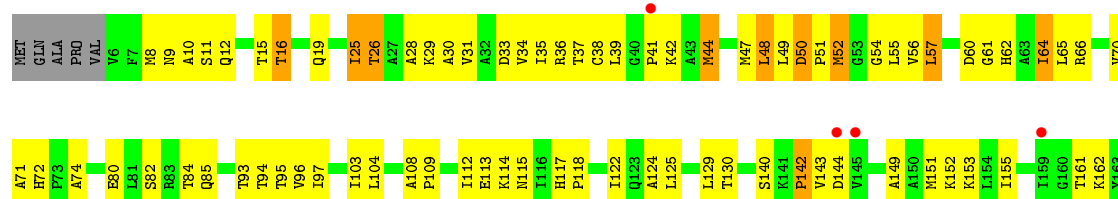
• Molecule 2: T-complex protein 1 subunit beta



• Molecule 2: T-complex protein 1 subunit beta



• Molecule 3: T-complex protein 1 subunit gamma



Chain c:

79% 7% 13%

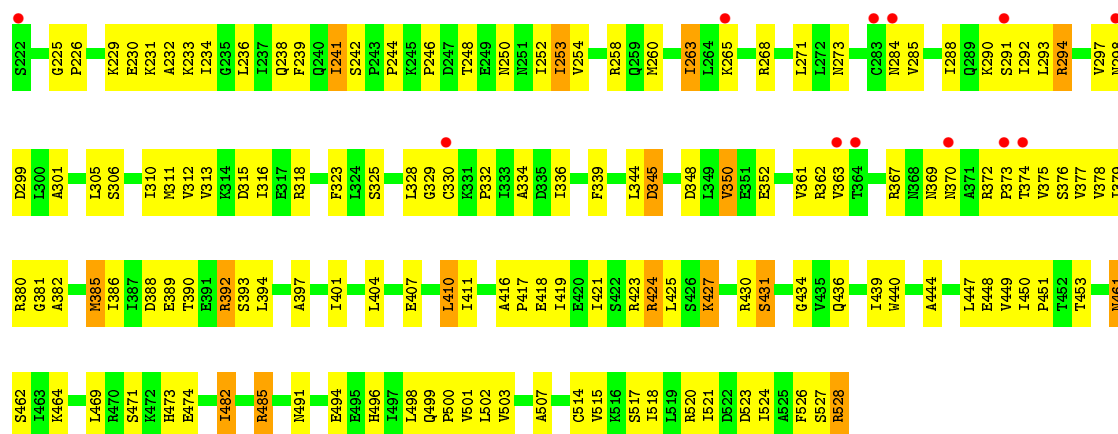
Legend:

- MET
- GLN
- ALA
- PRO
- VAL
- P1006
- F1007
- M1008
- T1016
- Q1019
- T1025
- T1026
- A1030
- R1036
- M1044
- L1048
- M1052
- L1057
- I1064
- P1142
- V1143
- D1144
- V1145
- E1145
- I1165
- K1170
- V1182
- R1183
- K1184
- D1185
- L1186
- GLY
- GLN
- THR
- VAL
- GLU
- GLY
- GLU
- PRO
- ASN
- PHE
- GLU
- I1198
- T1209
- P1210

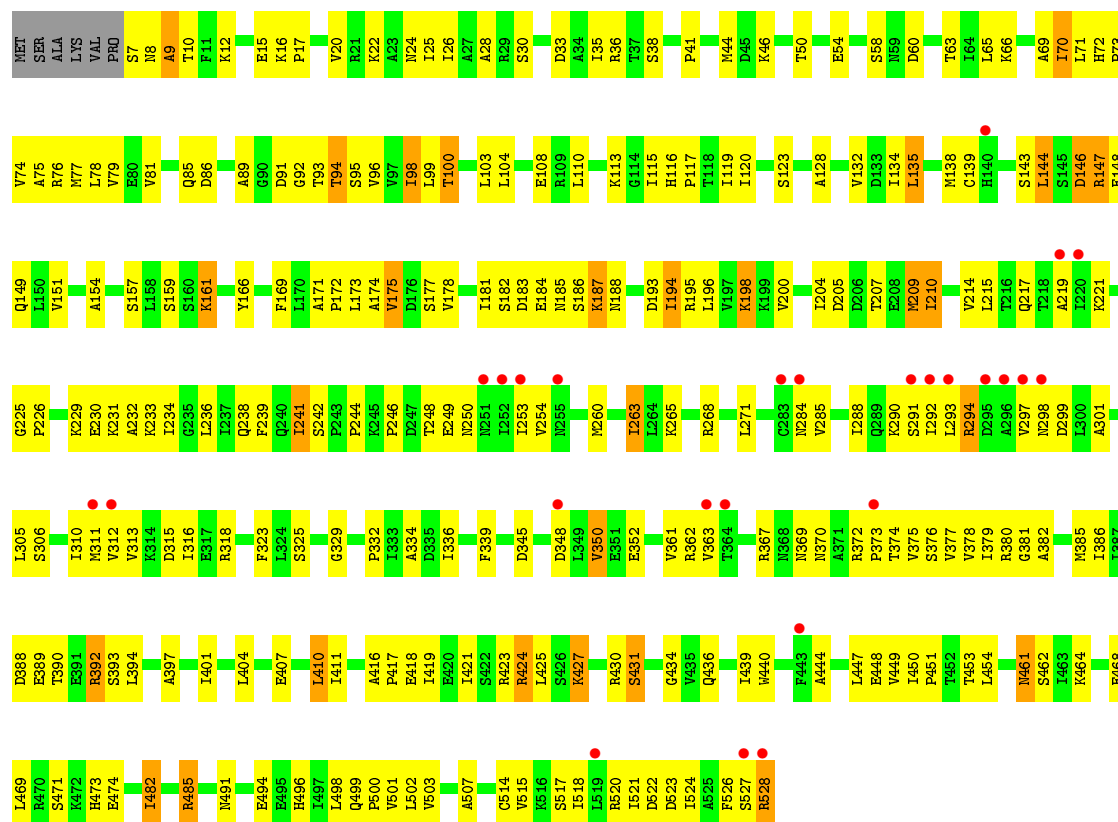
Chain k:

| Amino Acid | Percentage |
|------------|------------|
| Met | 2% |
| Ala | 79% |
| Val | 8% |
| Leu | 13% |

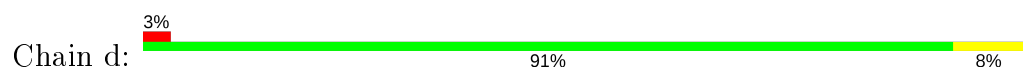
Chain D:

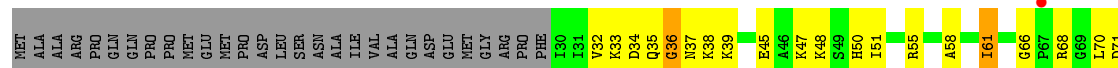


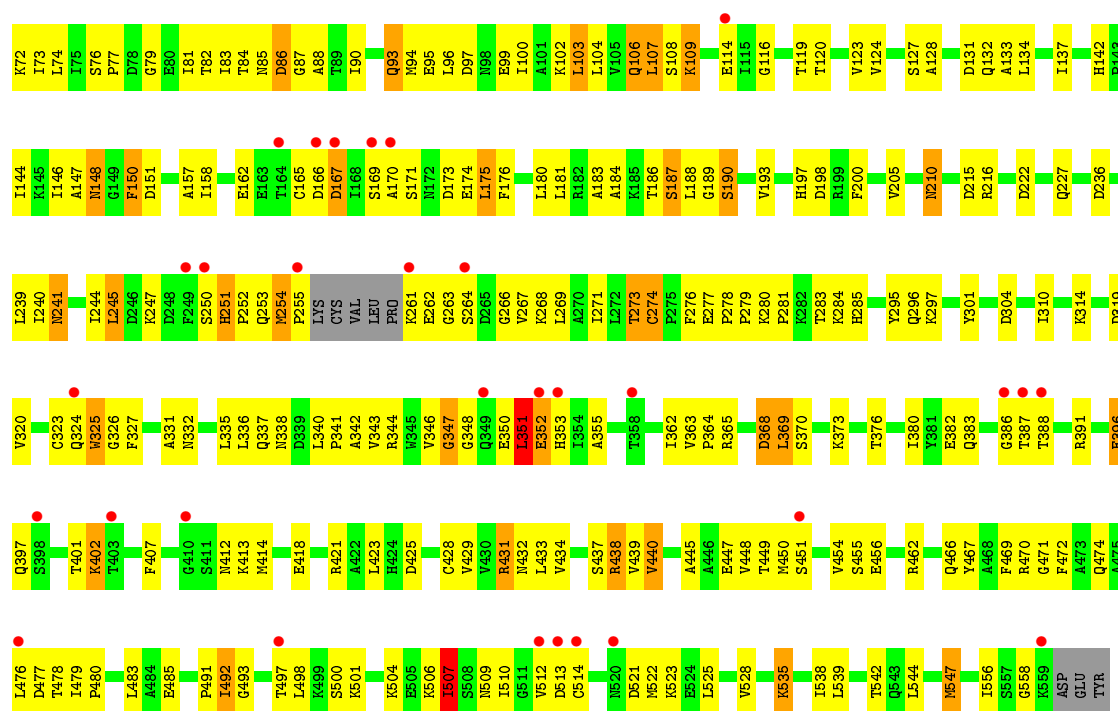
• Molecule 4: T-complex protein 1 subunit delta



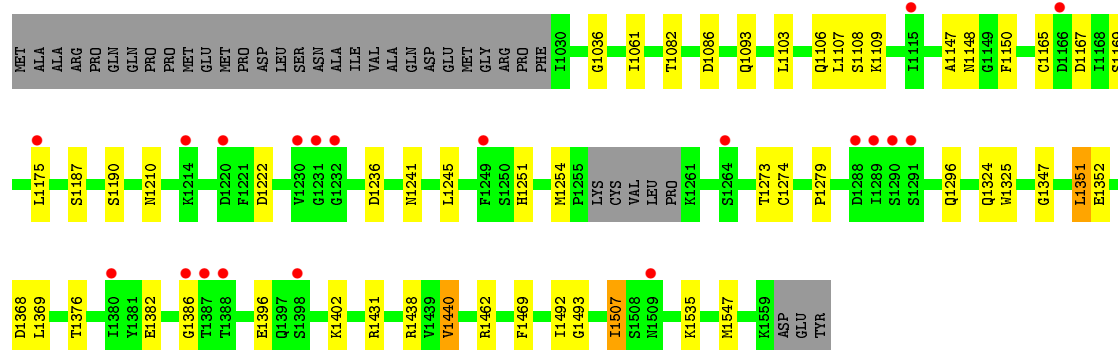
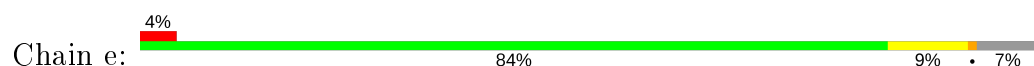
• Molecule 4: T-complex protein 1 subunit delta



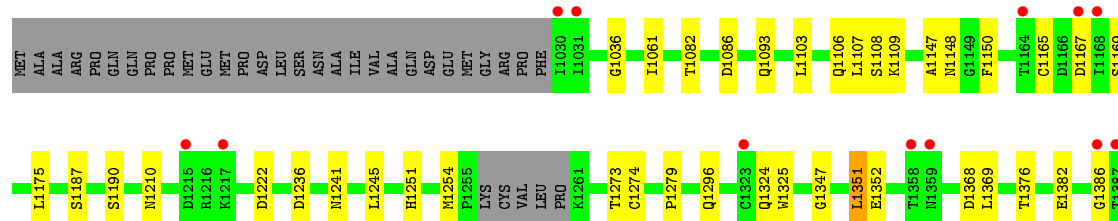
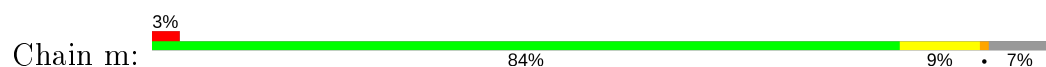




• Molecule 5: T-complex protein 1 subunit epsilon

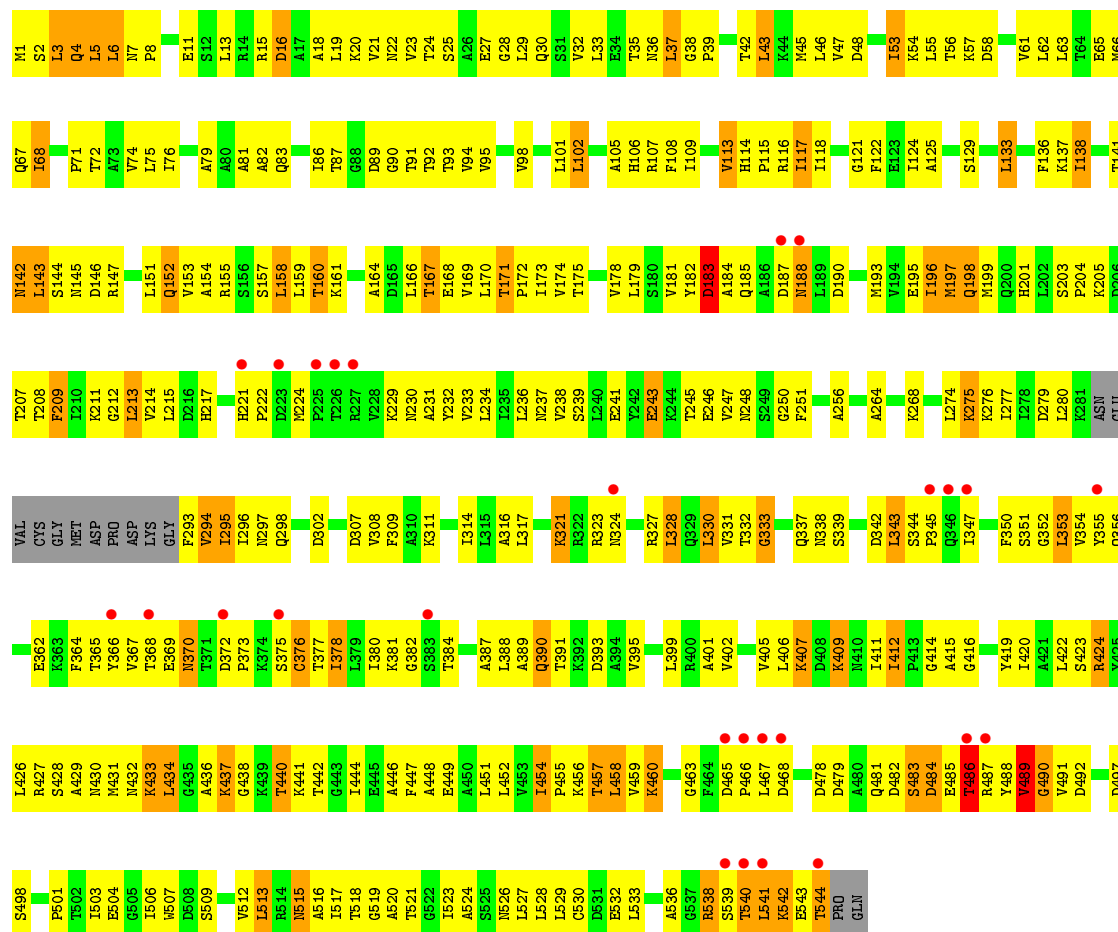


• Molecule 5: T-complex protein 1 subunit epsilon

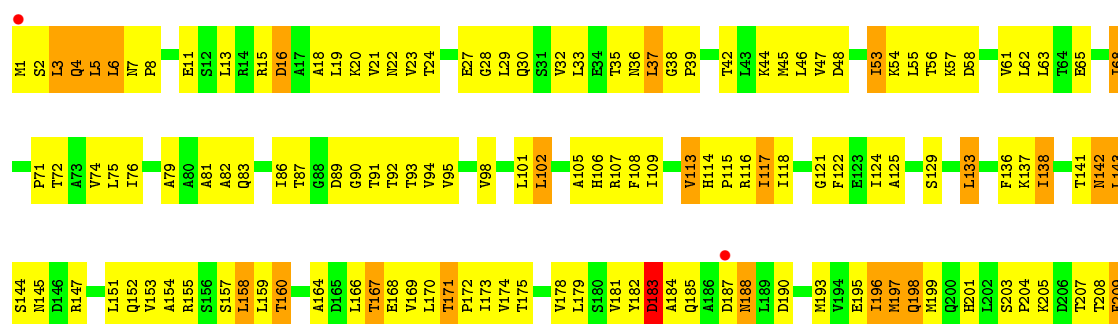


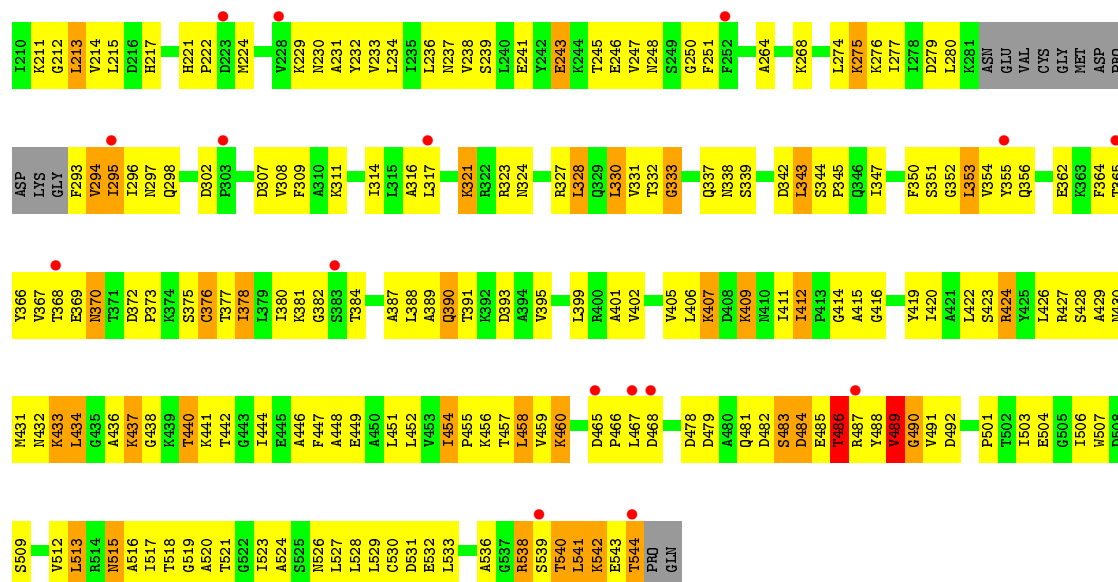


• Molecule 6: T-complex protein 1 subunit zeta

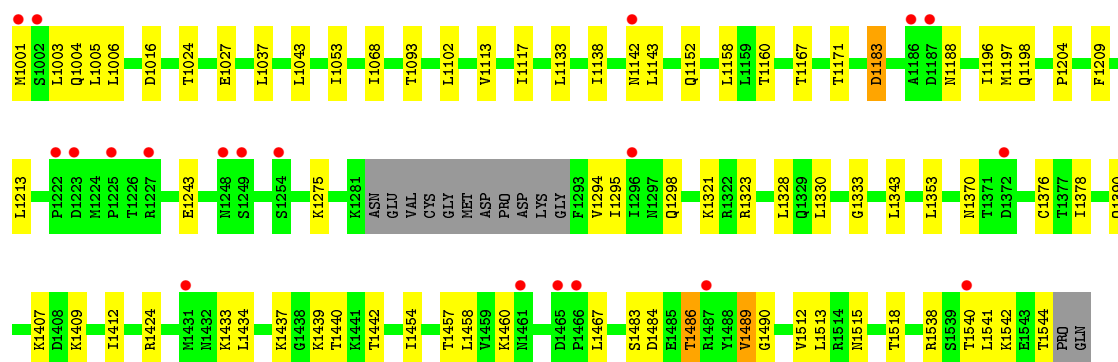
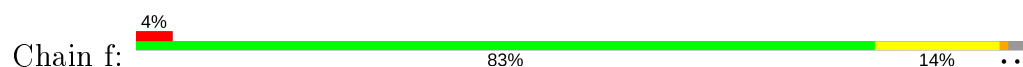


• Molecule 6: T-complex protein 1 subunit zeta

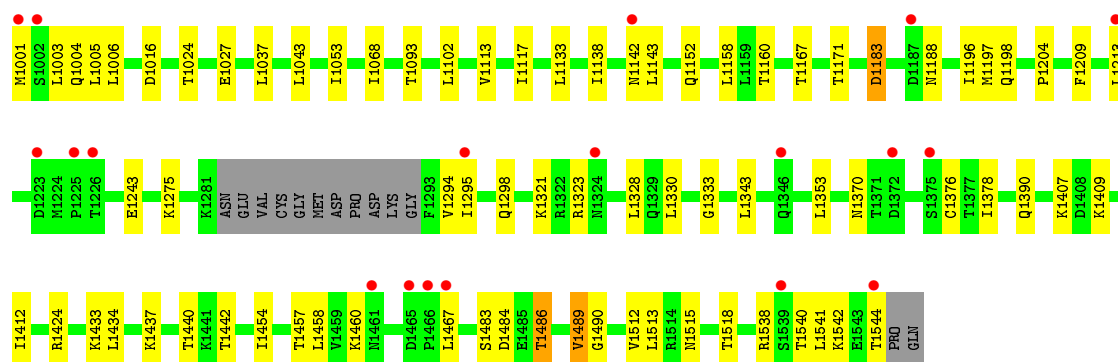
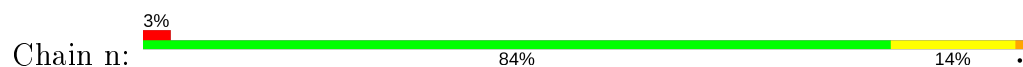




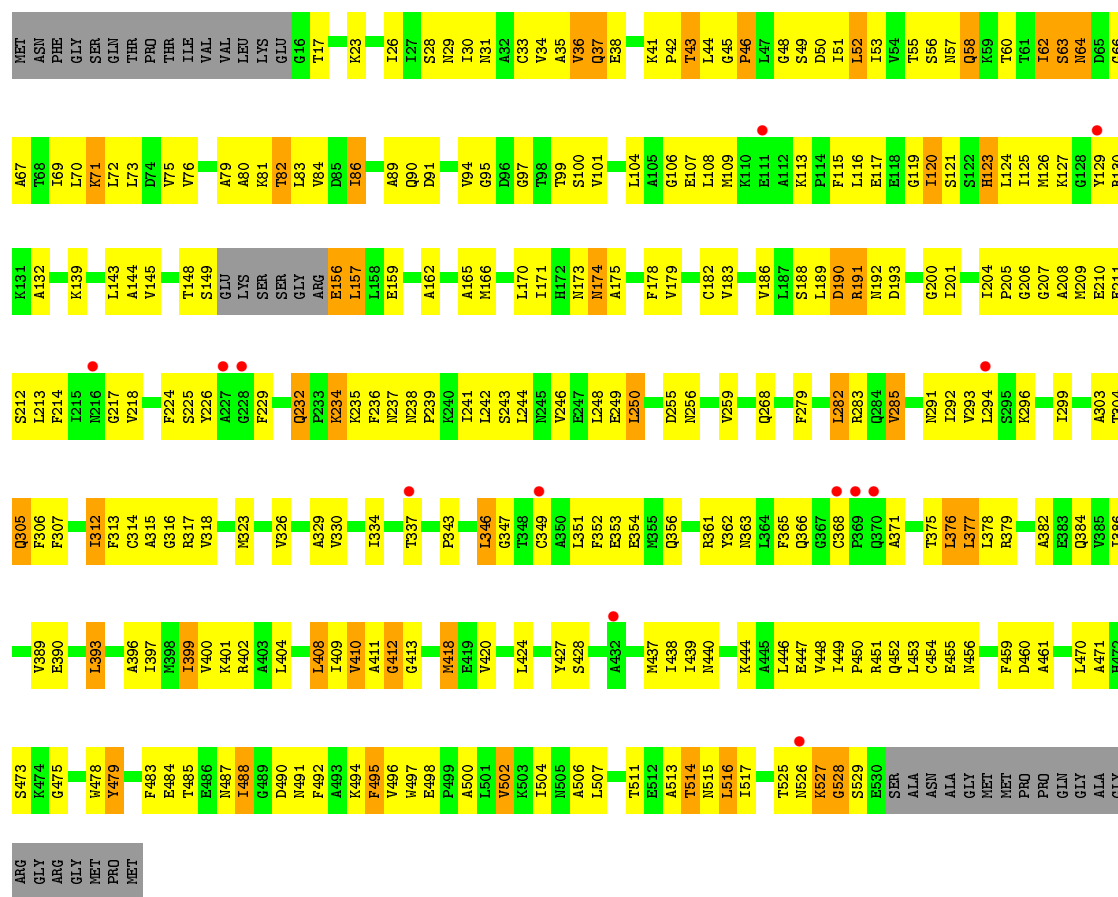
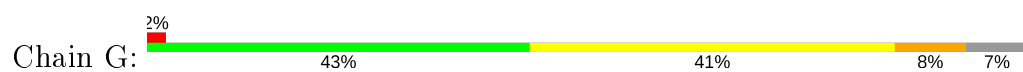
• Molecule 6: T-complex protein 1 subunit zeta



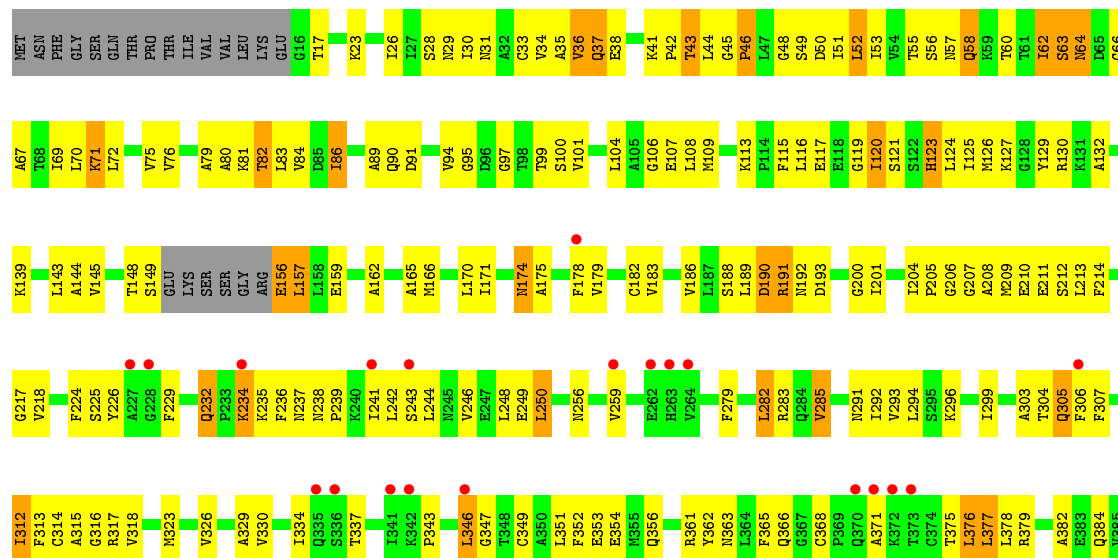
• Molecule 6: T-complex protein 1 subunit zeta

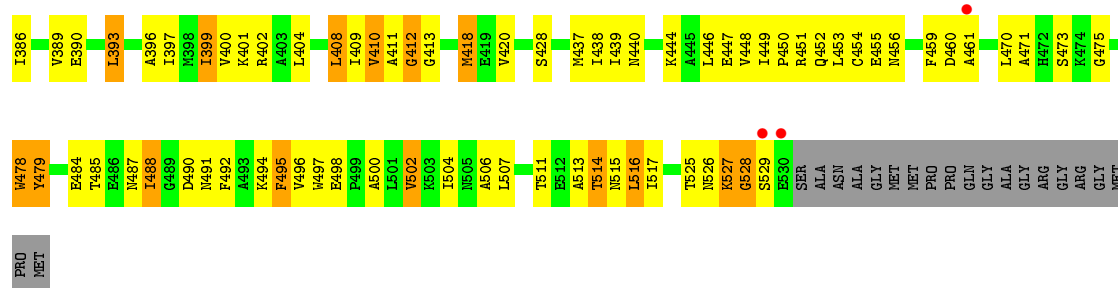


• Molecule 7: T-complex protein 1 subunit eta

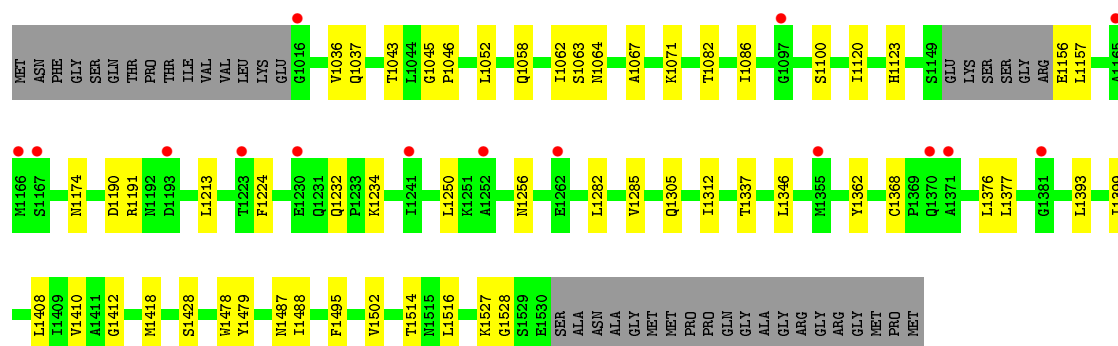
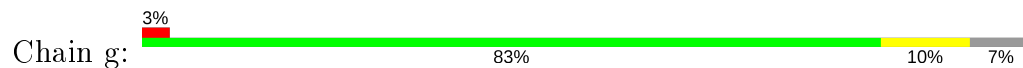


• Molecule 7: T-complex protein 1 subunit eta

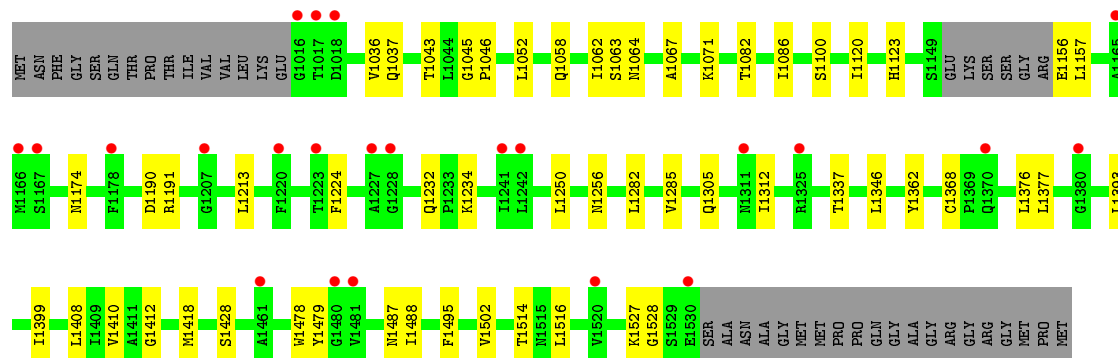
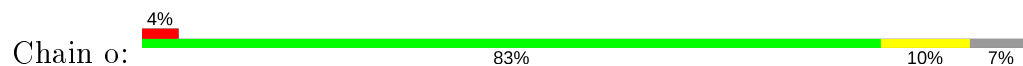




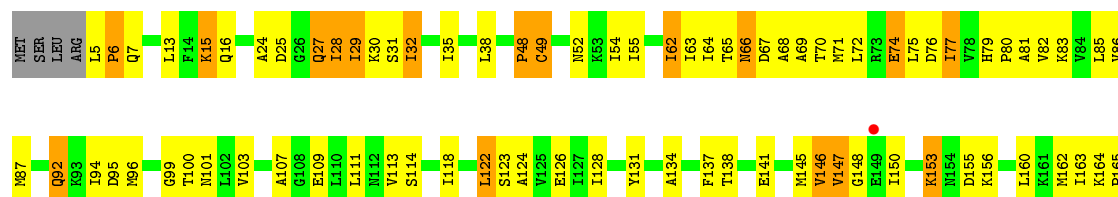
• Molecule 7: T-complex protein 1 subunit eta

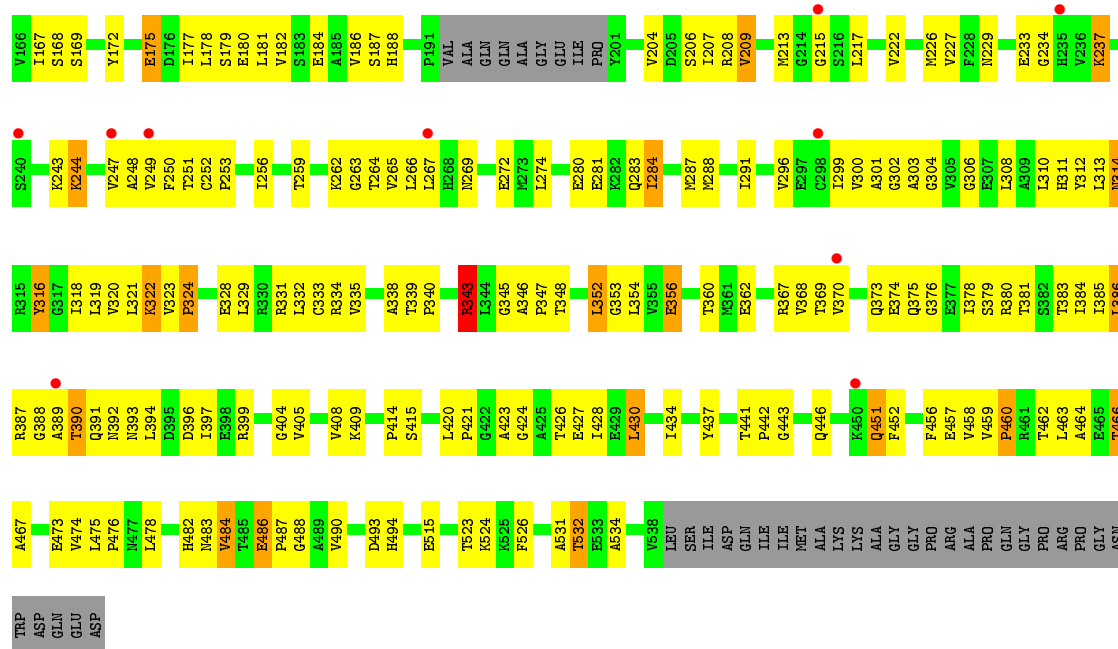


• Molecule 7: T-complex protein 1 subunit eta

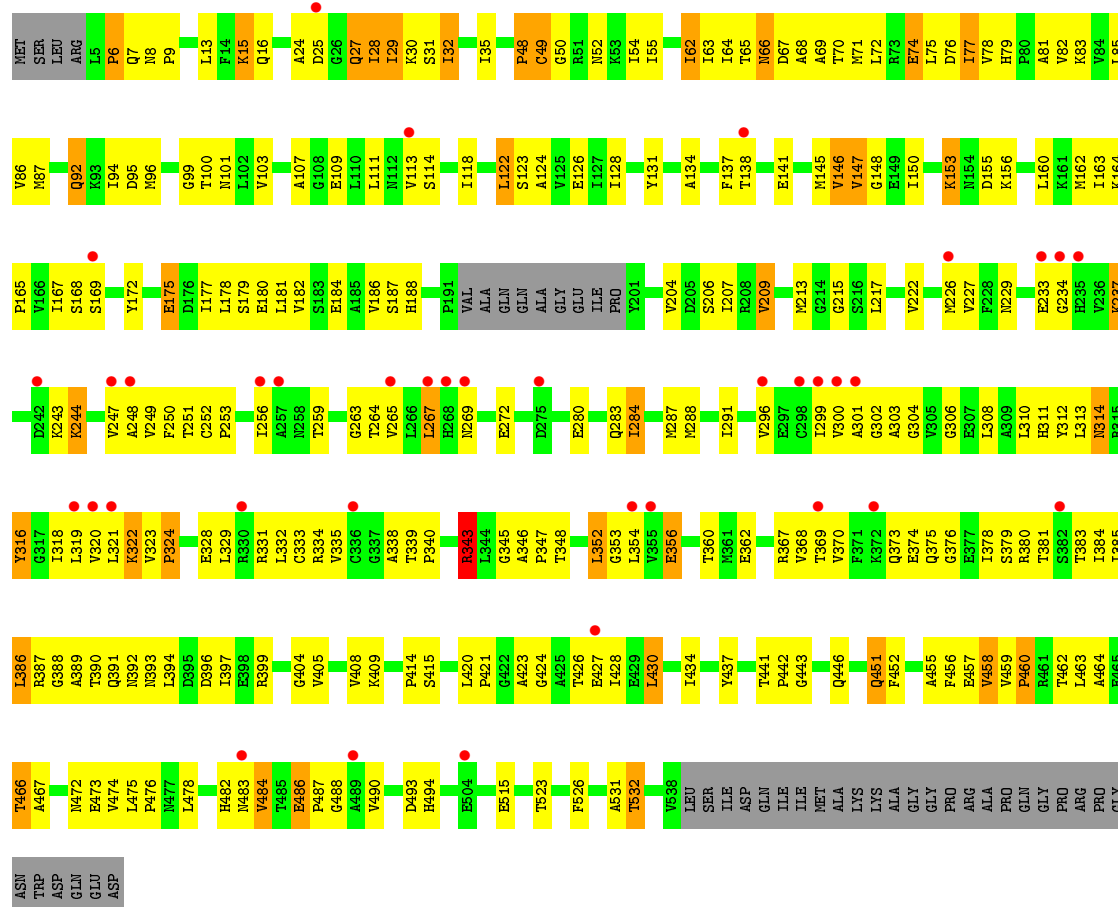


• Molecule 8: T-complex protein 1 subunit theta

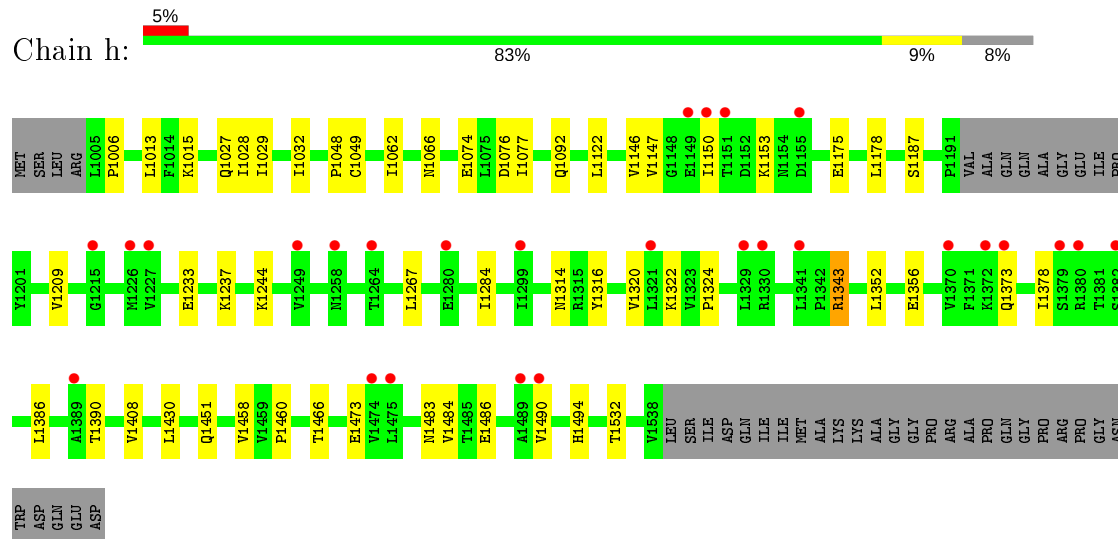




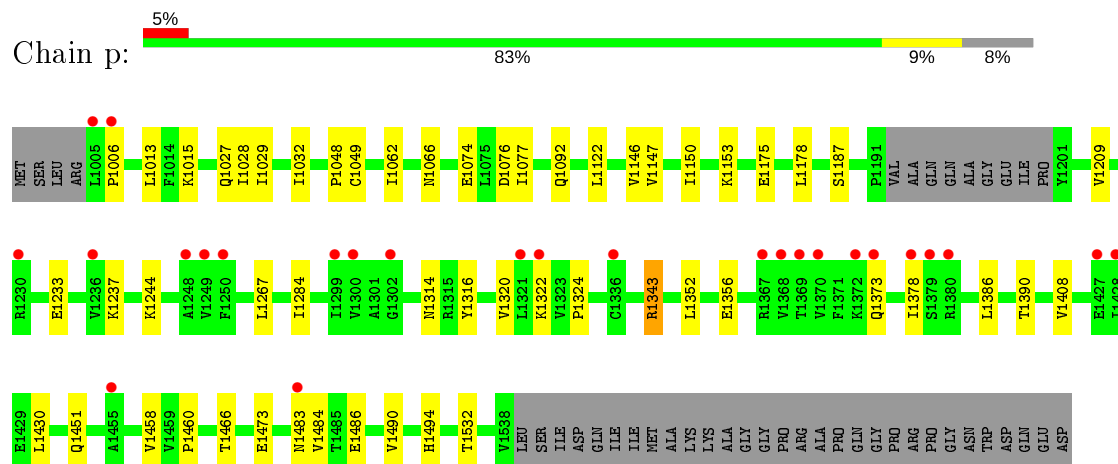
• Molecule 8: T-complex protein 1 subunit theta



- Molecule 8: T-complex protein 1 subunit theta



- Molecule 8: T-complex protein 1 subunit theta



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 159.10Å 162.54Å 268.10Å 85.23° 81.15° 61.17° | Depositor |
| Resolution (Å) | 89.95 – 3.80 89.95 – 3.80 | Depositor EDS |
| % Data completeness (in resolution range) | 91.6 (89.95-3.80) 91.6 (89.95-3.80) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | 0.08 | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 2.18 (at 3.78Å) | Xtriage |
| Refinement program | PHENIX (phenix.refine) | Depositor |
| R, R_{free} | 0.307 , 0.344 0.310 , 0.342 | Depositor DCC |
| R_{free} test set | 10483 reflections (5.00%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 112.3 | Xtriage |
| Anisotropy | 0.288 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.28 , 192.9 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$ | Xtriage |
| Estimated twinning fraction | 0.024 for -h,-h+k,-l | Xtriage |
| F_o, F_c correlation | 0.86 | EDS |
| Total number of atoms | 111235 | wwPDB-VP |
| Average B, all atoms (Å ²) | 141.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.01% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BEF, SO4, ADP

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 | 0.23 | 0/3515 | 0.47 | 1/4835 (0.0%) |
| 1 | I | 0.23 | 0/3515 | 0.47 | 1/4835 (0.0%) |
| 1 | a | 0.23 | 0/3515 | 0.47 | 1/4835 (0.0%) |
| 1 | i | 0.23 | 0/3515 | 0.47 | 1/4835 (0.0%) |
| 2 | B | 0.26 | 0/3480 | 0.49 | 0/4754 |
| 2 | J | 0.26 | 0/3480 | 0.49 | 0/4754 |
| 2 | b | 0.26 | 0/3481 | 0.49 | 0/4755 |
| 2 | j | 0.26 | 0/3478 | 0.49 | 0/4751 |
| 3 | C | 0.23 | 0/3421 | 0.46 | 0/4689 |
| 3 | K | 0.23 | 0/3422 | 0.46 | 0/4690 |
| 3 | c | 0.23 | 0/3424 | 0.46 | 0/4693 |
| 3 | k | 0.23 | 0/3424 | 0.46 | 0/4693 |
| 4 | D | 0.23 | 0/3421 | 0.46 | 2/4683 (0.0%) |
| 4 | L | 0.23 | 0/3421 | 0.45 | 1/4683 (0.0%) |
| 4 | d | 0.23 | 0/3421 | 0.45 | 1/4683 (0.0%) |
| 4 | l | 0.23 | 0/3421 | 0.45 | 1/4683 (0.0%) |
| 5 | E | 0.23 | 0/3466 | 0.46 | 0/4739 |
| 5 | M | 0.23 | 0/3466 | 0.46 | 0/4739 |
| 5 | e | 0.23 | 0/3466 | 0.46 | 0/4739 |
| 5 | m | 0.23 | 0/3466 | 0.46 | 0/4739 |
| 6 | F | 0.26 | 0/3663 | 0.52 | 1/5008 (0.0%) |
| 6 | N | 0.26 | 0/3660 | 0.52 | 1/5004 (0.0%) |
| 6 | f | 0.26 | 0/3665 | 0.52 | 1/5009 (0.0%) |
| 6 | n | 0.26 | 0/3661 | 0.52 | 1/5005 (0.0%) |
| 7 | G | 0.23 | 0/3342 | 0.46 | 0/4578 |
| 7 | O | 0.23 | 0/3339 | 0.45 | 0/4574 |
| 7 | g | 0.23 | 0/3339 | 0.45 | 0/4574 |
| 7 | o | 0.23 | 0/3339 | 0.45 | 0/4574 |
| 8 | H | 0.22 | 0/3522 | 0.42 | 0/4825 |
| 8 | P | 0.22 | 0/3522 | 0.42 | 0/4825 |
| 8 | h | 0.22 | 0/3519 | 0.42 | 0/4820 |
| 8 | p | 0.22 | 0/3522 | 0.42 | 0/4825 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------|-------------|------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| All | All | 0.24 | 0/111311 | 0.47 | 13/152428 (0.0%) |

There are no bond length outliers.

All (13) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | I | 437 | ALA | CB-CA-C | 8.54 | 122.92 | 110.10 |
| 1 | i | 1437 | ALA | CB-CA-C | 8.53 | 122.89 | 110.10 |
| 1 | A | 437 | ALA | CB-CA-C | 8.53 | 122.89 | 110.10 |
| 1 | a | 1437 | ALA | CB-CA-C | 8.52 | 122.88 | 110.10 |
| 4 | L | 350 | VAL | N-CA-C | -6.53 | 93.36 | 111.00 |
| 4 | d | 1350 | VAL | N-CA-C | -6.53 | 93.37 | 111.00 |
| 4 | l | 1350 | VAL | N-CA-C | -6.53 | 93.37 | 111.00 |
| 4 | D | 350 | VAL | N-CA-C | -6.52 | 93.41 | 111.00 |
| 6 | F | 275 | LYS | O-C-N | -5.79 | 113.43 | 122.70 |
| 6 | n | 1275 | LYS | O-C-N | -5.77 | 113.47 | 122.70 |
| 6 | f | 1275 | LYS | O-C-N | -5.77 | 113.47 | 122.70 |
| 6 | N | 275 | LYS | O-C-N | -5.76 | 113.49 | 122.70 |
| 4 | D | 345 | ASP | CB-CG-OD2 | 5.18 | 122.96 | 118.30 |

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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 | 3492 | 0 | 3026 | 298 | 0 |
| 1 | I | 3492 | 0 | 3026 | 291 | 0 |
| 1 | a | 3492 | 0 | 3026 | 0 | 0 |
| 1 | i | 3492 | 0 | 3026 | 0 | 0 |
| 2 | B | 3459 | 0 | 3146 | 476 | 0 |
| 2 | J | 3459 | 0 | 3146 | 479 | 0 |
| 2 | b | 3460 | 0 | 3148 | 0 | 0 |
| 2 | j | 3457 | 0 | 3139 | 0 | 0 |
| 3 | C | 3392 | 0 | 3019 | 295 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3 | K | 3393 | 0 | 3022 | 272 | 0 |
| 3 | c | 3395 | 0 | 3029 | 0 | 0 |
| 3 | k | 3395 | 0 | 3029 | 0 | 0 |
| 4 | D | 3398 | 0 | 3010 | 337 | 0 |
| 4 | L | 3398 | 0 | 3010 | 315 | 0 |
| 4 | d | 3398 | 0 | 3010 | 0 | 0 |
| 4 | l | 3398 | 0 | 3010 | 0 | 0 |
| 5 | E | 3437 | 0 | 2943 | 285 | 0 |
| 5 | M | 3437 | 0 | 2943 | 289 | 0 |
| 5 | e | 3437 | 0 | 2943 | 0 | 0 |
| 5 | m | 3437 | 0 | 2943 | 0 | 0 |
| 6 | F | 3631 | 0 | 3330 | 640 | 0 |
| 6 | N | 3628 | 0 | 3321 | 629 | 0 |
| 6 | f | 3633 | 0 | 3333 | 0 | 0 |
| 6 | n | 3629 | 0 | 3322 | 0 | 0 |
| 7 | G | 3317 | 0 | 2920 | 382 | 0 |
| 7 | O | 3314 | 0 | 2911 | 375 | 0 |
| 7 | g | 3314 | 0 | 2911 | 0 | 0 |
| 7 | o | 3314 | 0 | 2911 | 0 | 0 |
| 8 | H | 3487 | 0 | 3109 | 296 | 0 |
| 8 | P | 3487 | 0 | 3109 | 273 | 0 |
| 8 | h | 3485 | 0 | 3103 | 0 | 0 |
| 8 | p | 3487 | 0 | 3109 | 0 | 0 |
| 9 | A | 27 | 0 | 11 | 3 | 0 |
| 9 | B | 27 | 0 | 11 | 8 | 0 |
| 9 | C | 27 | 0 | 12 | 7 | 0 |
| 9 | D | 27 | 0 | 11 | 8 | 0 |
| 9 | E | 27 | 0 | 11 | 2 | 0 |
| 9 | F | 27 | 0 | 11 | 6 | 0 |
| 9 | G | 27 | 0 | 11 | 5 | 0 |
| 9 | H | 27 | 0 | 12 | 3 | 0 |
| 9 | J | 27 | 0 | 11 | 5 | 0 |
| 9 | L | 27 | 0 | 11 | 7 | 0 |
| 9 | M | 27 | 0 | 11 | 6 | 0 |
| 9 | N | 27 | 0 | 11 | 6 | 0 |
| 9 | P | 27 | 0 | 12 | 5 | 0 |
| 9 | a | 27 | 0 | 11 | 0 | 0 |
| 9 | b | 27 | 0 | 11 | 0 | 0 |
| 9 | e | 27 | 0 | 12 | 0 | 0 |
| 9 | f | 27 | 0 | 11 | 0 | 0 |
| 9 | g | 27 | 0 | 11 | 0 | 0 |
| 9 | h | 27 | 0 | 12 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 9 | k | 27 | 0 | 11 | 0 | 0 |
| 9 | l | 27 | 0 | 11 | 0 | 0 |
| 9 | m | 27 | 0 | 11 | 0 | 0 |
| 9 | n | 27 | 0 | 11 | 0 | 0 |
| 9 | p | 27 | 0 | 12 | 0 | 0 |
| 10 | A | 4 | 0 | 0 | 0 | 0 |
| 10 | B | 4 | 0 | 0 | 0 | 0 |
| 10 | C | 4 | 0 | 0 | 3 | 0 |
| 10 | D | 4 | 0 | 0 | 0 | 0 |
| 10 | E | 4 | 0 | 0 | 0 | 0 |
| 10 | F | 4 | 0 | 0 | 2 | 0 |
| 10 | G | 4 | 0 | 0 | 0 | 0 |
| 10 | H | 4 | 0 | 0 | 0 | 0 |
| 10 | J | 4 | 0 | 0 | 0 | 0 |
| 10 | L | 4 | 0 | 0 | 1 | 0 |
| 10 | M | 4 | 0 | 0 | 0 | 0 |
| 10 | N | 4 | 0 | 0 | 3 | 0 |
| 10 | P | 4 | 0 | 0 | 0 | 0 |
| 10 | a | 4 | 0 | 0 | 0 | 0 |
| 10 | b | 4 | 0 | 0 | 0 | 0 |
| 10 | e | 4 | 0 | 0 | 0 | 0 |
| 10 | f | 4 | 0 | 0 | 0 | 0 |
| 10 | g | 4 | 0 | 0 | 0 | 0 |
| 10 | h | 4 | 0 | 0 | 0 | 0 |
| 10 | k | 4 | 0 | 0 | 0 | 0 |
| 10 | l | 4 | 0 | 0 | 0 | 0 |
| 10 | m | 4 | 0 | 0 | 0 | 0 |
| 10 | n | 4 | 0 | 0 | 0 | 0 |
| 10 | p | 4 | 0 | 0 | 0 | 0 |
| 11 | I | 5 | 0 | 0 | 0 | 0 |
| 11 | K | 5 | 0 | 0 | 0 | 0 |
| 11 | O | 5 | 0 | 0 | 0 | 0 |
| 11 | c | 5 | 0 | 0 | 0 | 0 |
| 11 | d | 5 | 0 | 0 | 0 | 0 |
| 11 | i | 5 | 0 | 0 | 0 | 0 |
| 11 | j | 5 | 0 | 0 | 0 | 0 |
| 11 | o | 5 | 0 | 0 | 0 | 0 |
| 12 | B | 1 | 0 | 0 | 0 | 0 |
| 12 | E | 1 | 0 | 0 | 0 | 0 |
| 12 | G | 1 | 0 | 0 | 0 | 0 |
| 12 | M | 1 | 0 | 0 | 0 | 0 |
| 12 | e | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 12 | g | 1 | 0 | 0 | 0 | 0 |
| 12 | m | 1 | 0 | 0 | 0 | 0 |
| All | All | 111235 | 0 | 98253 | 5533 | 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 53.

All (5533) 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) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:4:GLN:HA | 2:B:5:ILE:CG1 | 1.37 | 1.53 |
| 2:J:4:GLN:HA | 2:J:5:ILE:CG1 | 1.37 | 1.48 |
| 6:N:36:ASN:HB3 | 6:N:57:LYS:NZ | 1.28 | 1.46 |
| 6:F:151:LEU:CD1 | 6:F:175:THR:CG2 | 1.90 | 1.46 |
| 6:N:151:LEU:CD1 | 6:N:175:THR:CG2 | 1.90 | 1.46 |
| 6:N:434:LEU:HD22 | 6:N:441:LYS:CB | 1.45 | 1.46 |
| 8:H:6:PRO:HG3 | 4:L:71:LEU:CB | 1.43 | 1.45 |
| 6:F:541:LEU:CB | 6:F:542:LYS:HA | 1.31 | 1.44 |
| 6:F:434:LEU:HD22 | 6:F:441:LYS:CB | 1.45 | 1.43 |
| 6:F:151:LEU:HD13 | 6:F:175:THR:CG2 | 0.95 | 1.43 |
| 6:F:36:ASN:HB3 | 6:F:57:LYS:NZ | 1.28 | 1.43 |
| 7:G:189:LEU:HA | 7:G:190:ASP:CB | 1.23 | 1.41 |
| 6:N:151:LEU:HD13 | 6:N:175:THR:CG2 | 0.95 | 1.41 |
| 6:N:541:LEU:CB | 6:N:542:LYS:HA | 1.30 | 1.41 |
| 6:F:352:GLY:CA | 6:F:369:GLU:O | 1.70 | 1.39 |
| 6:N:352:GLY:CA | 6:N:369:GLU:O | 1.70 | 1.39 |
| 7:O:189:LEU:HA | 7:O:190:ASP:CB | 1.23 | 1.39 |
| 4:D:71:LEU:CB | 8:P:6:PRO:HG3 | 1.51 | 1.38 |
| 6:F:541:LEU:HB2 | 6:F:542:LYS:CA | 1.51 | 1.37 |
| 6:F:117:ILE:CD1 | 5:M:34:ASP:HA | 1.51 | 1.35 |
| 2:J:4:GLN:CA | 2:J:5:ILE:HG12 | 1.59 | 1.33 |
| 2:B:4:GLN:CA | 2:B:5:ILE:HG12 | 1.59 | 1.32 |
| 6:N:541:LEU:HB2 | 6:N:542:LYS:CA | 1.51 | 1.31 |
| 6:N:151:LEU:CD1 | 6:N:175:THR:HG21 | 1.54 | 1.30 |
| 6:F:151:LEU:CD1 | 6:F:175:THR:HG21 | 1.54 | 1.29 |
| 8:H:6:PRO:CG | 4:L:71:LEU:CB | 2.10 | 1.29 |
| 7:O:516:LEU:C | 7:O:516:LEU:HD22 | 1.54 | 1.28 |
| 1:A:184:LEU:HD21 | 1:A:198:TYR:CD2 | 1.67 | 1.27 |
| 1:I:184:LEU:HD21 | 1:I:198:TYR:CD2 | 1.67 | 1.27 |
| 1:I:250:ASN:HB2 | 1:I:300:LYS:CB | 1.62 | 1.27 |
| 2:J:361:ALA:N | 2:J:362:GLY:HA2 | 1.31 | 1.27 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:250:ASN:HB2 | 1:A:300:LYS:CB | 1.62 | 1.26 |
| 6:F:36:ASN:CB | 6:F:57:LYS:HZ3 | 1.48 | 1.26 |
| 6:F:352:GLY:HA3 | 6:F:369:GLU:C | 1.54 | 1.25 |
| 7:O:235:LYS:HA | 7:O:352:PHE:O | 1.35 | 1.25 |
| 2:B:361:ALA:N | 2:B:362:GLY:HA2 | 1.31 | 1.25 |
| 7:G:235:LYS:HA | 7:G:352:PHE:O | 1.35 | 1.25 |
| 6:N:352:GLY:HA3 | 6:N:369:GLU:C | 1.54 | 1.25 |
| 6:N:352:GLY:O | 6:N:367:VAL:CG1 | 1.85 | 1.25 |
| 2:B:463:ILE:O | 2:B:467:ILE:CG1 | 1.85 | 1.24 |
| 6:N:94:VAL:O | 6:N:98:VAL:CG2 | 1.85 | 1.24 |
| 4:D:521:ILE:HA | 7:G:50:ASP:O | 1.37 | 1.24 |
| 6:F:352:GLY:O | 6:F:367:VAL:CG1 | 1.85 | 1.23 |
| 6:F:151:LEU:CD1 | 6:F:175:THR:HG23 | 1.60 | 1.23 |
| 6:F:94:VAL:O | 6:F:98:VAL:CG2 | 1.85 | 1.23 |
| 2:J:463:ILE:O | 2:J:467:ILE:CG1 | 1.85 | 1.23 |
| 7:O:189:LEU:CA | 7:O:190:ASP:CB | 2.14 | 1.23 |
| 2:J:463:ILE:O | 2:J:467:ILE:HG12 | 1.05 | 1.22 |
| 2:B:463:ILE:O | 2:B:467:ILE:HG12 | 1.06 | 1.22 |
| 6:F:90:GLY:O | 6:F:94:VAL:HG23 | 1.40 | 1.22 |
| 7:G:516:LEU:HD22 | 7:G:516:LEU:C | 1.54 | 1.22 |
| 1:I:184:LEU:HD21 | 1:I:198:TYR:CG | 1.75 | 1.21 |
| 7:G:189:LEU:CA | 7:G:190:ASP:CB | 2.14 | 1.21 |
| 4:L:521:ILE:HA | 7:O:50:ASP:O | 1.37 | 1.21 |
| 6:F:478:ASP:O | 6:F:482:ASP:CB | 1.90 | 1.20 |
| 1:A:184:LEU:HD21 | 1:A:198:TYR:CG | 1.75 | 1.20 |
| 6:N:478:ASP:O | 6:N:482:ASP:CB | 1.90 | 1.19 |
| 4:D:521:ILE:HD11 | 7:G:62:ILE:HD11 | 1.20 | 1.19 |
| 4:D:71:LEU:CB | 8:P:6:PRO:CG | 2.20 | 1.19 |
| 7:G:189:LEU:CA | 7:G:190:ASP:HB3 | 1.71 | 1.19 |
| 6:N:90:GLY:O | 6:N:94:VAL:HG23 | 1.40 | 1.18 |
| 6:N:151:LEU:CD1 | 6:N:175:THR:HG23 | 1.60 | 1.18 |
| 7:O:189:LEU:CA | 7:O:190:ASP:HB3 | 1.71 | 1.18 |
| 4:L:524:ILE:HA | 7:O:52:LEU:O | 1.41 | 1.17 |
| 4:L:524:ILE:HG12 | 7:O:52:LEU:CB | 1.72 | 1.17 |
| 3:C:457:ILE:HD13 | 3:C:467:LEU:HD13 | 1.26 | 1.17 |
| 2:J:4:GLN:HA | 2:J:5:ILE:CB | 1.73 | 1.16 |
| 6:N:36:ASN:CB | 6:N:57:LYS:HZ3 | 1.59 | 1.16 |
| 8:H:54:ILE:HG13 | 8:H:64:ILE:HG12 | 1.21 | 1.15 |
| 5:E:273:THR:HG22 | 5:E:364:PRO:HA | 1.29 | 1.15 |
| 2:B:4:GLN:HA | 2:B:5:ILE:CB | 1.73 | 1.15 |
| 6:F:94:VAL:O | 6:F:98:VAL:HG23 | 0.98 | 1.14 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:228:VAL:HG22 | 1:I:363:GLN:HE22 | 1.03 | 1.14 |
| 4:D:524:ILE:HG12 | 7:G:52:LEU:CB | 1.77 | 1.14 |
| 4:L:524:ILE:CG1 | 7:O:52:LEU:HB3 | 1.77 | 1.14 |
| 7:O:191:ARG:HE | 7:O:191:ARG:HA | 1.12 | 1.14 |
| 6:F:434:LEU:CD2 | 6:F:441:LYS:CB | 2.26 | 1.13 |
| 6:N:501:PRO:HB3 | 6:N:506:ILE:HB | 1.27 | 1.13 |
| 6:N:94:VAL:O | 6:N:98:VAL:HG23 | 0.98 | 1.13 |
| 3:C:230:VAL:HG11 | 3:C:302:SER:OG | 1.49 | 1.13 |
| 3:K:230:VAL:HG11 | 3:K:302:SER:OG | 1.49 | 1.13 |
| 5:E:34:ASP:HA | 6:N:117:ILE:CD1 | 1.78 | 1.12 |
| 6:N:434:LEU:CD2 | 6:N:441:LYS:CB | 2.27 | 1.12 |
| 7:G:94:VAL:HG21 | 7:G:502:VAL:HG22 | 1.17 | 1.12 |
| 1:A:228:VAL:HG22 | 1:A:363:GLN:HE22 | 1.03 | 1.12 |
| 4:D:520:ARG:O | 7:G:49:SER:HB3 | 1.47 | 1.12 |
| 2:B:200:GLY:HA3 | 2:B:369:LEU:HD23 | 1.30 | 1.12 |
| 6:N:478:ASP:O | 6:N:482:ASP:HB2 | 1.47 | 1.12 |
| 6:F:166:LEU:O | 6:F:167:THR:HG23 | 1.48 | 1.12 |
| 7:O:94:VAL:HG21 | 7:O:502:VAL:HG22 | 1.17 | 1.11 |
| 6:N:166:LEU:O | 6:N:167:THR:HG23 | 1.48 | 1.11 |
| 8:P:206:SER:HB2 | 8:P:381:THR:HG22 | 1.32 | 1.11 |
| 5:M:273:THR:HG22 | 5:M:364:PRO:HA | 1.29 | 1.11 |
| 6:N:434:LEU:HD23 | 6:N:434:LEU:H | 0.98 | 1.11 |
| 4:D:521:ILE:CD1 | 7:G:62:ILE:HD11 | 1.79 | 1.11 |
| 6:F:434:LEU:HD23 | 6:F:434:LEU:H | 0.98 | 1.11 |
| 2:J:357:SER:HB3 | 2:J:360:LYS:CB | 1.79 | 1.11 |
| 4:L:521:ILE:HD11 | 7:O:62:ILE:HD11 | 1.28 | 1.11 |
| 8:P:54:ILE:HG13 | 8:P:64:ILE:HG12 | 1.21 | 1.11 |
| 6:F:274:LEU:HD21 | 6:F:308:VAL:HG11 | 1.31 | 1.11 |
| 6:N:274:LEU:HD21 | 6:N:308:VAL:HG11 | 1.31 | 1.11 |
| 6:F:53:ILE:HD12 | 6:F:53:ILE:O | 1.49 | 1.10 |
| 2:B:422:ILE:HB | 2:B:427:SER:HB2 | 1.28 | 1.10 |
| 2:B:357:SER:HB3 | 2:B:360:LYS:CB | 1.79 | 1.10 |
| 6:F:478:ASP:O | 6:F:482:ASP:HB2 | 1.47 | 1.10 |
| 2:J:200:GLY:HA3 | 2:J:369:LEU:HD23 | 1.30 | 1.10 |
| 6:N:143:LEU:HD13 | 6:N:145:ASN:H | 0.94 | 1.10 |
| 1:A:494:ARG:CB | 1:A:495:ARG:CA | 2.29 | 1.10 |
| 2:J:29:VAL:O | 2:J:33:VAL:HG22 | 1.50 | 1.10 |
| 6:N:53:ILE:O | 6:N:53:ILE:HD12 | 1.49 | 1.09 |
| 2:B:29:VAL:O | 2:B:33:VAL:HG22 | 1.50 | 1.09 |
| 1:I:494:ARG:CB | 1:I:495:ARG:CA | 2.30 | 1.09 |
| 1:A:9:ARG:CB | 1:A:10:SER:CA | 2.30 | 1.09 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:N:3:LEU:N | 6:N:4:GLN:HB2 | 1.68 | 1.09 |
| 6:F:83:GLN:HG3 | 6:F:94:VAL:HG21 | 1.32 | 1.09 |
| 1:I:9:ARG:CB | 1:I:10:SER:CA | 2.30 | 1.09 |
| 7:G:191:ARG:HE | 7:G:191:ARG:HA | 1.12 | 1.09 |
| 3:K:457:ILE:HD13 | 3:K:467:LEU:HD13 | 1.26 | 1.09 |
| 2:J:422:ILE:HB | 2:J:427:SER:HB2 | 1.28 | 1.09 |
| 5:M:273:THR:CG2 | 5:M:364:PRO:HA | 1.81 | 1.09 |
| 7:O:189:LEU:HA | 7:O:190:ASP:HB2 | 1.26 | 1.08 |
| 6:F:3:LEU:N | 6:F:4:GLN:HB2 | 1.68 | 1.08 |
| 4:L:521:ILE:HD11 | 7:O:62:ILE:CD1 | 1.82 | 1.08 |
| 5:E:186:THR:HG21 | 5:E:528:VAL:O | 1.51 | 1.08 |
| 4:L:521:ILE:CD1 | 7:O:62:ILE:HD11 | 1.82 | 1.08 |
| 5:E:273:THR:CG2 | 5:E:364:PRO:HA | 1.81 | 1.08 |
| 5:M:186:THR:HG21 | 5:M:528:VAL:O | 1.51 | 1.08 |
| 6:N:352:GLY:HA3 | 6:N:369:GLU:O | 0.90 | 1.08 |
| 3:C:264:GLU:O | 3:C:265:LYS:HG3 | 1.54 | 1.08 |
| 4:D:521:ILE:HD11 | 7:G:62:ILE:CD1 | 1.82 | 1.08 |
| 1:I:90:GLN:HG3 | 1:I:101:VAL:HG21 | 1.27 | 1.08 |
| 1:A:90:GLN:HG3 | 1:A:101:VAL:HG21 | 1.27 | 1.08 |
| 8:H:206:SER:HB2 | 8:H:381:THR:HG22 | 1.32 | 1.08 |
| 4:D:524:ILE:CG1 | 7:G:52:LEU:HB3 | 1.84 | 1.07 |
| 4:L:250:ASN:HA | 7:O:259:VAL:HG12 | 1.35 | 1.07 |
| 5:E:34:ASP:HA | 6:N:117:ILE:HD11 | 1.11 | 1.07 |
| 6:F:143:LEU:HD13 | 6:F:145:ASN:H | 0.93 | 1.07 |
| 6:F:539:SER:HB3 | 6:F:542:LYS:HD2 | 1.37 | 1.07 |
| 8:H:237:LYS:HB3 | 8:H:314:ASN:CB | 1.84 | 1.07 |
| 2:J:242:LYS:NZ | 2:J:247:GLY:O | 1.86 | 1.07 |
| 6:F:352:GLY:HA3 | 6:F:369:GLU:O | 0.90 | 1.07 |
| 4:D:72:HIS:HB2 | 4:D:75:ALA:HB3 | 1.35 | 1.07 |
| 6:F:501:PRO:HB3 | 6:F:506:ILE:HB | 1.27 | 1.07 |
| 7:G:189:LEU:HA | 7:G:190:ASP:HB2 | 1.26 | 1.07 |
| 6:N:539:SER:HB3 | 6:N:542:LYS:HD2 | 1.37 | 1.07 |
| 8:P:237:LYS:HB3 | 8:P:314:ASN:CB | 1.85 | 1.07 |
| 7:G:188:SER:O | 7:G:190:ASP:HB2 | 1.54 | 1.06 |
| 1:A:93:GLU:CB | 1:A:94:ILE:HD12 | 1.86 | 1.06 |
| 2:B:5:ILE:O | 3:C:71:ALA:N | 1.87 | 1.06 |
| 8:H:482:HIS:O | 8:H:484:VAL:N | 1.89 | 1.06 |
| 2:B:242:LYS:NZ | 2:B:247:GLY:O | 1.86 | 1.06 |
| 6:N:83:GLN:HG3 | 6:N:94:VAL:HG21 | 1.32 | 1.06 |
| 6:F:489:VAL:O | 6:F:490:GLY:O | 1.72 | 1.06 |
| 1:I:93:GLU:CB | 1:I:94:ILE:HD12 | 1.85 | 1.06 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:513:ASN:O | 2:B:514:ILE:HD13 | 1.56 | 1.05 |
| 6:N:489:VAL:O | 6:N:490:GLY:O | 1.72 | 1.05 |
| 1:A:9:ARG:CB | 1:A:10:SER:HA | 1.84 | 1.05 |
| 6:N:430:ASN:HA | 6:N:433:LYS:HG2 | 1.05 | 1.05 |
| 7:O:188:SER:O | 7:O:190:ASP:HB2 | 1.54 | 1.05 |
| 8:P:482:HIS:O | 8:P:484:VAL:N | 1.89 | 1.05 |
| 1:A:517:VAL:O | 1:A:518:LEU:HG | 1.56 | 1.05 |
| 6:F:133:LEU:HD12 | 6:F:422:LEU:HD21 | 1.37 | 1.05 |
| 1:I:9:ARG:CB | 1:I:10:SER:HA | 1.83 | 1.05 |
| 6:F:430:ASN:HA | 6:F:433:LYS:HG2 | 1.05 | 1.05 |
| 6:F:434:LEU:N | 6:F:434:LEU:HD23 | 1.62 | 1.04 |
| 8:H:243:LYS:O | 8:H:244:LYS:HG2 | 1.57 | 1.04 |
| 1:I:494:ARG:CB | 1:I:495:ARG:HA | 1.87 | 1.04 |
| 6:F:430:ASN:HA | 6:F:433:LYS:CG | 1.86 | 1.04 |
| 8:P:237:LYS:HB3 | 8:P:314:ASN:HB2 | 1.39 | 1.04 |
| 7:G:226:TYR:CD1 | 7:G:229:PHE:O | 2.10 | 1.04 |
| 1:I:517:VAL:O | 1:I:518:LEU:HG | 1.56 | 1.04 |
| 2:J:513:ASN:O | 2:J:514:ILE:HD13 | 1.56 | 1.04 |
| 3:K:264:GLU:O | 3:K:265:LYS:HG3 | 1.54 | 1.04 |
| 4:L:520:ARG:O | 7:O:49:SER:HB3 | 1.57 | 1.04 |
| 8:H:237:LYS:HB3 | 8:H:314:ASN:HB2 | 1.39 | 1.04 |
| 6:N:430:ASN:HA | 6:N:433:LYS:CG | 1.86 | 1.04 |
| 5:M:401:THR:O | 5:M:402:LYS:HE2 | 1.58 | 1.04 |
| 6:N:430:ASN:O | 6:N:433:LYS:HB2 | 1.55 | 1.03 |
| 6:N:5:LEU:HA | 6:N:6:LEU:CB | 1.86 | 1.03 |
| 8:P:243:LYS:O | 8:P:244:LYS:HG2 | 1.57 | 1.03 |
| 6:F:5:LEU:HA | 6:F:6:LEU:CB | 1.86 | 1.03 |
| 3:K:302:SER:O | 3:K:303:ASP:HB2 | 1.59 | 1.03 |
| 5:M:184:ALA:O | 5:M:188:LEU:N | 1.91 | 1.03 |
| 1:A:494:ARG:CB | 1:A:495:ARG:HA | 1.86 | 1.03 |
| 4:D:524:ILE:HA | 7:G:52:LEU:O | 1.56 | 1.03 |
| 2:B:361:ALA:N | 2:B:362:GLY:CA | 2.22 | 1.03 |
| 6:F:430:ASN:O | 6:F:433:LYS:HB2 | 1.55 | 1.03 |
| 4:L:72:HIS:HB2 | 4:L:75:ALA:HB3 | 1.35 | 1.03 |
| 6:N:434:LEU:HD23 | 6:N:434:LEU:N | 1.62 | 1.03 |
| 6:F:2:SER:C | 6:F:4:GLN:HB2 | 1.77 | 1.03 |
| 2:B:142:ASN:HB2 | 2:B:143:SER:HA | 1.41 | 1.03 |
| 7:O:226:TYR:CD1 | 7:O:229:PHE:O | 2.10 | 1.03 |
| 5:E:401:THR:O | 5:E:402:LYS:HE2 | 1.58 | 1.02 |
| 6:N:2:SER:C | 6:N:4:GLN:HB2 | 1.77 | 1.02 |
| 5:E:350:GLU:O | 5:E:352:GLU:N | 1.92 | 1.02 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:M:350:GLU:O | 5:M:352:GLU:N | 1.92 | 1.02 |
| 6:N:133:LEU:HD12 | 6:N:422:LEU:HD21 | 1.37 | 1.02 |
| 1:I:228:VAL:HG22 | 1:I:363:GLN:NE2 | 1.75 | 1.02 |
| 6:F:158:LEU:HD12 | 6:F:158:LEU:O | 1.60 | 1.02 |
| 6:N:352:GLY:O | 6:N:367:VAL:HG13 | 1.57 | 1.01 |
| 2:J:361:ALA:N | 2:J:362:GLY:CA | 2.22 | 1.01 |
| 1:A:228:VAL:HG22 | 1:A:363:GLN:NE2 | 1.75 | 1.01 |
| 5:E:184:ALA:O | 5:E:188:LEU:N | 1.91 | 1.01 |
| 6:F:352:GLY:O | 6:F:367:VAL:HG13 | 1.57 | 1.01 |
| 7:G:42:PRO:O | 7:G:48:GLY:HA2 | 1.59 | 1.01 |
| 6:F:167:THR:HB | 6:F:169:VAL:N | 1.76 | 1.00 |
| 6:N:158:LEU:O | 6:N:158:LEU:HD12 | 1.60 | 1.00 |
| 6:N:167:THR:HB | 6:N:169:VAL:N | 1.76 | 1.00 |
| 3:C:298:GLU:C | 3:C:319:ARG:CB | 2.30 | 1.00 |
| 3:C:234:MET:HB3 | 3:C:310:LEU:HD22 | 1.44 | 1.00 |
| 2:J:4:GLN:CA | 2:J:5:ILE:HG23 | 1.91 | 1.00 |
| 4:L:134:ILE:HD11 | 4:L:424:ARG:HD3 | 1.41 | 1.00 |
| 3:K:298:GLU:C | 3:K:319:ARG:CB | 2.30 | 1.00 |
| 6:N:143:LEU:HD13 | 6:N:145:ASN:N | 1.76 | 1.00 |
| 7:O:42:PRO:O | 7:O:48:GLY:HA2 | 1.59 | 0.99 |
| 6:F:434:LEU:HA | 6:F:441:LYS:CB | 1.93 | 0.99 |
| 2:B:4:GLN:CA | 2:B:5:ILE:HG23 | 1.91 | 0.99 |
| 6:F:143:LEU:HD13 | 6:F:145:ASN:N | 1.75 | 0.99 |
| 6:F:434:LEU:O | 6:F:438:GLY:N | 1.95 | 0.99 |
| 6:N:434:LEU:HA | 6:N:441:LYS:CB | 1.92 | 0.99 |
| 6:F:540:THR:O | 6:F:542:LYS:HG2 | 1.62 | 0.99 |
| 1:I:9:ARG:CB | 1:I:10:SER:C | 2.31 | 0.99 |
| 6:N:434:LEU:O | 6:N:438:GLY:N | 1.95 | 0.99 |
| 7:O:516:LEU:HD13 | 7:O:517:ILE:HG12 | 1.44 | 0.99 |
| 3:C:302:SER:O | 3:C:303:ASP:HB2 | 1.59 | 0.99 |
| 2:J:142:ASN:HB2 | 2:J:143:SER:HA | 1.41 | 0.99 |
| 2:B:490:SER:O | 2:B:493:LEU:HG | 1.63 | 0.99 |
| 6:F:16:ASP:HA | 6:F:19:LEU:HD12 | 1.44 | 0.99 |
| 7:G:516:LEU:HD13 | 7:G:517:ILE:HG12 | 1.44 | 0.98 |
| 2:J:490:SER:O | 2:J:493:LEU:HG | 1.63 | 0.98 |
| 7:O:516:LEU:C | 7:O:516:LEU:CD2 | 2.30 | 0.98 |
| 1:A:9:ARG:CB | 1:A:10:SER:C | 2.31 | 0.98 |
| 4:D:70:ILE:HG12 | 4:D:70:ILE:O | 1.63 | 0.98 |
| 3:K:265:LYS:NZ | 3:K:268:ASP:HB3 | 1.79 | 0.98 |
| 8:H:423:ALA:HA | 9:H:601:ADP:H2' | 1.45 | 0.98 |
| 6:N:540:THR:O | 6:N:542:LYS:HG2 | 1.62 | 0.98 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:H:124:ALA:O | 8:H:128:ILE:HG13 | 1.63 | 0.98 |
| 4:D:134:ILE:HD11 | 4:D:424:ARG:HD3 | 1.41 | 0.98 |
| 6:F:540:THR:C | 6:F:541:LEU:HD22 | 1.84 | 0.98 |
| 2:J:8:ASP:HB3 | 2:J:9:GLN:HA | 1.43 | 0.98 |
| 2:B:8:ASP:HB3 | 2:B:9:GLN:HA | 1.43 | 0.97 |
| 2:J:260:GLN:HA | 2:J:263:LYS:HD2 | 1.46 | 0.97 |
| 6:N:540:THR:C | 6:N:541:LEU:HD22 | 1.84 | 0.97 |
| 3:C:265:LYS:NZ | 3:C:268:ASP:HB3 | 1.79 | 0.97 |
| 4:L:524:ILE:CA | 7:O:52:LEU:O | 2.12 | 0.97 |
| 7:O:516:LEU:CD1 | 7:O:517:ILE:HG12 | 1.94 | 0.97 |
| 6:N:3:LEU:HD12 | 6:N:5:LEU:HD23 | 1.46 | 0.97 |
| 4:L:70:ILE:HG12 | 4:L:70:ILE:O | 1.63 | 0.97 |
| 2:B:260:GLN:HA | 2:B:263:LYS:HD2 | 1.46 | 0.97 |
| 7:G:94:VAL:CG2 | 7:G:502:VAL:HG22 | 1.93 | 0.97 |
| 6:F:43:LEU:HD23 | 6:F:57:LYS:HB2 | 1.44 | 0.97 |
| 6:N:16:ASP:HA | 6:N:19:LEU:HD12 | 1.44 | 0.97 |
| 6:F:117:ILE:HD11 | 5:M:34:ASP:CA | 1.93 | 0.97 |
| 6:F:434:LEU:CA | 6:F:441:LYS:CB | 2.43 | 0.97 |
| 3:K:234:MET:HB3 | 3:K:310:LEU:HD22 | 1.44 | 0.97 |
| 3:K:298:GLU:O | 3:K:319:ARG:CB | 2.13 | 0.97 |
| 1:A:184:LEU:CD2 | 1:A:198:TYR:CD2 | 2.49 | 0.96 |
| 2:J:202:LYS:O | 2:J:370:ARG:HA | 1.64 | 0.96 |
| 2:B:202:LYS:O | 2:B:370:ARG:HA | 1.64 | 0.96 |
| 2:J:4:GLN:CA | 2:J:5:ILE:CG1 | 2.30 | 0.96 |
| 5:M:88:ALA:HB2 | 5:M:119:THR:HB | 1.46 | 0.96 |
| 7:O:94:VAL:CG2 | 7:O:502:VAL:HG22 | 1.93 | 0.96 |
| 5:E:88:ALA:HB2 | 5:E:119:THR:HB | 1.46 | 0.96 |
| 6:N:434:LEU:CA | 6:N:441:LYS:CB | 2.43 | 0.96 |
| 7:G:43:THR:HG22 | 7:G:64:ASN:HB3 | 1.45 | 0.96 |
| 4:D:254:VAL:HG22 | 8:H:265:VAL:HA | 1.47 | 0.96 |
| 5:M:66:GLY:H | 9:M:601:ADP:H5'1 | 1.30 | 0.96 |
| 3:K:269:TRP:HH2 | 6:N:248:ASN:H | 0.97 | 0.96 |
| 2:J:514:ILE:HD12 | 3:K:47:MET:HB3 | 1.48 | 0.96 |
| 6:N:154:ALA:CB | 6:N:402:VAL:HG23 | 1.96 | 0.96 |
| 3:C:298:GLU:O | 3:C:319:ARG:CB | 2.13 | 0.96 |
| 6:F:154:ALA:CB | 6:F:402:VAL:HG23 | 1.96 | 0.96 |
| 7:G:516:LEU:CD1 | 7:G:517:ILE:HG12 | 1.94 | 0.96 |
| 6:F:117:ILE:CD1 | 5:M:34:ASP:CA | 2.43 | 0.95 |
| 6:F:117:ILE:HD11 | 5:M:34:ASP:HA | 0.97 | 0.95 |
| 7:O:90:GLN:HG3 | 7:O:101:VAL:HG21 | 1.48 | 0.95 |
| 8:P:124:ALA:O | 8:P:128:ILE:HG13 | 1.63 | 0.95 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:F:3:LEU:HD12 | 6:F:5:LEU:HD23 | 1.46 | 0.95 |
| 6:F:43:LEU:CD2 | 6:F:57:LYS:HB2 | 1.96 | 0.95 |
| 6:N:36:ASN:CB | 6:N:57:LYS:NZ | 2.24 | 0.95 |
| 1:A:494:ARG:CB | 1:A:495:ARG:C | 2.35 | 0.95 |
| 1:I:184:LEU:CD2 | 1:I:198:TYR:CD2 | 2.49 | 0.95 |
| 4:D:521:ILE:CA | 7:G:50:ASP:O | 2.14 | 0.95 |
| 1:I:494:ARG:CB | 1:I:495:ARG:C | 2.35 | 0.95 |
| 7:O:235:LYS:CA | 7:O:352:PHE:O | 2.15 | 0.95 |
| 7:O:43:THR:HG22 | 7:O:64:ASN:HB3 | 1.45 | 0.94 |
| 6:N:541:LEU:CB | 6:N:542:LYS:CA | 2.22 | 0.94 |
| 6:F:465:ASP:HA | 6:F:466:PRO:C | 1.88 | 0.94 |
| 2:J:263:LYS:NZ | 3:K:266:GLU:HB3 | 1.81 | 0.94 |
| 3:C:335:THR:HB | 8:H:237:LYS:HE2 | 1.48 | 0.94 |
| 5:E:253:GLN:CB | 5:E:254:MET:CB | 2.46 | 0.94 |
| 8:H:316:TYR:H | 8:H:316:TYR:HD2 | 1.15 | 0.94 |
| 5:M:253:GLN:CB | 5:M:254:MET:CB | 2.46 | 0.94 |
| 6:N:465:ASP:HA | 6:N:466:PRO:C | 1.88 | 0.94 |
| 8:P:316:TYR:H | 8:P:316:TYR:HD2 | 1.15 | 0.94 |
| 5:M:107:LEU:HD22 | 5:M:544:LEU:HG | 1.49 | 0.94 |
| 1:A:494:ARG:CB | 1:A:496:SER:N | 2.30 | 0.94 |
| 4:D:523:ASP:O | 7:G:51:ILE:HG23 | 1.67 | 0.94 |
| 2:J:70:ASP:HB2 | 6:N:5:LEU:HD22 | 1.49 | 0.94 |
| 6:F:420:ILE:CG2 | 6:F:482:ASP:OD1 | 2.15 | 0.94 |
| 1:I:494:ARG:CB | 1:I:496:SER:N | 2.30 | 0.94 |
| 7:G:235:LYS:CA | 7:G:352:PHE:O | 2.15 | 0.93 |
| 7:G:516:LEU:CD2 | 7:G:516:LEU:C | 2.30 | 0.93 |
| 8:H:237:LYS:CB | 8:H:314:ASN:HB3 | 1.98 | 0.93 |
| 7:O:191:ARG:NE | 7:O:192:ASN:H | 1.65 | 0.93 |
| 6:N:420:ILE:CG2 | 6:N:482:ASP:OD1 | 2.15 | 0.93 |
| 2:B:4:GLN:CA | 2:B:5:ILE:CG1 | 2.30 | 0.93 |
| 7:G:516:LEU:HD22 | 7:G:517:ILE:N | 1.83 | 0.93 |
| 2:J:251:LYS:H | 6:N:251:PHE:HA | 1.32 | 0.93 |
| 6:N:434:LEU:CD2 | 6:N:434:LEU:N | 2.30 | 0.93 |
| 2:J:127:ALA:HB2 | 2:J:430:VAL:HG22 | 1.51 | 0.93 |
| 3:K:57:LEU:HD23 | 3:K:57:LEU:N | 1.83 | 0.93 |
| 7:O:513:ALA:O | 7:O:516:LEU:HD13 | 1.68 | 0.93 |
| 8:P:237:LYS:CB | 8:P:314:ASN:HB3 | 1.98 | 0.93 |
| 2:B:459:LEU:HD22 | 2:B:472:LEU:HG | 1.51 | 0.93 |
| 3:C:42:LYS:CB | 3:C:460:ALA:HA | 1.98 | 0.93 |
| 4:D:524:ILE:HG12 | 7:G:52:LEU:HB3 | 0.94 | 0.93 |
| 3:K:42:LYS:CB | 3:K:460:ALA:HA | 1.98 | 0.93 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:433:LEU:O | 1:A:437:ALA:N | 2.01 | 0.93 |
| 6:F:424:ARG:HE | 6:F:424:ARG:HA | 1.33 | 0.93 |
| 6:F:434:LEU:N | 6:F:434:LEU:CD2 | 2.30 | 0.93 |
| 6:N:53:ILE:C | 6:N:53:ILE:HD12 | 1.89 | 0.93 |
| 7:G:471:ALA:O | 7:G:475:GLY:CA | 2.17 | 0.93 |
| 7:G:513:ALA:O | 7:G:516:LEU:HD13 | 1.68 | 0.93 |
| 6:F:195:GLU:HB3 | 6:F:377:THR:HG22 | 1.51 | 0.93 |
| 6:F:409:LYS:HD3 | 6:F:409:LYS:H | 1.34 | 0.93 |
| 2:J:459:LEU:HD22 | 2:J:472:LEU:HG | 1.51 | 0.93 |
| 7:G:191:ARG:NE | 7:G:192:ASN:H | 1.65 | 0.92 |
| 3:C:57:LEU:N | 3:C:57:LEU:HD23 | 1.83 | 0.92 |
| 1:I:350:PHE:HE2 | 1:I:354:TYR:HB2 | 1.34 | 0.92 |
| 1:I:433:LEU:O | 1:I:437:ALA:N | 2.01 | 0.92 |
| 4:L:523:ASP:O | 7:O:51:ILE:HG23 | 1.69 | 0.92 |
| 2:B:442:THR:HG23 | 2:B:452:SER:HB2 | 1.50 | 0.92 |
| 4:L:210:ILE:HB | 4:L:376:SER:O | 1.69 | 0.92 |
| 6:N:409:LYS:HD3 | 6:N:409:LYS:H | 1.34 | 0.92 |
| 6:N:424:ARG:HE | 6:N:424:ARG:HA | 1.33 | 0.92 |
| 7:O:471:ALA:O | 7:O:475:GLY:N | 2.02 | 0.92 |
| 6:F:434:LEU:CD2 | 6:F:434:LEU:H | 1.80 | 0.92 |
| 2:J:442:THR:HG23 | 2:J:452:SER:HB2 | 1.50 | 0.92 |
| 7:O:516:LEU:HD22 | 7:O:517:ILE:N | 1.83 | 0.92 |
| 6:F:541:LEU:CB | 6:F:542:LYS:CA | 2.22 | 0.92 |
| 4:D:254:VAL:HG11 | 4:D:260:MET:SD | 2.09 | 0.92 |
| 5:E:107:LEU:HD22 | 5:E:544:LEU:HG | 1.49 | 0.92 |
| 4:L:254:VAL:HG11 | 4:L:260:MET:SD | 2.09 | 0.92 |
| 7:G:90:GLN:HG3 | 7:G:101:VAL:HG21 | 1.48 | 0.92 |
| 8:H:209:VAL:HG22 | 8:H:386:LEU:HD11 | 1.52 | 0.92 |
| 6:N:195:GLU:HB3 | 6:N:377:THR:HG22 | 1.51 | 0.92 |
| 7:O:471:ALA:O | 7:O:475:GLY:CA | 2.17 | 0.92 |
| 1:A:250:ASN:CB | 1:A:300:LYS:CB | 2.47 | 0.91 |
| 1:A:228:VAL:CG2 | 1:A:363:GLN:HE22 | 1.82 | 0.91 |
| 6:F:53:ILE:C | 6:F:53:ILE:HD12 | 1.89 | 0.91 |
| 2:B:127:ALA:HB2 | 2:B:430:VAL:HG22 | 1.51 | 0.91 |
| 2:B:21:SER:HG | 1:I:8:SER:N | 1.67 | 0.91 |
| 1:I:228:VAL:CG2 | 1:I:363:GLN:HE22 | 1.82 | 0.91 |
| 5:E:166:ASP:N | 5:E:167:ASP:HB2 | 1.86 | 0.91 |
| 4:D:210:ILE:HB | 4:D:376:SER:O | 1.69 | 0.91 |
| 6:N:151:LEU:HD13 | 6:N:175:THR:HG23 | 0.91 | 0.91 |
| 6:N:36:ASN:HB3 | 6:N:57:LYS:HZ1 | 1.29 | 0.91 |
| 7:G:471:ALA:O | 7:G:475:GLY:N | 2.02 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:250:ASN:CB | 1:I:300:LYS:CB | 2.47 | 0.91 |
| 2:J:3:VAL:O | 2:J:5:ILE:HG21 | 1.71 | 0.91 |
| 2:B:27:ILE:HD12 | 2:B:104:ARG:HH11 | 1.36 | 0.91 |
| 2:B:29:VAL:O | 2:B:33:VAL:CG2 | 2.19 | 0.91 |
| 2:J:27:ILE:HD12 | 2:J:104:ARG:HH11 | 1.36 | 0.91 |
| 4:L:521:ILE:CA | 7:O:50:ASP:O | 2.18 | 0.91 |
| 8:H:113:VAL:HG12 | 8:H:451:GLN:HG3 | 1.53 | 0.91 |
| 6:F:159:LEU:HA | 6:F:164:ALA:CB | 2.01 | 0.90 |
| 6:N:434:LEU:N | 6:N:441:LYS:CB | 2.34 | 0.90 |
| 2:J:422:ILE:CG2 | 2:J:427:SER:HB3 | 2.02 | 0.90 |
| 3:C:264:GLU:C | 3:C:265:LYS:HG3 | 1.91 | 0.90 |
| 2:B:3:VAL:O | 2:B:5:ILE:HG21 | 1.71 | 0.90 |
| 7:G:191:ARG:NE | 7:G:191:ARG:HA | 1.85 | 0.90 |
| 8:P:237:LYS:CB | 8:P:314:ASN:CB | 2.49 | 0.90 |
| 6:F:209:PHE:HE2 | 6:F:376:CYS:HG | 0.92 | 0.90 |
| 8:H:463:LEU:O | 8:H:466:THR:OG1 | 1.87 | 0.90 |
| 6:N:354:VAL:HG13 | 6:N:367:VAL:HG22 | 1.53 | 0.90 |
| 7:O:316:GLY:O | 7:O:317:ARG:HB3 | 1.71 | 0.90 |
| 1:A:350:PHE:HE2 | 1:A:354:TYR:HB2 | 1.34 | 0.90 |
| 6:N:159:LEU:HA | 6:N:164:ALA:CB | 2.01 | 0.90 |
| 2:B:3:VAL:O | 2:B:5:ILE:HD13 | 1.72 | 0.90 |
| 6:F:434:LEU:N | 6:F:441:LYS:CB | 2.34 | 0.90 |
| 8:P:463:LEU:O | 8:P:466:THR:OG1 | 1.87 | 0.90 |
| 3:C:265:LYS:HZ3 | 3:C:268:ASP:HB3 | 1.35 | 0.89 |
| 6:F:354:VAL:HG13 | 6:F:367:VAL:HG22 | 1.53 | 0.89 |
| 5:M:166:ASP:N | 5:M:167:ASP:HB2 | 1.85 | 0.89 |
| 5:M:32:VAL:HG22 | 5:M:33:LYS:H | 1.34 | 0.89 |
| 6:F:109:ILE:HG13 | 5:M:39:LYS:HZ3 | 1.35 | 0.89 |
| 2:J:70:ASP:CB | 6:N:5:LEU:HD22 | 2.02 | 0.89 |
| 7:O:191:ARG:HA | 7:O:191:ARG:NE | 1.85 | 0.89 |
| 8:P:209:VAL:HG22 | 8:P:386:LEU:HD11 | 1.52 | 0.89 |
| 2:B:422:ILE:CG2 | 2:B:427:SER:HB3 | 2.02 | 0.89 |
| 3:K:41:PRO:HA | 3:K:161:THR:CG2 | 2.02 | 0.89 |
| 2:B:4:GLN:HA | 2:B:5:ILE:HG12 | 0.90 | 0.89 |
| 6:F:151:LEU:HD13 | 6:F:175:THR:HG23 | 0.91 | 0.89 |
| 2:J:29:VAL:O | 2:J:33:VAL:CG2 | 2.19 | 0.89 |
| 1:A:156:LEU:HD13 | 1:A:185:LEU:HD11 | 1.54 | 0.89 |
| 7:G:316:GLY:O | 7:G:317:ARG:HB3 | 1.71 | 0.89 |
| 8:H:6:PRO:CB | 4:L:71:LEU:CB | 2.51 | 0.89 |
| 3:C:41:PRO:HA | 3:C:161:THR:CG2 | 2.02 | 0.89 |
| 4:L:521:ILE:CG1 | 7:O:62:ILE:HD11 | 2.01 | 0.89 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:242:LYS:CE | 2:B:247:GLY:H | 1.86 | 0.89 |
| 2:B:72:PRO:HB3 | 3:C:47:MET:HE3 | 1.55 | 0.89 |
| 6:F:452:LEU:C | 6:F:455:PRO:HD2 | 1.93 | 0.89 |
| 6:N:83:GLN:CG | 6:N:94:VAL:HG21 | 2.02 | 0.89 |
| 8:P:113:VAL:HG12 | 8:P:451:GLN:HG3 | 1.54 | 0.88 |
| 1:I:90:GLN:CG | 1:I:101:VAL:HG21 | 2.03 | 0.88 |
| 2:J:3:VAL:O | 2:J:5:ILE:HD13 | 1.72 | 0.88 |
| 6:N:430:ASN:CA | 6:N:433:LYS:HG2 | 2.00 | 0.88 |
| 5:E:174:GLU:O | 5:E:175:LEU:HG | 1.74 | 0.88 |
| 2:J:242:LYS:CE | 2:J:247:GLY:H | 1.86 | 0.88 |
| 6:N:143:LEU:CD1 | 6:N:145:ASN:H | 1.85 | 0.88 |
| 8:P:6:PRO:HB2 | 8:P:7:GLN:HG3 | 1.55 | 0.88 |
| 8:H:388:GLY:HA3 | 8:H:394:LEU:HD21 | 1.53 | 0.88 |
| 1:I:350:PHE:CE2 | 1:I:354:TYR:HB2 | 2.09 | 0.88 |
| 2:J:4:GLN:HA | 2:J:5:ILE:HG12 | 0.89 | 0.88 |
| 6:N:452:LEU:C | 6:N:455:PRO:HD2 | 1.93 | 0.88 |
| 6:F:83:GLN:CG | 6:F:94:VAL:HG21 | 2.02 | 0.88 |
| 5:M:173:ASP:HB3 | 5:M:437:SER:CB | 2.04 | 0.88 |
| 5:E:32:VAL:HG22 | 5:E:33:LYS:H | 1.34 | 0.88 |
| 3:K:265:LYS:HZ3 | 3:K:268:ASP:HB3 | 1.34 | 0.88 |
| 6:N:209:PHE:HE2 | 6:N:376:CYS:HG | 0.92 | 0.88 |
| 1:A:90:GLN:CG | 1:A:101:VAL:HG21 | 2.03 | 0.88 |
| 5:M:174:GLU:O | 5:M:175:LEU:HG | 1.74 | 0.88 |
| 5:E:320:VAL:HG22 | 5:E:341:PRO:HD2 | 1.56 | 0.88 |
| 8:H:237:LYS:CB | 8:H:314:ASN:CB | 2.49 | 0.88 |
| 6:N:330:LEU:HD12 | 6:N:375:SER:HB3 | 1.57 | 0.88 |
| 6:N:541:LEU:HB3 | 6:N:542:LYS:HA | 1.56 | 0.88 |
| 2:B:514:ILE:HD12 | 3:C:47:MET:HB3 | 1.56 | 0.87 |
| 6:F:330:LEU:HD12 | 6:F:375:SER:HB3 | 1.56 | 0.87 |
| 7:G:188:SER:C | 7:G:190:ASP:HB2 | 1.95 | 0.87 |
| 1:I:156:LEU:HD13 | 1:I:185:LEU:HD11 | 1.54 | 0.87 |
| 2:B:474:LEU:HG | 9:B:601:ADP:C2 | 2.09 | 0.87 |
| 3:C:230:VAL:CG1 | 3:C:302:SER:OG | 2.22 | 0.87 |
| 3:K:230:VAL:CG1 | 3:K:302:SER:OG | 2.22 | 0.87 |
| 3:K:269:TRP:CZ3 | 6:N:247:VAL:HB | 2.09 | 0.87 |
| 3:C:329:ALA:HB1 | 3:C:334:ALA:O | 1.73 | 0.87 |
| 6:F:430:ASN:CA | 6:F:433:LYS:HG2 | 2.00 | 0.87 |
| 7:O:188:SER:C | 7:O:190:ASP:HB2 | 1.95 | 0.87 |
| 2:J:285:ILE:HD11 | 2:J:289:LEU:HD23 | 1.56 | 0.87 |
| 6:N:362:GLU:HG2 | 6:N:364:PHE:CE2 | 2.10 | 0.87 |
| 6:F:38:GLY:H | 9:F:601:ADP:H5'1 | 1.36 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:G:43:THR:CG2 | 7:G:64:ASN:HB3 | 2.05 | 0.87 |
| 5:E:173:ASP:HB3 | 5:E:437:SER:CB | 2.04 | 0.87 |
| 7:O:170:LEU:O | 7:O:170:LEU:HD23 | 1.75 | 0.87 |
| 1:A:350:PHE:CE2 | 1:A:354:TYR:HB2 | 2.09 | 0.86 |
| 2:B:285:ILE:HD11 | 2:B:289:LEU:HD23 | 1.56 | 0.86 |
| 8:H:204:VAL:HG13 | 8:H:405:VAL:HG12 | 1.57 | 0.86 |
| 6:N:5:LEU:HA | 6:N:6:LEU:HB3 | 1.57 | 0.86 |
| 6:N:5:LEU:HB2 | 6:N:6:LEU:O | 1.75 | 0.86 |
| 7:O:43:THR:CG2 | 7:O:64:ASN:HB3 | 2.05 | 0.86 |
| 6:F:143:LEU:CD1 | 6:F:145:ASN:H | 1.85 | 0.86 |
| 3:K:15:THR:O | 3:K:16:THR:O | 1.93 | 0.86 |
| 8:P:388:GLY:HA3 | 8:P:394:LEU:HD21 | 1.54 | 0.86 |
| 6:F:362:GLU:HG2 | 6:F:364:PHE:CE2 | 2.10 | 0.86 |
| 2:J:208:LEU:HD13 | 2:J:366:THR:HG22 | 1.56 | 0.86 |
| 6:F:117:ILE:HG12 | 5:M:33:LYS:HE2 | 1.56 | 0.86 |
| 3:K:264:GLU:C | 3:K:265:LYS:HG3 | 1.91 | 0.86 |
| 7:O:148:THR:O | 7:O:149:SER:HB3 | 1.75 | 0.86 |
| 3:C:129:LEU:HG | 3:C:514:ILE:HG21 | 1.57 | 0.86 |
| 3:K:129:LEU:HG | 3:K:514:ILE:HG21 | 1.57 | 0.86 |
| 8:P:24:ALA:HA | 8:P:531:ALA:O | 1.76 | 0.86 |
| 6:F:154:ALA:CB | 6:F:402:VAL:CG2 | 2.54 | 0.86 |
| 6:F:411:ILE:HG22 | 6:F:412:ILE:H | 1.39 | 0.86 |
| 8:H:6:PRO:HB2 | 8:H:7:GLN:HG3 | 1.55 | 0.86 |
| 5:E:401:THR:C | 5:E:402:LYS:HG3 | 1.96 | 0.85 |
| 6:F:151:LEU:HD13 | 6:F:175:THR:HG21 | 0.86 | 0.85 |
| 6:F:541:LEU:HB3 | 6:F:542:LYS:HA | 1.56 | 0.85 |
| 5:M:320:VAL:HG22 | 5:M:341:PRO:HD2 | 1.56 | 0.85 |
| 6:N:411:ILE:HG22 | 6:N:412:ILE:H | 1.39 | 0.85 |
| 3:C:15:THR:O | 3:C:16:THR:O | 1.93 | 0.85 |
| 5:E:166:ASP:CA | 5:E:167:ASP:HB2 | 2.06 | 0.85 |
| 6:F:5:LEU:HA | 6:F:6:LEU:HB3 | 1.57 | 0.85 |
| 7:G:516:LEU:HD22 | 7:G:516:LEU:O | 1.76 | 0.85 |
| 3:K:329:ALA:HB1 | 3:K:334:ALA:O | 1.73 | 0.85 |
| 4:L:185:ASN:N | 4:L:186:SER:C | 2.30 | 0.85 |
| 4:L:72:HIS:CB | 4:L:75:ALA:HB3 | 2.05 | 0.85 |
| 6:F:5:LEU:HB2 | 6:F:6:LEU:O | 1.75 | 0.85 |
| 7:G:189:LEU:O | 7:G:189:LEU:HD12 | 1.77 | 0.85 |
| 2:J:208:LEU:HD11 | 2:J:364:ALA:HB1 | 1.59 | 0.85 |
| 6:N:154:ALA:CB | 6:N:402:VAL:CG2 | 2.54 | 0.85 |
| 6:N:243:GLU:HA | 6:N:243:GLU:OE2 | 1.76 | 0.85 |
| 4:D:520:ARG:O | 7:G:49:SER:CB | 2.23 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:185:ASN:N | 4:D:186:SER:C | 2.30 | 0.85 |
| 2:B:208:LEU:HD11 | 2:B:364:ALA:HB1 | 1.59 | 0.85 |
| 2:B:211:GLY:HA3 | 2:B:355:LYS:O | 1.77 | 0.85 |
| 2:B:245:ILE:O | 2:B:246:PHE:CD2 | 2.30 | 0.85 |
| 2:B:422:ILE:CB | 2:B:427:SER:HB2 | 2.07 | 0.85 |
| 4:D:72:HIS:CB | 4:D:75:ALA:HB3 | 2.05 | 0.85 |
| 7:G:148:THR:O | 7:G:149:SER:HB3 | 1.75 | 0.85 |
| 6:N:75:LEU:HD13 | 6:N:527:LEU:HD21 | 1.59 | 0.85 |
| 1:A:88:GLN:O | 1:A:92:ARG:HD2 | 1.76 | 0.85 |
| 6:N:151:LEU:HD13 | 6:N:175:THR:HG21 | 0.86 | 0.85 |
| 6:N:224:MET:HE1 | 6:N:316:ALA:H | 1.42 | 0.85 |
| 1:A:93:GLU:CB | 1:A:94:ILE:CD1 | 2.55 | 0.85 |
| 2:J:422:ILE:CB | 2:J:427:SER:HB2 | 2.07 | 0.85 |
| 8:H:346:ALA:N | 8:H:347:PRO:HD3 | 1.92 | 0.85 |
| 8:H:24:ALA:HA | 8:H:531:ALA:O | 1.76 | 0.85 |
| 2:J:72:PRO:O | 2:J:76:VAL:HG23 | 1.76 | 0.85 |
| 2:B:72:PRO:O | 2:B:76:VAL:HG23 | 1.76 | 0.84 |
| 5:E:104:LEU:HD21 | 5:E:123:VAL:HG13 | 1.58 | 0.84 |
| 4:L:285:VAL:HA | 4:L:311:MET:O | 1.78 | 0.84 |
| 5:M:166:ASP:CA | 5:M:167:ASP:HB2 | 2.07 | 0.84 |
| 8:P:204:VAL:HG13 | 8:P:405:VAL:HG12 | 1.57 | 0.84 |
| 7:O:189:LEU:HD12 | 7:O:189:LEU:O | 1.77 | 0.84 |
| 7:O:516:LEU:HD22 | 7:O:516:LEU:O | 1.76 | 0.84 |
| 4:D:330:CYS:CB | 4:D:345:ASP:OD1 | 2.25 | 0.84 |
| 4:L:521:ILE:CD1 | 7:O:62:ILE:CD1 | 2.48 | 0.84 |
| 6:F:75:LEU:HD13 | 6:F:527:LEU:HD21 | 1.59 | 0.84 |
| 2:J:245:ILE:O | 2:J:246:PHE:CD2 | 2.30 | 0.84 |
| 6:N:3:LEU:N | 6:N:4:GLN:CB | 2.41 | 0.84 |
| 7:O:109:MET:CG | 7:O:514:THR:HG22 | 2.08 | 0.84 |
| 7:O:189:LEU:CA | 7:O:190:ASP:HB2 | 1.94 | 0.84 |
| 4:D:330:CYS:CB | 4:D:345:ASP:CG | 2.45 | 0.84 |
| 7:G:170:LEU:O | 7:G:170:LEU:HD23 | 1.75 | 0.84 |
| 1:I:158:ASN:HB3 | 1:I:516:GLY:O | 1.77 | 0.84 |
| 1:I:88:GLN:O | 1:I:92:ARG:HD2 | 1.76 | 0.84 |
| 7:O:186:VAL:HG21 | 7:O:400:VAL:CG2 | 2.08 | 0.84 |
| 4:D:250:ASN:HA | 7:G:259:VAL:HG12 | 1.60 | 0.84 |
| 4:D:285:VAL:HA | 4:D:311:MET:O | 1.78 | 0.84 |
| 6:N:424:ARG:HG2 | 6:N:483:SER:HA | 1.60 | 0.84 |
| 6:F:36:ASN:HB3 | 6:F:57:LYS:HZ1 | 1.41 | 0.84 |
| 1:I:93:GLU:CB | 1:I:94:ILE:CD1 | 2.54 | 0.84 |
| 4:D:71:LEU:CB | 8:P:6:PRO:CB | 2.55 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:329:PHE:C | 2:B:329:PHE:CD2 | 2.51 | 0.84 |
| 6:F:35:THR:HG22 | 6:F:42:THR:O | 1.78 | 0.84 |
| 4:L:524:ILE:HG12 | 7:O:52:LEU:HB3 | 0.87 | 0.84 |
| 4:D:185:ASN:CB | 4:D:186:SER:HB2 | 2.08 | 0.83 |
| 4:D:524:ILE:CA | 7:G:52:LEU:O | 2.24 | 0.83 |
| 2:J:361:ALA:H | 2:J:362:GLY:HA2 | 1.01 | 0.83 |
| 5:M:104:LEU:HD21 | 5:M:123:VAL:HG13 | 1.58 | 0.83 |
| 5:M:401:THR:C | 5:M:402:LYS:HG3 | 1.97 | 0.83 |
| 6:N:415:ALA:HB2 | 6:N:506:ILE:HG21 | 1.57 | 0.83 |
| 2:B:88:VAL:HG13 | 2:B:393:GLN:HE22 | 1.43 | 0.83 |
| 5:E:84:THR:HG22 | 5:E:86:ASP:H | 1.42 | 0.83 |
| 6:F:3:LEU:N | 6:F:4:GLN:CB | 2.41 | 0.83 |
| 7:G:109:MET:CG | 7:G:514:THR:HG22 | 2.08 | 0.83 |
| 7:O:94:VAL:HG21 | 7:O:502:VAL:CG2 | 2.06 | 0.83 |
| 4:L:151:VAL:HG22 | 4:L:175:VAL:HG21 | 1.58 | 0.83 |
| 2:B:320:VAL:HG21 | 2:B:337:LEU:CB | 2.09 | 0.83 |
| 6:F:539:SER:CB | 6:F:542:LYS:HD2 | 2.09 | 0.83 |
| 4:D:254:VAL:HG21 | 8:H:265:VAL:HG22 | 1.60 | 0.83 |
| 8:P:346:ALA:N | 8:P:347:PRO:HD3 | 1.92 | 0.83 |
| 7:G:186:VAL:HG21 | 7:G:400:VAL:CG2 | 2.08 | 0.83 |
| 1:A:264:ILE:HD11 | 7:G:259:VAL:HG23 | 1.61 | 0.83 |
| 6:N:382:GLY:HA3 | 6:N:388:LEU:HD21 | 1.61 | 0.83 |
| 6:N:56:THR:HB | 6:N:390:GLN:NE2 | 1.94 | 0.83 |
| 6:N:35:THR:HG22 | 6:N:42:THR:O | 1.78 | 0.83 |
| 3:K:430:LYS:O | 3:K:433:GLN:HG3 | 1.78 | 0.83 |
| 6:N:539:SER:CB | 6:N:542:LYS:HD2 | 2.09 | 0.83 |
| 7:G:186:VAL:HG21 | 7:G:400:VAL:HG21 | 1.59 | 0.83 |
| 7:O:175:ALA:O | 7:O:179:VAL:HG23 | 1.79 | 0.83 |
| 2:B:37:LEU:HA | 9:B:601:ADP:H5'1 | 1.61 | 0.83 |
| 6:F:243:GLU:OE2 | 6:F:243:GLU:HA | 1.76 | 0.83 |
| 6:F:415:ALA:HB2 | 6:F:506:ILE:HG21 | 1.58 | 0.83 |
| 5:M:84:THR:HG22 | 5:M:86:ASP:H | 1.42 | 0.83 |
| 7:O:189:LEU:HA | 7:O:190:ASP:HB3 | 0.83 | 0.83 |
| 4:D:521:ILE:CD1 | 7:G:62:ILE:CD1 | 2.50 | 0.82 |
| 7:G:175:ALA:O | 7:G:179:VAL:HG23 | 1.79 | 0.82 |
| 2:J:211:GLY:HA3 | 2:J:355:LYS:O | 1.77 | 0.82 |
| 5:M:173:ASP:HB3 | 5:M:437:SER:HB2 | 1.60 | 0.82 |
| 2:J:329:PHE:CD2 | 2:J:329:PHE:C | 2.51 | 0.82 |
| 1:A:158:ASN:HB3 | 1:A:516:GLY:O | 1.77 | 0.82 |
| 6:F:382:GLY:HA3 | 6:F:388:LEU:HD21 | 1.61 | 0.82 |
| 3:K:306:GLN:HA | 3:K:316:VAL:HG11 | 1.62 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:L:185:ASN:CB | 4:L:186:SER:HB2 | 2.08 | 0.82 |
| 6:F:56:THR:HB | 6:F:390:GLN:NE2 | 1.94 | 0.82 |
| 2:J:4:GLN:CA | 2:J:5:ILE:CB | 2.57 | 0.82 |
| 2:B:4:GLN:CA | 2:B:5:ILE:CG2 | 2.57 | 0.82 |
| 4:D:99:LEU:O | 4:D:103:LEU:HB2 | 1.79 | 0.82 |
| 6:F:3:LEU:HA | 6:F:5:LEU:HG | 1.60 | 0.82 |
| 2:J:176:LEU:HD23 | 2:J:208:LEU:HB2 | 1.60 | 0.82 |
| 2:J:88:VAL:HG13 | 2:J:393:GLN:HE22 | 1.43 | 0.82 |
| 2:J:4:GLN:CA | 2:J:5:ILE:CG2 | 2.57 | 0.82 |
| 2:B:361:ALA:H | 2:B:362:GLY:HA2 | 1.01 | 0.82 |
| 2:J:320:VAL:HG21 | 2:J:337:LEU:CB | 2.09 | 0.82 |
| 3:C:306:GLN:HA | 3:C:316:VAL:HG11 | 1.62 | 0.82 |
| 3:C:493:ASP:HB3 | 3:C:495:VAL:HG12 | 1.62 | 0.82 |
| 4:D:151:VAL:HG22 | 4:D:175:VAL:HG21 | 1.58 | 0.82 |
| 4:D:134:ILE:HD11 | 4:D:424:ARG:CD | 2.09 | 0.82 |
| 4:D:521:ILE:HG23 | 7:G:51:ILE:HA | 1.61 | 0.82 |
| 1:I:12:THR:HG21 | 5:M:97:ASP:H | 1.45 | 0.82 |
| 7:O:186:VAL:HG21 | 7:O:400:VAL:HG21 | 1.59 | 0.82 |
| 3:C:430:LYS:O | 3:C:433:GLN:HG3 | 1.79 | 0.82 |
| 7:G:189:LEU:HA | 7:G:190:ASP:HB3 | 0.83 | 0.82 |
| 6:N:540:THR:C | 6:N:541:LEU:CD2 | 2.47 | 0.82 |
| 4:D:521:ILE:HG23 | 7:G:50:ASP:O | 1.80 | 0.82 |
| 7:G:191:ARG:CD | 7:G:192:ASN:H | 1.92 | 0.81 |
| 8:H:74:GLU:HA | 8:H:74:GLU:OE1 | 1.78 | 0.81 |
| 7:O:191:ARG:CD | 7:O:192:ASN:H | 1.92 | 0.81 |
| 4:D:246:PRO:HB2 | 4:D:250:ASN:OD1 | 1.80 | 0.81 |
| 6:F:430:ASN:O | 6:F:433:LYS:N | 2.12 | 0.81 |
| 2:J:249:LYS:O | 6:N:250:GLY:N | 2.12 | 0.81 |
| 2:J:361:ALA:H | 2:J:362:GLY:CA | 1.86 | 0.81 |
| 7:G:94:VAL:HG21 | 7:G:502:VAL:CG2 | 2.06 | 0.81 |
| 3:K:506:LYS:HA | 3:K:506:LYS:HE2 | 1.63 | 0.81 |
| 8:P:74:GLU:HA | 8:P:74:GLU:OE1 | 1.79 | 0.81 |
| 2:B:4:GLN:N | 2:B:5:ILE:HG23 | 1.96 | 0.81 |
| 6:F:424:ARG:HG2 | 6:F:483:SER:HA | 1.60 | 0.81 |
| 6:F:478:ASP:O | 6:F:482:ASP:HB3 | 1.80 | 0.81 |
| 4:L:134:ILE:HD11 | 4:L:424:ARG:CD | 2.09 | 0.81 |
| 5:M:166:ASP:CB | 5:M:167:ASP:HB2 | 2.11 | 0.81 |
| 6:F:143:LEU:HA | 6:F:145:ASN:N | 1.95 | 0.81 |
| 5:M:368:ASP:O | 5:M:370:SER:N | 2.13 | 0.81 |
| 5:M:401:THR:O | 5:M:402:LYS:HG3 | 1.81 | 0.81 |
| 6:N:430:ASN:O | 6:N:433:LYS:N | 2.12 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:E:173:ASP:HB3 | 5:E:437:SER:HB2 | 1.60 | 0.81 |
| 6:F:540:THR:C | 6:F:541:LEU:CD2 | 2.47 | 0.81 |
| 2:J:426:LYS:O | 2:J:429:ALA:HB3 | 1.81 | 0.81 |
| 6:N:3:LEU:HA | 6:N:5:LEU:HG | 1.60 | 0.81 |
| 8:P:206:SER:CB | 8:P:381:THR:HG22 | 2.11 | 0.81 |
| 2:B:426:LYS:O | 2:B:429:ALA:HB3 | 1.81 | 0.81 |
| 2:B:4:GLN:HA | 2:B:5:ILE:CG2 | 2.11 | 0.81 |
| 5:E:166:ASP:CB | 5:E:167:ASP:HB2 | 2.10 | 0.81 |
| 5:E:401:THR:O | 5:E:402:LYS:HG3 | 1.81 | 0.81 |
| 6:F:5:LEU:HA | 6:F:6:LEU:HB2 | 1.62 | 0.81 |
| 7:G:145:VAL:O | 7:G:408:LEU:HA | 1.80 | 0.81 |
| 7:G:171:ILE:HG23 | 7:G:178:PHE:CD2 | 2.16 | 0.81 |
| 2:J:4:GLN:N | 2:J:5:ILE:HG23 | 1.96 | 0.81 |
| 6:N:2:SER:HA | 6:N:3:LEU:HB2 | 1.63 | 0.81 |
| 4:D:499:GLN:HE22 | 9:D:601:ADP:H2' | 1.45 | 0.81 |
| 3:K:41:PRO:HA | 3:K:161:THR:HG22 | 1.63 | 0.81 |
| 3:K:493:ASP:HB3 | 3:K:495:VAL:HG12 | 1.62 | 0.81 |
| 4:L:99:LEU:O | 4:L:103:LEU:HB2 | 1.79 | 0.81 |
| 6:N:541:LEU:N | 6:N:541:LEU:HD22 | 1.95 | 0.81 |
| 6:N:452:LEU:O | 6:N:455:PRO:HD2 | 1.80 | 0.81 |
| 7:O:120:ILE:HD13 | 7:O:120:ILE:H | 1.46 | 0.81 |
| 2:J:263:LYS:HZ3 | 3:K:266:GLU:HB3 | 1.43 | 0.81 |
| 2:J:4:GLN:HA | 2:J:5:ILE:CG2 | 2.11 | 0.81 |
| 7:O:171:ILE:HG23 | 7:O:178:PHE:CD2 | 2.16 | 0.81 |
| 8:P:360:THR:HG22 | 8:P:369:THR:HG22 | 1.63 | 0.81 |
| 2:B:4:GLN:CA | 2:B:5:ILE:CB | 2.58 | 0.81 |
| 5:E:368:ASP:O | 5:E:370:SER:N | 2.13 | 0.81 |
| 7:G:232:GLN:CG | 7:G:313:PHE:HA | 2.10 | 0.81 |
| 2:B:176:LEU:HD23 | 2:B:208:LEU:HB2 | 1.60 | 0.80 |
| 6:F:195:GLU:HG2 | 6:F:197:MET:SD | 2.21 | 0.80 |
| 7:G:248:LEU:CB | 7:G:299:ILE:HD12 | 2.11 | 0.80 |
| 4:D:71:LEU:CB | 8:P:6:PRO:HB3 | 2.12 | 0.80 |
| 1:A:517:VAL:O | 1:A:518:LEU:CG | 2.28 | 0.80 |
| 2:B:242:LYS:HB2 | 3:C:269:TRP:HZ2 | 1.45 | 0.80 |
| 8:H:360:THR:HG22 | 8:H:369:THR:HG22 | 1.63 | 0.80 |
| 4:L:246:PRO:HB2 | 4:L:250:ASN:OD1 | 1.80 | 0.80 |
| 6:N:143:LEU:HA | 6:N:145:ASN:N | 1.95 | 0.80 |
| 5:E:245:LEU:HD13 | 5:E:247:LYS:H | 1.47 | 0.80 |
| 7:G:412:GLY:O | 7:G:491:ASN:ND2 | 2.14 | 0.80 |
| 1:I:224:LEU:CD1 | 1:I:226:CYS:HB2 | 2.11 | 0.80 |
| 3:K:457:ILE:CD1 | 3:K:467:LEU:HD13 | 2.11 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:264:ILE:HD11 | 7:O:259:VAL:HG23 | 1.62 | 0.80 |
| 6:F:452:LEU:O | 6:F:455:PRO:HD2 | 1.80 | 0.80 |
| 6:F:541:LEU:N | 6:F:541:LEU:HD22 | 1.95 | 0.80 |
| 1:I:9:ARG:CB | 1:I:10:SER:O | 2.30 | 0.80 |
| 2:J:4:GLN:C | 2:J:5:ILE:HG23 | 2.02 | 0.80 |
| 7:O:145:VAL:O | 7:O:408:LEU:HA | 1.81 | 0.80 |
| 4:D:230:GLU:O | 4:D:348:ASP:O | 2.00 | 0.80 |
| 5:E:401:THR:O | 5:E:402:LYS:CG | 2.30 | 0.80 |
| 6:F:215:LEU:HB3 | 6:F:217:HIS:HD2 | 1.46 | 0.80 |
| 7:G:189:LEU:CA | 7:G:190:ASP:HB2 | 1.94 | 0.80 |
| 4:D:521:ILE:CG1 | 7:G:62:ILE:HD11 | 2.11 | 0.80 |
| 4:L:72:HIS:O | 4:L:76:ARG:CB | 2.30 | 0.80 |
| 1:I:517:VAL:O | 1:I:518:LEU:CG | 2.28 | 0.80 |
| 7:O:248:LEU:CB | 7:O:299:ILE:HD12 | 2.11 | 0.80 |
| 8:H:206:SER:CB | 8:H:381:THR:HG22 | 2.11 | 0.80 |
| 5:M:401:THR:O | 5:M:402:LYS:CG | 2.30 | 0.80 |
| 4:D:323:PHE:HA | 4:D:374:THR:HG21 | 1.64 | 0.80 |
| 2:J:250:PHE:HA | 6:N:250:GLY:O | 1.81 | 0.80 |
| 2:J:132:LEU:HD21 | 2:J:495:ARG:HG3 | 1.64 | 0.80 |
| 2:B:233:ILE:O | 2:B:325:VAL:HB | 1.82 | 0.80 |
| 2:B:361:ALA:H | 2:B:362:GLY:CA | 1.86 | 0.80 |
| 3:C:506:LYS:HA | 3:C:506:LYS:HE2 | 1.63 | 0.80 |
| 5:E:401:THR:O | 5:E:402:LYS:CE | 2.30 | 0.80 |
| 4:L:336:ILE:O | 4:L:336:ILE:HG22 | 1.81 | 0.80 |
| 6:N:195:GLU:HG2 | 6:N:197:MET:SD | 2.21 | 0.80 |
| 7:O:232:GLN:CG | 7:O:313:PHE:HA | 2.10 | 0.80 |
| 1:A:224:LEU:CD1 | 1:A:226:CYS:HB2 | 2.11 | 0.80 |
| 6:N:5:LEU:HA | 6:N:6:LEU:HB2 | 1.62 | 0.80 |
| 4:D:72:HIS:O | 4:D:76:ARG:CB | 2.30 | 0.79 |
| 6:F:276:LYS:O | 6:F:279:ASP:CB | 2.30 | 0.79 |
| 6:F:2:SER:HA | 6:F:3:LEU:HB2 | 1.63 | 0.79 |
| 7:G:191:ARG:NE | 7:G:192:ASN:N | 2.30 | 0.79 |
| 7:O:191:ARG:NE | 7:O:192:ASN:N | 2.30 | 0.79 |
| 7:O:412:GLY:O | 7:O:491:ASN:ND2 | 2.14 | 0.79 |
| 8:P:24:ALA:O | 8:P:28:ILE:CG1 | 2.30 | 0.79 |
| 1:A:9:ARG:CB | 1:A:10:SER:O | 2.30 | 0.79 |
| 2:B:463:ILE:C | 2:B:467:ILE:HG12 | 2.01 | 0.79 |
| 7:G:191:ARG:HE | 7:G:191:ARG:CA | 1.94 | 0.79 |
| 8:H:24:ALA:O | 8:H:28:ILE:HG12 | 1.82 | 0.79 |
| 6:N:276:LYS:O | 6:N:279:ASP:CB | 2.30 | 0.79 |
| 6:N:46:LEU:N | 6:N:54:LYS:O | 2.14 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:82:SER:HB2 | 3:C:97:ILE:HD11 | 1.64 | 0.79 |
| 7:G:188:SER:O | 7:G:190:ASP:CB | 2.28 | 0.79 |
| 8:H:49:CYS:O | 8:H:466:THR:HB | 1.83 | 0.79 |
| 5:M:509:ASN:HB3 | 5:M:521:ASP:HB3 | 1.64 | 0.79 |
| 2:B:4:GLN:C | 2:B:5:ILE:HG23 | 2.02 | 0.79 |
| 3:K:264:GLU:O | 3:K:265:LYS:CG | 2.30 | 0.79 |
| 6:N:215:LEU:HB3 | 6:N:217:HIS:HD2 | 1.46 | 0.79 |
| 2:B:295:GLU:C | 6:F:337:GLN:HE22 | 1.86 | 0.79 |
| 1:I:180:VAL:HG13 | 1:I:406:LEU:HD23 | 1.63 | 0.79 |
| 2:J:463:ILE:C | 2:J:467:ILE:HG12 | 2.01 | 0.79 |
| 8:P:49:CYS:O | 8:P:466:THR:HB | 1.82 | 0.79 |
| 2:B:3:VAL:O | 2:B:5:ILE:CD1 | 2.30 | 0.79 |
| 2:B:475:ASN:HD22 | 2:B:475:ASN:H | 1.28 | 0.79 |
| 8:H:24:ALA:O | 8:H:28:ILE:CG1 | 2.30 | 0.79 |
| 1:I:93:GLU:C | 1:I:94:ILE:HD12 | 2.03 | 0.79 |
| 3:K:82:SER:HB2 | 3:K:97:ILE:HD11 | 1.64 | 0.79 |
| 4:L:230:GLU:O | 4:L:348:ASP:O | 2.00 | 0.79 |
| 6:N:478:ASP:O | 6:N:482:ASP:HB3 | 1.80 | 0.79 |
| 4:L:250:ASN:HA | 7:O:259:VAL:CG1 | 2.12 | 0.79 |
| 6:F:433:LYS:CG | 6:F:444:ILE:HG21 | 2.13 | 0.79 |
| 7:G:120:ILE:HD13 | 7:G:120:ILE:H | 1.46 | 0.79 |
| 2:J:233:ILE:O | 2:J:325:VAL:HB | 1.82 | 0.79 |
| 2:J:3:VAL:O | 2:J:5:ILE:CG2 | 2.30 | 0.79 |
| 2:J:475:ASN:HD22 | 2:J:475:ASN:H | 1.28 | 0.79 |
| 7:O:191:ARG:HE | 7:O:191:ARG:CA | 1.94 | 0.79 |
| 7:O:455:GLU:HG3 | 7:O:461:ALA:CB | 2.13 | 0.79 |
| 1:A:180:VAL:HG13 | 1:A:406:LEU:HD23 | 1.63 | 0.79 |
| 2:B:206:SER:HB3 | 2:B:368:VAL:HG13 | 1.65 | 0.79 |
| 2:B:132:LEU:HD21 | 2:B:495:ARG:HG3 | 1.64 | 0.79 |
| 2:B:3:VAL:O | 2:B:5:ILE:CG2 | 2.30 | 0.79 |
| 4:D:524:ILE:HG23 | 7:G:52:LEU:O | 1.82 | 0.79 |
| 2:J:37:LEU:HA | 9:J:601:ADP:H5'1 | 1.65 | 0.79 |
| 7:O:125:ILE:HA | 7:O:438:ILE:HG12 | 1.65 | 0.79 |
| 2:B:70:ASP:HB2 | 6:F:5:LEU:HD22 | 1.65 | 0.79 |
| 3:C:41:PRO:HA | 3:C:161:THR:HG22 | 1.63 | 0.79 |
| 3:C:457:ILE:CD1 | 3:C:467:LEU:HD13 | 2.11 | 0.79 |
| 1:A:123:THR:HG21 | 5:E:68:ARG:HE | 1.46 | 0.79 |
| 6:F:117:ILE:HD12 | 5:M:34:ASP:O | 1.81 | 0.79 |
| 5:M:245:LEU:HD13 | 5:M:247:LYS:H | 1.47 | 0.79 |
| 5:M:253:GLN:CA | 5:M:254:MET:CB | 2.61 | 0.79 |
| 6:N:501:PRO:HB3 | 6:N:506:ILE:CB | 2.11 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:N:53:ILE:CD1 | 6:N:53:ILE:O | 2.30 | 0.79 |
| 7:O:378:LEU:HD11 | 7:O:393:LEU:HD12 | 1.65 | 0.79 |
| 2:B:3:VAL:O | 2:B:5:ILE:CG1 | 2.32 | 0.78 |
| 6:N:433:LYS:CG | 6:N:444:ILE:HG21 | 2.13 | 0.78 |
| 8:P:24:ALA:O | 8:P:28:ILE:HG12 | 1.82 | 0.78 |
| 2:J:3:VAL:O | 2:J:5:ILE:CD1 | 2.30 | 0.78 |
| 7:O:191:ARG:CA | 7:O:191:ARG:NE | 2.46 | 0.78 |
| 4:D:336:ILE:O | 4:D:336:ILE:HG22 | 1.81 | 0.78 |
| 6:F:501:PRO:HB3 | 6:F:506:ILE:CB | 2.12 | 0.78 |
| 2:J:3:VAL:O | 2:J:5:ILE:CG1 | 2.31 | 0.78 |
| 7:O:188:SER:O | 7:O:190:ASP:CB | 2.28 | 0.78 |
| 7:O:191:ARG:CZ | 7:O:192:ASN:H | 1.97 | 0.78 |
| 5:E:253:GLN:CA | 5:E:254:MET:CB | 2.61 | 0.78 |
| 1:A:12:THR:HG21 | 5:E:97:ASP:H | 1.47 | 0.78 |
| 4:L:323:PHE:HA | 4:L:374:THR:HG21 | 1.64 | 0.78 |
| 6:N:36:ASN:HA | 6:N:57:LYS:HD2 | 1.66 | 0.78 |
| 8:H:206:SER:HB2 | 8:H:381:THR:CG2 | 2.13 | 0.78 |
| 5:E:166:ASP:HB3 | 5:E:167:ASP:HB2 | 1.66 | 0.78 |
| 7:G:191:ARG:NE | 7:G:191:ARG:CA | 2.46 | 0.78 |
| 2:J:329:PHE:O | 2:J:329:PHE:HD2 | 1.67 | 0.78 |
| 2:J:469:THR:O | 2:J:470:SER:HB2 | 1.82 | 0.78 |
| 5:M:401:THR:O | 5:M:402:LYS:CE | 2.30 | 0.78 |
| 6:N:35:THR:CG2 | 6:N:42:THR:O | 2.32 | 0.78 |
| 5:E:509:ASN:HB3 | 5:E:521:ASP:HB3 | 1.64 | 0.78 |
| 6:F:331:VAL:HG12 | 6:F:332:THR:HG23 | 1.65 | 0.78 |
| 6:N:221:HIS:HB2 | 6:N:224:MET:HG3 | 1.66 | 0.78 |
| 6:N:331:VAL:HG12 | 6:N:332:THR:HG23 | 1.65 | 0.78 |
| 2:B:72:PRO:HB3 | 3:C:47:MET:CE | 2.13 | 0.78 |
| 4:D:292:ILE:H | 4:D:293:LEU:HA | 1.48 | 0.78 |
| 7:G:455:GLU:HG3 | 7:G:461:ALA:CB | 2.13 | 0.78 |
| 8:H:6:PRO:HB3 | 4:L:71:LEU:CB | 2.11 | 0.78 |
| 7:G:212:SER:HB3 | 7:G:378:LEU:HA | 1.66 | 0.78 |
| 2:J:208:LEU:HD12 | 2:J:209:ASP:H | 1.48 | 0.78 |
| 2:B:492:LYS:HE2 | 2:B:493:LEU:H | 1.48 | 0.77 |
| 6:F:36:ASN:HA | 6:F:57:LYS:HD2 | 1.66 | 0.77 |
| 4:D:241:ILE:O | 4:D:299:ASP:HB2 | 1.83 | 0.77 |
| 4:L:292:ILE:H | 4:L:293:LEU:HA | 1.48 | 0.77 |
| 5:M:88:ALA:HB1 | 5:M:109:LYS:NZ | 2.00 | 0.77 |
| 5:M:166:ASP:HB3 | 5:M:167:ASP:HB2 | 1.66 | 0.77 |
| 1:A:93:GLU:C | 1:A:94:ILE:HD12 | 2.03 | 0.77 |
| 6:F:151:LEU:HD12 | 6:F:175:THR:HG21 | 1.65 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:L:241:ILE:O | 4:L:299:ASP:HB2 | 1.83 | 0.77 |
| 6:N:395:VAL:O | 6:N:399:LEU:HB2 | 1.85 | 0.77 |
| 4:L:521:ILE:HG23 | 7:O:51:ILE:HA | 1.66 | 0.77 |
| 7:G:191:ARG:CZ | 7:G:192:ASN:H | 1.97 | 0.77 |
| 7:G:378:LEU:HD11 | 7:G:393:LEU:HD12 | 1.65 | 0.77 |
| 3:C:264:GLU:O | 3:C:265:LYS:CG | 2.30 | 0.77 |
| 6:N:539:SER:CB | 6:N:542:LYS:CD | 2.62 | 0.77 |
| 2:B:208:LEU:HD12 | 2:B:209:ASP:H | 1.48 | 0.77 |
| 2:B:469:THR:O | 2:B:470:SER:HB2 | 1.82 | 0.77 |
| 3:C:452:ILE:O | 3:C:456:LEU:HB2 | 1.84 | 0.77 |
| 3:C:42:LYS:O | 3:C:459:ASN:HB3 | 1.85 | 0.77 |
| 6:F:224:MET:HE1 | 6:F:316:ALA:H | 1.49 | 0.77 |
| 1:I:123:THR:HG21 | 5:M:68:ARG:HE | 1.49 | 0.77 |
| 7:O:212:SER:HB3 | 7:O:378:LEU:HA | 1.66 | 0.77 |
| 2:B:463:ILE:O | 2:B:467:ILE:N | 2.18 | 0.77 |
| 6:F:395:VAL:O | 6:F:399:LEU:HB2 | 1.85 | 0.77 |
| 7:G:125:ILE:HA | 7:G:438:ILE:HG12 | 1.65 | 0.77 |
| 8:P:430:LEU:O | 8:P:434:ILE:HG12 | 1.84 | 0.77 |
| 2:B:329:PHE:O | 2:B:329:PHE:HD2 | 1.67 | 0.77 |
| 5:E:449:THR:HG22 | 5:E:507:ILE:HB | 1.65 | 0.77 |
| 6:F:420:ILE:HA | 6:F:423:SER:HB3 | 1.67 | 0.77 |
| 6:F:35:THR:CG2 | 6:F:42:THR:O | 2.32 | 0.77 |
| 7:G:30:ILE:HD12 | 7:G:109:MET:HB3 | 1.65 | 0.77 |
| 2:J:492:LYS:HE2 | 2:J:493:LEU:H | 1.48 | 0.77 |
| 3:K:452:ILE:O | 3:K:456:LEU:HB2 | 1.84 | 0.77 |
| 6:N:430:ASN:O | 6:N:433:LYS:CB | 2.33 | 0.77 |
| 4:D:292:ILE:N | 4:D:293:LEU:HA | 1.98 | 0.77 |
| 6:F:46:LEU:N | 6:F:54:LYS:O | 2.14 | 0.77 |
| 1:I:184:LEU:O | 1:I:184:LEU:HD23 | 1.85 | 0.77 |
| 6:F:221:HIS:HB2 | 6:F:224:MET:HG3 | 1.66 | 0.76 |
| 7:G:513:ALA:O | 7:G:516:LEU:CD1 | 2.33 | 0.76 |
| 4:L:416:ALA:HB3 | 4:L:417:PRO:HD3 | 1.66 | 0.76 |
| 4:D:416:ALA:HB3 | 4:D:417:PRO:HD3 | 1.66 | 0.76 |
| 5:E:348:GLY:O | 5:E:351:LEU:CD1 | 2.33 | 0.76 |
| 2:B:70:ASP:CB | 6:F:5:LEU:HD22 | 2.15 | 0.76 |
| 8:H:430:LEU:O | 8:H:434:ILE:HG12 | 1.84 | 0.76 |
| 4:L:184:GLU:CA | 4:L:186:SER:O | 2.33 | 0.76 |
| 5:M:509:ASN:OD1 | 5:M:523:LYS:HB2 | 1.86 | 0.76 |
| 6:N:420:ILE:HA | 6:N:423:SER:HB3 | 1.67 | 0.76 |
| 8:P:206:SER:HB2 | 8:P:381:THR:CG2 | 2.13 | 0.76 |
| 6:F:539:SER:CB | 6:F:542:LYS:CD | 2.62 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:412:SER:O | 2:J:416:ASP:HB2 | 1.86 | 0.76 |
| 4:L:292:ILE:N | 4:L:293:LEU:HA | 1.98 | 0.76 |
| 7:O:513:ALA:O | 7:O:516:LEU:CD1 | 2.33 | 0.76 |
| 1:A:431:ILE:HG12 | 1:A:482:ALA:HB2 | 1.68 | 0.76 |
| 4:D:334:ALA:HB3 | 7:G:305:GLN:HB2 | 1.64 | 0.76 |
| 8:H:237:LYS:HB2 | 8:H:314:ASN:HB3 | 1.65 | 0.76 |
| 2:B:412:SER:O | 2:B:416:ASP:HB2 | 1.86 | 0.76 |
| 6:F:430:ASN:O | 6:F:433:LYS:CB | 2.33 | 0.76 |
| 2:J:463:ILE:O | 2:J:467:ILE:N | 2.18 | 0.76 |
| 5:M:348:GLY:O | 5:M:351:LEU:CD1 | 2.33 | 0.76 |
| 5:M:449:THR:HG22 | 5:M:507:ILE:HB | 1.65 | 0.76 |
| 6:N:478:ASP:O | 6:N:482:ASP:N | 2.19 | 0.76 |
| 5:E:509:ASN:OD1 | 5:E:523:LYS:HB2 | 1.86 | 0.76 |
| 6:F:526:ASN:HA | 6:F:529:LEU:HD12 | 1.67 | 0.76 |
| 3:K:42:LYS:O | 3:K:459:ASN:HB3 | 1.85 | 0.76 |
| 4:L:268:ARG:HA | 4:L:271:LEU:HD23 | 1.68 | 0.76 |
| 4:L:36:ARG:HE | 4:L:98:ILE:HG23 | 1.51 | 0.76 |
| 1:A:184:LEU:HD23 | 1:A:184:LEU:O | 1.85 | 0.76 |
| 1:A:169:ILE:HD11 | 1:A:398:MET:HA | 1.68 | 0.76 |
| 6:F:159:LEU:HA | 6:F:164:ALA:HB1 | 1.68 | 0.76 |
| 7:G:447:GLU:O | 7:G:450:PRO:HD2 | 1.86 | 0.76 |
| 2:J:422:ILE:CG2 | 2:J:427:SER:CB | 2.63 | 0.76 |
| 3:K:56:VAL:C | 3:K:57:LEU:HD23 | 2.06 | 0.76 |
| 5:M:73:ILE:HG12 | 5:M:83:ILE:HG12 | 1.67 | 0.76 |
| 2:B:201:GLY:H | 6:F:86:ILE:HD12 | 1.49 | 0.76 |
| 2:B:473:ASP:OD2 | 2:B:476:ASN:O | 2.04 | 0.76 |
| 2:J:473:ASP:OD2 | 2:J:476:ASN:O | 2.04 | 0.76 |
| 2:J:493:LEU:HD12 | 2:J:494:LYS:N | 2.01 | 0.76 |
| 7:O:30:ILE:HD12 | 7:O:109:MET:HB3 | 1.65 | 0.76 |
| 7:O:471:ALA:O | 7:O:475:GLY:HA3 | 1.85 | 0.76 |
| 8:P:237:LYS:HB2 | 8:P:314:ASN:HB3 | 1.65 | 0.76 |
| 2:B:422:ILE:CG2 | 2:B:427:SER:CB | 2.63 | 0.76 |
| 5:E:88:ALA:HB1 | 5:E:109:LYS:NZ | 2.00 | 0.76 |
| 1:I:350:PHE:HD2 | 1:I:351:GLU:N | 1.83 | 0.76 |
| 6:N:159:LEU:HA | 6:N:164:ALA:HB1 | 1.68 | 0.76 |
| 6:N:352:GLY:O | 6:N:367:VAL:HG12 | 1.86 | 0.76 |
| 7:O:447:GLU:O | 7:O:450:PRO:HD2 | 1.86 | 0.76 |
| 7:O:448:VAL:HG12 | 7:O:452:GLN:HE22 | 1.51 | 0.76 |
| 6:F:352:GLY:O | 6:F:367:VAL:HG12 | 1.86 | 0.76 |
| 6:N:159:LEU:HA | 6:N:164:ALA:HB2 | 1.66 | 0.76 |
| 4:D:184:GLU:CA | 4:D:186:SER:O | 2.33 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:72:PRO:HG3 | 3:C:49:LEU:HD11 | 1.68 | 0.75 |
| 3:C:129:LEU:HB2 | 3:C:514:ILE:HD13 | 1.69 | 0.75 |
| 6:F:213:LEU:HD23 | 6:F:377:THR:HG23 | 1.68 | 0.75 |
| 7:O:238:ASN:N | 7:O:239:PRO:HD3 | 2.01 | 0.75 |
| 5:E:187:SER:OG | 5:E:429:VAL:HG21 | 1.86 | 0.75 |
| 5:E:73:ILE:HG12 | 5:E:83:ILE:HG12 | 1.67 | 0.75 |
| 6:F:478:ASP:O | 6:F:482:ASP:N | 2.19 | 0.75 |
| 1:I:543:THR:HB | 5:M:72:LYS:HD3 | 1.67 | 0.75 |
| 6:N:526:ASN:HA | 6:N:529:LEU:HD12 | 1.68 | 0.75 |
| 8:P:316:TYR:CD2 | 8:P:316:TYR:N | 2.54 | 0.75 |
| 1:A:226:CYS:SG | 1:A:318:VAL:CG1 | 2.75 | 0.75 |
| 2:B:208:LEU:HD12 | 2:B:209:ASP:N | 2.01 | 0.75 |
| 2:B:493:LEU:HD12 | 2:B:494:LYS:N | 2.01 | 0.75 |
| 6:F:154:ALA:HB2 | 6:F:402:VAL:CG2 | 2.16 | 0.75 |
| 2:J:165:ILE:HG12 | 6:N:529:LEU:HD13 | 1.68 | 0.75 |
| 1:A:221:GLY:HA2 | 1:A:382:SER:HB2 | 1.68 | 0.75 |
| 3:C:56:VAL:C | 3:C:57:LEU:HD23 | 2.06 | 0.75 |
| 7:G:238:ASN:N | 7:G:239:PRO:HD3 | 2.01 | 0.75 |
| 2:J:208:LEU:HD12 | 2:J:209:ASP:N | 2.01 | 0.75 |
| 3:K:104:LEU:HD11 | 3:K:520:LEU:HD12 | 1.69 | 0.75 |
| 8:P:72:LEU:HD13 | 8:P:86:VAL:HG22 | 1.69 | 0.75 |
| 1:A:456:LEU:O | 1:A:460:LYS:HG2 | 1.86 | 0.75 |
| 1:A:8:SER:N | 2:J:21:SER:HG | 1.84 | 0.75 |
| 4:D:36:ARG:HE | 4:D:98:ILE:HG23 | 1.51 | 0.75 |
| 7:G:448:VAL:HG12 | 7:G:452:GLN:HE22 | 1.51 | 0.75 |
| 3:K:129:LEU:HB2 | 3:K:514:ILE:HD13 | 1.69 | 0.75 |
| 5:E:39:LYS:HZ3 | 6:N:109:ILE:HG13 | 1.51 | 0.75 |
| 6:N:154:ALA:HB2 | 6:N:402:VAL:CG2 | 2.16 | 0.75 |
| 6:F:465:ASP:HA | 6:F:466:PRO:O | 1.86 | 0.75 |
| 6:F:53:ILE:CD1 | 6:F:53:ILE:O | 2.30 | 0.75 |
| 6:F:159:LEU:HA | 6:F:164:ALA:HB2 | 1.66 | 0.75 |
| 7:G:377:LEU:HD13 | 7:G:377:LEU:H | 1.51 | 0.75 |
| 1:I:431:ILE:HG12 | 1:I:482:ALA:HB2 | 1.68 | 0.75 |
| 1:A:543:THR:HB | 5:E:72:LYS:HD3 | 1.67 | 0.74 |
| 2:B:295:GLU:HB2 | 6:F:337:GLN:NE2 | 2.02 | 0.74 |
| 7:G:33:CYS:SG | 7:G:83:LEU:HD11 | 2.27 | 0.74 |
| 3:K:306:GLN:O | 3:K:310:LEU:HG | 1.87 | 0.74 |
| 5:M:492:ILE:H | 5:M:492:ILE:HD12 | 1.52 | 0.74 |
| 6:N:13:LEU:HD13 | 6:N:21:VAL:HG21 | 1.69 | 0.74 |
| 6:N:395:VAL:O | 6:N:399:LEU:CB | 2.35 | 0.74 |
| 7:O:413:GLY:HA3 | 7:O:491:ASN:HD21 | 1.52 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:306:GLN:O | 3:C:310:LEU:HG | 1.87 | 0.74 |
| 4:D:268:ARG:HA | 4:D:271:LEU:HD23 | 1.68 | 0.74 |
| 7:G:471:ALA:O | 7:G:475:GLY:HA3 | 1.85 | 0.74 |
| 1:I:115:LEU:HD21 | 1:I:446:LEU:HD22 | 1.69 | 0.74 |
| 1:I:221:GLY:HA2 | 1:I:382:SER:HB2 | 1.68 | 0.74 |
| 1:I:226:CYS:SG | 1:I:318:VAL:CG1 | 2.75 | 0.74 |
| 6:F:117:ILE:HD12 | 5:M:34:ASP:HA | 1.64 | 0.74 |
| 7:O:488:ILE:H | 7:O:488:ILE:HD12 | 1.52 | 0.74 |
| 8:P:114:SER:O | 8:P:118:ILE:HG13 | 1.87 | 0.74 |
| 8:H:72:LEU:HD13 | 8:H:86:VAL:HG22 | 1.69 | 0.74 |
| 8:P:204:VAL:CG1 | 8:P:405:VAL:HG12 | 2.16 | 0.74 |
| 1:A:350:PHE:HD2 | 1:A:351:GLU:N | 1.83 | 0.74 |
| 1:A:357:LEU:HB2 | 1:A:378:SER:HB3 | 1.69 | 0.74 |
| 3:C:104:LEU:HD11 | 3:C:520:LEU:HD12 | 1.69 | 0.74 |
| 4:D:119:ILE:HG23 | 4:D:436:GLN:HA | 1.68 | 0.74 |
| 5:M:187:SER:OG | 5:M:429:VAL:HG21 | 1.86 | 0.74 |
| 6:F:43:LEU:HD21 | 6:F:161:LYS:HA | 1.68 | 0.74 |
| 4:L:25:ILE:HD13 | 4:L:108:GLU:HB2 | 1.70 | 0.74 |
| 2:B:451:ASP:O | 2:B:455:LEU:HB2 | 1.88 | 0.74 |
| 6:F:395:VAL:O | 6:F:399:LEU:CB | 2.35 | 0.74 |
| 6:F:3:LEU:HD12 | 6:F:5:LEU:CD2 | 2.17 | 0.74 |
| 2:B:4:GLN:O | 3:C:72:HIS:HB2 | 1.87 | 0.74 |
| 2:J:422:ILE:HG22 | 2:J:427:SER:HB3 | 1.68 | 0.74 |
| 6:N:201:HIS:HB3 | 6:N:381:LYS:NZ | 2.03 | 0.74 |
| 7:O:33:CYS:SG | 7:O:83:LEU:HD11 | 2.27 | 0.74 |
| 7:G:109:MET:SD | 7:G:514:THR:CG2 | 2.76 | 0.74 |
| 7:G:498:GLU:OE2 | 9:G:601:ADP:H1' | 1.88 | 0.74 |
| 8:H:204:VAL:CG1 | 8:H:405:VAL:HG12 | 2.16 | 0.74 |
| 5:M:355:ALA:HB3 | 6:N:222:PRO:HG2 | 1.68 | 0.74 |
| 2:B:242:LYS:HE2 | 2:B:246:PHE:HA | 1.69 | 0.74 |
| 2:B:422:ILE:HG22 | 2:B:427:SER:HB3 | 1.68 | 0.74 |
| 7:G:330:VAL:HG12 | 7:G:347:GLY:HA3 | 1.69 | 0.74 |
| 1:I:169:ILE:HD11 | 1:I:398:MET:HA | 1.68 | 0.74 |
| 2:J:451:ASP:O | 2:J:455:LEU:HB2 | 1.88 | 0.74 |
| 3:C:329:ALA:O | 3:C:333:GLY:N | 2.21 | 0.74 |
| 6:F:13:LEU:HD13 | 6:F:21:VAL:HG21 | 1.69 | 0.74 |
| 7:G:488:ILE:HD12 | 7:G:488:ILE:H | 1.52 | 0.74 |
| 2:B:242:LYS:CE | 2:B:247:GLY:N | 2.50 | 0.73 |
| 3:C:501:GLU:OE2 | 9:C:1101:ADP:H3' | 1.87 | 0.73 |
| 6:F:138:ILE:HG22 | 6:F:138:ILE:O | 1.87 | 0.73 |
| 7:G:44:LEU:HD12 | 7:G:452:GLN:HB2 | 1.68 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:187:VAL:CG2 | 1:I:383:SER:HB3 | 2.18 | 0.73 |
| 1:I:63:THR:HG22 | 1:I:65:ASP:H | 1.52 | 0.73 |
| 6:N:155:ARG:CB | 6:N:171:THR:CG2 | 2.66 | 0.73 |
| 7:O:44:LEU:HD12 | 7:O:452:GLN:HB2 | 1.68 | 0.73 |
| 8:P:345:GLY:C | 8:P:347:PRO:HD3 | 2.08 | 0.73 |
| 1:A:115:LEU:HD21 | 1:A:446:LEU:HD22 | 1.69 | 0.73 |
| 2:B:232:LEU:HB3 | 2:B:283:THR:HG22 | 1.68 | 0.73 |
| 7:G:413:GLY:HA3 | 7:G:491:ASN:HD21 | 1.52 | 0.73 |
| 4:L:120:ILE:HG12 | 4:L:439:ILE:HG21 | 1.68 | 0.73 |
| 4:L:336:ILE:O | 4:L:336:ILE:CG2 | 2.35 | 0.73 |
| 6:N:213:LEU:HD23 | 6:N:377:THR:HG23 | 1.68 | 0.73 |
| 6:N:465:ASP:HA | 6:N:466:PRO:O | 1.86 | 0.73 |
| 4:D:421:ILE:O | 4:D:425:LEU:HG | 1.88 | 0.73 |
| 8:H:316:TYR:N | 8:H:316:TYR:CD2 | 2.54 | 0.73 |
| 1:I:456:LEU:O | 1:I:460:LYS:HG2 | 1.86 | 0.73 |
| 6:N:138:ILE:O | 6:N:138:ILE:HG22 | 1.87 | 0.73 |
| 7:O:377:LEU:H | 7:O:377:LEU:HD13 | 1.51 | 0.73 |
| 7:O:143:LEU:HD13 | 7:O:411:ALA:HB3 | 1.70 | 0.73 |
| 1:A:30:VAL:O | 1:A:33:THR:HG22 | 1.87 | 0.73 |
| 1:A:63:THR:HG22 | 1:A:65:ASP:H | 1.52 | 0.73 |
| 4:D:336:ILE:CG2 | 4:D:336:ILE:O | 2.35 | 0.73 |
| 8:H:316:TYR:N | 8:H:316:TYR:HD2 | 1.87 | 0.73 |
| 2:J:232:LEU:HB3 | 2:J:283:THR:HG22 | 1.68 | 0.73 |
| 4:L:485:ARG:H | 4:L:485:ARG:HD2 | 1.54 | 0.73 |
| 6:N:166:LEU:O | 6:N:167:THR:CG2 | 2.33 | 0.73 |
| 7:O:330:VAL:HG12 | 7:O:347:GLY:HA3 | 1.69 | 0.73 |
| 8:P:163:ILE:HG23 | 8:P:179:SER:HB2 | 1.71 | 0.73 |
| 8:P:77:ILE:HD13 | 8:P:77:ILE:H | 1.53 | 0.73 |
| 4:D:25:ILE:HD13 | 4:D:108:GLU:HB2 | 1.70 | 0.73 |
| 7:G:479:TYR:HA | 7:G:490:ASP:HA | 1.70 | 0.73 |
| 1:I:267:PRO:HA | 1:I:268:GLU:CB | 2.19 | 0.73 |
| 1:I:357:LEU:HB2 | 1:I:378:SER:HB3 | 1.69 | 0.73 |
| 1:A:187:VAL:CG2 | 1:A:383:SER:HB3 | 2.18 | 0.73 |
| 4:D:120:ILE:HG12 | 4:D:439:ILE:HG21 | 1.68 | 0.73 |
| 8:H:114:SER:O | 8:H:118:ILE:HG13 | 1.87 | 0.73 |
| 3:K:329:ALA:O | 3:K:333:GLY:N | 2.21 | 0.73 |
| 2:B:285:ILE:CD1 | 2:B:289:LEU:HD23 | 2.19 | 0.73 |
| 4:D:183:ASP:O | 4:D:187:LYS:HG2 | 1.88 | 0.73 |
| 2:J:242:LYS:HE2 | 2:J:246:PHE:HA | 1.69 | 0.73 |
| 5:M:142:HIS:O | 5:M:146:ILE:HG13 | 1.89 | 0.73 |
| 6:N:3:LEU:HD12 | 6:N:5:LEU:CD2 | 2.17 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:O:109:MET:SD | 7:O:514:THR:CG2 | 2.76 | 0.73 |
| 8:P:204:VAL:HG21 | 8:P:409:LYS:CB | 2.19 | 0.73 |
| 2:B:71:ASN:OD1 | 2:B:73:ALA:N | 2.22 | 0.73 |
| 6:F:155:ARG:CB | 6:F:171:THR:CG2 | 2.66 | 0.73 |
| 6:F:201:HIS:HB3 | 6:F:381:LYS:NZ | 2.03 | 0.73 |
| 6:F:193:MET:CE | 6:F:330:LEU:HD11 | 2.19 | 0.73 |
| 8:H:345:GLY:C | 8:H:347:PRO:HD3 | 2.08 | 0.73 |
| 8:H:77:ILE:H | 8:H:77:ILE:HD13 | 1.53 | 0.73 |
| 2:J:242:LYS:CE | 2:J:247:GLY:N | 2.50 | 0.73 |
| 4:D:254:VAL:CG2 | 8:H:265:VAL:HG22 | 2.18 | 0.73 |
| 2:J:57:THR:HG21 | 2:J:382:ARG:HD3 | 1.71 | 0.73 |
| 3:K:518:CYS:O | 3:K:522:ARG:HG3 | 1.89 | 0.73 |
| 4:L:183:ASP:O | 4:L:187:LYS:HG2 | 1.88 | 0.73 |
| 6:N:193:MET:CE | 6:N:330:LEU:HD11 | 2.19 | 0.73 |
| 8:P:54:ILE:CG1 | 8:P:64:ILE:HG12 | 2.13 | 0.73 |
| 4:D:258:ARG:HD2 | 8:H:283:GLN:HE21 | 1.54 | 0.73 |
| 5:E:142:HIS:O | 5:E:146:ILE:HG13 | 1.89 | 0.73 |
| 2:J:285:ILE:CD1 | 2:J:289:LEU:HD23 | 2.19 | 0.73 |
| 6:N:411:ILE:HG22 | 6:N:412:ILE:N | 2.04 | 0.73 |
| 2:B:411:MET:HB2 | 2:B:437:LEU:HD13 | 1.70 | 0.72 |
| 7:G:55:THR:HG21 | 7:G:72:LEU:HB3 | 1.70 | 0.72 |
| 6:N:167:THR:HB | 6:N:168:GLU:C | 2.09 | 0.72 |
| 6:N:193:MET:HE3 | 6:N:330:LEU:HD11 | 1.71 | 0.72 |
| 7:G:143:LEU:HD13 | 7:G:411:ALA:HB3 | 1.70 | 0.72 |
| 5:M:479:ILE:O | 5:M:483:LEU:HB2 | 1.89 | 0.72 |
| 1:I:17:GLY:HA3 | 5:M:95:GLU:OE2 | 1.88 | 0.72 |
| 3:C:518:CYS:O | 3:C:522:ARG:HG3 | 1.89 | 0.72 |
| 5:E:479:ILE:O | 5:E:483:LEU:HB2 | 1.89 | 0.72 |
| 5:E:492:ILE:HD11 | 2:J:115:ILE:HG12 | 1.71 | 0.72 |
| 6:F:143:LEU:CD2 | 6:F:145:ASN:HB3 | 2.19 | 0.72 |
| 6:F:540:THR:HB | 6:F:541:LEU:HD22 | 1.72 | 0.72 |
| 8:H:234:GLY:HA2 | 8:H:310:LEU:HD11 | 1.69 | 0.72 |
| 8:H:63:ILE:HD12 | 8:H:74:GLU:HG3 | 1.70 | 0.72 |
| 4:L:421:ILE:O | 4:L:425:LEU:HG | 1.89 | 0.72 |
| 8:P:28:ILE:O | 8:P:32:ILE:HB | 1.89 | 0.72 |
| 6:F:167:THR:HB | 6:F:168:GLU:C | 2.09 | 0.72 |
| 6:F:5:LEU:CA | 6:F:6:LEU:CB | 2.66 | 0.72 |
| 4:L:119:ILE:HG23 | 4:L:436:GLN:HA | 1.68 | 0.72 |
| 8:H:6:PRO:HG2 | 4:L:71:LEU:HA | 1.71 | 0.72 |
| 1:I:122:PRO:HG3 | 5:M:70:LEU:HD11 | 1.71 | 0.72 |
| 6:N:352:GLY:C | 6:N:369:GLU:O | 2.27 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:O:479:TYR:HA | 7:O:490:ASP:HA | 1.70 | 0.72 |
| 4:L:524:ILE:HG23 | 7:O:52:LEU:O | 1.88 | 0.72 |
| 2:B:475:ASN:ND2 | 2:B:475:ASN:N | 2.38 | 0.72 |
| 5:E:492:ILE:H | 5:E:492:ILE:HD12 | 1.52 | 0.72 |
| 6:F:108:PHE:CZ | 6:F:118:ILE:HG13 | 2.25 | 0.72 |
| 6:F:352:GLY:C | 6:F:369:GLU:O | 2.27 | 0.72 |
| 2:J:5:ILE:O | 3:K:70:VAL:HA | 1.88 | 0.72 |
| 2:J:263:LYS:NZ | 3:K:266:GLU:CB | 2.53 | 0.72 |
| 1:I:156:LEU:HD22 | 1:I:181:VAL:HG13 | 1.71 | 0.72 |
| 1:I:30:VAL:O | 1:I:33:THR:HG22 | 1.87 | 0.72 |
| 2:J:411:MET:HB2 | 2:J:437:LEU:HD13 | 1.70 | 0.72 |
| 2:J:242:LYS:HB2 | 3:K:269:TRP:HZ2 | 1.55 | 0.72 |
| 6:N:540:THR:HB | 6:N:541:LEU:HD22 | 1.72 | 0.72 |
| 8:P:234:GLY:HA2 | 8:P:310:LEU:HD11 | 1.69 | 0.72 |
| 2:B:164:LYS:O | 2:B:166:LEU:N | 2.22 | 0.72 |
| 6:F:420:ILE:HG21 | 6:F:482:ASP:OD1 | 1.89 | 0.72 |
| 7:G:191:ARG:HD3 | 7:G:192:ASN:H | 1.55 | 0.72 |
| 7:G:232:GLN:HG2 | 7:G:313:PHE:HA | 1.72 | 0.72 |
| 8:H:204:VAL:HG21 | 8:H:409:LYS:CB | 2.19 | 0.72 |
| 2:J:71:ASN:OD1 | 2:J:73:ALA:N | 2.22 | 0.72 |
| 7:O:205:PRO:HA | 7:O:386:ILE:HD11 | 1.71 | 0.72 |
| 1:A:267:PRO:HA | 1:A:268:GLU:CB | 2.19 | 0.72 |
| 3:C:114:LYS:HA | 3:C:115:ASN:CB | 2.20 | 0.72 |
| 3:C:322:LYS:HG3 | 3:C:323:SER:H | 1.55 | 0.72 |
| 4:D:207:THR:HG22 | 4:D:380:ARG:H | 1.54 | 0.72 |
| 6:F:411:ILE:HG22 | 6:F:412:ILE:N | 2.04 | 0.72 |
| 2:J:164:LYS:O | 2:J:166:LEU:N | 2.22 | 0.72 |
| 2:J:198:ILE:O | 2:J:377:LEU:HD21 | 1.89 | 0.72 |
| 3:K:322:LYS:HG3 | 3:K:323:SER:H | 1.55 | 0.72 |
| 2:J:4:GLN:HG2 | 3:K:72:HIS:HB2 | 1.72 | 0.72 |
| 6:N:143:LEU:CD2 | 6:N:145:ASN:HB3 | 2.19 | 0.72 |
| 2:B:357:SER:O | 2:B:360:LYS:CB | 2.38 | 0.72 |
| 2:J:357:SER:O | 2:J:360:LYS:CB | 2.38 | 0.72 |
| 4:L:207:THR:HG22 | 4:L:380:ARG:H | 1.54 | 0.72 |
| 3:C:291:ARG:N | 3:C:292:PRO:HD3 | 2.05 | 0.71 |
| 7:O:56:SER:HA | 7:O:57:ASN:O | 1.90 | 0.71 |
| 6:F:166:LEU:O | 6:F:167:THR:CG2 | 2.33 | 0.71 |
| 8:H:163:ILE:HG23 | 8:H:179:SER:HB2 | 1.70 | 0.71 |
| 8:H:28:ILE:O | 8:H:32:ILE:HB | 1.89 | 0.71 |
| 2:B:251:LYS:H | 6:F:251:PHE:HA | 1.55 | 0.71 |
| 4:D:404:LEU:O | 4:D:407:GLU:O | 2.08 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:N:108:PHE:CZ | 6:N:118:ILE:HG13 | 2.25 | 0.71 |
| 7:G:43:THR:HB | 7:G:99:THR:HG21 | 1.72 | 0.71 |
| 7:G:56:SER:HA | 7:G:57:ASN:O | 1.90 | 0.71 |
| 2:J:373:THR:O | 2:J:376:THR:HG22 | 1.91 | 0.71 |
| 6:N:151:LEU:HD12 | 6:N:175:THR:HG21 | 1.66 | 0.71 |
| 8:P:63:ILE:HD12 | 8:P:74:GLU:HG3 | 1.70 | 0.71 |
| 3:K:51:PRO:O | 3:K:52:MET:HG3 | 1.90 | 0.71 |
| 7:O:55:THR:HG21 | 7:O:72:LEU:HB3 | 1.71 | 0.71 |
| 2:B:345:GLU:O | 2:B:351:GLN:CB | 2.39 | 0.71 |
| 2:B:4:GLN:HG2 | 3:C:72:HIS:HB2 | 1.72 | 0.71 |
| 1:I:184:LEU:HD23 | 1:I:184:LEU:C | 2.10 | 0.71 |
| 4:L:210:ILE:O | 4:L:375:VAL:CG1 | 2.39 | 0.71 |
| 5:M:558:GLY:HA2 | 6:N:48:ASP:HB2 | 1.72 | 0.71 |
| 6:N:539:SER:HB3 | 6:N:542:LYS:CD | 2.15 | 0.71 |
| 3:C:51:PRO:O | 3:C:52:MET:HG3 | 1.90 | 0.71 |
| 5:E:319:ASP:O | 5:E:340:LEU:HB2 | 1.91 | 0.71 |
| 7:G:226:TYR:CE1 | 7:G:229:PHE:O | 2.44 | 0.71 |
| 7:G:232:GLN:HG3 | 7:G:313:PHE:HA | 1.73 | 0.71 |
| 1:I:16:GLY:HA3 | 1:I:548:ASP:HB3 | 1.73 | 0.71 |
| 3:K:225:LEU:HD13 | 3:K:320:VAL:HG13 | 1.73 | 0.71 |
| 6:N:154:ALA:HB1 | 6:N:402:VAL:HG23 | 1.73 | 0.71 |
| 6:N:203:SER:O | 6:N:205:LYS:N | 2.24 | 0.71 |
| 6:N:5:LEU:CB | 6:N:6:LEU:O | 2.38 | 0.71 |
| 1:A:12:THR:HG22 | 1:A:13:LEU:HD23 | 1.73 | 0.71 |
| 1:A:184:LEU:HD23 | 1:A:184:LEU:C | 2.10 | 0.71 |
| 1:A:350:PHE:HD2 | 1:A:351:GLU:H | 1.37 | 0.71 |
| 2:B:57:THR:HG21 | 2:B:382:ARG:HD3 | 1.71 | 0.71 |
| 4:D:328:LEU:CB | 4:D:345:ASP:OD2 | 2.38 | 0.71 |
| 4:D:485:ARG:H | 4:D:485:ARG:HD2 | 1.54 | 0.71 |
| 5:M:319:ASP:O | 5:M:340:LEU:HB2 | 1.91 | 0.71 |
| 7:O:226:TYR:CE1 | 7:O:229:PHE:O | 2.44 | 0.71 |
| 7:O:232:GLN:HG2 | 7:O:313:PHE:HA | 1.72 | 0.71 |
| 4:D:71:LEU:HA | 8:P:6:PRO:HG2 | 1.73 | 0.71 |
| 1:A:230:SER:O | 1:A:233:MET:HG3 | 1.91 | 0.71 |
| 1:A:16:GLY:HA3 | 1:A:548:ASP:HB3 | 1.73 | 0.71 |
| 2:B:373:THR:O | 2:B:376:THR:HG22 | 1.91 | 0.71 |
| 1:I:418:VAL:HG12 | 1:I:419:VAL:H | 1.56 | 0.71 |
| 1:I:101:VAL:HG22 | 1:I:527:SER:HB2 | 1.71 | 0.71 |
| 3:K:114:LYS:HA | 3:K:115:ASN:CB | 2.20 | 0.71 |
| 6:N:433:LYS:HG3 | 6:N:444:ILE:HG21 | 1.73 | 0.71 |
| 1:A:418:VAL:HG12 | 1:A:419:VAL:H | 1.56 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:198:ILE:O | 2:B:377:LEU:HD21 | 1.89 | 0.71 |
| 4:D:46:LYS:HG3 | 8:H:532:THR:HG23 | 1.71 | 0.71 |
| 8:H:243:LYS:C | 8:H:244:LYS:HG2 | 2.12 | 0.71 |
| 1:I:350:PHE:C | 1:I:351:GLU:OE2 | 2.30 | 0.71 |
| 4:L:134:ILE:CD1 | 4:L:424:ARG:HD3 | 2.20 | 0.71 |
| 6:F:209:PHE:HE2 | 6:F:376:CYS:SG | 2.10 | 0.70 |
| 2:J:237:THR:H | 2:J:287:ARG:HD2 | 1.56 | 0.70 |
| 2:J:475:ASN:N | 2:J:475:ASN:ND2 | 2.38 | 0.70 |
| 6:N:209:PHE:HE2 | 6:N:376:CYS:SG | 2.10 | 0.70 |
| 3:K:269:TRP:HZ3 | 6:N:247:VAL:HB | 1.54 | 0.70 |
| 7:O:232:GLN:HG3 | 7:O:313:PHE:HA | 1.73 | 0.70 |
| 6:F:203:SER:O | 6:F:205:LYS:N | 2.24 | 0.70 |
| 6:F:5:LEU:CB | 6:F:6:LEU:O | 2.38 | 0.70 |
| 1:I:94:ILE:HG22 | 1:I:96:ASP:H | 1.56 | 0.70 |
| 2:B:242:LYS:NZ | 2:B:247:GLY:H | 1.90 | 0.70 |
| 2:B:30:GLY:HA2 | 2:B:33:VAL:HG23 | 1.73 | 0.70 |
| 4:D:210:ILE:O | 4:D:375:VAL:CG1 | 2.39 | 0.70 |
| 8:P:291:ILE:HD11 | 8:P:345:GLY:HA2 | 1.74 | 0.70 |
| 2:B:237:THR:H | 2:B:287:ARG:HD2 | 1.56 | 0.70 |
| 2:B:131:ALA:HB1 | 2:B:411:MET:HB3 | 1.73 | 0.70 |
| 4:D:482:ILE:H | 4:D:482:ILE:HD13 | 1.57 | 0.70 |
| 6:F:154:ALA:HB1 | 6:F:402:VAL:HG23 | 1.73 | 0.70 |
| 2:B:295:GLU:OE1 | 6:F:339:SER:HB3 | 1.91 | 0.70 |
| 3:K:225:LEU:HD13 | 3:K:320:VAL:CG1 | 2.22 | 0.70 |
| 8:P:243:LYS:C | 8:P:244:LYS:HG2 | 2.12 | 0.70 |
| 2:B:475:ASN:ND2 | 2:B:475:ASN:H | 1.89 | 0.70 |
| 6:F:16:ASP:HA | 6:F:19:LEU:CD1 | 2.20 | 0.70 |
| 8:H:333:CYS:SG | 8:H:340:PRO:HD3 | 2.32 | 0.70 |
| 1:I:12:THR:HG22 | 1:I:13:LEU:HD23 | 1.73 | 0.70 |
| 6:N:420:ILE:HG21 | 6:N:482:ASP:OD1 | 1.89 | 0.70 |
| 6:N:5:LEU:CA | 6:N:6:LEU:CB | 2.66 | 0.70 |
| 7:O:43:THR:HB | 7:O:99:THR:HG21 | 1.72 | 0.70 |
| 2:B:30:GLY:HA2 | 2:B:33:VAL:CG2 | 2.22 | 0.70 |
| 3:C:225:LEU:HD13 | 3:C:320:VAL:CG1 | 2.22 | 0.70 |
| 2:J:345:GLU:O | 2:J:351:GLN:CB | 2.39 | 0.70 |
| 4:L:521:ILE:CG2 | 7:O:52:LEU:H | 2.05 | 0.70 |
| 5:M:253:GLN:N | 5:M:254:MET:CB | 2.54 | 0.70 |
| 5:M:509:ASN:O | 5:M:522:MET:N | 2.24 | 0.70 |
| 7:O:396:ALA:O | 7:O:399:ILE:HG22 | 1.92 | 0.70 |
| 1:A:101:VAL:HG22 | 1:A:527:SER:HB2 | 1.71 | 0.70 |
| 4:D:184:GLU:HA | 4:D:186:SER:O | 1.91 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:207:THR:HG22 | 4:D:380:ARG:N | 2.06 | 0.70 |
| 6:F:245:THR:OG1 | 6:F:247:VAL:HG22 | 1.91 | 0.70 |
| 2:J:39:PRO:HA | 2:J:163:SER:HA | 1.74 | 0.70 |
| 4:L:404:LEU:O | 4:L:407:GLU:O | 2.08 | 0.70 |
| 8:H:6:PRO:CG | 4:L:71:LEU:CA | 2.69 | 0.70 |
| 5:M:104:LEU:HA | 5:M:107:LEU:HD23 | 1.73 | 0.70 |
| 2:J:295:GLU:C | 6:N:337:GLN:HE22 | 1.94 | 0.70 |
| 7:G:58:GLN:NE2 | 8:P:6:PRO:O | 2.24 | 0.70 |
| 1:A:350:PHE:C | 1:A:351:GLU:OE2 | 2.30 | 0.70 |
| 5:E:509:ASN:O | 5:E:522:MET:N | 2.24 | 0.70 |
| 6:F:37:LEU:HD13 | 6:F:458:LEU:HA | 1.73 | 0.70 |
| 8:H:475:LEU:HB2 | 8:H:476:PRO:HD3 | 1.74 | 0.70 |
| 2:J:131:ALA:HB1 | 2:J:411:MET:HB3 | 1.73 | 0.70 |
| 3:K:125:LEU:HD22 | 3:K:445:VAL:HG23 | 1.74 | 0.70 |
| 3:K:291:ARG:N | 3:K:292:PRO:HD3 | 2.05 | 0.70 |
| 4:L:482:ILE:H | 4:L:482:ILE:HD13 | 1.57 | 0.70 |
| 6:N:245:THR:OG1 | 6:N:247:VAL:HG22 | 1.91 | 0.70 |
| 6:N:7:ASN:OD1 | 6:N:8:PRO:N | 2.25 | 0.70 |
| 8:P:333:CYS:SG | 8:P:340:PRO:HD3 | 2.32 | 0.70 |
| 1:A:156:LEU:HD22 | 1:A:181:VAL:HG13 | 1.71 | 0.70 |
| 2:B:83:VAL:HG21 | 3:C:384:GLY:O | 1.91 | 0.70 |
| 5:E:319:ASP:O | 5:E:340:LEU:CB | 2.40 | 0.70 |
| 1:I:12:THR:HB | 1:I:13:LEU:HB2 | 1.74 | 0.70 |
| 2:J:206:SER:HB3 | 2:J:368:VAL:HG13 | 1.73 | 0.70 |
| 2:J:242:LYS:NZ | 2:J:247:GLY:H | 1.90 | 0.70 |
| 4:L:184:GLU:HA | 4:L:186:SER:O | 1.91 | 0.70 |
| 4:L:207:THR:HG22 | 4:L:380:ARG:N | 2.06 | 0.70 |
| 7:O:121:SER:HB2 | 7:O:124:LEU:HD23 | 1.74 | 0.70 |
| 2:B:31:ASP:OD1 | 2:B:31:ASP:C | 2.30 | 0.70 |
| 2:B:3:VAL:C | 2:B:5:ILE:CG2 | 2.61 | 0.70 |
| 6:F:113:VAL:HB | 6:F:118:ILE:HD11 | 1.73 | 0.70 |
| 2:J:3:VAL:C | 2:J:5:ILE:CG2 | 2.61 | 0.70 |
| 4:L:521:ILE:HG12 | 7:O:62:ILE:HD11 | 1.73 | 0.70 |
| 6:N:113:VAL:HB | 6:N:118:ILE:HD11 | 1.73 | 0.70 |
| 2:B:263:LYS:NZ | 3:C:266:GLU:HB3 | 2.06 | 0.69 |
| 5:E:253:GLN:N | 5:E:254:MET:CB | 2.54 | 0.69 |
| 6:F:154:ALA:HB2 | 6:F:402:VAL:HG23 | 1.73 | 0.69 |
| 6:F:36:ASN:CB | 6:F:57:LYS:NZ | 2.24 | 0.69 |
| 7:G:121:SER:HB2 | 7:G:124:LEU:HD23 | 1.74 | 0.69 |
| 7:G:205:PRO:HA | 7:G:386:ILE:HD11 | 1.71 | 0.69 |
| 2:J:31:ASP:OD1 | 2:J:31:ASP:C | 2.30 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:N:158:LEU:O | 6:N:158:LEU:CD1 | 2.39 | 0.69 |
| 6:N:434:LEU:O | 6:N:437:LYS:C | 2.30 | 0.69 |
| 8:P:475:LEU:HB2 | 8:P:476:PRO:HD3 | 1.74 | 0.69 |
| 2:B:414:ALA:O | 2:B:417:THR:HG22 | 1.92 | 0.69 |
| 2:B:422:ILE:HB | 2:B:427:SER:CB | 2.15 | 0.69 |
| 3:C:299:LYS:CA | 3:C:319:ARG:CB | 2.70 | 0.69 |
| 6:F:433:LYS:HG3 | 6:F:444:ILE:HG13 | 1.74 | 0.69 |
| 5:M:35:GLN:CD | 5:M:36:GLY:HA3 | 2.13 | 0.69 |
| 6:N:37:LEU:HD13 | 6:N:458:LEU:HA | 1.74 | 0.69 |
| 7:O:191:ARG:HD3 | 7:O:192:ASN:H | 1.55 | 0.69 |
| 1:A:299:THR:HG23 | 1:A:326:LEU:HD12 | 1.74 | 0.69 |
| 2:B:328:THR:O | 2:B:329:PHE:CG | 2.46 | 0.69 |
| 5:E:104:LEU:HA | 5:E:107:LEU:HD23 | 1.73 | 0.69 |
| 6:F:434:LEU:O | 6:F:437:LYS:C | 2.30 | 0.69 |
| 4:L:166:TYR:O | 4:L:169:PHE:HB3 | 1.92 | 0.69 |
| 3:C:265:LYS:NZ | 3:C:268:ASP:CB | 2.55 | 0.69 |
| 4:D:254:VAL:HG22 | 8:H:264:THR:O | 1.92 | 0.69 |
| 6:F:321:LYS:HA | 6:F:321:LYS:HE3 | 1.75 | 0.69 |
| 1:I:224:LEU:HD11 | 1:I:226:CYS:HB2 | 1.75 | 0.69 |
| 2:J:328:THR:O | 2:J:329:PHE:CG | 2.45 | 0.69 |
| 6:N:353:LEU:O | 6:N:367:VAL:CG1 | 2.40 | 0.69 |
| 8:P:237:LYS:HB3 | 8:P:314:ASN:HB3 | 1.63 | 0.69 |
| 3:C:416:GLY:HA2 | 9:C:1101:ADP:H2' | 1.74 | 0.69 |
| 4:D:169:PHE:O | 4:D:173:LEU:HD13 | 1.92 | 0.69 |
| 4:L:521:ILE:HG21 | 7:O:52:LEU:H | 1.56 | 0.69 |
| 6:N:433:LYS:HG3 | 6:N:444:ILE:HG13 | 1.74 | 0.69 |
| 3:C:225:LEU:HD13 | 3:C:320:VAL:HG13 | 1.73 | 0.69 |
| 4:D:265:LYS:NZ | 8:H:343:ARG:HD3 | 2.07 | 0.69 |
| 1:I:230:SER:O | 1:I:233:MET:HG3 | 1.91 | 0.69 |
| 1:I:299:THR:HG23 | 1:I:326:LEU:HD12 | 1.75 | 0.69 |
| 2:J:311:PHE:O | 2:J:315:GLU:HG2 | 1.93 | 0.69 |
| 2:B:32:LEU:CD1 | 6:F:532:GLU:OE2 | 2.41 | 0.69 |
| 4:D:404:LEU:HD22 | 4:D:410:LEU:HG | 1.74 | 0.69 |
| 4:D:134:ILE:CD1 | 4:D:424:ARG:HD3 | 2.20 | 0.69 |
| 8:H:153:LYS:H | 8:H:153:LYS:HD2 | 1.56 | 0.69 |
| 2:J:30:GLY:HA2 | 2:J:33:VAL:CG2 | 2.22 | 0.69 |
| 2:J:459:LEU:HB2 | 2:J:472:LEU:HD21 | 1.73 | 0.69 |
| 7:O:109:MET:HG2 | 7:O:514:THR:HG22 | 1.74 | 0.69 |
| 7:O:148:THR:O | 7:O:149:SER:CB | 2.40 | 0.69 |
| 2:B:257:LYS:HA | 2:B:260:GLN:HB3 | 1.75 | 0.69 |
| 4:D:159:SER:O | 4:D:161:LYS:HD3 | 1.93 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:166:TYR:O | 4:D:169:PHE:HB3 | 1.92 | 0.69 |
| 5:E:166:ASP:HB3 | 5:E:167:ASP:CB | 2.23 | 0.69 |
| 5:E:35:GLN:CD | 5:E:36:GLY:HA3 | 2.13 | 0.69 |
| 6:F:167:THR:HA | 6:F:168:GLU:HB3 | 1.75 | 0.69 |
| 8:H:291:ILE:HD11 | 8:H:345:GLY:HA2 | 1.73 | 0.69 |
| 1:I:350:PHE:HD2 | 1:I:351:GLU:H | 1.37 | 0.69 |
| 2:J:475:ASN:H | 2:J:475:ASN:ND2 | 1.89 | 0.69 |
| 6:N:433:LYS:HG2 | 6:N:444:ILE:HG21 | 1.74 | 0.69 |
| 8:P:153:LYS:H | 8:P:153:LYS:HD2 | 1.56 | 0.69 |
| 2:B:32:LEU:HG | 6:F:532:GLU:OE1 | 1.92 | 0.69 |
| 4:D:15:GLU:O | 4:D:523:ASP:OD2 | 2.11 | 0.69 |
| 6:F:539:SER:HB3 | 6:F:542:LYS:CD | 2.15 | 0.69 |
| 7:G:148:THR:O | 7:G:149:SER:CB | 2.40 | 0.69 |
| 8:H:335:VAL:HG13 | 8:H:379:SER:HB3 | 1.75 | 0.69 |
| 8:H:346:ALA:N | 8:H:347:PRO:CD | 2.56 | 0.69 |
| 2:J:328:THR:O | 2:J:329:PHE:CD1 | 2.46 | 0.69 |
| 3:C:467:LEU:O | 3:C:471:LEU:HB2 | 1.93 | 0.69 |
| 5:E:544:LEU:HD23 | 6:F:384:THR:HG21 | 1.73 | 0.69 |
| 6:F:433:LYS:HG3 | 6:F:444:ILE:HG21 | 1.73 | 0.69 |
| 7:G:396:ALA:O | 7:G:399:ILE:HG22 | 1.92 | 0.69 |
| 3:K:299:LYS:CA | 3:K:319:ARG:CB | 2.70 | 0.69 |
| 5:M:319:ASP:O | 5:M:340:LEU:CB | 2.40 | 0.69 |
| 2:B:459:LEU:HB2 | 2:B:472:LEU:HD21 | 1.73 | 0.69 |
| 3:C:125:LEU:HD22 | 3:C:445:VAL:HG23 | 1.74 | 0.69 |
| 6:F:158:LEU:O | 6:F:158:LEU:CD1 | 2.39 | 0.69 |
| 6:F:354:VAL:HG22 | 6:F:367:VAL:HG13 | 1.75 | 0.69 |
| 6:F:209:PHE:HB2 | 6:F:378:ILE:HB | 1.75 | 0.69 |
| 2:J:30:GLY:HA2 | 2:J:33:VAL:HG23 | 1.73 | 0.69 |
| 3:K:299:LYS:N | 3:K:319:ARG:CB | 2.55 | 0.69 |
| 4:L:520:ARG:O | 7:O:49:SER:CB | 2.36 | 0.69 |
| 1:A:224:LEU:HD11 | 1:A:226:CYS:HB2 | 1.75 | 0.68 |
| 1:A:94:ILE:HG22 | 1:A:96:ASP:H | 1.56 | 0.68 |
| 2:B:39:PRO:HA | 2:B:163:SER:HA | 1.74 | 0.68 |
| 6:F:353:LEU:O | 6:F:367:VAL:CG1 | 2.40 | 0.68 |
| 7:G:450:PRO:HA | 7:G:453:LEU:HD12 | 1.75 | 0.68 |
| 7:G:94:VAL:HG13 | 7:G:95:GLY:H | 1.59 | 0.68 |
| 2:J:360:LYS:C | 2:J:362:GLY:HA2 | 2.12 | 0.68 |
| 3:K:467:LEU:O | 3:K:471:LEU:HB2 | 1.93 | 0.68 |
| 1:A:12:THR:HB | 1:A:13:LEU:HB2 | 1.74 | 0.68 |
| 1:A:94:ILE:HG12 | 1:A:523:SER:HA | 1.75 | 0.68 |
| 2:B:328:THR:O | 2:B:329:PHE:CD1 | 2.46 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:299:LYS:N | 3:C:319:ARG:CB | 2.55 | 0.68 |
| 5:E:251:HIS:O | 5:E:253:GLN:N | 2.25 | 0.68 |
| 2:J:83:VAL:HG21 | 3:K:384:GLY:O | 1.92 | 0.68 |
| 5:M:74:LEU:HG | 5:M:93:GLN:HB3 | 1.75 | 0.68 |
| 6:N:154:ALA:HB2 | 6:N:402:VAL:HG23 | 1.73 | 0.68 |
| 8:P:346:ALA:N | 8:P:347:PRO:CD | 2.56 | 0.68 |
| 6:F:420:ILE:HG22 | 6:F:482:ASP:OD1 | 1.94 | 0.68 |
| 2:J:30:GLY:CA | 2:J:33:VAL:HG23 | 2.24 | 0.68 |
| 4:L:169:PHE:O | 4:L:173:LEU:HD13 | 1.92 | 0.68 |
| 8:P:316:TYR:HD2 | 8:P:316:TYR:N | 1.87 | 0.68 |
| 8:P:6:PRO:HB3 | 8:P:7:GLN:HA | 1.75 | 0.68 |
| 1:A:66:GLY:O | 1:A:69:ILE:HG22 | 1.94 | 0.68 |
| 4:D:71:LEU:CA | 8:P:6:PRO:CG | 2.71 | 0.68 |
| 2:J:422:ILE:HG22 | 2:J:424:GLY:N | 2.08 | 0.68 |
| 2:J:4:GLN:CB | 2:J:5:ILE:HG12 | 2.24 | 0.68 |
| 4:L:159:SER:O | 4:L:161:LYS:HD3 | 1.93 | 0.68 |
| 4:L:404:LEU:HD22 | 4:L:410:LEU:HG | 1.74 | 0.68 |
| 6:N:141:THR:HB | 6:N:409:LYS:HG3 | 1.75 | 0.68 |
| 6:N:330:LEU:HB2 | 6:N:375:SER:OG | 1.93 | 0.68 |
| 2:B:30:GLY:CA | 2:B:33:VAL:HG23 | 2.24 | 0.68 |
| 5:E:74:LEU:HG | 5:E:93:GLN:HB3 | 1.75 | 0.68 |
| 6:F:141:THR:HB | 6:F:409:LYS:HG3 | 1.75 | 0.68 |
| 6:F:233:VAL:HG13 | 6:F:351:SER:HB3 | 1.76 | 0.68 |
| 6:F:433:LYS:HG2 | 6:F:444:ILE:HG21 | 1.74 | 0.68 |
| 7:G:109:MET:HG2 | 7:G:514:THR:HG22 | 1.74 | 0.68 |
| 2:J:285:ILE:HD11 | 2:J:289:LEU:CD2 | 2.24 | 0.68 |
| 2:J:402:LEU:HD21 | 2:J:483:ARG:HG3 | 1.74 | 0.68 |
| 6:N:354:VAL:HG22 | 6:N:367:VAL:HG13 | 1.75 | 0.68 |
| 4:D:184:GLU:C | 4:D:186:SER:O | 2.32 | 0.68 |
| 6:F:7:ASN:OD1 | 6:F:8:PRO:N | 2.25 | 0.68 |
| 8:H:283:GLN:O | 8:H:287:MET:HG2 | 1.93 | 0.68 |
| 8:P:24:ALA:HB2 | 8:P:531:ALA:HB1 | 1.76 | 0.68 |
| 2:B:402:LEU:HD21 | 2:B:483:ARG:HG3 | 1.74 | 0.68 |
| 4:D:178:VAL:HG11 | 4:D:401:ILE:HD11 | 1.76 | 0.68 |
| 4:D:461:ASN:HB3 | 4:D:464:LYS:HG2 | 1.75 | 0.68 |
| 8:H:249:VAL:HG22 | 8:H:300:VAL:HB | 1.75 | 0.68 |
| 2:J:295:GLU:OE2 | 6:N:338:ASN:HB2 | 1.92 | 0.68 |
| 2:J:414:ALA:O | 2:J:417:THR:HG22 | 1.92 | 0.68 |
| 5:M:166:ASP:HB3 | 5:M:167:ASP:CB | 2.23 | 0.68 |
| 1:A:289:ILE:HA | 1:A:293:ALA:HB2 | 1.76 | 0.68 |
| 2:B:19:ARG:NH2 | 2:B:512:ASP:H | 1.92 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:181:ILE:HD13 | 4:D:373:PRO:O | 1.94 | 0.68 |
| 4:L:178:VAL:HG11 | 4:L:401:ILE:HD11 | 1.76 | 0.68 |
| 6:N:154:ALA:O | 6:N:157:SER:OG | 2.12 | 0.68 |
| 8:H:291:ILE:HD12 | 8:H:347:PRO:CG | 2.24 | 0.68 |
| 8:H:131:TYR:HD2 | 8:H:452:PHE:HD2 | 1.42 | 0.68 |
| 3:K:250:LEU:HG | 3:K:301:VAL:CB | 2.23 | 0.68 |
| 4:L:15:GLU:O | 4:L:523:ASP:OD2 | 2.11 | 0.68 |
| 3:C:250:LEU:HG | 3:C:301:VAL:CB | 2.23 | 0.68 |
| 5:E:34:ASP:O | 6:N:117:ILE:HD12 | 1.94 | 0.68 |
| 6:F:43:LEU:HD23 | 6:F:57:LYS:CB | 2.20 | 0.68 |
| 3:K:332:THR:HB | 3:K:349:GLY:HA3 | 1.76 | 0.68 |
| 4:L:521:ILE:HG23 | 7:O:50:ASP:O | 1.94 | 0.68 |
| 7:O:409:ILE:HG22 | 7:O:410:VAL:H | 1.59 | 0.68 |
| 8:P:291:ILE:HD12 | 8:P:347:PRO:CG | 2.24 | 0.68 |
| 2:B:285:ILE:HD11 | 2:B:289:LEU:CD2 | 2.24 | 0.67 |
| 6:F:352:GLY:O | 6:F:353:LEU:C | 2.33 | 0.67 |
| 8:H:6:PRO:HB3 | 8:H:7:GLN:HA | 1.76 | 0.67 |
| 1:I:66:GLY:O | 1:I:69:ILE:HG22 | 1.94 | 0.67 |
| 2:J:257:LYS:HA | 2:J:260:GLN:HB3 | 1.75 | 0.67 |
| 4:L:184:GLU:C | 4:L:186:SER:O | 2.32 | 0.67 |
| 6:N:167:THR:HA | 6:N:168:GLU:HB3 | 1.75 | 0.67 |
| 7:O:42:PRO:O | 7:O:48:GLY:CA | 2.40 | 0.67 |
| 7:O:94:VAL:HG13 | 7:O:95:GLY:H | 1.59 | 0.67 |
| 2:B:311:PHE:O | 2:B:315:GLU:HG2 | 1.93 | 0.67 |
| 3:C:332:THR:HB | 3:C:349:GLY:HA3 | 1.76 | 0.67 |
| 5:E:88:ALA:HB1 | 5:E:109:LYS:HZ1 | 1.60 | 0.67 |
| 6:F:330:LEU:HB2 | 6:F:375:SER:OG | 1.93 | 0.67 |
| 6:F:352:GLY:O | 6:F:367:VAL:HG11 | 1.91 | 0.67 |
| 7:G:241:ILE:HB | 7:G:330:VAL:HG11 | 1.77 | 0.67 |
| 7:G:448:VAL:HG12 | 7:G:452:GLN:NE2 | 2.09 | 0.67 |
| 7:G:492:PHE:HA | 7:G:497:TRP:HE1 | 1.59 | 0.67 |
| 6:N:423:SER:O | 6:N:427:ARG:HG3 | 1.94 | 0.67 |
| 2:B:243:VAL:HG12 | 2:B:245:ILE:H | 1.59 | 0.67 |
| 3:C:94:THR:HG23 | 10:C:1102:BEF:F1 | 1.82 | 0.67 |
| 4:D:241:ILE:HD12 | 4:D:241:ILE:H | 1.60 | 0.67 |
| 6:F:170:LEU:O | 6:F:173:ILE:HG22 | 1.94 | 0.67 |
| 1:I:289:ILE:HA | 1:I:293:ALA:HB2 | 1.76 | 0.67 |
| 1:I:64:ASN:ND2 | 1:I:166:SER:O | 2.27 | 0.67 |
| 6:N:501:PRO:CB | 6:N:506:ILE:HB | 2.17 | 0.67 |
| 7:O:241:ILE:HB | 7:O:330:VAL:HG11 | 1.77 | 0.67 |
| 7:O:450:PRO:HA | 7:O:453:LEU:HD12 | 1.75 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:P:249:VAL:HG22 | 8:P:300:VAL:HB | 1.76 | 0.67 |
| 2:B:237:THR:N | 2:B:287:ARG:HG3 | 2.10 | 0.67 |
| 2:B:422:ILE:HG22 | 2:B:424:GLY:N | 2.08 | 0.67 |
| 8:H:54:ILE:CG1 | 8:H:64:ILE:HG12 | 2.13 | 0.67 |
| 1:I:94:ILE:HG12 | 1:I:523:SER:HA | 1.75 | 0.67 |
| 2:J:422:ILE:HB | 2:J:427:SER:CB | 2.15 | 0.67 |
| 6:N:209:PHE:HB2 | 6:N:378:ILE:HB | 1.75 | 0.67 |
| 8:P:283:GLN:O | 8:P:287:MET:HG2 | 1.93 | 0.67 |
| 1:A:64:ASN:ND2 | 1:A:166:SER:O | 2.27 | 0.67 |
| 2:B:295:GLU:OE2 | 6:F:338:ASN:HB2 | 1.93 | 0.67 |
| 4:D:521:ILE:CG2 | 7:G:50:ASP:O | 2.42 | 0.67 |
| 7:G:162:ALA:HB3 | 7:G:179:VAL:HG13 | 1.77 | 0.67 |
| 4:L:100:THR:HG22 | 4:L:515:VAL:HG13 | 1.77 | 0.67 |
| 5:E:34:ASP:CA | 6:N:117:ILE:CD1 | 2.66 | 0.67 |
| 6:N:321:LYS:HA | 6:N:321:LYS:HE3 | 1.75 | 0.67 |
| 6:F:224:MET:CE | 6:F:316:ALA:H | 2.06 | 0.67 |
| 4:D:69:ALA:O | 8:H:15:LYS:HE2 | 1.94 | 0.67 |
| 8:H:334:ARG:HG2 | 8:H:380:ARG:HB3 | 1.77 | 0.67 |
| 1:I:66:GLY:H | 1:I:99:THR:HG22 | 1.60 | 0.67 |
| 2:J:19:ARG:NH2 | 2:J:512:ASP:H | 1.92 | 0.67 |
| 3:K:108:ALA:N | 3:K:109:PRO:HD2 | 2.10 | 0.67 |
| 5:M:251:HIS:O | 5:M:253:GLN:N | 2.24 | 0.67 |
| 6:N:485:GLU:HB3 | 6:N:488:TYR:CB | 2.24 | 0.67 |
| 1:A:66:GLY:H | 1:A:99:THR:HG22 | 1.60 | 0.67 |
| 4:D:100:THR:HG22 | 4:D:515:VAL:HG13 | 1.77 | 0.67 |
| 6:F:151:LEU:HB3 | 6:F:175:THR:OG1 | 1.95 | 0.67 |
| 7:G:282:LEU:HD22 | 7:G:307:PHE:HB3 | 1.76 | 0.67 |
| 1:I:348:GLU:CB | 1:I:349:THR:HA | 2.25 | 0.67 |
| 6:N:170:LEU:O | 6:N:173:ILE:HG22 | 1.94 | 0.67 |
| 7:O:492:PHE:HA | 7:O:497:TRP:HE1 | 1.59 | 0.67 |
| 8:P:335:VAL:HG13 | 8:P:379:SER:HB3 | 1.75 | 0.67 |
| 2:B:34:LYS:O | 2:B:36:THR:N | 2.27 | 0.67 |
| 6:F:485:GLU:HB3 | 6:F:488:TYR:CB | 2.25 | 0.67 |
| 4:L:181:ILE:HD13 | 4:L:373:PRO:O | 1.94 | 0.67 |
| 4:L:461:ASN:HB3 | 4:L:464:LYS:HG2 | 1.75 | 0.67 |
| 6:N:16:ASP:HA | 6:N:19:LEU:CD1 | 2.20 | 0.67 |
| 6:N:280:LEU:HD23 | 6:N:280:LEU:H | 1.60 | 0.67 |
| 7:O:282:LEU:HD22 | 7:O:307:PHE:HB3 | 1.76 | 0.67 |
| 4:D:528:ARG:H | 4:D:528:ARG:HE | 1.43 | 0.67 |
| 6:F:187:ASP:O | 6:F:188:ASN:CB | 2.43 | 0.67 |
| 6:F:423:SER:O | 6:F:427:ARG:HG3 | 1.94 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:H:6:PRO:O | 7:O:58:GLN:NE2 | 2.28 | 0.67 |
| 6:N:187:ASP:O | 6:N:188:ASN:CB | 2.43 | 0.67 |
| 7:O:162:ALA:HB3 | 7:O:179:VAL:HG13 | 1.77 | 0.67 |
| 4:D:233:LYS:HA | 4:D:345:ASP:O | 1.95 | 0.67 |
| 5:E:355:ALA:HB3 | 6:F:222:PRO:HG2 | 1.76 | 0.67 |
| 1:I:250:ASN:CG | 1:I:250:ASN:O | 2.32 | 0.67 |
| 4:L:9:ALA:HB1 | 7:O:76:VAL:H | 1.60 | 0.67 |
| 8:P:334:ARG:HG2 | 8:P:380:ARG:HB3 | 1.77 | 0.67 |
| 3:C:467:LEU:HD21 | 3:C:491:ILE:HG21 | 1.78 | 0.66 |
| 6:F:195:GLU:OE1 | 6:F:197:MET:SD | 2.53 | 0.66 |
| 1:I:397:GLU:HG2 | 1:I:400:ARG:HH11 | 1.61 | 0.66 |
| 1:A:507:GLY:O | 1:A:508:LYS:CB | 2.43 | 0.66 |
| 7:G:91:ASP:O | 7:G:95:GLY:HA2 | 1.95 | 0.66 |
| 2:J:237:THR:N | 2:J:287:ARG:HG3 | 2.10 | 0.66 |
| 4:L:24:ASN:HD21 | 4:L:524:ILE:HD11 | 1.60 | 0.66 |
| 6:N:224:MET:CE | 6:N:316:ALA:H | 2.06 | 0.66 |
| 7:O:448:VAL:HG12 | 7:O:452:GLN:NE2 | 2.09 | 0.66 |
| 7:O:108:LEU:HD11 | 7:O:511:THR:HG22 | 1.77 | 0.66 |
| 1:A:118:ASN:C | 1:A:119:LYS:HD2 | 2.16 | 0.66 |
| 1:A:348:GLU:CB | 1:A:349:THR:HA | 2.25 | 0.66 |
| 2:B:206:SER:CB | 2:B:368:VAL:HG13 | 2.26 | 0.66 |
| 2:B:329:PHE:C | 2:B:329:PHE:HD2 | 1.96 | 0.66 |
| 2:B:360:LYS:C | 2:B:362:GLY:HA2 | 2.12 | 0.66 |
| 4:D:24:ASN:HD21 | 4:D:524:ILE:HD11 | 1.60 | 0.66 |
| 9:D:601:ADP:O3' | 9:D:601:ADP:H8 | 1.78 | 0.66 |
| 7:G:483:PHE:CB | 9:G:601:ADP:HN62 | 2.08 | 0.66 |
| 8:H:24:ALA:HB2 | 8:H:531:ALA:HB1 | 1.76 | 0.66 |
| 2:J:409:MET:HE2 | 2:J:409:MET:HA | 1.76 | 0.66 |
| 3:K:265:LYS:NZ | 3:K:268:ASP:CB | 2.55 | 0.66 |
| 3:K:467:LEU:HD21 | 3:K:491:ILE:HG21 | 1.77 | 0.66 |
| 4:L:241:ILE:H | 4:L:241:ILE:HD12 | 1.60 | 0.66 |
| 8:P:131:TYR:HD2 | 8:P:452:PHE:HD2 | 1.42 | 0.66 |
| 6:F:543:GLU:O | 6:F:544:THR:C | 2.33 | 0.66 |
| 7:G:343:PRO:HA | 7:G:346:LEU:HD21 | 1.78 | 0.66 |
| 7:G:410:VAL:HG12 | 7:G:498:GLU:O | 1.95 | 0.66 |
| 4:L:24:ASN:HA | 4:L:74:VAL:HG21 | 1.77 | 0.66 |
| 2:J:49:ALA:HB1 | 6:N:538:ARG:HB2 | 1.78 | 0.66 |
| 7:O:317:ARG:HG3 | 7:O:317:ARG:O | 1.94 | 0.66 |
| 1:A:397:GLU:HG2 | 1:A:400:ARG:HH11 | 1.61 | 0.66 |
| 2:B:23:PHE:HA | 2:B:103:LEU:HD13 | 1.77 | 0.66 |
| 2:B:255:THR:HA | 2:B:258:LEU:HD13 | 1.77 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:4:GLN:CB | 2:B:5:ILE:HG12 | 2.24 | 0.66 |
| 2:B:165:ILE:HG12 | 6:F:529:LEU:HD13 | 1.76 | 0.66 |
| 7:G:317:ARG:O | 7:G:317:ARG:HG3 | 1.95 | 0.66 |
| 8:H:204:VAL:HG13 | 8:H:405:VAL:CG1 | 2.25 | 0.66 |
| 4:D:44:MET:HG3 | 8:H:531:ALA:HB3 | 1.77 | 0.66 |
| 1:I:431:ILE:HG12 | 1:I:482:ALA:CB | 2.25 | 0.66 |
| 2:J:422:ILE:O | 2:J:423:ASP:CG | 2.34 | 0.66 |
| 2:J:463:ILE:O | 2:J:467:ILE:CA | 2.44 | 0.66 |
| 4:L:528:ARG:H | 4:L:528:ARG:HE | 1.43 | 0.66 |
| 6:N:352:GLY:O | 6:N:353:LEU:C | 2.33 | 0.66 |
| 6:N:541:LEU:HB3 | 6:N:543:GLU:H | 1.60 | 0.66 |
| 4:L:233:LYS:HA | 4:L:345:ASP:O | 1.95 | 0.66 |
| 4:D:252:ILE:HB | 8:H:262:LYS:O | 1.96 | 0.66 |
| 6:F:451:LEU:O | 6:F:455:PRO:CD | 2.44 | 0.66 |
| 6:N:75:LEU:HD22 | 6:N:527:LEU:HD11 | 1.78 | 0.66 |
| 7:O:516:LEU:HD11 | 7:O:517:ILE:HG12 | 1.75 | 0.66 |
| 4:L:254:VAL:HG22 | 8:P:265:VAL:HA | 1.77 | 0.66 |
| 2:B:444:LEU:HD21 | 9:B:601:ADP:H1' | 1.78 | 0.66 |
| 6:F:541:LEU:HB3 | 6:F:543:GLU:H | 1.60 | 0.66 |
| 7:G:409:ILE:HG22 | 7:G:410:VAL:H | 1.59 | 0.66 |
| 3:K:297:THR:O | 3:K:319:ARG:HA | 1.96 | 0.66 |
| 6:N:233:VAL:HG13 | 6:N:351:SER:HB3 | 1.76 | 0.66 |
| 7:O:410:VAL:HG12 | 7:O:498:GLU:O | 1.95 | 0.66 |
| 8:P:6:PRO:CB | 8:P:7:GLN:HA | 2.26 | 0.66 |
| 1:A:54:VAL:HG12 | 1:A:56:ASP:H | 1.60 | 0.66 |
| 1:A:65:ASP:HB3 | 1:A:68:THR:OG1 | 1.96 | 0.66 |
| 7:G:108:LEU:HD11 | 7:G:511:THR:HG22 | 1.77 | 0.66 |
| 1:I:118:ASN:C | 1:I:119:LYS:HD2 | 2.16 | 0.66 |
| 5:M:55:ARG:HG3 | 5:M:131:ASP:OD2 | 1.96 | 0.66 |
| 5:M:350:GLU:HA | 5:M:352:GLU:OE2 | 1.96 | 0.66 |
| 7:O:75:VAL:HG21 | 7:O:84:VAL:HG21 | 1.78 | 0.66 |
| 7:O:91:ASP:O | 7:O:95:GLY:HA2 | 1.95 | 0.66 |
| 1:A:183:ALA:HB1 | 1:A:383:SER:CB | 2.26 | 0.66 |
| 1:A:431:ILE:HG12 | 1:A:482:ALA:CB | 2.25 | 0.66 |
| 5:E:55:ARG:HG3 | 5:E:131:ASP:OD2 | 1.96 | 0.66 |
| 6:F:280:LEU:H | 6:F:280:LEU:HD23 | 1.59 | 0.66 |
| 7:G:70:LEU:HB3 | 7:G:84:VAL:HG13 | 1.78 | 0.66 |
| 8:H:6:PRO:CB | 8:H:7:GLN:HA | 2.26 | 0.66 |
| 2:J:243:VAL:HG12 | 2:J:245:ILE:H | 1.60 | 0.66 |
| 2:J:255:THR:HA | 2:J:258:LEU:HD13 | 1.77 | 0.66 |
| 2:J:3:VAL:O | 2:J:5:ILE:HG12 | 1.96 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:N:151:LEU:HB3 | 6:N:175:THR:OG1 | 1.95 | 0.66 |
| 6:N:420:ILE:HG22 | 6:N:482:ASP:OD1 | 1.94 | 0.66 |
| 8:P:24:ALA:CA | 8:P:531:ALA:O | 2.43 | 0.66 |
| 8:P:94:ILE:HD12 | 8:P:95:ASP:H | 1.61 | 0.66 |
| 1:A:250:ASN:CG | 1:A:250:ASN:O | 2.32 | 0.65 |
| 3:C:108:ALA:N | 3:C:109:PRO:HD2 | 2.10 | 0.65 |
| 5:M:66:GLY:N | 9:M:601:ADP:H5'1 | 2.07 | 0.65 |
| 7:O:90:GLN:CG | 7:O:101:VAL:HG21 | 2.24 | 0.65 |
| 6:F:193:MET:HE2 | 6:F:330:LEU:HD11 | 1.76 | 0.65 |
| 6:F:75:LEU:HD22 | 6:F:527:LEU:HD11 | 1.78 | 0.65 |
| 6:N:195:GLU:OE1 | 6:N:197:MET:SD | 2.53 | 0.65 |
| 6:N:543:GLU:O | 6:N:544:THR:C | 2.33 | 0.65 |
| 4:D:185:ASN:N | 4:D:186:SER:O | 2.30 | 0.65 |
| 6:F:154:ALA:O | 6:F:157:SER:OG | 2.12 | 0.65 |
| 8:H:94:ILE:HD12 | 8:H:95:ASP:H | 1.61 | 0.65 |
| 2:J:263:LYS:HZ1 | 3:K:266:GLU:CB | 2.09 | 0.65 |
| 2:J:300:ASP:O | 2:J:301:LEU:CB | 2.44 | 0.65 |
| 6:N:451:LEU:O | 6:N:455:PRO:CD | 2.44 | 0.65 |
| 2:B:5:ILE:HG13 | 2:B:6:PHE:N | 2.09 | 0.65 |
| 4:D:254:VAL:CG2 | 8:H:265:VAL:HA | 2.25 | 0.65 |
| 1:I:183:ALA:HB1 | 1:I:383:SER:CB | 2.26 | 0.65 |
| 2:J:319:LEU:HD21 | 2:J:357:SER:OG | 1.97 | 0.65 |
| 2:J:492:LYS:HE2 | 2:J:493:LEU:N | 2.12 | 0.65 |
| 6:N:353:LEU:O | 6:N:367:VAL:HG13 | 1.97 | 0.65 |
| 2:B:422:ILE:O | 2:B:423:ASP:CG | 2.34 | 0.65 |
| 4:D:297:VAL:HB | 4:D:298:ASN:HA | 1.78 | 0.65 |
| 8:H:24:ALA:CA | 8:H:531:ALA:O | 2.43 | 0.65 |
| 3:K:269:TRP:HH2 | 6:N:248:ASN:N | 1.82 | 0.65 |
| 3:K:57:LEU:N | 3:K:57:LEU:CD2 | 2.57 | 0.65 |
| 6:N:540:THR:HB | 6:N:541:LEU:CD2 | 2.25 | 0.65 |
| 2:B:402:LEU:HD11 | 2:B:483:ARG:HE | 1.62 | 0.65 |
| 3:C:122:ILE:HD13 | 3:C:522:ARG:HG2 | 1.79 | 0.65 |
| 7:G:75:VAL:HG21 | 7:G:84:VAL:HG21 | 1.78 | 0.65 |
| 8:H:250:PHE:HE2 | 8:H:299:ILE:HD12 | 1.62 | 0.65 |
| 1:I:65:ASP:HB3 | 1:I:68:THR:OG1 | 1.96 | 0.65 |
| 2:J:459:LEU:HD22 | 2:J:472:LEU:CG | 2.26 | 0.65 |
| 4:L:297:VAL:HB | 4:L:298:ASN:HA | 1.78 | 0.65 |
| 6:N:53:ILE:CD1 | 6:N:53:ILE:C | 2.62 | 0.65 |
| 8:P:250:PHE:HE2 | 8:P:299:ILE:HD12 | 1.61 | 0.65 |
| 1:I:187:VAL:HG23 | 1:I:383:SER:HB3 | 1.79 | 0.65 |
| 1:I:507:GLY:O | 1:I:508:LYS:CB | 2.43 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------------------|--------------------------|-------------------|
| 2:J:23:PHE:HA | 2:J:103:LEU:HD13 | 1.77 | 0.65 |
| 2:J:393:GLN:HB3 | 2:J:492:LYS:HE3 | 1.79 | 0.65 |
| 2:J:5:ILE:HG13 | 2:J:6:PHE:N | 2.09 | 0.65 |
| 3:K:255:GLY:H | 3:K:259:THR:HG21 | 1.62 | 0.65 |
| 8:P:300:VAL:HG11 | 8:P:332:LEU:HD21 | 1.79 | 0.65 |
| 4:D:330:CYS:CB | 4:D:345:ASP:OD2 | 2.44 | 0.65 |
| 6:F:540:THR:HB | 6:F:541:LEU:CD2 | 2.25 | 0.65 |
| 7:G:86:ILE:HA | 7:G:89:ALA:HB3 | 1.79 | 0.65 |
| 1:I:54:VAL:HG12 | 1:I:56:ASP:H | 1.60 | 0.65 |
| 6:N:540:THR:O | 6:N:542:LYS:CG | 2.44 | 0.65 |
| 7:O:70:LEU:HB3 | 7:O:84:VAL:HG13 | 1.78 | 0.65 |
| 2:B:319:LEU:HD21 | 2:B:357:SER:OG | 1.97 | 0.65 |
| 2:B:278:LYS:HA | 2:B:333:SER:HB3 | 1.79 | 0.65 |
| 2:B:8:ASP:CB | 2:B:9:GLN:HA | 2.22 | 0.65 |
| 4:D:24:ASN:HA | 4:D:74:VAL:HG21 | 1.77 | 0.65 |
| 4:D:217:GLN:NE2 | 4:D:316:ILE:HA | 2.12 | 0.65 |
| 6:F:174:VAL:HG13 | 6:F:399:LEU:HD13 | 1.77 | 0.65 |
| 7:G:446:LEU:HD21 | 7:G:507:LEU:HD23 | 1.78 | 0.65 |
| 2:J:409:MET:HB3 | 2:J:463:ILE:HD13 | 1.78 | 0.65 |
| 4:L:154:ALA:HB2 | 4:L:175:VAL:HG13 | 1.79 | 0.65 |
| 4:L:38:SER:HB3 | 4:L:46:LYS:HZ3 | 1.61 | 0.65 |
| 7:O:56:SER:HA | 7:O:57:ASN:C | 2.17 | 0.65 |
| 3:C:161:THR:H | 3:C:165:ILE:HG13 | 1.62 | 0.65 |
| 3:C:297:THR:O | 3:C:319:ARG:HA | 1.96 | 0.65 |
| 5:E:350:GLU:HA | 5:E:352:GLU:OE2 | 1.96 | 0.65 |
| 6:F:539:SER:HB2 | 6:F:542:LYS:CD | 2.27 | 0.65 |
| 7:G:454:CYS:HB2 | 7:G:461:ALA:CB | 2.27 | 0.65 |
| 2:J:27:ILE:CD1 | 2:J:104:ARG:HH11 | 2.09 | 0.65 |
| 2:J:230:LYS:HA | 2:J:337:LEU:O | 1.97 | 0.65 |
| 2:J:402:LEU:HD11 | 2:J:483:ARG:HE | 1.62 | 0.65 |
| 7:O:83:LEU:HD23 | 7:O:86:ILE:HD11 | 1.78 | 0.65 |
| 2:B:21:SER:OG | 1:I:8:SER:N | 2.30 | 0.64 |
| 2:J:45:LEU:HB2 | 6:N:533:LEU:CB | 2.27 | 0.64 |
| 4:L:185:ASN:N | 4:L:186:SER:O | 2.30 | 0.64 |
| 4:L:214:VAL:HG22 | 4:L:362:ARG:HG2 | 1.80 | 0.64 |
| 4:L:38:SER:HB3 | 4:L:46:LYS:NZ | 2.12 | 0.64 |
| 1:A:45:GLY:H | 9:A:601:ADP:H5 ¹ | 1.63 | 0.64 |
| 2:B:206:SER:HB2 | 2:B:368:VAL:HG22 | 1.78 | 0.64 |
| 2:B:300:ASP:O | 2:B:301:LEU:CB | 2.44 | 0.64 |
| 2:B:463:ILE:O | 2:B:467:ILE:CA | 2.44 | 0.64 |
| 2:B:492:LYS:HE2 | 2:B:493:LEU:N | 2.12 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:255:GLY:H | 3:C:259:THR:HG21 | 1.62 | 0.64 |
| 4:D:226:PRO:HB2 | 4:D:311:MET:HG2 | 1.79 | 0.64 |
| 4:D:38:SER:HB3 | 4:D:46:LYS:NZ | 2.12 | 0.64 |
| 4:D:521:ILE:HG21 | 7:G:52:LEU:H | 1.61 | 0.64 |
| 6:F:241:GLU:HA | 6:F:302:ASP:OD2 | 1.98 | 0.64 |
| 2:J:197:LYS:HB3 | 2:J:381:GLU:OE1 | 1.97 | 0.64 |
| 3:K:124:ALA:HB1 | 3:K:441:PRO:HB2 | 1.79 | 0.64 |
| 7:O:446:LEU:HD21 | 7:O:507:LEU:HD23 | 1.78 | 0.64 |
| 4:L:524:ILE:HG23 | 7:O:52:LEU:HD22 | 1.80 | 0.64 |
| 4:D:239:PHE:H | 4:D:288:ILE:HD12 | 1.62 | 0.64 |
| 7:G:90:GLN:CG | 7:G:101:VAL:HG21 | 2.24 | 0.64 |
| 7:G:235:LYS:CB | 7:G:352:PHE:O | 2.46 | 0.64 |
| 3:K:269:TRP:CH2 | 6:N:248:ASN:N | 2.60 | 0.64 |
| 4:L:217:GLN:NE2 | 4:L:316:ILE:HA | 2.12 | 0.64 |
| 4:L:410:LEU:HD13 | 4:L:498:LEU:HD22 | 1.78 | 0.64 |
| 6:N:143:LEU:HD22 | 6:N:145:ASN:HB3 | 1.79 | 0.64 |
| 1:A:187:VAL:HG23 | 1:A:383:SER:HB3 | 1.79 | 0.64 |
| 2:B:230:LYS:HA | 2:B:337:LEU:O | 1.98 | 0.64 |
| 2:B:8:ASP:HA | 2:B:10:VAL:HG23 | 1.80 | 0.64 |
| 6:F:419:TYR:CZ | 6:F:513:LEU:HD21 | 2.32 | 0.64 |
| 6:F:53:ILE:CD1 | 6:F:53:ILE:C | 2.62 | 0.64 |
| 7:G:83:LEU:HD23 | 7:G:86:ILE:HD11 | 1.78 | 0.64 |
| 2:J:357:SER:C | 2:J:360:LYS:CB | 2.66 | 0.64 |
| 2:J:408:GLU:HG2 | 2:J:440:LEU:HB3 | 1.78 | 0.64 |
| 5:E:39:LYS:HE2 | 6:N:109:ILE:O | 1.96 | 0.64 |
| 6:N:419:TYR:CZ | 6:N:513:LEU:HD21 | 2.32 | 0.64 |
| 1:A:184:LEU:HD21 | 1:A:198:TYR:CB | 2.28 | 0.64 |
| 2:B:232:LEU:HD21 | 2:B:325:VAL:HG21 | 1.79 | 0.64 |
| 2:B:393:GLN:HB3 | 2:B:492:LYS:HE3 | 1.79 | 0.64 |
| 6:F:434:LEU:O | 6:F:438:GLY:CA | 2.45 | 0.64 |
| 7:G:42:PRO:O | 7:G:48:GLY:CA | 2.40 | 0.64 |
| 2:J:232:LEU:HD21 | 2:J:325:VAL:HG21 | 1.80 | 0.64 |
| 4:L:239:PHE:H | 4:L:288:ILE:HD12 | 1.62 | 0.64 |
| 4:L:226:PRO:HB2 | 4:L:311:MET:HG2 | 1.80 | 0.64 |
| 2:J:295:GLU:HB2 | 6:N:337:GLN:NE2 | 2.12 | 0.64 |
| 6:N:414:GLY:O | 6:N:415:ALA:HB3 | 1.97 | 0.64 |
| 7:O:239:PRO:HA | 7:O:291:ASN:HD21 | 1.63 | 0.64 |
| 8:P:168:SER:HB3 | 8:P:175:GLU:HB3 | 1.80 | 0.64 |
| 1:A:218:LEU:HD22 | 1:A:219:VAL:H | 1.63 | 0.64 |
| 2:B:409:MET:HB3 | 2:B:463:ILE:HD13 | 1.78 | 0.64 |
| 4:D:214:VAL:HG22 | 4:D:362:ARG:HG2 | 1.80 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:410:LEU:HD13 | 4:D:498:LEU:HD22 | 1.78 | 0.64 |
| 4:D:134:ILE:HD11 | 4:D:424:ARG:CG | 2.28 | 0.64 |
| 5:E:166:ASP:H | 5:E:167:ASP:HB2 | 1.60 | 0.64 |
| 7:G:239:PRO:HA | 7:G:291:ASN:HD21 | 1.63 | 0.64 |
| 7:G:56:SER:HA | 7:G:57:ASN:C | 2.16 | 0.64 |
| 2:J:8:ASP:HA | 2:J:10:VAL:HG23 | 1.79 | 0.64 |
| 3:K:122:ILE:HD13 | 3:K:522:ARG:HG2 | 1.79 | 0.64 |
| 6:N:174:VAL:HG13 | 6:N:399:LEU:HD13 | 1.78 | 0.64 |
| 7:G:109:MET:HG2 | 7:G:514:THR:CG2 | 2.28 | 0.64 |
| 7:G:516:LEU:HD11 | 7:G:517:ILE:HG12 | 1.75 | 0.64 |
| 3:K:161:THR:H | 3:K:165:ILE:HG13 | 1.62 | 0.64 |
| 4:L:134:ILE:HD11 | 4:L:424:ARG:CG | 2.28 | 0.64 |
| 6:N:434:LEU:O | 6:N:438:GLY:CA | 2.45 | 0.64 |
| 7:O:343:PRO:HA | 7:O:346:LEU:HD21 | 1.78 | 0.64 |
| 7:O:454:CYS:HB2 | 7:O:461:ALA:CB | 2.27 | 0.64 |
| 2:B:197:LYS:HB3 | 2:B:381:GLU:OE1 | 1.97 | 0.64 |
| 3:C:93:THR:HG22 | 10:C:1102:BEF:F2 | 1.87 | 0.64 |
| 4:D:499:GLN:NE2 | 9:D:601:ADP:H2' | 2.12 | 0.64 |
| 6:F:353:LEU:O | 6:F:367:VAL:HG13 | 1.97 | 0.64 |
| 2:J:201:GLY:H | 6:N:86:ILE:HD12 | 1.63 | 0.64 |
| 5:M:66:GLY:H | 9:M:601:ADP:C5' | 2.05 | 0.64 |
| 6:N:538:ARG:HH11 | 6:N:538:ARG:CG | 2.11 | 0.64 |
| 7:O:191:ARG:CD | 7:O:192:ASN:N | 2.61 | 0.64 |
| 7:O:86:ILE:HA | 7:O:89:ALA:HB3 | 1.79 | 0.64 |
| 1:A:517:VAL:C | 1:A:518:LEU:HG | 2.18 | 0.64 |
| 2:B:4:GLN:HB2 | 3:C:71:ALA:HB3 | 1.80 | 0.64 |
| 4:D:154:ALA:HB2 | 4:D:175:VAL:HG13 | 1.79 | 0.64 |
| 2:J:465:ASN:OD1 | 2:J:465:ASN:C | 2.36 | 0.64 |
| 4:L:367:ARG:C | 4:L:369:ASN:H | 2.01 | 0.64 |
| 6:N:83:GLN:HG3 | 6:N:94:VAL:CG2 | 2.18 | 0.64 |
| 1:A:66:GLY:N | 1:A:99:THR:HG22 | 2.12 | 0.64 |
| 3:C:223:VAL:HG12 | 3:C:224:LEU:H | 1.63 | 0.64 |
| 5:E:33:LYS:HE2 | 6:N:117:ILE:HG12 | 1.79 | 0.64 |
| 5:E:128:ALA:HB2 | 5:E:478:THR:HG21 | 1.80 | 0.64 |
| 6:F:23:VAL:HG11 | 6:F:106:HIS:CB | 2.28 | 0.64 |
| 6:F:331:VAL:O | 6:F:332:THR:OG1 | 2.12 | 0.64 |
| 1:I:66:GLY:N | 1:I:99:THR:HG22 | 2.12 | 0.64 |
| 2:J:278:LYS:HA | 2:J:333:SER:HB3 | 1.79 | 0.64 |
| 2:J:411:MET:O | 2:J:415:VAL:HG23 | 1.98 | 0.64 |
| 5:M:401:THR:O | 5:M:402:LYS:CB | 2.46 | 0.64 |
| 6:N:352:GLY:O | 6:N:367:VAL:HG11 | 1.91 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:O:317:ARG:O | 7:O:317:ARG:CG | 2.46 | 0.64 |
| 2:B:357:SER:C | 2:B:360:LYS:CB | 2.66 | 0.63 |
| 3:C:124:ALA:HB1 | 3:C:441:PRO:HB2 | 1.79 | 0.63 |
| 1:I:540:ARG:O | 5:M:70:LEU:HB3 | 1.98 | 0.63 |
| 2:J:329:PHE:HD2 | 2:J:329:PHE:C | 1.95 | 0.63 |
| 5:M:166:ASP:H | 5:M:167:ASP:HB2 | 1.60 | 0.63 |
| 8:P:430:LEU:HD13 | 8:P:434:ILE:HD11 | 1.79 | 0.63 |
| 3:C:391:GLU:O | 3:C:395:ASN:HB2 | 1.99 | 0.63 |
| 4:D:210:ILE:O | 4:D:375:VAL:HG13 | 1.98 | 0.63 |
| 6:F:538:ARG:HH11 | 6:F:538:ARG:CG | 2.11 | 0.63 |
| 1:I:218:LEU:HD22 | 1:I:219:VAL:H | 1.63 | 0.63 |
| 2:J:251:LYS:N | 6:N:251:PHE:HA | 2.10 | 0.63 |
| 2:B:411:MET:O | 2:B:415:VAL:HG23 | 1.98 | 0.63 |
| 7:G:317:ARG:O | 7:G:317:ARG:CG | 2.46 | 0.63 |
| 3:K:335:THR:HB | 8:P:237:LYS:HE2 | 1.80 | 0.63 |
| 4:D:252:ILE:O | 8:H:263:GLY:HA2 | 1.99 | 0.63 |
| 6:N:159:LEU:O | 6:N:160:THR:CB | 2.46 | 0.63 |
| 6:N:241:GLU:HA | 6:N:302:ASP:OD2 | 1.98 | 0.63 |
| 7:O:235:LYS:CB | 7:O:352:PHE:O | 2.46 | 0.63 |
| 2:B:408:GLU:HG2 | 2:B:440:LEU:HB3 | 1.78 | 0.63 |
| 3:C:35:ILE:HD11 | 3:C:65:LEU:HG | 1.80 | 0.63 |
| 6:F:106:HIS:O | 6:F:109:ILE:HG12 | 1.97 | 0.63 |
| 6:F:83:GLN:HG3 | 6:F:94:VAL:CG2 | 2.18 | 0.63 |
| 8:H:300:VAL:HG11 | 8:H:332:LEU:HD21 | 1.79 | 0.63 |
| 8:H:430:LEU:HD13 | 8:H:434:ILE:HD11 | 1.79 | 0.63 |
| 1:I:158:ASN:ND2 | 1:I:516:GLY:HA2 | 2.13 | 0.63 |
| 6:N:433:LYS:HB3 | 6:N:441:LYS:HA | 1.80 | 0.63 |
| 6:N:539:SER:HB2 | 6:N:542:LYS:CD | 2.27 | 0.63 |
| 7:O:282:LEU:HD21 | 7:O:306:PHE:HB2 | 1.80 | 0.63 |
| 2:B:236:THR:OG1 | 2:B:327:SER:HA | 1.99 | 0.63 |
| 5:E:283:THR:HG22 | 5:E:284:LYS:H | 1.64 | 0.63 |
| 6:F:143:LEU:HD22 | 6:F:145:ASN:HB3 | 1.79 | 0.63 |
| 6:F:330:LEU:CB | 6:F:375:SER:OG | 2.47 | 0.63 |
| 1:I:115:LEU:HD13 | 1:I:125:ILE:HD11 | 1.81 | 0.63 |
| 6:N:331:VAL:O | 6:N:332:THR:OG1 | 2.12 | 0.63 |
| 7:O:237:ASN:C | 7:O:239:PRO:HD3 | 2.18 | 0.63 |
| 8:P:204:VAL:HG13 | 8:P:405:VAL:CG1 | 2.25 | 0.63 |
| 2:B:465:ASN:OD1 | 2:B:465:ASN:C | 2.36 | 0.63 |
| 6:F:159:LEU:O | 6:F:160:THR:CB | 2.46 | 0.63 |
| 7:G:191:ARG:CZ | 7:G:192:ASN:N | 2.61 | 0.63 |
| 1:I:517:VAL:C | 1:I:518:LEU:HG | 2.18 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:210:GLU:OE1 | 2:J:357:SER:O | 2.17 | 0.63 |
| 2:J:492:LYS:H | 2:J:492:LYS:NZ | 1.97 | 0.63 |
| 5:M:283:THR:HG22 | 5:M:284:LYS:H | 1.64 | 0.63 |
| 6:N:106:HIS:O | 6:N:109:ILE:HG12 | 1.97 | 0.63 |
| 6:N:330:LEU:CB | 6:N:375:SER:OG | 2.47 | 0.63 |
| 7:O:189:LEU:N | 7:O:190:ASP:HB2 | 2.14 | 0.63 |
| 7:O:109:MET:HG2 | 7:O:514:THR:CG2 | 2.28 | 0.63 |
| 7:O:109:MET:SD | 7:O:514:THR:HG22 | 2.39 | 0.63 |
| 1:I:55:ASP:HA | 7:O:527:LYS:HB3 | 1.80 | 0.63 |
| 1:A:458:ILE:HB | 1:A:459:PRO:HD3 | 1.81 | 0.63 |
| 2:B:230:LYS:H | 2:B:281:ILE:HG22 | 1.62 | 0.63 |
| 2:B:3:VAL:O | 2:B:5:ILE:HG12 | 1.96 | 0.63 |
| 4:D:367:ARG:C | 4:D:369:ASN:H | 2.01 | 0.63 |
| 7:G:191:ARG:CD | 7:G:192:ASN:N | 2.61 | 0.63 |
| 7:G:498:GLU:HG2 | 9:G:601:ADP:O2' | 1.99 | 0.63 |
| 8:H:168:SER:HB3 | 8:H:175:GLU:HB3 | 1.80 | 0.63 |
| 2:J:34:LYS:O | 2:J:36:THR:N | 2.27 | 0.63 |
| 5:M:104:LEU:CD2 | 5:M:123:VAL:HG13 | 2.27 | 0.63 |
| 6:N:23:VAL:HG11 | 6:N:106:HIS:CB | 2.28 | 0.63 |
| 7:O:304:THR:HA | 7:O:307:PHE:HE2 | 1.63 | 0.63 |
| 6:F:203:SER:C | 6:F:205:LYS:H | 2.03 | 0.63 |
| 6:F:414:GLY:O | 6:F:415:ALA:HB3 | 1.98 | 0.63 |
| 1:I:228:VAL:CG2 | 1:I:363:GLN:NE2 | 2.49 | 0.63 |
| 2:J:422:ILE:HG21 | 2:J:427:SER:HB3 | 1.79 | 0.63 |
| 2:J:98:LEU:O | 2:J:102:LEU:HB2 | 1.99 | 0.63 |
| 4:L:528:ARG:NE | 4:L:528:ARG:H | 1.97 | 0.63 |
| 5:M:383:GLN:O | 5:M:391:ARG:CB | 2.47 | 0.63 |
| 5:M:128:ALA:HB2 | 5:M:478:THR:HG21 | 1.80 | 0.63 |
| 6:N:108:PHE:CE2 | 6:N:118:ILE:HG13 | 2.34 | 0.63 |
| 1:A:115:LEU:HD13 | 1:A:125:ILE:HD11 | 1.81 | 0.62 |
| 2:B:210:GLU:OE1 | 2:B:357:SER:O | 2.17 | 0.62 |
| 4:D:528:ARG:H | 4:D:528:ARG:NE | 1.97 | 0.62 |
| 7:G:237:ASN:C | 7:G:239:PRO:HD3 | 2.18 | 0.62 |
| 7:G:304:THR:HA | 7:G:307:PHE:HE2 | 1.63 | 0.62 |
| 2:J:246:PHE:C | 2:J:246:PHE:CD1 | 2.73 | 0.62 |
| 4:L:292:ILE:HG13 | 4:L:293:LEU:HA | 1.81 | 0.62 |
| 1:A:158:ASN:ND2 | 1:A:516:GLY:HA2 | 2.13 | 0.62 |
| 2:B:38:GLY:HA3 | 2:B:474:LEU:CD1 | 2.29 | 0.62 |
| 5:E:273:THR:HG22 | 5:E:363:VAL:O | 1.99 | 0.62 |
| 6:F:109:ILE:HG13 | 5:M:39:LYS:NZ | 2.11 | 0.62 |
| 7:G:409:ILE:HG22 | 7:G:410:VAL:N | 2.14 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:H:227:VAL:HG21 | 8:H:385:ILE:HD11 | 1.81 | 0.62 |
| 2:J:230:LYS:H | 2:J:281:ILE:HG22 | 1.62 | 0.62 |
| 2:J:436:ALA:O | 2:J:439:GLN:HB3 | 1.99 | 0.62 |
| 3:K:35:ILE:HD11 | 3:K:65:LEU:HG | 1.80 | 0.62 |
| 7:O:214:PHE:HD1 | 7:O:376:LEU:HB3 | 1.64 | 0.62 |
| 7:O:79:ALA:O | 7:O:82:THR:HG22 | 1.99 | 0.62 |
| 8:P:227:VAL:HG21 | 8:P:385:ILE:HD11 | 1.81 | 0.62 |
| 6:F:481:GLN:O | 6:F:489:VAL:HG21 | 1.99 | 0.62 |
| 7:G:126:MET:HE3 | 7:G:515:ASN:HA | 1.82 | 0.62 |
| 4:D:292:ILE:HG13 | 4:D:293:LEU:HA | 1.82 | 0.62 |
| 5:E:174:GLU:O | 5:E:175:LEU:CG | 2.47 | 0.62 |
| 5:E:337:GLN:C | 5:E:338:ASN:HD22 | 2.03 | 0.62 |
| 7:G:109:MET:SD | 7:G:514:THR:HG22 | 2.39 | 0.62 |
| 2:J:38:GLY:HA3 | 2:J:474:LEU:CD1 | 2.29 | 0.62 |
| 3:K:223:VAL:HG12 | 3:K:224:LEU:H | 1.63 | 0.62 |
| 4:L:375:VAL:HG12 | 4:L:376:SER:H | 1.64 | 0.62 |
| 1:A:184:LEU:CD2 | 1:A:198:TYR:CG | 2.69 | 0.62 |
| 2:B:246:PHE:CD1 | 2:B:246:PHE:C | 2.73 | 0.62 |
| 2:B:98:LEU:O | 2:B:102:LEU:HB2 | 1.99 | 0.62 |
| 4:D:185:ASN:H | 4:D:186:SER:C | 2.02 | 0.62 |
| 5:E:401:THR:O | 5:E:402:LYS:CB | 2.46 | 0.62 |
| 7:G:226:TYR:CE1 | 7:G:229:PHE:C | 2.73 | 0.62 |
| 8:H:375:GLN:N | 8:H:376:GLY:HA3 | 2.14 | 0.62 |
| 3:K:391:GLU:O | 3:K:395:ASN:HB2 | 1.98 | 0.62 |
| 4:L:210:ILE:O | 4:L:375:VAL:HG13 | 1.98 | 0.62 |
| 6:N:173:ILE:HD11 | 6:N:209:PHE:HB3 | 1.82 | 0.62 |
| 7:O:409:ILE:HG22 | 7:O:410:VAL:N | 2.14 | 0.62 |
| 8:P:24:ALA:O | 8:P:28:ILE:HG13 | 1.99 | 0.62 |
| 8:P:227:VAL:HG22 | 8:P:370:VAL:HG12 | 1.81 | 0.62 |
| 3:C:142:PRO:HB3 | 3:C:410:PRO:HB2 | 1.81 | 0.62 |
| 8:H:227:VAL:HG22 | 8:H:370:VAL:HG12 | 1.81 | 0.62 |
| 8:H:441:THR:O | 8:H:446:GLN:HG2 | 2.00 | 0.62 |
| 1:I:224:LEU:HD13 | 1:I:226:CYS:HB2 | 1.81 | 0.62 |
| 2:J:236:THR:OG1 | 2:J:327:SER:HA | 1.99 | 0.62 |
| 5:M:483:LEU:HD11 | 9:M:601:ADP:O4' | 1.99 | 0.62 |
| 5:M:88:ALA:HB1 | 5:M:109:LYS:HZ1 | 1.64 | 0.62 |
| 1:A:224:LEU:HD13 | 1:A:226:CYS:HB2 | 1.81 | 0.62 |
| 2:B:464:TYR:O | 2:B:467:ILE:HD11 | 2.00 | 0.62 |
| 6:F:501:PRO:CB | 6:F:506:ILE:HB | 2.17 | 0.62 |
| 6:F:540:THR:O | 6:F:542:LYS:CG | 2.44 | 0.62 |
| 7:G:282:LEU:HD21 | 7:G:306:PHE:HB2 | 1.80 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:G:214:PHE:HD1 | 7:G:376:LEU:HB3 | 1.64 | 0.62 |
| 1:I:184:LEU:CD2 | 1:I:198:TYR:CG | 2.69 | 0.62 |
| 1:I:480:TYR:O | 1:I:483:ALA:HB3 | 2.00 | 0.62 |
| 1:A:470:SER:H | 3:K:115:ASN:CB | 2.13 | 0.62 |
| 3:K:495:VAL:HG23 | 3:K:500:TRP:HH2 | 1.65 | 0.62 |
| 6:N:481:GLN:O | 6:N:489:VAL:HG21 | 1.99 | 0.62 |
| 2:J:375:GLN:NE2 | 6:N:75:LEU:HD12 | 2.14 | 0.62 |
| 7:O:226:TYR:CE1 | 7:O:229:PHE:C | 2.73 | 0.62 |
| 2:B:436:ALA:O | 2:B:439:GLN:HB3 | 2.00 | 0.62 |
| 4:D:375:VAL:HG12 | 4:D:376:SER:H | 1.64 | 0.62 |
| 5:E:133:ALA:O | 5:E:137:ILE:HG13 | 1.99 | 0.62 |
| 5:E:210:ASN:HD22 | 5:E:210:ASN:H | 1.48 | 0.62 |
| 6:F:155:ARG:CB | 6:F:171:THR:HG21 | 2.30 | 0.62 |
| 6:F:353:LEU:HB2 | 6:F:368:THR:OG1 | 2.00 | 0.62 |
| 7:G:189:LEU:N | 7:G:190:ASP:HB2 | 2.14 | 0.62 |
| 7:G:413:GLY:HA3 | 7:G:491:ASN:ND2 | 2.15 | 0.62 |
| 1:I:458:ILE:HB | 1:I:459:PRO:HD3 | 1.81 | 0.62 |
| 3:K:223:VAL:HG11 | 3:K:328:ILE:CG1 | 2.29 | 0.62 |
| 3:K:31:VAL:HG11 | 3:K:70:VAL:HG11 | 1.81 | 0.62 |
| 6:N:92:THR:CG2 | 10:N:602:BEF:F3 | 2.37 | 0.62 |
| 2:B:492:LYS:NZ | 2:B:492:LYS:H | 1.97 | 0.62 |
| 3:C:223:VAL:HG11 | 3:C:328:ILE:CG1 | 2.29 | 0.62 |
| 3:C:62:HIS:O | 3:C:66:ARG:HG3 | 2.00 | 0.62 |
| 5:E:383:GLN:O | 5:E:391:ARG:CB | 2.47 | 0.62 |
| 1:A:122:PRO:HG3 | 5:E:70:LEU:HD11 | 1.82 | 0.62 |
| 8:H:131:TYR:CD2 | 8:H:452:PHE:HD2 | 2.17 | 0.62 |
| 2:J:8:ASP:CB | 2:J:9:GLN:HA | 2.22 | 0.62 |
| 3:K:264:GLU:C | 3:K:265:LYS:CG | 2.62 | 0.62 |
| 5:M:273:THR:HG22 | 5:M:363:VAL:O | 1.99 | 0.62 |
| 7:O:43:THR:HG22 | 7:O:64:ASN:CB | 2.27 | 0.62 |
| 3:C:462:GLY:O | 3:C:464:PRO:HD3 | 1.99 | 0.62 |
| 5:E:348:GLY:O | 5:E:351:LEU:HD11 | 2.00 | 0.62 |
| 1:I:233:MET:HG2 | 1:I:311:VAL:HG22 | 1.82 | 0.62 |
| 3:K:142:PRO:HB3 | 3:K:410:PRO:HB2 | 1.81 | 0.62 |
| 5:M:50:HIS:HB3 | 5:M:100:ILE:HG21 | 1.82 | 0.62 |
| 3:C:495:VAL:HG23 | 3:C:500:TRP:HH2 | 1.65 | 0.61 |
| 5:E:39:LYS:NZ | 6:N:109:ILE:HG13 | 2.14 | 0.61 |
| 7:G:307:PHE:HD1 | 7:G:312:ILE:HG23 | 1.64 | 0.61 |
| 4:D:521:ILE:HG23 | 7:G:51:ILE:CA | 2.29 | 0.61 |
| 8:H:24:ALA:O | 8:H:28:ILE:HG13 | 1.99 | 0.61 |
| 8:H:335:VAL:HG22 | 8:H:379:SER:HB2 | 1.82 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:266:ASP:N | 1:I:267:PRO:HD2 | 2.15 | 0.61 |
| 5:M:133:ALA:O | 5:M:137:ILE:HG13 | 1.99 | 0.61 |
| 8:P:109:GLU:O | 8:P:113:VAL:HG23 | 2.00 | 0.61 |
| 1:A:118:ASN:O | 1:A:119:LYS:HG2 | 2.00 | 0.61 |
| 3:C:50:ASP:HB2 | 3:C:51:PRO:HD2 | 1.82 | 0.61 |
| 5:E:104:LEU:CD2 | 5:E:123:VAL:HG13 | 2.27 | 0.61 |
| 5:E:183:ALA:O | 5:E:187:SER:HB2 | 2.00 | 0.61 |
| 6:F:515:ASN:HD22 | 6:F:516:ALA:N | 1.99 | 0.61 |
| 1:I:187:VAL:HG21 | 1:I:383:SER:HB3 | 1.83 | 0.61 |
| 5:M:348:GLY:O | 5:M:351:LEU:HD11 | 2.00 | 0.61 |
| 6:N:229:LYS:HA | 6:N:353:LEU:HD23 | 1.82 | 0.61 |
| 8:P:441:THR:O | 8:P:446:GLN:HG2 | 1.99 | 0.61 |
| 1:A:228:VAL:CG2 | 1:A:363:GLN:NE2 | 2.49 | 0.61 |
| 2:B:263:LYS:HZ3 | 3:C:266:GLU:HB3 | 1.62 | 0.61 |
| 6:F:133:LEU:HD12 | 6:F:422:LEU:CD2 | 2.24 | 0.61 |
| 7:G:165:ALA:HB2 | 7:G:399:ILE:HG21 | 1.82 | 0.61 |
| 7:G:79:ALA:O | 7:G:82:THR:HG22 | 1.99 | 0.61 |
| 1:I:118:ASN:O | 1:I:119:LYS:HG2 | 2.00 | 0.61 |
| 1:I:90:GLN:OE1 | 1:I:96:ASP:O | 2.17 | 0.61 |
| 2:J:509:LEU:HD23 | 2:J:509:LEU:O | 2.00 | 0.61 |
| 3:K:50:ASP:HB2 | 3:K:51:PRO:HD2 | 1.82 | 0.61 |
| 5:M:174:GLU:O | 5:M:175:LEU:CG | 2.47 | 0.61 |
| 6:N:353:LEU:HB2 | 6:N:368:THR:OG1 | 2.00 | 0.61 |
| 7:O:239:PRO:HD2 | 7:O:349:CYS:O | 2.01 | 0.61 |
| 7:O:413:GLY:HA3 | 7:O:491:ASN:ND2 | 2.15 | 0.61 |
| 1:A:233:MET:HG2 | 1:A:311:VAL:HG22 | 1.82 | 0.61 |
| 3:C:31:VAL:HG11 | 3:C:70:VAL:HG11 | 1.81 | 0.61 |
| 5:E:433:LEU:HD11 | 5:E:439:VAL:HG13 | 1.82 | 0.61 |
| 6:F:108:PHE:CE2 | 6:F:118:ILE:HG13 | 2.34 | 0.61 |
| 7:G:37:GLN:HE21 | 7:G:38:GLU:N | 1.98 | 0.61 |
| 3:K:512:THR:HG23 | 8:P:389:ALA:HB1 | 1.82 | 0.61 |
| 5:M:337:GLN:C | 5:M:338:ASN:HD22 | 2.03 | 0.61 |
| 6:N:203:SER:C | 6:N:205:LYS:H | 2.03 | 0.61 |
| 7:O:191:ARG:CZ | 7:O:192:ASN:N | 2.61 | 0.61 |
| 8:P:375:GLN:N | 8:P:376:GLY:HA3 | 2.14 | 0.61 |
| 2:B:437:LEU:O | 2:B:441:PRO:HD2 | 2.01 | 0.61 |
| 5:E:273:THR:HG22 | 5:E:364:PRO:CA | 2.20 | 0.61 |
| 6:F:433:LYS:HB3 | 6:F:441:LYS:HA | 1.80 | 0.61 |
| 7:G:239:PRO:HD2 | 7:G:349:CYS:O | 2.01 | 0.61 |
| 6:N:36:ASN:HB3 | 6:N:57:LYS:HZ3 | 0.81 | 0.61 |
| 6:N:454:ILE:N | 6:N:455:PRO:CD | 2.64 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:540:ARG:O | 5:E:70:LEU:HB3 | 2.00 | 0.61 |
| 3:C:41:PRO:HA | 3:C:161:THR:HG21 | 1.82 | 0.61 |
| 4:D:524:ILE:CG2 | 7:G:52:LEU:O | 2.47 | 0.61 |
| 6:F:454:ILE:N | 6:F:455:PRO:CD | 2.64 | 0.61 |
| 8:H:109:GLU:O | 8:H:113:VAL:HG23 | 2.00 | 0.61 |
| 2:J:203:LEU:O | 2:J:204:SER:CB | 2.49 | 0.61 |
| 3:K:149:ALA:HA | 3:K:152:LYS:HG3 | 1.83 | 0.61 |
| 3:K:462:GLY:O | 3:K:464:PRO:HD3 | 1.99 | 0.61 |
| 6:N:178:VAL:O | 6:N:182:TYR:N | 2.34 | 0.61 |
| 1:A:218:LEU:HD13 | 1:A:219:VAL:N | 2.16 | 0.61 |
| 3:C:149:ALA:HA | 3:C:152:LYS:HG3 | 1.83 | 0.61 |
| 6:F:7:ASN:OD1 | 6:F:8:PRO:HD2 | 1.99 | 0.61 |
| 1:I:348:GLU:N | 1:I:349:THR:HB | 2.16 | 0.61 |
| 1:I:70:LEU:HD23 | 1:I:73:LEU:HD22 | 1.83 | 0.61 |
| 5:M:183:ALA:O | 5:M:187:SER:HB2 | 2.00 | 0.61 |
| 7:O:307:PHE:HD1 | 7:O:312:ILE:HG23 | 1.64 | 0.61 |
| 8:P:131:TYR:CD2 | 8:P:452:PHE:HD2 | 2.17 | 0.61 |
| 8:P:335:VAL:HG22 | 8:P:379:SER:HB2 | 1.82 | 0.61 |
| 1:A:266:ASP:N | 1:A:267:PRO:HD2 | 2.15 | 0.61 |
| 1:A:348:GLU:N | 1:A:349:THR:HB | 2.16 | 0.61 |
| 4:D:499:GLN:HE22 | 9:D:601:ADP:C2' | 2.13 | 0.61 |
| 6:F:173:ILE:HD11 | 6:F:209:PHE:HB3 | 1.82 | 0.61 |
| 6:F:178:VAL:O | 6:F:182:TYR:N | 2.34 | 0.61 |
| 6:F:437:LYS:HE2 | 6:F:437:LYS:HA | 1.83 | 0.61 |
| 7:G:43:THR:HG22 | 7:G:64:ASN:CB | 2.27 | 0.61 |
| 1:I:218:LEU:HD13 | 1:I:219:VAL:N | 2.16 | 0.61 |
| 1:I:258:MET:HA | 1:I:258:MET:HE3 | 1.82 | 0.61 |
| 3:K:96:VAL:HG13 | 3:K:513:ALA:HB2 | 1.83 | 0.61 |
| 3:C:299:LYS:HA | 3:C:319:ARG:CB | 2.31 | 0.61 |
| 2:B:72:PRO:CB | 3:C:47:MET:CE | 2.79 | 0.61 |
| 4:D:485:ARG:NH2 | 9:D:601:ADP:HN62 | 1.99 | 0.61 |
| 6:F:108:PHE:CE2 | 6:F:118:ILE:HG21 | 2.36 | 0.61 |
| 6:F:98:VAL:HG22 | 6:F:520:ALA:HA | 1.83 | 0.61 |
| 2:J:3:VAL:C | 2:J:5:ILE:HG23 | 2.21 | 0.61 |
| 3:K:62:HIS:O | 3:K:66:ARG:HG3 | 2.00 | 0.61 |
| 6:N:437:LYS:HA | 6:N:437:LYS:HE2 | 1.83 | 0.61 |
| 6:N:7:ASN:OD1 | 6:N:8:PRO:CD | 2.49 | 0.61 |
| 6:N:7:ASN:OD1 | 6:N:8:PRO:HD2 | 1.99 | 0.61 |
| 1:A:73:LEU:O | 1:A:74:ASP:HB3 | 2.01 | 0.61 |
| 7:G:94:VAL:HG13 | 7:G:95:GLY:N | 2.16 | 0.61 |
| 2:J:464:TYR:O | 2:J:467:ILE:HD11 | 2.00 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:K:54:GLY:O | 3:K:56:VAL:HG23 | 2.01 | 0.61 |
| 6:N:35:THR:CG2 | 6:N:42:THR:H | 2.14 | 0.61 |
| 1:A:480:TYR:O | 1:A:483:ALA:HB3 | 2.00 | 0.60 |
| 2:B:3:VAL:C | 2:B:5:ILE:HG23 | 2.21 | 0.60 |
| 2:B:509:LEU:HD23 | 2:B:509:LEU:O | 2.00 | 0.60 |
| 3:C:142:PRO:HG3 | 3:C:411:SER:HA | 1.83 | 0.60 |
| 6:F:478:ASP:C | 6:F:482:ASP:HB2 | 2.21 | 0.60 |
| 8:H:138:THR:HG22 | 8:H:434:ILE:HD12 | 1.83 | 0.60 |
| 1:I:184:LEU:HD21 | 1:I:198:TYR:CB | 2.28 | 0.60 |
| 6:N:458:LEU:HD12 | 6:N:458:LEU:O | 2.01 | 0.60 |
| 2:B:232:LEU:HD22 | 2:B:233:ILE:N | 2.16 | 0.60 |
| 2:B:424:GLY:O | 2:B:427:SER:CB | 2.49 | 0.60 |
| 6:F:198:GLN:HE21 | 6:F:198:GLN:N | 1.99 | 0.60 |
| 1:I:233:MET:HE2 | 1:I:315:ILE:O | 2.01 | 0.60 |
| 2:J:30:GLY:C | 2:J:33:VAL:HG23 | 2.22 | 0.60 |
| 2:J:424:GLY:O | 2:J:427:SER:CB | 2.49 | 0.60 |
| 3:K:142:PRO:HG3 | 3:K:411:SER:HA | 1.83 | 0.60 |
| 2:J:295:GLU:OE1 | 6:N:339:SER:HB3 | 2.01 | 0.60 |
| 6:N:465:ASP:CA | 6:N:466:PRO:C | 2.68 | 0.60 |
| 8:P:269:ASN:H | 8:P:272:GLU:HG3 | 1.66 | 0.60 |
| 2:B:27:ILE:CD1 | 2:B:104:ARG:HH11 | 2.09 | 0.60 |
| 2:B:397:GLU:OE1 | 2:B:399:ARG:HG3 | 2.01 | 0.60 |
| 2:B:422:ILE:HG21 | 2:B:427:SER:HB3 | 1.79 | 0.60 |
| 2:B:459:LEU:HD22 | 2:B:472:LEU:CG | 2.26 | 0.60 |
| 6:F:264:ALA:O | 6:F:268:LYS:HG2 | 2.02 | 0.60 |
| 6:F:35:THR:CG2 | 6:F:42:THR:H | 2.14 | 0.60 |
| 6:F:478:ASP:O | 6:F:482:ASP:CA | 2.49 | 0.60 |
| 7:G:420:VAL:O | 7:G:424:LEU:HG | 2.01 | 0.60 |
| 5:M:100:ILE:HA | 5:M:103:LEU:HD12 | 1.83 | 0.60 |
| 6:N:133:LEU:HD12 | 6:N:422:LEU:CD2 | 2.24 | 0.60 |
| 6:N:515:ASN:HD22 | 6:N:516:ALA:N | 1.99 | 0.60 |
| 3:C:512:THR:HG23 | 8:H:389:ALA:HB1 | 1.83 | 0.60 |
| 5:E:50:HIS:HB3 | 5:E:100:ILE:HG21 | 1.82 | 0.60 |
| 6:F:229:LYS:HA | 6:F:353:LEU:HD23 | 1.82 | 0.60 |
| 6:F:458:LEU:HD12 | 6:F:458:LEU:O | 2.01 | 0.60 |
| 1:I:73:LEU:O | 1:I:74:ASP:HB3 | 2.00 | 0.60 |
| 2:J:357:SER:CB | 2:J:360:LYS:CB | 2.69 | 0.60 |
| 2:J:38:GLY:HA3 | 2:J:474:LEU:HD11 | 1.83 | 0.60 |
| 5:M:433:LEU:HD11 | 5:M:439:VAL:HG13 | 1.82 | 0.60 |
| 2:B:384:LEU:O | 2:B:387:ALA:HB3 | 2.01 | 0.60 |
| 4:D:284:ASN:O | 4:D:310:ILE:HG23 | 2.01 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:F:151:LEU:O | 6:F:171:THR:CG2 | 2.50 | 0.60 |
| 3:K:15:THR:O | 3:K:16:THR:C | 2.39 | 0.60 |
| 3:K:299:LYS:HA | 3:K:319:ARG:CB | 2.31 | 0.60 |
| 3:K:9:ASN:ND2 | 3:K:10:ALA:N | 2.50 | 0.60 |
| 4:L:284:ASN:O | 4:L:310:ILE:HG23 | 2.01 | 0.60 |
| 6:N:108:PHE:CE2 | 6:N:118:ILE:HG21 | 2.36 | 0.60 |
| 7:O:174:ASN:OD1 | 7:O:174:ASN:N | 2.33 | 0.60 |
| 7:O:94:VAL:HG13 | 7:O:95:GLY:N | 2.16 | 0.60 |
| 1:A:90:GLN:OE1 | 1:A:96:ASP:O | 2.17 | 0.60 |
| 3:C:9:ASN:ND2 | 3:C:10:ALA:N | 2.50 | 0.60 |
| 6:F:7:ASN:OD1 | 6:F:8:PRO:CD | 2.49 | 0.60 |
| 7:G:293:VAL:HG13 | 7:G:312:ILE:HD11 | 1.84 | 0.60 |
| 1:I:113:ASN:HA | 1:I:116:VAL:HG22 | 1.83 | 0.60 |
| 1:I:65:ASP:O | 1:I:69:ILE:HB | 2.01 | 0.60 |
| 3:K:223:VAL:HG11 | 3:K:328:ILE:HG13 | 1.83 | 0.60 |
| 6:N:160:THR:H | 6:N:164:ALA:HB3 | 1.67 | 0.60 |
| 6:N:98:VAL:HG22 | 6:N:520:ALA:HA | 1.83 | 0.60 |
| 6:N:61:VAL:HG12 | 6:N:62:LEU:HD23 | 1.84 | 0.60 |
| 7:O:516:LEU:CD2 | 7:O:516:LEU:O | 2.46 | 0.60 |
| 8:P:182:VAL:O | 8:P:186:VAL:HG23 | 2.02 | 0.60 |
| 2:B:200:GLY:O | 2:B:371:GLY:N | 2.28 | 0.60 |
| 2:B:326:VAL:HG13 | 3:C:304:LEU:HD22 | 1.83 | 0.60 |
| 2:B:487:ILE:HD12 | 9:B:601:ADP:N6 | 2.17 | 0.60 |
| 3:C:266:GLU:CD | 3:C:266:GLU:H | 2.05 | 0.60 |
| 8:H:182:VAL:O | 8:H:186:VAL:HG23 | 2.02 | 0.60 |
| 2:J:397:GLU:OE1 | 2:J:399:ARG:HG3 | 2.02 | 0.60 |
| 6:N:198:GLN:N | 6:N:198:GLN:HE21 | 1.99 | 0.60 |
| 6:N:233:VAL:HG12 | 6:N:294:VAL:HG22 | 1.84 | 0.60 |
| 6:N:430:ASN:HA | 6:N:433:LYS:CB | 2.32 | 0.60 |
| 1:A:187:VAL:HG21 | 1:A:383:SER:HB3 | 1.83 | 0.60 |
| 3:C:96:VAL:HG13 | 3:C:513:ALA:HB2 | 1.83 | 0.60 |
| 6:F:233:VAL:HG12 | 6:F:294:VAL:HG22 | 1.84 | 0.60 |
| 6:F:125:ALA:HB2 | 6:F:444:ILE:HG23 | 1.82 | 0.60 |
| 6:F:485:GLU:HB2 | 6:F:488:TYR:O | 2.01 | 0.60 |
| 7:G:208:ALA:HB3 | 7:G:211:GLU:HG3 | 1.84 | 0.60 |
| 7:G:109:MET:CG | 7:G:514:THR:CG2 | 2.79 | 0.60 |
| 2:J:384:LEU:O | 2:J:387:ALA:HB3 | 2.01 | 0.60 |
| 2:J:437:LEU:O | 2:J:441:PRO:HD2 | 2.00 | 0.60 |
| 4:L:524:ILE:CG2 | 7:O:52:LEU:O | 2.50 | 0.60 |
| 5:M:210:ASN:H | 5:M:210:ASN:HD22 | 1.48 | 0.60 |
| 6:N:155:ARG:CB | 6:N:171:THR:HG21 | 2.30 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:N:264:ALA:O | 6:N:268:LYS:HG2 | 2.02 | 0.60 |
| 6:N:389:ALA:O | 6:N:393:ASP:OD2 | 2.20 | 0.60 |
| 7:O:37:GLN:HE21 | 7:O:38:GLU:N | 1.98 | 0.60 |
| 1:A:183:ALA:HB1 | 1:A:383:SER:OG | 2.02 | 0.60 |
| 2:B:203:LEU:O | 2:B:204:SER:CB | 2.49 | 0.60 |
| 2:B:27:ILE:HD12 | 2:B:104:ARG:HD2 | 1.84 | 0.60 |
| 3:C:229:VAL:HG12 | 3:C:230:VAL:N | 2.17 | 0.60 |
| 3:C:42:LYS:CB | 3:C:460:ALA:CA | 2.75 | 0.60 |
| 6:F:170:LEU:HA | 6:F:173:ILE:HG22 | 1.84 | 0.60 |
| 6:F:61:VAL:HG12 | 6:F:62:LEU:HD23 | 1.84 | 0.60 |
| 3:K:457:ILE:CD1 | 3:K:467:LEU:HD22 | 2.31 | 0.60 |
| 6:N:151:LEU:CG | 6:N:175:THR:HG23 | 2.32 | 0.60 |
| 6:N:38:GLY:H | 9:N:601:ADP:H5'1 | 1.66 | 0.60 |
| 8:P:162:MET:O | 8:P:165:PRO:HD2 | 2.02 | 0.60 |
| 8:P:459:VAL:O | 8:P:463:LEU:HD23 | 2.02 | 0.60 |
| 2:B:30:GLY:C | 2:B:33:VAL:HG23 | 2.22 | 0.60 |
| 3:C:54:GLY:O | 3:C:56:VAL:HG23 | 2.01 | 0.60 |
| 4:D:38:SER:HB3 | 4:D:46:LYS:HZ3 | 1.65 | 0.60 |
| 5:E:323:CYS:O | 5:E:344:ARG:HA | 2.02 | 0.60 |
| 6:F:389:ALA:O | 6:F:393:ASP:OD2 | 2.20 | 0.60 |
| 7:G:191:ARG:HD3 | 7:G:192:ASN:N | 2.16 | 0.60 |
| 1:I:183:ALA:HB1 | 1:I:383:SER:OG | 2.02 | 0.60 |
| 4:L:210:ILE:O | 4:L:375:VAL:HG12 | 2.02 | 0.60 |
| 5:M:273:THR:HG21 | 5:M:364:PRO:HA | 1.78 | 0.60 |
| 7:O:165:ALA:HB2 | 7:O:399:ILE:HG21 | 1.82 | 0.60 |
| 8:P:153:LYS:H | 8:P:153:LYS:CD | 2.15 | 0.60 |
| 1:A:333:THR:HB | 1:A:357:LEU:H | 1.67 | 0.59 |
| 3:C:15:THR:O | 3:C:16:THR:C | 2.39 | 0.59 |
| 6:F:352:GLY:O | 6:F:353:LEU:O | 2.20 | 0.59 |
| 6:F:430:ASN:C | 6:F:433:LYS:H | 2.05 | 0.59 |
| 8:H:162:MET:O | 8:H:165:PRO:HD2 | 2.02 | 0.59 |
| 3:C:258:GLN:O | 8:H:264:THR:HB | 2.02 | 0.59 |
| 3:K:229:VAL:HG12 | 3:K:230:VAL:N | 2.17 | 0.59 |
| 8:P:362:GLU:HG2 | 8:P:367:ARG:HA | 1.82 | 0.59 |
| 3:C:457:ILE:CD1 | 3:C:467:LEU:HD22 | 2.31 | 0.59 |
| 4:D:71:LEU:HA | 8:P:6:PRO:CG | 2.31 | 0.59 |
| 6:F:415:ALA:CB | 6:F:506:ILE:HG21 | 2.30 | 0.59 |
| 1:I:333:THR:HB | 1:I:357:LEU:H | 1.67 | 0.59 |
| 1:I:50:ASP:CG | 1:I:64:ASN:HB2 | 2.23 | 0.59 |
| 5:M:281:PRO:HD2 | 5:M:285:HIS:HB3 | 1.84 | 0.59 |
| 6:N:478:ASP:C | 6:N:482:ASP:HB2 | 2.20 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:N:485:GLU:HB2 | 6:N:488:TYR:O | 2.01 | 0.59 |
| 7:O:293:VAL:HG13 | 7:O:312:ILE:HD11 | 1.83 | 0.59 |
| 1:A:65:ASP:O | 1:A:69:ILE:HB | 2.01 | 0.59 |
| 2:B:213:ILE:H | 2:B:213:ILE:HD12 | 1.67 | 0.59 |
| 5:E:39:LYS:HZ3 | 6:N:109:ILE:CG1 | 2.15 | 0.59 |
| 6:F:201:HIS:HB3 | 6:F:381:LYS:CE | 2.32 | 0.59 |
| 6:F:92:THR:HG21 | 10:F:602:BEF:F3 | 1.92 | 0.59 |
| 7:G:174:ASN:OD1 | 7:G:174:ASN:N | 2.34 | 0.59 |
| 8:H:153:LYS:H | 8:H:153:LYS:CD | 2.15 | 0.59 |
| 8:H:177:ILE:O | 8:H:180:GLU:HB2 | 2.03 | 0.59 |
| 1:I:97:GLY:O | 1:I:101:VAL:HG23 | 2.02 | 0.59 |
| 3:K:42:LYS:CB | 3:K:460:ALA:CA | 2.75 | 0.59 |
| 5:M:351:LEU:HD13 | 5:M:351:LEU:H | 1.67 | 0.59 |
| 5:M:74:LEU:CD1 | 5:M:93:GLN:HB3 | 2.33 | 0.59 |
| 6:N:167:THR:HB | 6:N:169:VAL:H | 1.66 | 0.59 |
| 6:N:151:LEU:O | 6:N:171:THR:CG2 | 2.50 | 0.59 |
| 7:O:189:LEU:CD1 | 7:O:189:LEU:O | 2.50 | 0.59 |
| 7:O:401:LYS:HG3 | 7:O:402:ARG:N | 2.17 | 0.59 |
| 8:P:138:THR:HG22 | 8:P:434:ILE:HD12 | 1.83 | 0.59 |
| 1:A:97:GLY:O | 1:A:101:VAL:HG23 | 2.02 | 0.59 |
| 1:A:113:ASN:HA | 1:A:116:VAL:HG22 | 1.83 | 0.59 |
| 3:C:275:ILE:HA | 8:H:274:LEU:HD21 | 1.84 | 0.59 |
| 3:C:57:LEU:CD2 | 3:C:57:LEU:N | 2.57 | 0.59 |
| 4:D:238:GLN:HB2 | 4:D:290:LYS:HE3 | 1.84 | 0.59 |
| 6:F:430:ASN:HA | 6:F:433:LYS:CB | 2.32 | 0.59 |
| 4:D:81:VAL:HG22 | 7:G:382:ALA:HB2 | 1.84 | 0.59 |
| 4:L:185:ASN:H | 4:L:186:SER:C | 2.02 | 0.59 |
| 5:M:368:ASP:O | 5:M:369:LEU:C | 2.41 | 0.59 |
| 5:M:55:ARG:HH21 | 5:M:134:LEU:HD13 | 1.67 | 0.59 |
| 6:N:478:ASP:O | 6:N:482:ASP:CA | 2.49 | 0.59 |
| 7:O:109:MET:CG | 7:O:514:THR:CG2 | 2.79 | 0.59 |
| 8:P:146:VAL:HG13 | 8:P:147:VAL:H | 1.68 | 0.59 |
| 8:P:177:ILE:O | 8:P:180:GLU:HB2 | 2.03 | 0.59 |
| 4:L:44:MET:HG3 | 8:P:531:ALA:HB3 | 1.83 | 0.59 |
| 1:A:70:LEU:HD23 | 1:A:73:LEU:HD22 | 1.83 | 0.59 |
| 3:C:223:VAL:HG11 | 3:C:328:ILE:HG13 | 1.83 | 0.59 |
| 6:F:201:HIS:HB3 | 6:F:381:LYS:HZ3 | 1.66 | 0.59 |
| 6:F:485:GLU:HG3 | 6:F:489:VAL:HB | 1.85 | 0.59 |
| 8:H:362:GLU:HG2 | 8:H:367:ARG:HA | 1.82 | 0.59 |
| 8:H:459:VAL:O | 8:H:463:LEU:HD23 | 2.02 | 0.59 |
| 1:I:159:ILE:HD11 | 1:I:418:VAL:HG11 | 1.84 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:418:VAL:HG12 | 1:I:419:VAL:N | 2.17 | 0.59 |
| 3:K:41:PRO:HA | 3:K:161:THR:HG21 | 1.82 | 0.59 |
| 4:L:12:LYS:HD3 | 4:L:526:PHE:O | 2.01 | 0.59 |
| 4:L:254:VAL:HG23 | 4:L:254:VAL:O | 2.01 | 0.59 |
| 4:D:12:LYS:HD3 | 4:D:526:PHE:O | 2.01 | 0.59 |
| 5:E:241:ASN:ND2 | 5:E:241:ASN:O | 2.34 | 0.59 |
| 5:E:368:ASP:O | 5:E:369:LEU:C | 2.41 | 0.59 |
| 6:N:125:ALA:HB2 | 6:N:444:ILE:HG23 | 1.82 | 0.59 |
| 8:P:322:LYS:O | 8:P:324:PRO:HD3 | 2.02 | 0.59 |
| 1:A:50:ASP:CG | 1:A:64:ASN:HB2 | 2.23 | 0.59 |
| 1:A:73:LEU:O | 1:A:74:ASP:CB | 2.50 | 0.59 |
| 4:D:336:ILE:HG23 | 4:D:339:PHE:HB3 | 1.85 | 0.59 |
| 4:D:379:ILE:H | 4:D:379:ILE:HD12 | 1.68 | 0.59 |
| 5:E:351:LEU:HD13 | 5:E:351:LEU:H | 1.67 | 0.59 |
| 8:H:269:ASN:H | 8:H:272:GLU:HG3 | 1.66 | 0.59 |
| 8:H:322:LYS:O | 8:H:324:PRO:HD3 | 2.02 | 0.59 |
| 1:I:73:LEU:O | 1:I:74:ASP:CB | 2.50 | 0.59 |
| 2:J:27:ILE:HD12 | 2:J:104:ARG:HD2 | 1.83 | 0.59 |
| 3:K:266:GLU:H | 3:K:266:GLU:CD | 2.05 | 0.59 |
| 3:K:414:PRO:O | 3:K:418:ALA:HB3 | 2.03 | 0.59 |
| 4:L:336:ILE:HG23 | 4:L:339:PHE:HB3 | 1.85 | 0.59 |
| 5:M:32:VAL:HG22 | 5:M:33:LYS:N | 2.13 | 0.59 |
| 1:A:164:MET:O | 1:A:167:LYS:CB | 2.51 | 0.59 |
| 2:B:326:VAL:HG22 | 3:C:304:LEU:HD22 | 1.85 | 0.59 |
| 4:D:521:ILE:CG2 | 7:G:52:LEU:H | 2.15 | 0.59 |
| 5:E:74:LEU:CD1 | 5:E:93:GLN:HB3 | 2.32 | 0.59 |
| 7:G:238:ASN:N | 7:G:239:PRO:CD | 2.66 | 0.59 |
| 8:H:94:ILE:HD12 | 8:H:95:ASP:N | 2.18 | 0.59 |
| 2:J:32:LEU:CD1 | 6:N:532:GLU:OE2 | 2.51 | 0.59 |
| 6:N:201:HIS:HB3 | 6:N:381:LYS:CE | 2.33 | 0.59 |
| 6:N:540:THR:O | 6:N:541:LEU:HD23 | 2.03 | 0.59 |
| 7:O:191:ARG:HD3 | 7:O:192:ASN:N | 2.16 | 0.59 |
| 3:C:414:PRO:O | 3:C:418:ALA:HB3 | 2.03 | 0.59 |
| 4:D:330:CYS:N | 4:D:345:ASP:OD2 | 2.36 | 0.59 |
| 4:D:103:LEU:HD13 | 4:D:515:VAL:HG21 | 1.85 | 0.59 |
| 5:E:240:ILE:HG12 | 5:E:244:ILE:CG2 | 2.32 | 0.59 |
| 5:E:335:LEU:HD22 | 5:E:340:LEU:HD11 | 1.84 | 0.59 |
| 6:F:109:ILE:O | 5:M:39:LYS:HE2 | 2.02 | 0.59 |
| 2:J:232:LEU:HD22 | 2:J:233:ILE:N | 2.17 | 0.59 |
| 6:N:352:GLY:O | 6:N:353:LEU:O | 2.20 | 0.59 |
| 3:C:112:ILE:C | 3:C:114:LYS:H | 2.06 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:264:GLU:C | 3:C:265:LYS:CG | 2.62 | 0.59 |
| 3:C:508:GLN:HG2 | 8:H:215:GLY:HA2 | 1.85 | 0.59 |
| 5:E:281:PRO:HD2 | 5:E:285:HIS:HB3 | 1.84 | 0.59 |
| 5:E:373:LYS:HE2 | 6:F:311:LYS:NZ | 2.18 | 0.59 |
| 6:F:433:LYS:HG3 | 6:F:444:ILE:CG1 | 2.33 | 0.59 |
| 6:F:43:LEU:CD2 | 6:F:57:LYS:CB | 2.78 | 0.59 |
| 8:H:288:MET:CE | 8:H:313:LEU:HG | 2.33 | 0.59 |
| 8:H:217:LEU:HA | 8:H:387:ARG:O | 2.03 | 0.59 |
| 5:M:544:LEU:HD23 | 6:N:384:THR:HG21 | 1.85 | 0.59 |
| 6:N:201:HIS:HB3 | 6:N:381:LYS:HE2 | 1.85 | 0.59 |
| 7:O:484:GLU:CB | 7:O:485:THR:HA | 2.32 | 0.59 |
| 3:C:151:MET:O | 3:C:155:ILE:HG12 | 2.04 | 0.58 |
| 3:C:265:LYS:O | 3:C:268:ASP:OD1 | 2.21 | 0.58 |
| 5:E:100:ILE:HA | 5:E:103:LEU:HD12 | 1.83 | 0.58 |
| 5:E:55:ARG:HH21 | 5:E:134:LEU:HD13 | 1.67 | 0.58 |
| 6:F:160:THR:H | 6:F:164:ALA:HB3 | 1.67 | 0.58 |
| 6:F:57:LYS:HG2 | 6:F:57:LYS:O | 2.03 | 0.58 |
| 4:L:128:ALA:O | 4:L:132:VAL:HG23 | 2.03 | 0.58 |
| 5:M:350:GLU:C | 5:M:352:GLU:N | 2.55 | 0.58 |
| 4:L:334:ALA:HB3 | 7:O:305:GLN:HB2 | 1.84 | 0.58 |
| 1:A:17:GLY:HA3 | 5:E:95:GLU:OE2 | 2.03 | 0.58 |
| 6:F:33:LEU:HD21 | 6:F:63:LEU:HD21 | 1.85 | 0.58 |
| 5:E:544:LEU:HD23 | 6:F:384:THR:CG2 | 2.33 | 0.58 |
| 7:G:189:LEU:O | 7:G:189:LEU:CD1 | 2.50 | 0.58 |
| 2:J:463:ILE:HG13 | 2:J:468:SER:HA | 1.85 | 0.58 |
| 3:K:151:MET:O | 3:K:155:ILE:HG12 | 2.04 | 0.58 |
| 6:N:433:LYS:HG3 | 6:N:444:ILE:CG1 | 2.33 | 0.58 |
| 6:N:485:GLU:HG3 | 6:N:489:VAL:HB | 1.85 | 0.58 |
| 7:O:455:GLU:CG | 7:O:461:ALA:CB | 2.81 | 0.58 |
| 8:P:94:ILE:HD12 | 8:P:95:ASP:N | 2.18 | 0.58 |
| 6:F:280:LEU:HD13 | 6:F:343:LEU:HD21 | 1.85 | 0.58 |
| 1:I:55:ASP:HB2 | 1:I:59:ASP:HB2 | 1.85 | 0.58 |
| 2:J:213:ILE:H | 2:J:213:ILE:HD12 | 1.67 | 0.58 |
| 3:K:112:ILE:C | 3:K:114:LYS:H | 2.06 | 0.58 |
| 5:M:240:ILE:HG12 | 5:M:244:ILE:CG2 | 2.32 | 0.58 |
| 6:N:201:HIS:CB | 6:N:381:LYS:HE2 | 2.34 | 0.58 |
| 6:N:424:ARG:NE | 6:N:424:ARG:HA | 2.12 | 0.58 |
| 7:O:125:ILE:HG22 | 7:O:129:TYR:CE2 | 2.38 | 0.58 |
| 2:B:357:SER:CB | 2:B:360:LYS:CB | 2.69 | 0.58 |
| 2:B:422:ILE:CB | 2:B:427:SER:CB | 2.79 | 0.58 |
| 4:D:147:ARG:HG2 | 4:D:148:GLU:N | 2.18 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:110:LEU:HD13 | 4:D:439:ILE:HD12 | 1.85 | 0.58 |
| 5:E:253:GLN:H | 5:E:254:MET:CB | 2.16 | 0.58 |
| 6:F:465:ASP:CA | 6:F:466:PRO:C | 2.68 | 0.58 |
| 8:H:48:PRO:HA | 8:H:169:SER:O | 2.04 | 0.58 |
| 1:I:164:MET:O | 1:I:167:LYS:CB | 2.51 | 0.58 |
| 3:K:452:ILE:HB | 3:K:453:PRO:HD3 | 1.85 | 0.58 |
| 4:L:298:ASN:HB3 | 4:L:299:ASP:HA | 1.84 | 0.58 |
| 8:P:222:VAL:HG22 | 8:P:384:ILE:HG23 | 1.86 | 0.58 |
| 8:P:217:LEU:HA | 8:P:387:ARG:O | 2.03 | 0.58 |
| 1:A:333:THR:HG22 | 1:A:377:THR:HG22 | 1.86 | 0.58 |
| 3:C:452:ILE:HB | 3:C:453:PRO:HD3 | 1.85 | 0.58 |
| 4:D:254:VAL:O | 4:D:254:VAL:HG23 | 2.02 | 0.58 |
| 7:G:218:VAL:HA | 7:G:375:THR:HG21 | 1.86 | 0.58 |
| 8:H:69:ALA:HB2 | 8:H:100:THR:HB | 1.85 | 0.58 |
| 2:J:373:THR:CG2 | 2:J:375:GLN:HG2 | 2.34 | 0.58 |
| 4:L:238:GLN:HB2 | 4:L:290:LYS:HE3 | 1.84 | 0.58 |
| 5:M:335:LEU:HD22 | 5:M:340:LEU:HD11 | 1.84 | 0.58 |
| 6:F:109:ILE:CG1 | 5:M:39:LYS:HZ3 | 2.13 | 0.58 |
| 6:N:155:ARG:CB | 6:N:171:THR:OG1 | 2.52 | 0.58 |
| 1:A:159:ILE:HD11 | 1:A:418:VAL:HG11 | 1.84 | 0.58 |
| 1:A:247:LEU:O | 1:A:298:THR:HA | 2.04 | 0.58 |
| 2:B:373:THR:CG2 | 2:B:375:GLN:HG2 | 2.34 | 0.58 |
| 2:B:407:ALA:O | 2:B:410:VAL:HG12 | 2.03 | 0.58 |
| 2:B:463:ILE:O | 2:B:467:ILE:CB | 2.52 | 0.58 |
| 2:B:38:GLY:HA3 | 2:B:474:LEU:HD11 | 1.84 | 0.58 |
| 3:C:296:ILE:HG23 | 3:C:320:VAL:HG21 | 1.85 | 0.58 |
| 4:D:128:ALA:O | 4:D:132:VAL:HG23 | 2.03 | 0.58 |
| 4:D:182:SER:HB2 | 4:D:187:LYS:HE2 | 1.85 | 0.58 |
| 4:D:521:ILE:HG12 | 7:G:62:ILE:HD11 | 1.86 | 0.58 |
| 6:F:32:VAL:HB | 6:F:33:LEU:HD22 | 1.86 | 0.58 |
| 6:F:201:HIS:CB | 6:F:381:LYS:HE2 | 2.34 | 0.58 |
| 6:F:201:HIS:HB3 | 6:F:381:LYS:HE2 | 1.85 | 0.58 |
| 7:G:125:ILE:HG22 | 7:G:129:TYR:CE2 | 2.38 | 0.58 |
| 8:H:427:GLU:HG2 | 8:H:459:VAL:HG21 | 1.85 | 0.58 |
| 2:J:32:LEU:HG | 6:N:532:GLU:OE1 | 2.04 | 0.58 |
| 5:M:323:CYS:O | 5:M:344:ARG:HA | 2.02 | 0.58 |
| 6:N:57:LYS:O | 6:N:57:LYS:HG2 | 2.03 | 0.58 |
| 1:A:463:ALA:HB1 | 1:A:470:SER:HB2 | 1.86 | 0.58 |
| 2:B:285:ILE:HD13 | 2:B:285:ILE:N | 2.19 | 0.58 |
| 2:B:159:THR:HG21 | 2:B:488:VAL:H | 1.69 | 0.58 |
| 4:D:104:LEU:HD11 | 4:D:518:ILE:HD12 | 1.86 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:171:ALA:HB3 | 4:D:172:PRO:HD3 | 1.86 | 0.58 |
| 4:D:210:ILE:O | 4:D:375:VAL:HG12 | 2.02 | 0.58 |
| 6:F:401:ALA:O | 6:F:405:VAL:HG23 | 2.04 | 0.58 |
| 6:F:125:ALA:HA | 6:F:426:LEU:HD21 | 1.85 | 0.58 |
| 6:F:541:LEU:HB2 | 6:F:542:LYS:CB | 2.32 | 0.58 |
| 7:G:376:LEU:HD23 | 7:G:376:LEU:H | 1.69 | 0.58 |
| 2:J:200:GLY:O | 2:J:371:GLY:N | 2.28 | 0.58 |
| 5:M:253:GLN:H | 5:M:254:MET:CB | 2.16 | 0.58 |
| 5:M:448:VAL:HG21 | 5:M:498:LEU:HD13 | 1.86 | 0.58 |
| 6:N:175:THR:O | 6:N:179:LEU:HG | 2.04 | 0.58 |
| 6:N:33:LEU:HD21 | 6:N:63:LEU:HD21 | 1.85 | 0.58 |
| 6:N:343:LEU:HG | 6:N:344:SER:HB3 | 1.85 | 0.58 |
| 6:N:56:THR:HG22 | 6:N:390:GLN:HB2 | 1.86 | 0.58 |
| 7:O:208:ALA:HB3 | 7:O:211:GLU:HG3 | 1.84 | 0.58 |
| 7:O:376:LEU:HD23 | 7:O:376:LEU:H | 1.69 | 0.58 |
| 7:O:126:MET:HE3 | 7:O:515:ASN:HA | 1.86 | 0.58 |
| 3:C:514:ILE:HA | 3:C:517:ALA:HB3 | 1.86 | 0.58 |
| 4:D:258:ARG:HD2 | 8:H:283:GLN:NE2 | 2.19 | 0.58 |
| 6:F:151:LEU:O | 6:F:171:THR:HG22 | 2.04 | 0.58 |
| 6:F:155:ARG:CB | 6:F:171:THR:OG1 | 2.52 | 0.58 |
| 6:F:433:LYS:C | 6:F:441:LYS:CB | 2.72 | 0.58 |
| 7:G:401:LYS:HG3 | 7:G:402:ARG:N | 2.17 | 0.58 |
| 8:H:68:ALA:H | 8:H:101:ASN:HD21 | 1.49 | 0.58 |
| 1:I:247:LEU:O | 1:I:298:THR:HA | 2.04 | 0.58 |
| 6:N:433:LYS:C | 6:N:441:LYS:CB | 2.72 | 0.58 |
| 8:P:288:MET:CE | 8:P:313:LEU:HG | 2.32 | 0.58 |
| 1:A:209:HIS:HE1 | 7:G:89:ALA:HB2 | 1.69 | 0.58 |
| 4:D:215:LEU:HB3 | 4:D:217:GLN:HG2 | 1.86 | 0.58 |
| 4:D:89:ALA:HB1 | 4:D:503:VAL:HG22 | 1.85 | 0.58 |
| 5:E:273:THR:HG21 | 5:E:364:PRO:HA | 1.78 | 0.58 |
| 6:F:343:LEU:HG | 6:F:344:SER:HB3 | 1.85 | 0.58 |
| 6:F:540:THR:O | 6:F:541:LEU:HD23 | 2.03 | 0.58 |
| 1:I:333:THR:HG22 | 1:I:377:THR:HG22 | 1.86 | 0.58 |
| 1:I:93:GLU:CA | 1:I:94:ILE:HD12 | 2.34 | 0.58 |
| 3:K:296:ILE:HG23 | 3:K:320:VAL:HG21 | 1.85 | 0.58 |
| 4:L:16:LYS:O | 4:L:20:VAL:HG23 | 2.04 | 0.58 |
| 6:N:415:ALA:CB | 6:N:506:ILE:HG21 | 2.30 | 0.58 |
| 6:N:125:ALA:HA | 6:N:426:LEU:HD21 | 1.86 | 0.58 |
| 6:N:447:PHE:CE2 | 6:N:451:LEU:HD11 | 2.39 | 0.58 |
| 7:O:218:VAL:HA | 7:O:375:THR:HG21 | 1.86 | 0.58 |
| 1:A:55:ASP:HB2 | 1:A:59:ASP:HB2 | 1.85 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:88:VAL:HA | 2:B:393:GLN:NE2 | 2.19 | 0.58 |
| 3:C:255:GLY:N | 3:C:259:THR:HG21 | 2.18 | 0.58 |
| 4:D:291:SER:HA | 4:D:315:ASP:HA | 1.86 | 0.58 |
| 7:G:484:GLU:CB | 7:G:485:THR:HA | 2.32 | 0.58 |
| 8:H:138:THR:HG22 | 8:H:434:ILE:CD1 | 2.34 | 0.58 |
| 8:H:222:VAL:HG22 | 8:H:384:ILE:HG23 | 1.86 | 0.58 |
| 4:L:182:SER:HB2 | 4:L:187:LYS:HE2 | 1.85 | 0.58 |
| 4:L:65:LEU:HD13 | 4:L:79:VAL:HG13 | 1.85 | 0.58 |
| 6:N:32:VAL:HB | 6:N:33:LEU:HD22 | 1.86 | 0.58 |
| 6:N:401:ALA:O | 6:N:405:VAL:HG23 | 2.04 | 0.58 |
| 6:N:411:ILE:CG2 | 6:N:412:ILE:H | 2.16 | 0.58 |
| 4:L:521:ILE:HG23 | 7:O:51:ILE:CA | 2.32 | 0.58 |
| 8:P:138:THR:HG22 | 8:P:434:ILE:CD1 | 2.34 | 0.58 |
| 8:P:213:MET:HE2 | 8:P:391:GLN:HG3 | 1.84 | 0.58 |
| 8:P:69:ALA:HB2 | 8:P:100:THR:HB | 1.85 | 0.58 |
| 1:A:93:GLU:CA | 1:A:94:ILE:HD12 | 2.34 | 0.57 |
| 2:B:250:PHE:HA | 6:F:250:GLY:O | 2.04 | 0.57 |
| 3:C:320:VAL:O | 3:C:321:LYS:C | 2.41 | 0.57 |
| 6:F:203:SER:C | 6:F:205:LYS:N | 2.58 | 0.57 |
| 2:B:375:GLN:NE2 | 6:F:75:LEU:HD12 | 2.19 | 0.57 |
| 8:H:146:VAL:HG13 | 8:H:147:VAL:H | 1.68 | 0.57 |
| 2:J:285:ILE:HD13 | 2:J:285:ILE:N | 2.19 | 0.57 |
| 2:J:407:ALA:O | 2:J:410:VAL:HG12 | 2.03 | 0.57 |
| 3:K:265:LYS:O | 3:K:268:ASP:OD1 | 2.21 | 0.57 |
| 4:L:379:ILE:HD12 | 4:L:379:ILE:H | 1.68 | 0.57 |
| 4:L:110:LEU:HD13 | 4:L:439:ILE:HD12 | 1.84 | 0.57 |
| 4:L:103:LEU:HD13 | 4:L:515:VAL:HG21 | 1.85 | 0.57 |
| 5:M:68:ARG:HD3 | 5:M:514:CYS:HB3 | 1.85 | 0.57 |
| 6:N:451:LEU:HD12 | 6:N:451:LEU:H | 1.69 | 0.57 |
| 7:O:238:ASN:N | 7:O:239:PRO:CD | 2.66 | 0.57 |
| 8:P:68:ALA:H | 8:P:101:ASN:HD21 | 1.49 | 0.57 |
| 8:P:48:PRO:HA | 8:P:169:SER:O | 2.04 | 0.57 |
| 2:B:30:GLY:O | 2:B:33:VAL:HG23 | 2.04 | 0.57 |
| 4:D:171:ALA:O | 4:D:175:VAL:HG22 | 2.04 | 0.57 |
| 7:G:393:LEU:HD22 | 7:G:397:ILE:HG13 | 1.85 | 0.57 |
| 1:I:350:PHE:CE2 | 1:I:354:TYR:CB | 2.85 | 0.57 |
| 3:K:255:GLY:N | 3:K:259:THR:HG21 | 2.18 | 0.57 |
| 4:L:305:LEU:HD21 | 4:L:312:VAL:HG21 | 1.85 | 0.57 |
| 6:N:221:HIS:HD2 | 6:N:224:MET:SD | 2.27 | 0.57 |
| 7:O:516:LEU:HD13 | 7:O:517:ILE:N | 2.20 | 0.57 |
| 1:A:418:VAL:HG12 | 1:A:419:VAL:N | 2.17 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:433:LEU:O | 1:A:437:ALA:HB3 | 2.05 | 0.57 |
| 2:B:263:LYS:HB3 | 2:B:267:GLU:OE2 | 2.04 | 0.57 |
| 4:D:16:LYS:O | 4:D:20:VAL:HG23 | 2.04 | 0.57 |
| 4:D:305:LEU:HD21 | 4:D:312:VAL:HG21 | 1.85 | 0.57 |
| 4:D:65:LEU:HD13 | 4:D:79:VAL:HG13 | 1.85 | 0.57 |
| 6:F:175:THR:O | 6:F:179:LEU:HG | 2.04 | 0.57 |
| 6:F:221:HIS:HD2 | 6:F:224:MET:SD | 2.27 | 0.57 |
| 6:F:447:PHE:CD2 | 6:F:451:LEU:HD11 | 2.39 | 0.57 |
| 6:F:451:LEU:HD12 | 6:F:451:LEU:H | 1.69 | 0.57 |
| 7:G:294:LEU:HD23 | 7:G:315:ALA:HB3 | 1.87 | 0.57 |
| 2:J:142:ASN:CB | 2:J:143:SER:HA | 2.18 | 0.57 |
| 2:J:30:GLY:O | 2:J:33:VAL:HG23 | 2.04 | 0.57 |
| 3:K:279:GLN:O | 3:K:283:MET:HG2 | 2.05 | 0.57 |
| 3:K:320:VAL:O | 3:K:321:LYS:C | 2.41 | 0.57 |
| 4:L:147:ARG:HG2 | 4:L:148:GLU:N | 2.18 | 0.57 |
| 4:L:171:ALA:HB3 | 4:L:172:PRO:HD3 | 1.86 | 0.57 |
| 5:M:267:VAL:HA | 5:M:319:ASP:OD2 | 2.04 | 0.57 |
| 5:M:273:THR:HG22 | 5:M:364:PRO:CA | 2.20 | 0.57 |
| 6:N:167:THR:CA | 6:N:168:GLU:HB3 | 2.35 | 0.57 |
| 6:N:231:ALA:HB1 | 6:N:293:PHE:N | 2.18 | 0.57 |
| 6:N:430:ASN:C | 6:N:433:LYS:HB2 | 2.24 | 0.57 |
| 2:B:373:THR:HG22 | 2:B:376:THR:N | 2.20 | 0.57 |
| 2:B:463:ILE:HG13 | 2:B:468:SER:HA | 1.85 | 0.57 |
| 2:B:72:PRO:CB | 3:C:47:MET:HE1 | 2.33 | 0.57 |
| 3:C:402:VAL:HG13 | 3:C:502:PRO:HG2 | 1.86 | 0.57 |
| 6:F:167:THR:HG21 | 6:F:169:VAL:HG23 | 1.86 | 0.57 |
| 7:G:282:LEU:O | 7:G:285:VAL:HG12 | 2.05 | 0.57 |
| 7:G:455:GLU:CG | 7:G:461:ALA:CB | 2.81 | 0.57 |
| 7:G:516:LEU:HD13 | 7:G:517:ILE:N | 2.20 | 0.57 |
| 7:G:83:LEU:O | 7:G:86:ILE:HG13 | 2.04 | 0.57 |
| 1:I:90:GLN:HG3 | 1:I:101:VAL:CG2 | 2.19 | 0.57 |
| 2:J:116:HIS:HE1 | 2:J:118:GLN:CB | 2.18 | 0.57 |
| 9:L:601:ADP:O3B | 9:L:601:ADP:H5'2 | 2.04 | 0.57 |
| 5:M:241:ASN:O | 5:M:241:ASN:ND2 | 2.34 | 0.57 |
| 6:N:170:LEU:HA | 6:N:173:ILE:HG22 | 1.84 | 0.57 |
| 6:N:430:ASN:C | 6:N:433:LYS:H | 2.05 | 0.57 |
| 7:O:83:LEU:O | 7:O:86:ILE:HG13 | 2.04 | 0.57 |
| 3:C:9:ASN:HD22 | 3:C:10:ALA:H | 1.53 | 0.57 |
| 4:D:298:ASN:HB3 | 4:D:299:ASP:HA | 1.84 | 0.57 |
| 6:F:231:ALA:HB1 | 6:F:293:PHE:N | 2.18 | 0.57 |
| 2:J:373:THR:HG22 | 2:J:376:THR:N | 2.20 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:K:353:GLY:H | 3:K:370:ASN:HB3 | 1.70 | 0.57 |
| 4:L:171:ALA:O | 4:L:175:VAL:HG22 | 2.05 | 0.57 |
| 4:L:89:ALA:HB1 | 4:L:503:VAL:HG22 | 1.85 | 0.57 |
| 6:N:151:LEU:O | 6:N:171:THR:HG22 | 2.04 | 0.57 |
| 6:N:447:PHE:CD2 | 6:N:451:LEU:HD11 | 2.39 | 0.57 |
| 1:A:182:ASP:O | 1:A:186:ALA:HB3 | 2.05 | 0.57 |
| 2:B:329:PHE:O | 2:B:329:PHE:CD2 | 2.53 | 0.57 |
| 3:C:113:GLU:HB2 | 1:I:460:LYS:HD2 | 1.86 | 0.57 |
| 6:F:167:THR:CA | 6:F:168:GLU:HB3 | 2.34 | 0.57 |
| 6:F:193:MET:HE3 | 6:F:330:LEU:HD11 | 1.86 | 0.57 |
| 6:F:58:ASP:O | 6:F:62:LEU:HG | 2.04 | 0.57 |
| 8:H:486:GLU:H | 8:H:487:PRO:HA | 1.69 | 0.57 |
| 2:J:206:SER:CB | 2:J:368:VAL:HG13 | 2.34 | 0.57 |
| 2:J:68:PRO:HG2 | 6:N:536:ALA:HB2 | 1.86 | 0.57 |
| 5:M:509:ASN:CG | 5:M:523:LYS:HB2 | 2.24 | 0.57 |
| 4:D:328:LEU:C | 4:D:345:ASP:OD2 | 2.43 | 0.57 |
| 2:B:40:LYS:HZ1 | 6:F:117:ILE:HG13 | 1.68 | 0.57 |
| 6:F:56:THR:HG22 | 6:F:390:GLN:HB2 | 1.86 | 0.57 |
| 6:F:430:ASN:C | 6:F:433:LYS:HB2 | 2.24 | 0.57 |
| 7:G:516:LEU:O | 7:G:516:LEU:CD2 | 2.46 | 0.57 |
| 7:G:51:ILE:HG22 | 7:G:53:ILE:HG23 | 1.87 | 0.57 |
| 8:H:204:VAL:CG2 | 8:H:409:LYS:CB | 2.82 | 0.57 |
| 1:I:329:ILE:HD13 | 1:I:374:ILE:HD12 | 1.87 | 0.57 |
| 2:J:88:VAL:HA | 2:J:393:GLN:NE2 | 2.19 | 0.57 |
| 4:L:215:LEU:HB3 | 4:L:217:GLN:HG2 | 1.86 | 0.57 |
| 4:L:291:SER:HA | 4:L:315:ASP:HA | 1.86 | 0.57 |
| 4:L:41:PRO:HG2 | 9:L:601:ADP:C6 | 2.40 | 0.57 |
| 6:N:108:PHE:O | 6:N:113:VAL:HG23 | 2.04 | 0.57 |
| 5:M:352:GLU:HA | 6:N:222:PRO:HG3 | 1.86 | 0.57 |
| 7:O:393:LEU:HD22 | 7:O:397:ILE:HG13 | 1.85 | 0.57 |
| 7:O:494:LYS:O | 7:O:495:PHE:CB | 2.52 | 0.57 |
| 4:D:120:ILE:HA | 4:D:123:SER:HB3 | 1.87 | 0.57 |
| 5:E:448:VAL:HG21 | 5:E:498:LEU:HD13 | 1.86 | 0.57 |
| 6:F:108:PHE:O | 6:F:113:VAL:HG23 | 2.04 | 0.57 |
| 2:B:43:ASP:O | 6:F:530:CYS:HA | 2.04 | 0.57 |
| 1:I:433:LEU:O | 1:I:437:ALA:HB3 | 2.05 | 0.57 |
| 6:N:167:THR:HG21 | 6:N:169:VAL:HG23 | 1.86 | 0.57 |
| 6:N:280:LEU:HD13 | 6:N:343:LEU:HD21 | 1.85 | 0.57 |
| 6:N:485:GLU:O | 6:N:488:TYR:CB | 2.52 | 0.57 |
| 7:O:294:LEU:HD23 | 7:O:315:ALA:HB3 | 1.86 | 0.57 |
| 1:A:264:ILE:O | 1:A:265:ASP:HB3 | 2.05 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:33:THR:OG1 | 1:I:83:LEU:HD11 | 2.05 | 0.57 |
| 2:J:263:LYS:HB3 | 2:J:267:GLU:OE2 | 2.04 | 0.57 |
| 3:K:355:PHE:HB2 | 3:K:368:LEU:HD13 | 1.87 | 0.57 |
| 4:L:110:LEU:HD13 | 4:L:439:ILE:HG23 | 1.87 | 0.57 |
| 5:M:255:PRO:HG3 | 5:M:336:LEU:HA | 1.87 | 0.57 |
| 6:N:169:VAL:C | 6:N:172:PRO:HD2 | 2.26 | 0.57 |
| 8:P:54:ILE:HG13 | 8:P:64:ILE:CG1 | 2.15 | 0.57 |
| 1:A:252:GLN:HG3 | 1:A:253:LYS:N | 2.20 | 0.57 |
| 5:E:267:VAL:HA | 5:E:319:ASP:OD2 | 2.04 | 0.57 |
| 5:E:68:ARG:HD3 | 5:E:514:CYS:HB3 | 1.85 | 0.57 |
| 6:F:38:GLY:N | 9:F:601:ADP:H5'1 | 2.15 | 0.57 |
| 6:F:6:LEU:CD1 | 6:F:7:ASN:H | 2.18 | 0.57 |
| 1:I:183:ALA:HB1 | 1:I:383:SER:HB2 | 1.87 | 0.57 |
| 2:J:463:ILE:O | 2:J:467:ILE:CB | 2.52 | 0.57 |
| 2:J:91:GLY:HA2 | 9:J:601:ADP:O2A | 2.05 | 0.57 |
| 3:K:223:VAL:HG12 | 3:K:224:LEU:N | 2.20 | 0.57 |
| 3:K:402:VAL:HG13 | 3:K:502:PRO:HG2 | 1.86 | 0.57 |
| 4:L:177:SER:O | 4:L:181:ILE:HG12 | 2.05 | 0.57 |
| 6:N:45:MET:HA | 6:N:54:LYS:O | 2.05 | 0.57 |
| 6:N:56:THR:O | 6:N:62:LEU:HD21 | 2.05 | 0.57 |
| 6:N:58:ASP:O | 6:N:62:LEU:HG | 2.04 | 0.57 |
| 1:A:33:THR:OG1 | 1:A:83:LEU:HD11 | 2.05 | 0.56 |
| 2:B:245:ILE:O | 2:B:246:PHE:HD2 | 1.87 | 0.56 |
| 3:C:353:GLY:H | 3:C:370:ASN:HB3 | 1.70 | 0.56 |
| 6:F:447:PHE:CE2 | 6:F:451:LEU:HD11 | 2.39 | 0.56 |
| 6:F:452:LEU:O | 6:F:455:PRO:CD | 2.51 | 0.56 |
| 2:J:159:THR:HG21 | 2:J:488:VAL:H | 1.69 | 0.56 |
| 8:P:300:VAL:HG13 | 8:P:321:LEU:HB3 | 1.87 | 0.56 |
| 1:A:548:ASP:N | 1:A:548:ASP:OD2 | 2.37 | 0.56 |
| 2:B:230:LYS:H | 2:B:281:ILE:CG2 | 2.18 | 0.56 |
| 4:D:36:ARG:HE | 4:D:98:ILE:CG2 | 2.18 | 0.56 |
| 5:E:32:VAL:HG22 | 5:E:33:LYS:N | 2.14 | 0.56 |
| 6:F:29:LEU:O | 6:F:33:LEU:HD23 | 2.05 | 0.56 |
| 7:G:43:THR:CG2 | 7:G:64:ASN:CB | 2.83 | 0.56 |
| 1:I:252:GLN:HG3 | 1:I:253:LYS:N | 2.20 | 0.56 |
| 2:J:213:ILE:HG23 | 2:J:354:LEU:CD2 | 2.35 | 0.56 |
| 5:M:74:LEU:CG | 5:M:93:GLN:HB3 | 2.35 | 0.56 |
| 5:M:352:GLU:HA | 6:N:222:PRO:CG | 2.35 | 0.56 |
| 6:N:428:SER:O | 6:N:431:MET:HG2 | 2.06 | 0.56 |
| 3:C:80:GLU:O | 3:C:84:THR:HG23 | 2.05 | 0.56 |
| 6:F:169:VAL:C | 6:F:172:PRO:HD2 | 2.26 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:F:428:SER:O | 6:F:431:MET:HG2 | 2.05 | 0.56 |
| 6:F:56:THR:O | 6:F:62:LEU:HD21 | 2.05 | 0.56 |
| 1:A:55:ASP:HA | 7:G:527:LYS:HB3 | 1.86 | 0.56 |
| 1:I:264:ILE:O | 1:I:265:ASP:HB3 | 2.05 | 0.56 |
| 2:J:239:ASP:OD1 | 2:J:290:ILE:HB | 2.06 | 0.56 |
| 2:J:245:ILE:O | 2:J:246:PHE:HD2 | 1.87 | 0.56 |
| 3:K:118:PRO:O | 3:K:122:ILE:HG13 | 2.05 | 0.56 |
| 3:K:302:SER:O | 3:K:303:ASP:CB | 2.40 | 0.56 |
| 3:K:514:ILE:HA | 3:K:517:ALA:HB3 | 1.86 | 0.56 |
| 8:P:427:GLU:HG2 | 8:P:459:VAL:HG21 | 1.85 | 0.56 |
| 5:E:428:CYS:HA | 5:E:431:ARG:HG3 | 1.88 | 0.56 |
| 5:E:509:ASN:CG | 5:E:523:LYS:HB2 | 2.24 | 0.56 |
| 8:H:284:ILE:O | 8:H:288:MET:HG2 | 2.06 | 0.56 |
| 3:K:321:LYS:HB3 | 3:K:324:ASP:HB2 | 1.87 | 0.56 |
| 4:L:104:LEU:HD11 | 4:L:518:ILE:HD12 | 1.86 | 0.56 |
| 4:L:7:SER:HA | 7:O:35:ALA:HB1 | 1.86 | 0.56 |
| 5:M:252:PRO:HA | 5:M:255:PRO:C | 2.26 | 0.56 |
| 6:N:452:LEU:O | 6:N:455:PRO:CD | 2.51 | 0.56 |
| 7:O:109:MET:SD | 7:O:514:THR:HB | 2.45 | 0.56 |
| 7:O:51:ILE:HG22 | 7:O:53:ILE:HG23 | 1.87 | 0.56 |
| 1:A:266:ASP:N | 1:A:267:PRO:CD | 2.68 | 0.56 |
| 2:B:213:ILE:HG23 | 2:B:354:LEU:CD2 | 2.35 | 0.56 |
| 3:C:149:ALA:O | 3:C:153:LYS:HG2 | 2.05 | 0.56 |
| 3:C:279:GLN:O | 3:C:283:MET:HG2 | 2.05 | 0.56 |
| 7:G:494:LYS:O | 7:G:495:PHE:CB | 2.52 | 0.56 |
| 8:H:52:ASN:OD1 | 8:H:66:ASN:HB2 | 2.06 | 0.56 |
| 3:K:226:ASN:OD1 | 3:K:365:PHE:HA | 2.06 | 0.56 |
| 6:N:6:LEU:CD1 | 6:N:7:ASN:H | 2.18 | 0.56 |
| 8:P:204:VAL:CG2 | 8:P:409:LYS:CB | 2.82 | 0.56 |
| 8:P:486:GLU:H | 8:P:487:PRO:HA | 1.69 | 0.56 |
| 2:B:116:HIS:HE1 | 2:B:118:GLN:CB | 2.18 | 0.56 |
| 3:C:355:PHE:HB2 | 3:C:368:LEU:HD13 | 1.87 | 0.56 |
| 4:D:110:LEU:HD13 | 4:D:439:ILE:HG23 | 1.87 | 0.56 |
| 4:D:485:ARG:N | 4:D:485:ARG:HD2 | 2.20 | 0.56 |
| 5:E:255:PRO:HG3 | 5:E:336:LEU:HA | 1.87 | 0.56 |
| 6:F:485:GLU:O | 6:F:488:TYR:CB | 2.52 | 0.56 |
| 7:G:71:LYS:HD2 | 7:G:72:LEU:HD12 | 1.88 | 0.56 |
| 8:H:300:VAL:HG13 | 8:H:321:LEU:HB3 | 1.87 | 0.56 |
| 1:I:159:ILE:O | 1:I:162:THR:HG22 | 2.06 | 0.56 |
| 1:I:463:ALA:HB1 | 1:I:470:SER:HB2 | 1.86 | 0.56 |
| 2:J:237:THR:CB | 2:J:288:GLN:O | 2.54 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:K:80:GLU:O | 3:K:84:THR:HG23 | 2.05 | 0.56 |
| 4:L:209:MET:HA | 4:L:377:VAL:HG12 | 1.86 | 0.56 |
| 8:P:52:ASN:OD1 | 8:P:66:ASN:HB2 | 2.06 | 0.56 |
| 1:A:422:GLY:HA2 | 9:A:601:ADP:N3 | 2.20 | 0.56 |
| 2:B:237:THR:CB | 2:B:288:GLN:O | 2.54 | 0.56 |
| 2:B:242:LYS:HD3 | 3:C:269:TRP:CZ2 | 2.39 | 0.56 |
| 2:B:319:LEU:HD22 | 2:B:320:VAL:HG13 | 1.88 | 0.56 |
| 2:B:450:PHE:CB | 2:B:455:LEU:HD22 | 2.36 | 0.56 |
| 2:B:45:LEU:CD2 | 2:B:56:VAL:HG22 | 2.35 | 0.56 |
| 3:C:12:GLN:NE2 | 3:C:529:GLY:HA2 | 2.21 | 0.56 |
| 3:C:335:THR:O | 3:C:337:VAL:HG23 | 2.06 | 0.56 |
| 4:D:372:ARG:N | 4:D:373:PRO:HD3 | 2.21 | 0.56 |
| 8:H:68:ALA:O | 8:H:72:LEU:HG | 2.05 | 0.56 |
| 2:J:375:GLN:HE22 | 6:N:75:LEU:HB2 | 1.70 | 0.56 |
| 3:K:335:THR:O | 3:K:337:VAL:HG23 | 2.06 | 0.56 |
| 5:M:84:THR:HG22 | 5:M:86:ASP:N | 2.18 | 0.56 |
| 7:O:121:SER:HB3 | 7:O:123:HIS:CE1 | 2.41 | 0.56 |
| 7:O:282:LEU:O | 7:O:285:VAL:HG12 | 2.05 | 0.56 |
| 8:P:123:SER:OG | 8:P:126:GLU:HG3 | 2.06 | 0.56 |
| 1:A:76:GLN:O | 1:A:77:HIS:HB3 | 2.06 | 0.56 |
| 4:D:177:SER:O | 4:D:181:ILE:HG12 | 2.05 | 0.56 |
| 4:D:219:ALA:HB1 | 4:D:221:LYS:NZ | 2.20 | 0.56 |
| 6:F:143:LEU:HA | 6:F:144:SER:C | 2.24 | 0.56 |
| 6:F:154:ALA:HB2 | 6:F:402:VAL:HG22 | 1.87 | 0.56 |
| 6:F:424:ARG:HG2 | 6:F:483:SER:CA | 2.34 | 0.56 |
| 6:F:415:ALA:O | 6:F:491:VAL:HG23 | 2.06 | 0.56 |
| 7:G:323:MET:HA | 7:G:326:VAL:HG22 | 1.88 | 0.56 |
| 1:I:209:HIS:HE1 | 7:O:89:ALA:HB2 | 1.71 | 0.56 |
| 2:J:16:GLU:HG3 | 2:J:17:ASN:H | 1.70 | 0.56 |
| 3:K:9:ASN:HD22 | 3:K:10:ALA:H | 1.53 | 0.56 |
| 3:K:149:ALA:O | 3:K:153:LYS:HG2 | 2.05 | 0.56 |
| 6:N:143:LEU:CD1 | 6:N:145:ASN:CG | 2.74 | 0.56 |
| 6:N:29:LEU:O | 6:N:33:LEU:HD23 | 2.05 | 0.56 |
| 6:N:541:LEU:HB2 | 6:N:542:LYS:HA | 0.59 | 0.56 |
| 7:O:43:THR:CG2 | 7:O:64:ASN:CB | 2.83 | 0.56 |
| 8:P:284:ILE:O | 8:P:288:MET:HG2 | 2.05 | 0.56 |
| 1:A:183:ALA:HB1 | 1:A:383:SER:HB2 | 1.87 | 0.56 |
| 2:B:239:ASP:OD1 | 2:B:290:ILE:HB | 2.06 | 0.56 |
| 3:C:118:PRO:O | 3:C:122:ILE:HG13 | 2.05 | 0.56 |
| 2:B:32:LEU:HD12 | 6:F:532:GLU:OE2 | 2.05 | 0.56 |
| 7:G:23:LYS:HA | 7:G:26:ILE:CG2 | 2.36 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:37:LEU:HB2 | 2:J:444:LEU:HD13 | 1.87 | 0.56 |
| 2:J:47:GLN:OE1 | 2:J:54:CYS:HB3 | 2.05 | 0.56 |
| 3:K:264:GLU:O | 3:K:265:LYS:CB | 2.54 | 0.56 |
| 4:L:120:ILE:HA | 4:L:123:SER:HB3 | 1.87 | 0.56 |
| 4:L:219:ALA:HB1 | 4:L:221:LYS:NZ | 2.20 | 0.56 |
| 4:L:242:SER:O | 4:L:244:PRO:HD3 | 2.06 | 0.56 |
| 5:M:428:CYS:HA | 5:M:431:ARG:HG3 | 1.88 | 0.56 |
| 6:N:203:SER:C | 6:N:205:LYS:N | 2.58 | 0.56 |
| 1:A:187:VAL:HB | 1:A:382:SER:N | 2.21 | 0.56 |
| 3:C:223:VAL:HG12 | 3:C:224:LEU:N | 2.20 | 0.56 |
| 2:B:326:VAL:CG1 | 3:C:304:LEU:HD22 | 2.36 | 0.56 |
| 9:D:601:ADP:O3' | 9:D:601:ADP:C8 | 2.59 | 0.56 |
| 6:F:424:ARG:NH1 | 6:F:479:ASP:CB | 2.69 | 0.56 |
| 6:F:541:LEU:HB2 | 6:F:542:LYS:HA | 0.60 | 0.56 |
| 7:G:121:SER:HB3 | 7:G:123:HIS:CE1 | 2.41 | 0.56 |
| 7:G:420:VAL:HG23 | 7:G:446:LEU:HD13 | 1.88 | 0.56 |
| 2:J:402:LEU:HD21 | 2:J:483:ARG:CG | 2.36 | 0.56 |
| 2:J:450:PHE:CB | 2:J:455:LEU:HD22 | 2.36 | 0.56 |
| 6:N:47:VAL:HG12 | 6:N:48:ASP:H | 1.71 | 0.56 |
| 6:N:92:THR:HG21 | 10:N:602:BEF:F3 | 1.95 | 0.56 |
| 7:O:41:LYS:N | 7:O:42:PRO:CD | 2.69 | 0.56 |
| 8:P:25:ASP:HA | 8:P:28:ILE:HG13 | 1.87 | 0.56 |
| 8:P:323:VAL:O | 8:P:323:VAL:HG23 | 2.06 | 0.56 |
| 1:A:159:ILE:O | 1:A:162:THR:HG22 | 2.06 | 0.56 |
| 2:B:37:LEU:HB2 | 2:B:444:LEU:HD13 | 1.87 | 0.56 |
| 2:B:47:GLN:OE1 | 2:B:54:CYS:HB3 | 2.05 | 0.56 |
| 2:B:63:ILE:HG23 | 2:B:64:LEU:HG | 1.88 | 0.56 |
| 4:D:242:SER:O | 4:D:244:PRO:HD3 | 2.06 | 0.56 |
| 8:H:25:ASP:HA | 8:H:28:ILE:HG13 | 1.87 | 0.56 |
| 8:H:29:ILE:CG2 | 8:H:30:LYS:N | 2.69 | 0.56 |
| 1:I:266:ASP:N | 1:I:267:PRO:CD | 2.68 | 0.56 |
| 1:I:76:GLN:O | 1:I:77:HIS:HB3 | 2.06 | 0.56 |
| 2:J:230:LYS:H | 2:J:281:ILE:CG2 | 2.18 | 0.56 |
| 2:J:63:ILE:HG23 | 2:J:64:LEU:HG | 1.88 | 0.56 |
| 4:L:527:SER:HB3 | 4:L:528:ARG:HH21 | 1.71 | 0.56 |
| 6:N:540:THR:O | 6:N:541:LEU:CD2 | 2.54 | 0.56 |
| 7:O:323:MET:HA | 7:O:326:VAL:HG22 | 1.88 | 0.56 |
| 1:A:252:GLN:HG3 | 1:A:253:LYS:H | 1.71 | 0.55 |
| 1:A:329:ILE:HD13 | 1:A:374:ILE:HD12 | 1.87 | 0.55 |
| 2:B:16:GLU:HG3 | 2:B:17:ASN:H | 1.71 | 0.55 |
| 2:B:475:ASN:HD22 | 2:B:475:ASN:N | 1.92 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:402:LEU:HD11 | 2:B:483:ARG:HG3 | 1.88 | 0.55 |
| 5:E:252:PRO:HA | 5:E:255:PRO:C | 2.26 | 0.55 |
| 5:E:35:GLN:OE1 | 5:E:36:GLY:HA3 | 2.06 | 0.55 |
| 5:E:74:LEU:CG | 5:E:93:GLN:HB3 | 2.35 | 0.55 |
| 1:I:187:VAL:HB | 1:I:382:SER:N | 2.21 | 0.55 |
| 1:I:517:VAL:O | 1:I:518:LEU:CD2 | 2.54 | 0.55 |
| 2:J:5:ILE:O | 3:K:71:ALA:N | 2.39 | 0.55 |
| 4:L:372:ARG:N | 4:L:373:PRO:HD3 | 2.21 | 0.55 |
| 4:L:394:LEU:HA | 4:L:397:ALA:HB3 | 1.88 | 0.55 |
| 5:M:181:LEU:HA | 5:M:205:VAL:HG21 | 1.89 | 0.55 |
| 1:A:500:TYR:HA | 1:A:511:ASP:HA | 1.89 | 0.55 |
| 1:A:517:VAL:O | 1:A:518:LEU:CD2 | 2.54 | 0.55 |
| 3:C:321:LYS:HB3 | 3:C:324:ASP:HB2 | 1.87 | 0.55 |
| 3:C:226:ASN:OD1 | 3:C:365:PHE:HA | 2.06 | 0.55 |
| 5:E:350:GLU:C | 5:E:352:GLU:N | 2.55 | 0.55 |
| 6:F:45:MET:HA | 6:F:54:LYS:O | 2.05 | 0.55 |
| 6:F:47:VAL:HG12 | 6:F:48:ASP:H | 1.70 | 0.55 |
| 1:I:182:ASP:O | 1:I:186:ALA:HB3 | 2.05 | 0.55 |
| 3:K:482:THR:HA | 3:K:493:ASP:HA | 1.87 | 0.55 |
| 2:B:115:ILE:HG12 | 5:M:492:ILE:HD11 | 1.88 | 0.55 |
| 6:N:209:PHE:CZ | 6:N:211:LYS:HD2 | 2.41 | 0.55 |
| 6:N:68:ILE:HD13 | 6:N:74:VAL:HG22 | 1.89 | 0.55 |
| 1:A:350:PHE:CE2 | 1:A:354:TYR:CB | 2.85 | 0.55 |
| 3:C:322:LYS:HG3 | 3:C:323:SER:N | 2.21 | 0.55 |
| 4:D:209:MET:HA | 4:D:377:VAL:HG12 | 1.86 | 0.55 |
| 4:D:411:ILE:HG13 | 4:D:501:VAL:HG22 | 1.87 | 0.55 |
| 5:E:181:LEU:HA | 5:E:205:VAL:HG21 | 1.88 | 0.55 |
| 5:E:351:LEU:N | 5:E:351:LEU:HD13 | 2.22 | 0.55 |
| 6:F:151:LEU:CG | 6:F:175:THR:HG23 | 2.31 | 0.55 |
| 6:F:68:ILE:HD13 | 6:F:74:VAL:HG22 | 1.89 | 0.55 |
| 6:F:5:LEU:CB | 6:F:6:LEU:C | 2.75 | 0.55 |
| 7:G:58:GLN:HA | 7:G:58:GLN:NE2 | 2.22 | 0.55 |
| 2:J:511:VAL:HB | 2:J:514:ILE:HD11 | 1.88 | 0.55 |
| 3:K:506:LYS:O | 3:K:510:VAL:HG23 | 2.06 | 0.55 |
| 5:M:273:THR:CG2 | 5:M:364:PRO:CA | 2.72 | 0.55 |
| 1:I:273:ILE:HG21 | 5:M:295:TYR:CE2 | 2.41 | 0.55 |
| 5:M:351:LEU:HD13 | 5:M:351:LEU:N | 2.22 | 0.55 |
| 6:N:489:VAL:O | 6:N:490:GLY:C | 2.41 | 0.55 |
| 8:P:68:ALA:O | 8:P:72:LEU:HG | 2.06 | 0.55 |
| 2:B:402:LEU:HD21 | 2:B:483:ARG:CG | 2.36 | 0.55 |
| 2:B:3:VAL:C | 2:B:5:ILE:HG21 | 2.25 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:F:540:THR:O | 6:F:541:LEU:CD2 | 2.54 | 0.55 |
| 1:I:484:SER:OG | 1:I:498:ARG:CB | 2.55 | 0.55 |
| 2:J:319:LEU:HD22 | 2:J:320:VAL:HG13 | 1.88 | 0.55 |
| 4:L:521:ILE:HD11 | 7:O:62:ILE:HD12 | 1.82 | 0.55 |
| 7:O:23:LYS:HA | 7:O:26:ILE:CG2 | 2.36 | 0.55 |
| 7:O:492:PHE:HA | 7:O:497:TRP:NE1 | 2.21 | 0.55 |
| 8:P:29:ILE:CG2 | 8:P:30:LYS:N | 2.69 | 0.55 |
| 1:A:252:GLN:HB2 | 1:A:303:ASP:HB2 | 1.89 | 0.55 |
| 3:C:104:LEU:HD21 | 3:C:517:ALA:HA | 1.89 | 0.55 |
| 6:F:143:LEU:CD1 | 6:F:145:ASN:CG | 2.74 | 0.55 |
| 7:G:294:LEU:CD2 | 7:G:315:ALA:HB3 | 2.37 | 0.55 |
| 7:G:109:MET:SD | 7:G:514:THR:HB | 2.45 | 0.55 |
| 2:J:460:ARG:O | 2:J:463:ILE:HG22 | 2.07 | 0.55 |
| 2:J:402:LEU:HD11 | 2:J:483:ARG:HG3 | 1.88 | 0.55 |
| 4:L:524:ILE:HG22 | 4:L:524:ILE:O | 2.06 | 0.55 |
| 6:N:160:THR:H | 6:N:164:ALA:CB | 2.20 | 0.55 |
| 6:N:35:THR:HG22 | 6:N:42:THR:H | 1.72 | 0.55 |
| 6:N:424:ARG:NH1 | 6:N:479:ASP:CB | 2.69 | 0.55 |
| 6:N:415:ALA:O | 6:N:491:VAL:HG23 | 2.06 | 0.55 |
| 6:N:5:LEU:CB | 6:N:6:LEU:C | 2.75 | 0.55 |
| 1:A:484:SER:OG | 1:A:498:ARG:CB | 2.55 | 0.55 |
| 3:C:47:MET:HE2 | 3:C:49:LEU:HD21 | 1.87 | 0.55 |
| 4:D:207:THR:HB | 4:D:378:VAL:O | 2.07 | 0.55 |
| 6:F:209:PHE:CZ | 6:F:211:LYS:HD2 | 2.41 | 0.55 |
| 8:H:323:VAL:O | 8:H:323:VAL:HG23 | 2.06 | 0.55 |
| 1:I:252:GLN:HG3 | 1:I:253:LYS:H | 1.71 | 0.55 |
| 1:I:76:GLN:O | 1:I:77:HIS:CB | 2.55 | 0.55 |
| 2:J:45:LEU:CD2 | 2:J:56:VAL:HG22 | 2.36 | 0.55 |
| 4:L:298:ASN:CB | 4:L:299:ASP:HA | 2.37 | 0.55 |
| 4:L:485:ARG:N | 4:L:485:ARG:HD2 | 2.20 | 0.55 |
| 5:M:470:ARG:O | 5:M:474:GLN:HG3 | 2.07 | 0.55 |
| 7:O:115:PHE:O | 7:O:119:GLY:HA3 | 2.07 | 0.55 |
| 7:O:126:MET:HE2 | 7:O:126:MET:HA | 1.88 | 0.55 |
| 8:P:328:GLU:HG3 | 8:P:331:ARG:HH12 | 1.72 | 0.55 |
| 1:A:92:ARG:HB3 | 5:E:388:THR:HA | 1.89 | 0.55 |
| 3:C:482:THR:HA | 3:C:493:ASP:HA | 1.87 | 0.55 |
| 4:D:394:LEU:HA | 4:D:397:ALA:HB3 | 1.89 | 0.55 |
| 6:F:160:THR:H | 6:F:164:ALA:CB | 2.20 | 0.55 |
| 6:F:214:VAL:O | 6:F:215:LEU:HD23 | 2.06 | 0.55 |
| 6:F:92:THR:CG2 | 10:F:602:BEF:F3 | 2.44 | 0.55 |
| 7:G:34:VAL:O | 7:G:38:GLU:HG2 | 2.06 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:G:41:LYS:N | 7:G:42:PRO:CD | 2.69 | 0.55 |
| 3:K:508:GLN:HG2 | 8:P:215:GLY:HA2 | 1.89 | 0.55 |
| 3:K:104:LEU:HD21 | 3:K:517:ALA:HA | 1.89 | 0.55 |
| 6:N:143:LEU:HA | 6:N:144:SER:C | 2.24 | 0.55 |
| 8:P:146:VAL:C | 8:P:148:GLY:H | 2.10 | 0.55 |
| 2:B:229:ALA:HB3 | 2:B:339:GLU:O | 2.07 | 0.55 |
| 2:B:460:ARG:O | 2:B:463:ILE:HG22 | 2.07 | 0.55 |
| 3:C:264:GLU:O | 3:C:265:LYS:CB | 2.54 | 0.55 |
| 2:B:514:ILE:CD1 | 3:C:47:MET:HB3 | 2.35 | 0.55 |
| 5:E:173:ASP:HB3 | 5:E:437:SER:HB3 | 1.87 | 0.55 |
| 2:J:173:PHE:HA | 2:J:176:LEU:HD12 | 1.89 | 0.55 |
| 2:J:475:ASN:N | 2:J:475:ASN:HD22 | 1.92 | 0.55 |
| 2:J:4:GLN:N | 2:J:5:ILE:HG12 | 2.19 | 0.55 |
| 2:J:3:VAL:C | 2:J:5:ILE:HG21 | 2.24 | 0.55 |
| 3:K:322:LYS:HG3 | 3:K:323:SER:N | 2.21 | 0.55 |
| 4:L:207:THR:HB | 4:L:378:VAL:O | 2.07 | 0.55 |
| 4:L:410:LEU:HD22 | 4:L:498:LEU:HB3 | 1.89 | 0.55 |
| 6:N:195:GLU:CG | 6:N:197:MET:SD | 2.94 | 0.55 |
| 6:N:214:VAL:O | 6:N:215:LEU:HD23 | 2.07 | 0.55 |
| 6:N:277:ILE:HG21 | 6:N:295:ILE:HG13 | 1.89 | 0.55 |
| 4:L:81:VAL:HG22 | 7:O:382:ALA:HB2 | 1.89 | 0.55 |
| 7:O:386:ILE:O | 7:O:389:VAL:HB | 2.07 | 0.55 |
| 8:P:24:ALA:CB | 8:P:531:ALA:HB1 | 2.37 | 0.55 |
| 2:B:173:PHE:HA | 2:B:176:LEU:HD12 | 1.89 | 0.55 |
| 2:B:95:VAL:HG22 | 2:B:497:VAL:HG22 | 1.89 | 0.55 |
| 4:D:375:VAL:HG12 | 4:D:376:SER:N | 2.22 | 0.55 |
| 6:F:277:ILE:HG21 | 6:F:295:ILE:HG13 | 1.89 | 0.55 |
| 6:F:353:LEU:N | 6:F:369:GLU:HB3 | 2.22 | 0.55 |
| 6:F:372:ASP:N | 6:F:373:PRO:HD3 | 2.22 | 0.55 |
| 6:F:406:LEU:C | 6:F:407:LYS:HE3 | 2.27 | 0.55 |
| 3:C:275:ILE:CA | 8:H:274:LEU:HD21 | 2.37 | 0.55 |
| 2:J:39:PRO:HA | 2:J:163:SER:CA | 2.37 | 0.55 |
| 3:K:523:VAL:HA | 8:P:52:ASN:O | 2.06 | 0.55 |
| 5:M:35:GLN:OE1 | 5:M:36:GLY:HA3 | 2.06 | 0.55 |
| 6:N:171:THR:O | 6:N:175:THR:CB | 2.55 | 0.55 |
| 6:N:538:ARG:HH11 | 6:N:538:ARG:HG3 | 1.71 | 0.55 |
| 6:N:541:LEU:HB2 | 6:N:542:LYS:CB | 2.32 | 0.55 |
| 7:O:71:LYS:HD2 | 7:O:72:LEU:HD12 | 1.88 | 0.55 |
| 3:C:124:ALA:HB1 | 3:C:441:PRO:CB | 2.37 | 0.55 |
| 5:E:88:ALA:CB | 5:E:109:LYS:NZ | 2.68 | 0.55 |
| 6:F:199:MET:O | 6:F:381:LYS:CE | 2.55 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:F:538:ARG:HG3 | 6:F:538:ARG:HH11 | 1.71 | 0.55 |
| 8:H:123:SER:OG | 8:H:126:GLU:HG3 | 2.06 | 0.55 |
| 1:I:252:GLN:HB2 | 1:I:303:ASP:HB2 | 1.89 | 0.55 |
| 4:L:411:ILE:HG13 | 4:L:501:VAL:HG22 | 1.87 | 0.55 |
| 6:N:372:ASP:N | 6:N:373:PRO:HD3 | 2.22 | 0.55 |
| 7:O:455:GLU:HG3 | 7:O:461:ALA:HB2 | 1.88 | 0.55 |
| 7:O:58:GLN:HA | 7:O:58:GLN:NE2 | 2.22 | 0.55 |
| 1:A:460:LYS:HD2 | 3:K:113:GLU:HB2 | 1.89 | 0.54 |
| 1:A:94:ILE:HD11 | 1:A:526:LYS:HB2 | 1.89 | 0.54 |
| 2:B:422:ILE:HG21 | 2:B:427:SER:CB | 2.36 | 0.54 |
| 3:C:370:ASN:OD1 | 3:C:1054:GLY:HA2 | 2.07 | 0.54 |
| 4:D:214:VAL:HG13 | 4:D:362:ARG:HG2 | 1.89 | 0.54 |
| 4:D:196:LEU:HD22 | 4:D:377:VAL:CG2 | 2.37 | 0.54 |
| 4:D:524:ILE:HG22 | 4:D:524:ILE:O | 2.07 | 0.54 |
| 7:G:191:ARG:HB3 | 7:G:193:ASP:O | 2.07 | 0.54 |
| 7:G:440:ASN:O | 7:G:444:LYS:HD3 | 2.08 | 0.54 |
| 2:J:210:GLU:HB3 | 2:J:357:SER:O | 2.07 | 0.54 |
| 2:J:127:ALA:CB | 2:J:430:VAL:HG22 | 2.31 | 0.54 |
| 3:K:432:LYS:HA | 3:K:439:GLN:HE21 | 1.72 | 0.54 |
| 4:L:499:GLN:HE22 | 9:L:601:ADP:H1' | 1.72 | 0.54 |
| 6:N:33:LEU:HD22 | 6:N:33:LEU:N | 2.22 | 0.54 |
| 6:N:353:LEU:N | 6:N:369:GLU:HB3 | 2.22 | 0.54 |
| 2:B:192:HIS:CD2 | 2:B:193:ILE:HG23 | 2.42 | 0.54 |
| 2:B:511:VAL:HB | 2:B:514:ILE:HD11 | 1.88 | 0.54 |
| 4:D:418:GLU:HG2 | 4:D:450:ILE:HB | 1.89 | 0.54 |
| 4:D:70:ILE:HA | 8:H:15:LYS:HZ3 | 1.72 | 0.54 |
| 6:F:171:THR:O | 6:F:175:THR:CB | 2.55 | 0.54 |
| 6:F:215:LEU:HB3 | 6:F:217:HIS:CD2 | 2.36 | 0.54 |
| 1:I:548:ASP:OD2 | 1:I:548:ASP:N | 2.37 | 0.54 |
| 2:J:505:ALA:O | 2:J:509:LEU:HB2 | 2.07 | 0.54 |
| 4:L:418:GLU:HG2 | 4:L:450:ILE:HB | 1.89 | 0.54 |
| 6:N:199:MET:O | 6:N:381:LYS:CE | 2.55 | 0.54 |
| 6:N:424:ARG:HG2 | 6:N:483:SER:CA | 2.34 | 0.54 |
| 6:N:75:LEU:HD21 | 6:N:523:ILE:HG23 | 1.89 | 0.54 |
| 7:O:294:LEU:CD2 | 7:O:315:ALA:HB3 | 2.36 | 0.54 |
| 1:A:90:GLN:NE2 | 1:A:527:SER:HB3 | 2.22 | 0.54 |
| 2:B:4:GLN:N | 2:B:5:ILE:HG12 | 2.19 | 0.54 |
| 4:D:527:SER:HB3 | 4:D:528:ARG:HH21 | 1.71 | 0.54 |
| 5:E:470:ARG:O | 5:E:474:GLN:HG3 | 2.07 | 0.54 |
| 5:E:84:THR:HG23 | 5:E:418:GLU:OE2 | 2.08 | 0.54 |
| 6:F:324:ASN:O | 6:F:328:LEU:N | 2.33 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:F:75:LEU:HD21 | 6:F:523:ILE:HG23 | 1.89 | 0.54 |
| 8:H:138:THR:HG21 | 8:H:452:PHE:HE1 | 1.72 | 0.54 |
| 2:J:326:VAL:HG13 | 3:K:304:LEU:HD22 | 1.90 | 0.54 |
| 3:K:12:GLN:NE2 | 3:K:529:GLY:HA2 | 2.21 | 0.54 |
| 6:N:501:PRO:O | 6:N:504:GLU:N | 2.39 | 0.54 |
| 7:O:420:VAL:HG23 | 7:O:446:LEU:HD13 | 1.88 | 0.54 |
| 1:A:412:THR:OG1 | 1:A:520:PRO:HG3 | 2.08 | 0.54 |
| 2:B:284:PHE:HB3 | 2:B:305:SER:HB3 | 1.89 | 0.54 |
| 2:B:289:LEU:HD13 | 2:B:294:PRO:HG3 | 1.90 | 0.54 |
| 2:B:326:VAL:CG2 | 3:C:304:LEU:HD22 | 2.37 | 0.54 |
| 4:D:196:LEU:HD22 | 4:D:377:VAL:HG22 | 1.89 | 0.54 |
| 3:C:262:GLU:H | 8:H:266:LEU:HD11 | 1.73 | 0.54 |
| 2:J:284:PHE:HB3 | 2:J:305:SER:HB3 | 1.89 | 0.54 |
| 2:J:31:ASP:OD1 | 2:J:32:LEU:N | 2.40 | 0.54 |
| 2:J:196:ILE:O | 2:J:367:ILE:HA | 2.07 | 0.54 |
| 2:J:95:VAL:HG22 | 2:J:497:VAL:HG22 | 1.89 | 0.54 |
| 4:L:28:ALA:HB1 | 4:L:78:LEU:HD11 | 1.89 | 0.54 |
| 4:L:214:VAL:HG13 | 4:L:362:ARG:HG2 | 1.89 | 0.54 |
| 5:M:173:ASP:HB3 | 5:M:437:SER:HB3 | 1.87 | 0.54 |
| 6:N:155:ARG:CB | 6:N:171:THR:HG23 | 2.38 | 0.54 |
| 7:O:397:ILE:O | 7:O:400:VAL:HG22 | 2.07 | 0.54 |
| 4:L:46:LYS:HG3 | 8:P:532:THR:HG23 | 1.89 | 0.54 |
| 1:A:44:LEU:HD21 | 1:A:103:ILE:HD12 | 1.89 | 0.54 |
| 1:A:267:PRO:HB3 | 1:A:268:GLU:C | 2.28 | 0.54 |
| 2:B:504:ALA:O | 2:B:508:LEU:HB3 | 2.07 | 0.54 |
| 6:F:33:LEU:HD22 | 6:F:33:LEU:N | 2.21 | 0.54 |
| 6:F:35:THR:HG22 | 6:F:42:THR:H | 1.72 | 0.54 |
| 7:G:115:PHE:O | 7:G:119:GLY:HA3 | 2.07 | 0.54 |
| 1:I:500:TYR:HA | 1:I:511:ASP:HA | 1.89 | 0.54 |
| 2:J:192:HIS:CD2 | 2:J:193:ILE:HG23 | 2.42 | 0.54 |
| 3:K:370:ASN:OD1 | 3:K:1054:GLY:HA2 | 2.07 | 0.54 |
| 3:K:334:ALA:HB2 | 3:K:349:GLY:N | 2.23 | 0.54 |
| 5:M:476:LEU:HD11 | 5:M:538:ILE:HD11 | 1.90 | 0.54 |
| 6:N:488:TYR:O | 6:N:489:VAL:CB | 2.56 | 0.54 |
| 7:O:34:VAL:O | 7:O:38:GLU:HG2 | 2.06 | 0.54 |
| 1:A:76:GLN:O | 1:A:77:HIS:CB | 2.55 | 0.54 |
| 2:B:455:LEU:HG | 2:B:472:LEU:HD13 | 1.90 | 0.54 |
| 3:C:241:PRO:O | 3:C:350:THR:HG23 | 2.08 | 0.54 |
| 4:D:28:ALA:HB1 | 4:D:78:LEU:HD11 | 1.89 | 0.54 |
| 7:G:397:ILE:O | 7:G:400:VAL:HG22 | 2.07 | 0.54 |
| 8:H:131:TYR:HD2 | 8:H:452:PHE:CD2 | 2.24 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:515:GLU:OE2 | 8:H:390:THR:HG22 | 2.08 | 0.54 |
| 1:I:350:PHE:HE2 | 1:I:354:TYR:CB | 2.16 | 0.54 |
| 1:I:532:LEU:HD22 | 1:I:536:VAL:HG23 | 1.90 | 0.54 |
| 2:J:27:ILE:HA | 2:J:100:ALA:HB1 | 1.88 | 0.54 |
| 6:N:406:LEU:C | 6:N:407:LYS:HE3 | 2.27 | 0.54 |
| 6:N:434:LEU:O | 6:N:438:GLY:HA2 | 2.08 | 0.54 |
| 2:J:70:ASP:HB3 | 6:N:5:LEU:HD22 | 1.87 | 0.54 |
| 7:O:440:ASN:O | 7:O:444:LYS:HD3 | 2.08 | 0.54 |
| 8:P:288:MET:HE2 | 8:P:313:LEU:HG | 1.89 | 0.54 |
| 2:B:459:LEU:CD2 | 2:B:472:LEU:HG | 2.33 | 0.54 |
| 2:B:505:ALA:O | 2:B:509:LEU:HB2 | 2.07 | 0.54 |
| 3:C:334:ALA:HB2 | 3:C:349:GLY:N | 2.23 | 0.54 |
| 4:D:273:ASN:HD22 | 7:G:268:GLN:HE22 | 1.56 | 0.54 |
| 5:E:350:GLU:O | 5:E:351:LEU:C | 2.46 | 0.54 |
| 6:F:434:LEU:O | 6:F:438:GLY:HA2 | 2.08 | 0.54 |
| 6:F:501:PRO:O | 6:F:504:GLU:N | 2.39 | 0.54 |
| 8:H:237:LYS:HB2 | 8:H:314:ASN:CB | 2.31 | 0.54 |
| 1:I:431:ILE:HG13 | 1:I:435:ASN:HD22 | 1.73 | 0.54 |
| 2:J:245:ILE:O | 2:J:246:PHE:CB | 2.56 | 0.54 |
| 2:J:445:ALA:HB2 | 2:J:455:LEU:HD23 | 1.90 | 0.54 |
| 2:J:455:LEU:HG | 2:J:472:LEU:HD13 | 1.90 | 0.54 |
| 2:J:514:ILE:CD1 | 3:K:47:MET:HB3 | 2.30 | 0.54 |
| 5:M:88:ALA:CB | 5:M:109:LYS:NZ | 2.68 | 0.54 |
| 6:N:451:LEU:O | 6:N:455:PRO:HD3 | 2.07 | 0.54 |
| 7:O:241:ILE:HG12 | 7:O:292:ILE:HG23 | 1.89 | 0.54 |
| 8:P:131:TYR:HD2 | 8:P:452:PHE:CD2 | 2.24 | 0.54 |
| 1:A:350:PHE:CD2 | 1:A:351:GLU:N | 2.72 | 0.54 |
| 2:B:213:ILE:HG23 | 2:B:354:LEU:HD23 | 1.90 | 0.54 |
| 2:B:40:LYS:HA | 6:F:116:ARG:HG3 | 1.90 | 0.54 |
| 3:C:506:LYS:O | 3:C:510:VAL:HG23 | 2.06 | 0.54 |
| 6:F:155:ARG:CB | 6:F:171:THR:HG23 | 2.38 | 0.54 |
| 6:F:236:LEU:O | 6:F:297:ASN:HA | 2.08 | 0.54 |
| 6:F:481:GLN:O | 6:F:485:GLU:HG2 | 2.07 | 0.54 |
| 7:G:206:GLY:O | 7:G:379:ARG:HD2 | 2.07 | 0.54 |
| 7:G:455:GLU:HG3 | 7:G:461:ALA:HB2 | 1.88 | 0.54 |
| 2:J:242:LYS:HE2 | 2:J:247:GLY:H | 1.69 | 0.54 |
| 2:J:359:CYS:CB | 2:J:360:LYS:HA | 2.38 | 0.54 |
| 3:K:124:ALA:HB1 | 3:K:441:PRO:CB | 2.37 | 0.54 |
| 1:I:12:THR:HB | 5:M:96:LEU:HA | 1.90 | 0.54 |
| 6:N:125:ALA:CA | 6:N:426:LEU:HD21 | 2.38 | 0.54 |
| 7:O:208:ALA:HB1 | 7:O:210:GLU:OE1 | 2.08 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:P:138:THR:HG21 | 8:P:452:PHE:HE1 | 1.72 | 0.54 |
| 2:B:359:CYS:CB | 2:B:360:LYS:HA | 2.38 | 0.54 |
| 2:B:45:LEU:HB2 | 6:F:533:LEU:CB | 2.38 | 0.54 |
| 4:D:110:LEU:CD1 | 4:D:439:ILE:HG23 | 2.38 | 0.54 |
| 6:F:488:TYR:O | 6:F:489:VAL:CB | 2.56 | 0.54 |
| 2:B:49:ALA:HB1 | 6:F:538:ARG:HB2 | 1.90 | 0.54 |
| 2:J:213:ILE:HG23 | 2:J:354:LEU:HD23 | 1.90 | 0.54 |
| 5:M:188:LEU:CB | 5:M:197:HIS:HB2 | 2.38 | 0.54 |
| 6:N:154:ALA:HB2 | 6:N:402:VAL:HG22 | 1.87 | 0.54 |
| 6:N:15:ARG:O | 6:N:18:ALA:HB3 | 2.08 | 0.54 |
| 7:O:377:LEU:H | 7:O:377:LEU:CD1 | 2.19 | 0.54 |
| 2:B:27:ILE:HA | 2:B:100:ALA:HB1 | 1.88 | 0.54 |
| 2:B:210:GLU:HB3 | 2:B:357:SER:O | 2.07 | 0.54 |
| 2:B:409:MET:CE | 2:B:409:MET:HA | 2.38 | 0.54 |
| 3:C:457:ILE:HD11 | 3:C:467:LEU:HD22 | 1.90 | 0.54 |
| 5:E:355:ALA:HB2 | 5:E:362:ILE:HD11 | 1.90 | 0.54 |
| 5:E:61:ILE:O | 5:E:61:ILE:HD13 | 2.08 | 0.54 |
| 6:F:16:ASP:O | 6:F:19:LEU:HB2 | 2.08 | 0.54 |
| 6:F:43:LEU:HD22 | 6:F:57:LYS:HB2 | 1.84 | 0.54 |
| 7:G:208:ALA:HB1 | 7:G:210:GLU:OE1 | 2.08 | 0.54 |
| 7:G:174:ASN:ND2 | 7:G:209:MET:SD | 2.80 | 0.54 |
| 7:G:492:PHE:HA | 7:G:497:TRP:NE1 | 2.21 | 0.54 |
| 8:H:252:CYS:HB2 | 8:H:343:ARG:H | 1.73 | 0.54 |
| 8:H:24:ALA:CB | 8:H:531:ALA:O | 2.56 | 0.54 |
| 1:I:458:ILE:N | 1:I:458:ILE:HD12 | 2.24 | 0.54 |
| 1:I:90:GLN:NE2 | 1:I:527:SER:HB3 | 2.22 | 0.54 |
| 2:J:289:LEU:O | 2:J:289:LEU:HD12 | 2.08 | 0.54 |
| 2:J:289:LEU:HD13 | 2:J:294:PRO:HG3 | 1.90 | 0.54 |
| 4:L:521:ILE:CG2 | 7:O:50:ASP:O | 2.55 | 0.54 |
| 1:A:184:LEU:CD2 | 1:A:184:LEU:C | 2.76 | 0.53 |
| 1:A:36:VAL:HG13 | 1:A:70:LEU:HD22 | 1.89 | 0.53 |
| 4:D:258:ARG:CD | 8:H:283:GLN:HE21 | 2.20 | 0.53 |
| 4:D:423:ARG:HH12 | 4:D:473:HIS:CD2 | 2.26 | 0.53 |
| 4:D:485:ARG:HH22 | 9:D:601:ADP:HN62 | 1.55 | 0.53 |
| 5:E:88:ALA:CB | 5:E:119:THR:HB | 2.29 | 0.53 |
| 6:F:105:ALA:C | 6:F:107:ARG:H | 2.10 | 0.53 |
| 6:F:183:ASP:OD1 | 6:F:183:ASP:N | 2.41 | 0.53 |
| 6:F:451:LEU:O | 6:F:455:PRO:HD3 | 2.07 | 0.53 |
| 7:G:377:LEU:H | 7:G:377:LEU:CD1 | 2.19 | 0.53 |
| 7:G:386:ILE:O | 7:G:389:VAL:HB | 2.07 | 0.53 |
| 7:G:75:VAL:HG11 | 7:G:80:ALA:HB1 | 1.89 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:H:213:MET:HE2 | 8:H:391:GLN:HG3 | 1.89 | 0.53 |
| 8:H:288:MET:HE2 | 8:H:313:LEU:HG | 1.90 | 0.53 |
| 8:H:354:LEU:H | 8:H:354:LEU:HD23 | 1.73 | 0.53 |
| 1:I:267:PRO:HB3 | 1:I:268:GLU:C | 2.28 | 0.53 |
| 2:J:504:ALA:O | 2:J:508:LEU:HB3 | 2.07 | 0.53 |
| 3:K:241:PRO:O | 3:K:350:THR:HG23 | 2.08 | 0.53 |
| 4:L:196:LEU:HD22 | 4:L:377:VAL:HG22 | 1.89 | 0.53 |
| 6:N:16:ASP:O | 6:N:19:LEU:HB2 | 2.08 | 0.53 |
| 6:N:481:GLN:O | 6:N:485:GLU:HG2 | 2.08 | 0.53 |
| 8:P:24:ALA:CB | 8:P:531:ALA:O | 2.56 | 0.53 |
| 1:A:20:ILE:CB | 1:A:25:ILE:HG12 | 2.38 | 0.53 |
| 2:B:196:ILE:O | 2:B:367:ILE:HA | 2.09 | 0.53 |
| 4:D:410:LEU:HD22 | 4:D:498:LEU:HB3 | 1.89 | 0.53 |
| 6:F:125:ALA:CA | 6:F:426:LEU:HD21 | 2.38 | 0.53 |
| 7:G:420:VAL:CG2 | 7:G:446:LEU:HD13 | 2.38 | 0.53 |
| 1:I:363:GLN:HA | 1:I:372:ILE:HA | 1.90 | 0.53 |
| 2:J:422:ILE:HG21 | 2:J:427:SER:CB | 2.36 | 0.53 |
| 4:L:375:VAL:HG12 | 4:L:376:SER:N | 2.22 | 0.53 |
| 4:L:196:LEU:HD22 | 4:L:377:VAL:CG2 | 2.37 | 0.53 |
| 6:N:236:LEU:O | 6:N:297:ASN:HA | 2.08 | 0.53 |
| 6:N:57:LYS:O | 6:N:57:LYS:NZ | 2.40 | 0.53 |
| 8:P:354:LEU:H | 8:P:354:LEU:HD23 | 1.74 | 0.53 |
| 2:B:39:PRO:HA | 2:B:163:SER:CA | 2.37 | 0.53 |
| 2:B:31:ASP:OD1 | 2:B:32:LEU:N | 2.40 | 0.53 |
| 2:B:198:ILE:O | 2:B:377:LEU:CD2 | 2.55 | 0.53 |
| 5:E:476:LEU:HD11 | 5:E:538:ILE:HD11 | 1.90 | 0.53 |
| 8:H:24:ALA:CB | 8:H:531:ALA:HB1 | 2.37 | 0.53 |
| 1:I:412:THR:OG1 | 1:I:520:PRO:HG3 | 2.08 | 0.53 |
| 1:I:158:ASN:CG | 1:I:516:GLY:HA2 | 2.28 | 0.53 |
| 1:I:63:THR:HG22 | 1:I:65:ASP:N | 2.22 | 0.53 |
| 1:I:94:ILE:HD11 | 1:I:526:LYS:HB2 | 1.89 | 0.53 |
| 2:J:459:LEU:CD2 | 2:J:472:LEU:HG | 2.33 | 0.53 |
| 6:N:406:LEU:HB3 | 6:N:407:LYS:NZ | 2.24 | 0.53 |
| 7:O:75:VAL:HG11 | 7:O:80:ALA:HB1 | 1.89 | 0.53 |
| 8:P:428:ILE:HD13 | 8:P:478:LEU:HD13 | 1.89 | 0.53 |
| 5:E:81:ILE:HG22 | 5:E:414:MET:HE1 | 1.89 | 0.53 |
| 2:J:229:ALA:HB3 | 2:J:339:GLU:O | 2.07 | 0.53 |
| 2:J:49:ALA:HB2 | 6:N:536:ALA:O | 2.08 | 0.53 |
| 3:K:457:ILE:HD11 | 3:K:467:LEU:HD22 | 1.90 | 0.53 |
| 4:L:110:LEU:CD1 | 4:L:439:ILE:HG23 | 2.38 | 0.53 |
| 6:F:117:ILE:CG1 | 5:M:33:LYS:HE2 | 2.34 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:M:350:GLU:O | 5:M:351:LEU:C | 2.46 | 0.53 |
| 5:M:84:THR:HG23 | 5:M:418:GLU:OE2 | 2.08 | 0.53 |
| 8:P:229:ASN:HA | 8:P:368:VAL:HG22 | 1.90 | 0.53 |
| 8:P:420:LEU:HD23 | 8:P:421:PRO:N | 2.24 | 0.53 |
| 1:A:431:ILE:HG13 | 1:A:435:ASN:HD22 | 1.73 | 0.53 |
| 1:A:532:LEU:HD22 | 1:A:536:VAL:HG23 | 1.90 | 0.53 |
| 2:B:124:TYR:O | 2:B:128:SER:HB2 | 2.08 | 0.53 |
| 2:B:319:LEU:CD2 | 2:B:357:SER:OG | 2.57 | 0.53 |
| 2:B:127:ALA:CB | 2:B:430:VAL:HG22 | 2.31 | 0.53 |
| 3:C:432:LYS:HA | 3:C:439:GLN:HE21 | 1.72 | 0.53 |
| 6:F:35:THR:HG21 | 6:F:42:THR:O | 2.08 | 0.53 |
| 2:B:201:GLY:N | 6:F:86:ILE:HD12 | 2.21 | 0.53 |
| 7:G:225:SER:HB3 | 7:G:314:CYS:O | 2.09 | 0.53 |
| 7:G:201:ILE:HG21 | 7:G:390:GLU:HG3 | 1.90 | 0.53 |
| 8:H:420:LEU:HD23 | 8:H:421:PRO:N | 2.24 | 0.53 |
| 4:L:491:ASN:HB2 | 4:L:494:GLU:OE1 | 2.09 | 0.53 |
| 5:M:471:GLY:HA2 | 5:M:474:GLN:OE1 | 2.08 | 0.53 |
| 5:M:93:GLN:NE2 | 5:M:93:GLN:HA | 2.23 | 0.53 |
| 6:N:183:ASP:N | 6:N:183:ASP:OD1 | 2.41 | 0.53 |
| 7:O:206:GLY:O | 7:O:379:ARG:HD2 | 2.07 | 0.53 |
| 1:A:158:ASN:CG | 1:A:516:GLY:HA2 | 2.28 | 0.53 |
| 1:A:63:THR:HG22 | 1:A:65:ASP:N | 2.22 | 0.53 |
| 4:D:77:MET:CE | 7:G:384:GLN:HB2 | 2.39 | 0.53 |
| 6:F:105:ALA:HA | 6:F:108:PHE:CD2 | 2.44 | 0.53 |
| 6:F:36:ASN:HA | 6:F:57:LYS:CD | 2.38 | 0.53 |
| 6:F:416:GLY:HA2 | 6:F:419:TYR:CD2 | 2.44 | 0.53 |
| 6:F:437:LYS:HE2 | 6:F:437:LYS:CA | 2.33 | 0.53 |
| 8:H:27:GLN:O | 8:H:31:SER:N | 2.33 | 0.53 |
| 1:I:20:ILE:CB | 1:I:25:ILE:HG12 | 2.38 | 0.53 |
| 2:J:124:TYR:O | 2:J:128:SER:HB2 | 2.08 | 0.53 |
| 2:J:30:GLY:CA | 2:J:33:VAL:CG2 | 2.86 | 0.53 |
| 3:K:422:ALA:HA | 3:K:475:HIS:CE1 | 2.44 | 0.53 |
| 4:L:423:ARG:HH12 | 4:L:473:HIS:CD2 | 2.26 | 0.53 |
| 4:L:36:ARG:HE | 4:L:98:ILE:CG2 | 2.18 | 0.53 |
| 7:O:191:ARG:HB3 | 7:O:193:ASP:O | 2.08 | 0.53 |
| 3:C:269:TRP:HH2 | 6:F:248:ASN:H | 1.56 | 0.53 |
| 5:E:100:ILE:O | 5:E:103:LEU:HB2 | 2.08 | 0.53 |
| 5:E:58:ALA:CB | 5:E:127:SER:HB3 | 2.39 | 0.53 |
| 6:F:45:MET:HA | 6:F:55:LEU:HA | 1.91 | 0.53 |
| 1:I:44:LEU:HD21 | 1:I:103:ILE:HD12 | 1.89 | 0.53 |
| 2:J:45:LEU:HD12 | 6:N:533:LEU:HD13 | 1.91 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:K:413:SER:HB3 | 3:K:419:THR:HG21 | 1.91 | 0.53 |
| 4:L:249:GLU:O | 7:O:259:VAL:HG12 | 2.09 | 0.53 |
| 5:M:227:GLN:O | 5:M:407:PHE:HA | 2.09 | 0.53 |
| 5:M:350:GLU:C | 5:M:352:GLU:H | 2.11 | 0.53 |
| 5:M:58:ALA:CB | 5:M:127:SER:HB3 | 2.39 | 0.53 |
| 6:N:105:ALA:HA | 6:N:108:PHE:CD2 | 2.44 | 0.53 |
| 6:N:143:LEU:HD11 | 6:N:145:ASN:CG | 2.29 | 0.53 |
| 2:J:43:ASP:O | 6:N:530:CYS:HA | 2.09 | 0.53 |
| 2:B:376:THR:HA | 2:B:379:GLU:HB2 | 1.91 | 0.53 |
| 5:E:188:LEU:CB | 5:E:197:HIS:HB2 | 2.38 | 0.53 |
| 5:E:273:THR:CG2 | 5:E:364:PRO:CA | 2.72 | 0.53 |
| 6:F:15:ARG:O | 6:F:18:ALA:HB3 | 2.08 | 0.53 |
| 6:F:5:LEU:CA | 6:F:6:LEU:HB2 | 2.34 | 0.53 |
| 1:I:498:ARG:O | 1:I:499:ASN:CB | 2.56 | 0.53 |
| 5:M:81:ILE:HG22 | 5:M:414:MET:HE1 | 1.91 | 0.53 |
| 6:N:76:ILE:CG2 | 6:N:95:VAL:HG13 | 2.39 | 0.53 |
| 7:O:201:ILE:HG21 | 7:O:390:GLU:HG3 | 1.90 | 0.53 |
| 8:P:243:LYS:C | 8:P:244:LYS:CG | 2.77 | 0.53 |
| 1:A:363:GLN:HA | 1:A:372:ILE:HA | 1.90 | 0.53 |
| 2:B:91:GLY:HA2 | 9:B:601:ADP:PA | 2.48 | 0.53 |
| 4:D:263:ILE:HD13 | 4:D:263:ILE:O | 2.09 | 0.53 |
| 4:D:524:ILE:HG23 | 7:G:52:LEU:HD22 | 1.91 | 0.53 |
| 5:E:58:ALA:HB3 | 5:E:127:SER:HB3 | 1.91 | 0.53 |
| 8:H:237:LYS:HB3 | 8:H:314:ASN:HB3 | 1.63 | 0.53 |
| 1:I:184:LEU:CD2 | 1:I:184:LEU:C | 2.76 | 0.53 |
| 2:J:409:MET:CE | 2:J:409:MET:HA | 2.38 | 0.53 |
| 2:J:39:PRO:HD2 | 2:J:474:LEU:HD12 | 1.91 | 0.53 |
| 6:N:171:THR:N | 6:N:172:PRO:CD | 2.71 | 0.53 |
| 6:N:324:ASN:O | 6:N:328:LEU:N | 2.33 | 0.53 |
| 6:N:35:THR:HG21 | 6:N:42:THR:O | 2.08 | 0.53 |
| 8:P:67:ASP:HB3 | 8:P:70:THR:OG1 | 2.08 | 0.53 |
| 2:B:289:LEU:HD12 | 2:B:289:LEU:O | 2.08 | 0.53 |
| 3:C:422:ALA:HA | 3:C:475:HIS:CE1 | 2.44 | 0.53 |
| 4:D:491:ASN:HB2 | 4:D:494:GLU:OE1 | 2.09 | 0.53 |
| 6:F:167:THR:HB | 6:F:169:VAL:H | 1.66 | 0.53 |
| 6:F:171:THR:N | 6:F:172:PRO:CD | 2.71 | 0.53 |
| 6:F:195:GLU:CG | 6:F:197:MET:SD | 2.94 | 0.53 |
| 3:C:269:TRP:CZ3 | 6:F:247:VAL:HB | 2.44 | 0.53 |
| 6:F:345:PRO:O | 6:F:347:ILE:HG13 | 2.09 | 0.53 |
| 7:G:43:THR:HB | 7:G:99:THR:CG2 | 2.40 | 0.53 |
| 1:I:541:ILE:HD13 | 5:M:73:ILE:HG13 | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:544:MET:HG2 | 1:I:546:THR:HG23 | 1.90 | 0.53 |
| 2:J:164:LYS:O | 2:J:165:ILE:C | 2.48 | 0.53 |
| 5:M:61:ILE:O | 5:M:61:ILE:HD13 | 2.08 | 0.53 |
| 6:N:276:LYS:O | 6:N:279:ASP:N | 2.42 | 0.53 |
| 6:N:345:PRO:O | 6:N:347:ILE:HG13 | 2.09 | 0.53 |
| 9:N:601:ADP:C8 | 9:N:601:ADP:O2' | 2.62 | 0.53 |
| 1:A:544:MET:HG2 | 1:A:546:THR:HG23 | 1.90 | 0.52 |
| 2:B:39:PRO:HD2 | 2:B:474:LEU:HD12 | 1.91 | 0.52 |
| 4:D:195:ARG:O | 4:D:196:LEU:HD23 | 2.10 | 0.52 |
| 5:E:471:GLY:HA2 | 5:E:474:GLN:OE1 | 2.08 | 0.52 |
| 7:G:307:PHE:CD1 | 7:G:312:ILE:HG23 | 2.44 | 0.52 |
| 8:H:146:VAL:C | 8:H:148:GLY:H | 2.10 | 0.52 |
| 2:J:64:LEU:HD23 | 2:J:67:ILE:HD12 | 1.91 | 0.52 |
| 2:J:263:LYS:HZ1 | 3:K:266:GLU:HB3 | 1.66 | 0.52 |
| 5:M:310:ILE:HD11 | 5:M:331:ALA:HB1 | 1.91 | 0.52 |
| 7:O:225:SER:HB3 | 7:O:314:CYS:O | 2.09 | 0.52 |
| 7:O:377:LEU:O | 7:O:377:LEU:HD22 | 2.09 | 0.52 |
| 8:P:252:CYS:HB2 | 8:P:343:ARG:H | 1.73 | 0.52 |
| 1:A:498:ARG:O | 1:A:499:ASN:CB | 2.57 | 0.52 |
| 2:B:102:LEU:HD21 | 2:B:124:TYR:HD2 | 1.75 | 0.52 |
| 2:B:445:ALA:HB2 | 2:B:455:LEU:HD23 | 1.90 | 0.52 |
| 5:E:48:LYS:O | 5:E:51:ILE:HG22 | 2.09 | 0.52 |
| 6:F:352:GLY:CA | 6:F:369:GLU:C | 2.48 | 0.52 |
| 7:G:241:ILE:HG12 | 7:G:292:ILE:HG23 | 1.89 | 0.52 |
| 8:H:243:LYS:C | 8:H:244:LYS:CG | 2.77 | 0.52 |
| 8:H:328:GLU:HG3 | 8:H:331:ARG:HH12 | 1.72 | 0.52 |
| 1:I:501:GLY:HA3 | 1:I:512:GLU:CG | 2.39 | 0.52 |
| 2:J:106:ALA:HB1 | 2:J:509:LEU:HD11 | 1.91 | 0.52 |
| 4:L:310:ILE:HG22 | 4:L:312:VAL:HG23 | 1.92 | 0.52 |
| 5:M:100:ILE:O | 5:M:103:LEU:HB2 | 2.08 | 0.52 |
| 6:N:105:ALA:C | 6:N:107:ARG:H | 2.10 | 0.52 |
| 6:N:167:THR:OG1 | 6:N:169:VAL:HB | 2.09 | 0.52 |
| 6:N:231:ALA:O | 6:N:351:SER:OG | 2.22 | 0.52 |
| 6:N:45:MET:HA | 6:N:55:LEU:HA | 1.91 | 0.52 |
| 8:P:423:ALA:HA | 9:P:601:ADP:H2' | 1.90 | 0.52 |
| 2:B:88:VAL:HG13 | 2:B:393:GLN:NE2 | 2.21 | 0.52 |
| 5:E:498:LEU:HD11 | 5:E:512:VAL:HG23 | 1.91 | 0.52 |
| 5:E:74:LEU:HG | 5:E:93:GLN:CB | 2.39 | 0.52 |
| 5:E:84:THR:HG22 | 5:E:86:ASP:N | 2.19 | 0.52 |
| 7:G:66:GLY:HA2 | 7:G:69:ILE:HG22 | 1.92 | 0.52 |
| 8:H:428:ILE:HD13 | 8:H:478:LEU:HD13 | 1.90 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:36:VAL:HG13 | 1:I:70:LEU:HD22 | 1.89 | 0.52 |
| 4:L:241:ILE:HD13 | 4:L:292:ILE:HG23 | 1.92 | 0.52 |
| 6:N:129:SER:HB2 | 6:N:426:LEU:HD23 | 1.91 | 0.52 |
| 7:O:420:VAL:CG2 | 7:O:446:LEU:HD13 | 2.38 | 0.52 |
| 1:A:458:ILE:HD12 | 1:A:458:ILE:N | 2.24 | 0.52 |
| 2:B:407:ALA:O | 2:B:411:MET:HG2 | 2.10 | 0.52 |
| 4:D:198:LYS:H | 4:D:198:LYS:HD3 | 1.74 | 0.52 |
| 6:F:129:SER:HB2 | 6:F:426:LEU:HD23 | 1.91 | 0.52 |
| 6:F:406:LEU:HB3 | 6:F:407:LYS:NZ | 2.24 | 0.52 |
| 6:F:76:ILE:CG2 | 6:F:95:VAL:HG13 | 2.39 | 0.52 |
| 2:J:102:LEU:O | 2:J:105:GLU:HB2 | 2.10 | 0.52 |
| 2:J:514:ILE:HG22 | 2:J:515:ILE:N | 2.24 | 0.52 |
| 3:K:320:VAL:CG1 | 3:K:324:ASP:HB3 | 2.40 | 0.52 |
| 5:M:355:ALA:HB2 | 5:M:362:ILE:HD11 | 1.90 | 0.52 |
| 5:M:498:LEU:HD11 | 5:M:512:VAL:HG23 | 1.91 | 0.52 |
| 6:N:171:THR:O | 6:N:175:THR:OG1 | 2.24 | 0.52 |
| 5:M:544:LEU:HD23 | 6:N:384:THR:CG2 | 2.40 | 0.52 |
| 4:L:69:ALA:O | 8:P:15:LYS:HE2 | 2.09 | 0.52 |
| 8:P:463:LEU:HD11 | 9:P:601:ADP:H8 | 1.73 | 0.52 |
| 2:B:102:LEU:HD21 | 2:B:124:TYR:CD2 | 2.45 | 0.52 |
| 5:E:166:ASP:N | 5:E:167:ASP:CB | 2.66 | 0.52 |
| 5:E:186:THR:HG23 | 5:E:187:SER:N | 2.24 | 0.52 |
| 6:F:143:LEU:HD11 | 6:F:145:ASN:CG | 2.29 | 0.52 |
| 7:G:516:LEU:HD13 | 7:G:517:ILE:H | 1.75 | 0.52 |
| 8:H:160:LEU:HA | 8:H:163:ILE:HG22 | 1.92 | 0.52 |
| 8:H:54:ILE:HG13 | 8:H:64:ILE:CG1 | 2.15 | 0.52 |
| 2:J:102:LEU:HD21 | 2:J:124:TYR:CD2 | 2.45 | 0.52 |
| 2:J:245:ILE:O | 2:J:246:PHE:CG | 2.62 | 0.52 |
| 2:J:319:LEU:CD2 | 2:J:357:SER:OG | 2.57 | 0.52 |
| 5:M:48:LYS:O | 5:M:51:ILE:HG22 | 2.09 | 0.52 |
| 5:M:58:ALA:HB3 | 5:M:127:SER:HB3 | 1.91 | 0.52 |
| 7:O:91:ASP:O | 7:O:95:GLY:CA | 2.57 | 0.52 |
| 8:P:138:THR:HG21 | 8:P:452:PHE:CE1 | 2.45 | 0.52 |
| 8:P:160:LEU:HA | 8:P:163:ILE:HG22 | 1.92 | 0.52 |
| 2:B:295:GLU:HB2 | 6:F:337:GLN:CD | 2.29 | 0.52 |
| 2:B:106:ALA:HB1 | 2:B:509:LEU:HD11 | 1.91 | 0.52 |
| 3:C:320:VAL:CG1 | 3:C:324:ASP:HB3 | 2.40 | 0.52 |
| 3:C:413:SER:HB3 | 3:C:419:THR:HG21 | 1.91 | 0.52 |
| 3:C:341:GLU:OE1 | 8:H:281:GLU:OE1 | 2.28 | 0.52 |
| 4:L:195:ARG:O | 4:L:196:LEU:HD23 | 2.10 | 0.52 |
| 4:L:263:ILE:O | 4:L:263:ILE:HD13 | 2.09 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:L:85:GLN:NE2 | 4:L:507:ALA:HB2 | 2.25 | 0.52 |
| 5:E:37:ASN:HD22 | 6:N:114:HIS:CD2 | 2.27 | 0.52 |
| 6:N:436:ALA:HA | 6:N:437:LYS:HE2 | 1.92 | 0.52 |
| 2:B:153:LEU:HB3 | 2:B:178:THR:HG22 | 1.92 | 0.52 |
| 2:B:245:ILE:O | 2:B:246:PHE:CB | 2.56 | 0.52 |
| 2:B:30:GLY:CA | 2:B:33:VAL:CG2 | 2.86 | 0.52 |
| 3:C:320:VAL:O | 3:C:321:LYS:O | 2.28 | 0.52 |
| 4:D:219:ALA:HB1 | 4:D:221:LYS:HZ3 | 1.74 | 0.52 |
| 4:D:292:ILE:HG13 | 4:D:293:LEU:CA | 2.40 | 0.52 |
| 4:D:135:LEU:HD11 | 4:D:411:ILE:HD11 | 1.92 | 0.52 |
| 4:D:94:THR:O | 4:D:98:ILE:HG12 | 2.10 | 0.52 |
| 7:G:243:SER:HB2 | 7:G:334:ILE:HD13 | 1.92 | 0.52 |
| 7:G:91:ASP:O | 7:G:95:GLY:CA | 2.57 | 0.52 |
| 8:H:229:ASN:HA | 8:H:368:VAL:HG22 | 1.91 | 0.52 |
| 1:I:226:CYS:SG | 1:I:318:VAL:HG12 | 2.50 | 0.52 |
| 2:J:102:LEU:HD21 | 2:J:124:TYR:HD2 | 1.74 | 0.52 |
| 2:J:376:THR:HA | 2:J:379:GLU:HB2 | 1.91 | 0.52 |
| 2:J:159:THR:HG21 | 2:J:488:VAL:N | 2.25 | 0.52 |
| 3:K:60:ASP:OD1 | 3:K:93:THR:HG21 | 2.10 | 0.52 |
| 7:O:307:PHE:CD1 | 7:O:312:ILE:HG23 | 2.44 | 0.52 |
| 1:A:147:SER:OG | 1:A:418:VAL:HB | 2.10 | 0.52 |
| 1:A:344:LEU:CD1 | 1:A:345:GLU:H | 2.23 | 0.52 |
| 2:B:245:ILE:O | 2:B:246:PHE:CG | 2.62 | 0.52 |
| 2:B:64:LEU:HD23 | 2:B:67:ILE:HD12 | 1.91 | 0.52 |
| 2:B:68:PRO:HG2 | 6:F:536:ALA:HB2 | 1.92 | 0.52 |
| 4:D:178:VAL:CG1 | 4:D:401:ILE:HD11 | 2.40 | 0.52 |
| 4:D:85:GLN:NE2 | 4:D:507:ALA:HB2 | 2.25 | 0.52 |
| 6:F:16:ASP:CA | 6:F:19:LEU:HD12 | 2.28 | 0.52 |
| 6:F:420:ILE:CB | 6:F:482:ASP:OD1 | 2.58 | 0.52 |
| 6:F:515:ASN:ND2 | 6:F:516:ALA:N | 2.58 | 0.52 |
| 7:G:156:GLU:OE1 | 7:G:157:LEU:HB2 | 2.10 | 0.52 |
| 7:G:303:ALA:O | 7:G:307:PHE:HD2 | 1.93 | 0.52 |
| 8:H:138:THR:HG21 | 8:H:452:PHE:CE1 | 2.45 | 0.52 |
| 2:J:231:ILE:HD13 | 2:J:282:ASN:HB2 | 1.92 | 0.52 |
| 2:J:407:ALA:O | 2:J:411:MET:HG2 | 2.10 | 0.52 |
| 2:J:256:ALA:HB1 | 3:K:266:GLU:OE2 | 2.10 | 0.52 |
| 4:L:449:VAL:O | 4:L:453:THR:HG23 | 2.10 | 0.52 |
| 5:M:74:LEU:HG | 5:M:93:GLN:CB | 2.39 | 0.52 |
| 5:M:88:ALA:HB1 | 5:M:109:LYS:HZ2 | 1.72 | 0.52 |
| 6:N:420:ILE:CB | 6:N:482:ASP:OD1 | 2.58 | 0.52 |
| 1:A:501:GLY:HA3 | 1:A:512:GLU:CG | 2.39 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:102:LEU:O | 2:B:105:GLU:HB2 | 2.10 | 0.52 |
| 2:B:514:ILE:HG22 | 2:B:515:ILE:N | 2.24 | 0.52 |
| 3:C:165:ILE:HA | 3:C:168:SER:HB3 | 1.91 | 0.52 |
| 4:D:241:ILE:HD13 | 4:D:292:ILE:HG23 | 1.91 | 0.52 |
| 5:E:450:MET:HE3 | 5:E:454:VAL:HG23 | 1.92 | 0.52 |
| 6:F:137:LYS:O | 6:F:138:ILE:HB | 2.10 | 0.52 |
| 6:F:353:LEU:O | 6:F:367:VAL:HG12 | 2.09 | 0.52 |
| 6:F:57:LYS:O | 6:F:57:LYS:NZ | 2.40 | 0.52 |
| 7:G:424:LEU:O | 7:G:427:TYR:N | 2.43 | 0.52 |
| 2:J:141:ASP:CG | 2:J:142:ASN:H | 2.13 | 0.52 |
| 2:J:371:GLY:O | 2:J:372:ALA:C | 2.49 | 0.52 |
| 4:L:292:ILE:HG13 | 4:L:293:LEU:CA | 2.40 | 0.52 |
| 4:L:521:ILE:CD1 | 7:O:62:ILE:HD12 | 2.36 | 0.52 |
| 4:L:20:VAL:HG13 | 4:L:524:ILE:HD12 | 1.92 | 0.52 |
| 6:N:143:LEU:CD1 | 6:N:145:ASN:OD1 | 2.58 | 0.52 |
| 6:N:193:MET:HE2 | 6:N:330:LEU:HD11 | 1.92 | 0.52 |
| 6:N:342:ASP:O | 6:N:345:PRO:HD3 | 2.10 | 0.52 |
| 6:N:367:VAL:HG12 | 6:N:369:GLU:O | 2.10 | 0.52 |
| 6:N:36:ASN:HA | 6:N:57:LYS:CD | 2.38 | 0.52 |
| 6:N:488:TYR:O | 6:N:489:VAL:HB | 2.10 | 0.52 |
| 7:O:243:SER:HB2 | 7:O:334:ILE:HD13 | 1.92 | 0.52 |
| 7:O:303:ALA:O | 7:O:307:PHE:HD2 | 1.92 | 0.52 |
| 1:A:345:GLU:CD | 1:A:346:GLY:HA2 | 2.30 | 0.52 |
| 2:B:159:THR:HG21 | 2:B:488:VAL:N | 2.25 | 0.52 |
| 4:D:419:ILE:O | 4:D:423:ARG:HG3 | 2.09 | 0.52 |
| 5:E:93:GLN:NE2 | 5:E:93:GLN:HA | 2.23 | 0.52 |
| 6:F:143:LEU:HD13 | 6:F:145:ASN:CB | 2.40 | 0.52 |
| 8:H:243:LYS:HB3 | 8:H:244:LYS:CE | 2.40 | 0.52 |
| 8:H:67:ASP:HB3 | 8:H:70:THR:OG1 | 2.08 | 0.52 |
| 1:I:345:GLU:CD | 1:I:346:GLY:HA2 | 2.30 | 0.52 |
| 2:J:198:ILE:O | 2:J:377:LEU:CD2 | 2.55 | 0.52 |
| 4:L:419:ILE:O | 4:L:423:ARG:HG3 | 2.10 | 0.52 |
| 4:L:94:THR:O | 4:L:98:ILE:HG12 | 2.10 | 0.52 |
| 5:M:450:MET:HE3 | 5:M:454:VAL:HG23 | 1.92 | 0.52 |
| 6:N:416:GLY:HA2 | 6:N:419:TYR:CD2 | 2.44 | 0.52 |
| 7:O:516:LEU:HD13 | 7:O:517:ILE:H | 1.75 | 0.52 |
| 3:C:491:ILE:H | 3:C:491:ILE:HD13 | 1.75 | 0.51 |
| 3:C:104:LEU:CD1 | 3:C:520:LEU:HD12 | 2.39 | 0.51 |
| 4:D:310:ILE:HG22 | 4:D:312:VAL:HG23 | 1.91 | 0.51 |
| 5:E:509:ASN:O | 5:E:521:ASP:HA | 2.09 | 0.51 |
| 1:A:549:PRO:HA | 5:E:77:PRO:O | 2.10 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:F:143:LEU:CD1 | 6:F:145:ASN:OD1 | 2.58 | 0.51 |
| 6:F:167:THR:OG1 | 6:F:169:VAL:HB | 2.09 | 0.51 |
| 6:F:276:LYS:O | 6:F:279:ASP:N | 2.43 | 0.51 |
| 6:F:488:TYR:O | 6:F:489:VAL:HG12 | 2.10 | 0.51 |
| 6:F:92:THR:OG1 | 9:F:601:ADP:O2B | 2.28 | 0.51 |
| 7:G:377:LEU:O | 7:G:377:LEU:HD22 | 2.09 | 0.51 |
| 4:L:226:PRO:CB | 4:L:311:MET:HG2 | 2.40 | 0.51 |
| 6:N:201:HIS:HB3 | 6:N:381:LYS:HZ3 | 1.74 | 0.51 |
| 2:J:250:PHE:CA | 6:N:250:GLY:O | 2.56 | 0.51 |
| 6:N:406:LEU:HD22 | 6:N:407:LYS:HZ1 | 1.75 | 0.51 |
| 2:J:45:LEU:HB2 | 6:N:533:LEU:HB2 | 1.92 | 0.51 |
| 8:P:463:LEU:CD1 | 9:P:601:ADP:H8 | 2.23 | 0.51 |
| 2:B:141:ASP:CG | 2:B:142:ASN:H | 2.13 | 0.51 |
| 2:B:319:LEU:HD11 | 2:B:355:LYS:O | 2.10 | 0.51 |
| 4:D:226:PRO:CB | 4:D:311:MET:HG2 | 2.40 | 0.51 |
| 5:E:197:HIS:O | 5:E:200:PHE:N | 2.44 | 0.51 |
| 5:E:310:ILE:HD11 | 5:E:331:ALA:HB1 | 1.91 | 0.51 |
| 5:E:431:ARG:O | 5:E:434:VAL:HG12 | 2.10 | 0.51 |
| 6:F:356:GLN:CB | 6:F:365:THR:HG22 | 2.40 | 0.51 |
| 6:F:485:GLU:O | 6:F:486:THR:C | 2.48 | 0.51 |
| 6:F:488:TYR:O | 6:F:489:VAL:HB | 2.10 | 0.51 |
| 2:B:43:ASP:OD1 | 6:F:529:LEU:HD22 | 2.11 | 0.51 |
| 2:J:153:LEU:HB3 | 2:J:178:THR:HG22 | 1.92 | 0.51 |
| 7:O:225:SER:O | 7:O:226:TYR:HB3 | 2.10 | 0.51 |
| 7:O:242:LEU:HB2 | 7:O:293:VAL:HG12 | 1.93 | 0.51 |
| 3:C:38:CYS:HA | 3:C:44:MET:H | 1.75 | 0.51 |
| 5:E:197:HIS:O | 5:E:198:ASP:C | 2.49 | 0.51 |
| 6:F:39:PRO:HA | 6:F:160:THR:CB | 2.40 | 0.51 |
| 6:F:342:ASP:O | 6:F:345:PRO:HD3 | 2.10 | 0.51 |
| 4:D:192:ASN:HB2 | 7:G:361:ARG:HH21 | 1.76 | 0.51 |
| 3:K:250:LEU:HD23 | 3:K:250:LEU:N | 2.26 | 0.51 |
| 3:K:49:LEU:HD21 | 3:K:55:LEU:HD23 | 1.92 | 0.51 |
| 4:L:147:ARG:HG2 | 4:L:148:GLU:H | 1.74 | 0.51 |
| 5:M:431:ARG:O | 5:M:434:VAL:HG12 | 2.10 | 0.51 |
| 6:N:138:ILE:O | 6:N:138:ILE:CG2 | 2.58 | 0.51 |
| 6:N:356:GLN:CB | 6:N:365:THR:HG22 | 2.40 | 0.51 |
| 6:N:92:THR:HG23 | 10:N:602:BEF:F3 | 2.00 | 0.51 |
| 7:O:413:GLY:CA | 7:O:491:ASN:HD21 | 2.22 | 0.51 |
| 8:P:304:GLY:N | 8:P:323:VAL:HG11 | 2.26 | 0.51 |
| 2:B:164:LYS:O | 2:B:165:ILE:C | 2.48 | 0.51 |
| 2:B:242:LYS:HE2 | 2:B:247:GLY:H | 1.69 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:8:ASN:C | 4:D:10:THR:H | 2.14 | 0.51 |
| 5:E:76:SER:HB2 | 5:E:79:GLY:H | 1.75 | 0.51 |
| 6:F:129:SER:O | 6:F:422:LEU:HD23 | 2.10 | 0.51 |
| 7:G:418:MET:HE3 | 7:G:447:GLU:HG2 | 1.93 | 0.51 |
| 8:H:163:ILE:CG2 | 8:H:179:SER:HB2 | 2.40 | 0.51 |
| 2:J:88:VAL:HG13 | 2:J:393:GLN:NE2 | 2.21 | 0.51 |
| 3:K:165:ILE:HA | 3:K:168:SER:HB3 | 1.91 | 0.51 |
| 5:M:186:THR:HG23 | 5:M:187:SER:N | 2.24 | 0.51 |
| 5:M:197:HIS:O | 5:M:198:ASP:C | 2.49 | 0.51 |
| 5:M:76:SER:HB2 | 5:M:79:GLY:H | 1.75 | 0.51 |
| 6:N:488:TYR:O | 6:N:489:VAL:HG12 | 2.10 | 0.51 |
| 4:D:147:ARG:HG2 | 4:D:148:GLU:H | 1.74 | 0.51 |
| 4:D:390:THR:O | 4:D:394:LEU:HD23 | 2.10 | 0.51 |
| 5:E:341:PRO:O | 5:E:343:VAL:HG23 | 2.11 | 0.51 |
| 1:A:12:THR:HB | 5:E:96:LEU:HA | 1.91 | 0.51 |
| 6:F:143:LEU:HD13 | 6:F:145:ASN:OD1 | 2.10 | 0.51 |
| 6:F:92:THR:OG1 | 9:F:601:ADP:O3B | 2.28 | 0.51 |
| 7:G:242:LEU:HB2 | 7:G:293:VAL:HG12 | 1.92 | 0.51 |
| 8:H:452:PHE:CE1 | 8:H:456:PHE:HE2 | 2.28 | 0.51 |
| 2:J:319:LEU:HD11 | 2:J:355:LYS:O | 2.10 | 0.51 |
| 2:J:93:THR:HG21 | 9:J:601:ADP:O3B | 2.10 | 0.51 |
| 5:M:166:ASP:N | 5:M:167:ASP:CB | 2.66 | 0.51 |
| 5:M:197:HIS:O | 5:M:200:PHE:N | 2.44 | 0.51 |
| 6:N:424:ARG:HD3 | 6:N:483:SER:OG | 2.11 | 0.51 |
| 8:P:31:SER:O | 8:P:35:ILE:HG12 | 2.11 | 0.51 |
| 1:A:258:MET:HE3 | 1:A:258:MET:HA | 1.93 | 0.51 |
| 2:B:402:LEU:CD1 | 2:B:483:ARG:HE | 2.24 | 0.51 |
| 3:C:153:LYS:HD3 | 3:C:500:TRP:CD1 | 2.46 | 0.51 |
| 4:D:298:ASN:CB | 4:D:299:ASP:HA | 2.37 | 0.51 |
| 6:F:354:VAL:HA | 6:F:367:VAL:HA | 1.93 | 0.51 |
| 7:G:126:MET:CE | 7:G:126:MET:HA | 2.40 | 0.51 |
| 7:G:126:MET:HA | 7:G:126:MET:HE2 | 1.92 | 0.51 |
| 7:G:225:SER:O | 7:G:226:TYR:HB3 | 2.10 | 0.51 |
| 1:I:350:PHE:CD2 | 1:I:351:GLU:N | 2.72 | 0.51 |
| 2:J:46:LEU:HD11 | 2:J:63:ILE:HA | 1.93 | 0.51 |
| 3:K:320:VAL:O | 3:K:321:LYS:O | 2.28 | 0.51 |
| 3:K:47:MET:HE2 | 3:K:49:LEU:HD21 | 1.93 | 0.51 |
| 3:K:104:LEU:CD1 | 3:K:520:LEU:HD12 | 2.39 | 0.51 |
| 6:F:114:HIS:HA | 5:M:37:ASN:HB2 | 1.92 | 0.51 |
| 5:M:509:ASN:O | 5:M:521:ASP:HA | 2.09 | 0.51 |
| 6:N:143:LEU:HD13 | 6:N:145:ASN:CB | 2.40 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:N:209:PHE:HB2 | 6:N:378:ILE:CB | 2.40 | 0.51 |
| 6:N:56:THR:OG1 | 6:N:61:VAL:HG11 | 2.10 | 0.51 |
| 8:P:15:LYS:HE3 | 8:P:16:GLN:N | 2.26 | 0.51 |
| 8:P:163:ILE:CG2 | 8:P:179:SER:HB2 | 2.40 | 0.51 |
| 8:P:243:LYS:HB3 | 8:P:244:LYS:CE | 2.41 | 0.51 |
| 1:A:226:CYS:SG | 1:A:318:VAL:HG12 | 2.50 | 0.51 |
| 2:B:371:GLY:O | 2:B:372:ALA:C | 2.49 | 0.51 |
| 2:B:442:THR:HG23 | 2:B:452:SER:CB | 2.34 | 0.51 |
| 4:D:449:VAL:O | 4:D:453:THR:HG23 | 2.10 | 0.51 |
| 5:E:227:GLN:O | 5:E:407:PHE:HA | 2.09 | 0.51 |
| 5:E:55:ARG:NH2 | 5:E:134:LEU:HD13 | 2.26 | 0.51 |
| 7:G:292:ILE:HA | 7:G:313:PHE:O | 2.10 | 0.51 |
| 3:K:38:CYS:HA | 3:K:44:MET:H | 1.75 | 0.51 |
| 5:M:506:LYS:C | 5:M:507:ILE:HD12 | 2.31 | 0.51 |
| 6:N:167:THR:HG22 | 6:N:168:GLU:HB3 | 1.93 | 0.51 |
| 6:N:151:LEU:CD2 | 6:N:175:THR:HG23 | 2.41 | 0.51 |
| 7:O:126:MET:CE | 7:O:126:MET:HA | 2.40 | 0.51 |
| 7:O:156:GLU:OE1 | 7:O:157:LEU:HB2 | 2.10 | 0.51 |
| 7:O:459:PHE:HB3 | 7:O:460:ASP:HB3 | 1.93 | 0.51 |
| 8:P:250:PHE:CE2 | 8:P:299:ILE:HD12 | 2.45 | 0.51 |
| 3:C:109:PRO:O | 3:C:113:GLU:HG2 | 2.11 | 0.51 |
| 3:C:60:ASP:OD1 | 3:C:93:THR:HG21 | 2.10 | 0.51 |
| 4:D:221:LYS:HE2 | 4:D:225:GLY:CA | 2.41 | 0.51 |
| 6:F:167:THR:HG22 | 6:F:168:GLU:HB3 | 1.93 | 0.51 |
| 6:F:436:ALA:HA | 6:F:437:LYS:HE2 | 1.92 | 0.51 |
| 2:B:375:GLN:HE22 | 6:F:75:LEU:HB2 | 1.75 | 0.51 |
| 3:C:335:THR:CB | 8:H:237:LYS:HE2 | 2.30 | 0.51 |
| 1:I:147:SER:OG | 1:I:418:VAL:HB | 2.10 | 0.51 |
| 3:K:266:GLU:CD | 3:K:266:GLU:N | 2.64 | 0.51 |
| 3:K:491:ILE:H | 3:K:491:ILE:HD13 | 1.75 | 0.51 |
| 6:N:143:LEU:HD13 | 6:N:145:ASN:OD1 | 2.10 | 0.51 |
| 6:N:39:PRO:HA | 6:N:160:THR:CB | 2.41 | 0.51 |
| 6:N:230:ASN:H | 6:N:353:LEU:HD23 | 1.76 | 0.51 |
| 6:N:354:VAL:HA | 6:N:367:VAL:HA | 1.93 | 0.51 |
| 6:N:437:LYS:CA | 6:N:437:LYS:HE2 | 2.33 | 0.51 |
| 6:N:515:ASN:ND2 | 6:N:516:ALA:N | 2.58 | 0.51 |
| 5:E:483:LEU:HD11 | 9:E:601:ADP:H1' | 1.92 | 0.51 |
| 6:F:367:VAL:HG12 | 6:F:369:GLU:O | 2.10 | 0.51 |
| 8:H:304:GLY:N | 8:H:323:VAL:HG11 | 2.26 | 0.51 |
| 1:I:221:GLY:HA3 | 1:I:374:ILE:O | 2.11 | 0.51 |
| 1:I:225:ASN:HD22 | 1:I:225:ASN:C | 2.13 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:104:ILE:HG12 | 1:I:458:ILE:HD11 | 1.93 | 0.51 |
| 2:J:422:ILE:HG22 | 2:J:424:GLY:H | 1.75 | 0.51 |
| 3:K:109:PRO:O | 3:K:113:GLU:HG2 | 2.11 | 0.51 |
| 3:K:153:LYS:HD3 | 3:K:500:TRP:CD1 | 2.46 | 0.51 |
| 4:L:8:ASN:C | 4:L:10:THR:H | 2.14 | 0.51 |
| 5:M:45:GLU:C | 5:M:47:LYS:H | 2.14 | 0.51 |
| 6:N:129:SER:O | 6:N:422:LEU:HD23 | 2.10 | 0.51 |
| 6:N:16:ASP:CA | 6:N:19:LEU:HD12 | 2.28 | 0.51 |
| 6:N:484:ASP:OD1 | 6:N:484:ASP:N | 2.44 | 0.51 |
| 8:P:29:ILE:O | 8:P:32:ILE:HG22 | 2.11 | 0.51 |
| 1:A:159:ILE:HD12 | 1:A:412:THR:HG21 | 1.93 | 0.51 |
| 1:A:351:GLU:O | 1:A:353:SER:N | 2.44 | 0.51 |
| 6:F:151:LEU:CD2 | 6:F:175:THR:HG23 | 2.41 | 0.51 |
| 6:F:230:ASN:H | 6:F:353:LEU:HD23 | 1.76 | 0.51 |
| 3:C:269:TRP:HZ3 | 6:F:247:VAL:HB | 1.76 | 0.51 |
| 4:L:390:THR:O | 4:L:394:LEU:HD23 | 2.10 | 0.51 |
| 4:L:450:ILE:HB | 4:L:451:PRO:HD3 | 1.93 | 0.51 |
| 5:M:513:ASP:OD2 | 5:M:525:LEU:HD13 | 2.11 | 0.51 |
| 5:M:90:ILE:O | 5:M:94:MET:HG2 | 2.11 | 0.51 |
| 7:O:292:ILE:HA | 7:O:313:PHE:O | 2.10 | 0.51 |
| 7:O:62:ILE:O | 7:O:63:SER:HB3 | 2.11 | 0.51 |
| 2:B:46:LEU:HD11 | 2:B:63:ILE:HA | 1.93 | 0.50 |
| 3:C:266:GLU:CD | 3:C:266:GLU:N | 2.64 | 0.50 |
| 3:C:242:ARG:CB | 3:C:292:PRO:HA | 2.42 | 0.50 |
| 6:F:424:ARG:HD3 | 6:F:483:SER:OG | 2.11 | 0.50 |
| 6:F:433:LYS:O | 6:F:436:ALA:O | 2.30 | 0.50 |
| 6:F:56:THR:OG1 | 6:F:61:VAL:HG11 | 2.10 | 0.50 |
| 6:F:90:GLY:O | 6:F:94:VAL:CG2 | 2.34 | 0.50 |
| 2:J:242:LYS:HE3 | 2:J:247:GLY:N | 2.25 | 0.50 |
| 2:J:271:ASN:ND2 | 2:J:328:THR:OG1 | 2.44 | 0.50 |
| 2:J:46:LEU:HD11 | 2:J:63:ILE:HD12 | 1.93 | 0.50 |
| 4:L:198:LYS:HD3 | 4:L:198:LYS:H | 1.74 | 0.50 |
| 4:L:229:LYS:CB | 4:L:232:ALA:HB2 | 2.42 | 0.50 |
| 4:L:135:LEU:HD11 | 4:L:411:ILE:HD11 | 1.92 | 0.50 |
| 6:N:433:LYS:O | 6:N:436:ALA:O | 2.30 | 0.50 |
| 7:O:115:PHE:CD1 | 7:O:437:MET:HB3 | 2.46 | 0.50 |
| 7:O:66:GLY:HA2 | 7:O:69:ILE:HG22 | 1.92 | 0.50 |
| 8:P:452:PHE:CE1 | 8:P:456:PHE:HE2 | 2.28 | 0.50 |
| 1:A:225:ASN:HD22 | 1:A:225:ASN:C | 2.14 | 0.50 |
| 4:D:30:SER:O | 4:D:33:ASP:HB2 | 2.11 | 0.50 |
| 4:D:20:VAL:HG13 | 4:D:524:ILE:HD12 | 1.92 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:E:513:ASP:OD2 | 5:E:525:LEU:HD13 | 2.11 | 0.50 |
| 6:F:484:ASP:N | 6:F:484:ASP:OD1 | 2.44 | 0.50 |
| 8:H:226:MET:HA | 8:H:383:THR:OG1 | 2.11 | 0.50 |
| 1:I:351:GLU:O | 1:I:353:SER:N | 2.44 | 0.50 |
| 2:J:3:VAL:HB | 2:J:4:GLN:OE1 | 2.12 | 0.50 |
| 3:K:242:ARG:CB | 3:K:292:PRO:HA | 2.42 | 0.50 |
| 5:M:341:PRO:O | 5:M:343:VAL:HG23 | 2.11 | 0.50 |
| 6:N:137:LYS:O | 6:N:138:ILE:HB | 2.10 | 0.50 |
| 6:N:353:LEU:O | 6:N:367:VAL:HG12 | 2.09 | 0.50 |
| 6:N:485:GLU:O | 6:N:486:THR:C | 2.48 | 0.50 |
| 2:B:34:LYS:O | 2:B:37:LEU:HG | 2.12 | 0.50 |
| 2:B:490:SER:HB2 | 2:B:492:LYS:NZ | 2.26 | 0.50 |
| 4:D:115:ILE:HG21 | 4:D:439:ILE:HG13 | 1.94 | 0.50 |
| 4:L:386:ILE:C | 4:L:388:ASP:H | 2.15 | 0.50 |
| 4:L:418:GLU:HG3 | 4:L:447:LEU:O | 2.11 | 0.50 |
| 5:M:88:ALA:CB | 5:M:119:THR:HB | 2.29 | 0.50 |
| 6:N:440:THR:O | 6:N:444:ILE:HG12 | 2.12 | 0.50 |
| 5:M:556:ILE:HG23 | 6:N:47:VAL:HB | 1.93 | 0.50 |
| 7:O:346:LEU:HD23 | 7:O:346:LEU:H | 1.76 | 0.50 |
| 8:P:287:MET:O | 8:P:291:ILE:HG12 | 2.12 | 0.50 |
| 8:P:31:SER:CB | 8:P:79:HIS:HE1 | 2.24 | 0.50 |
| 1:A:221:GLY:HA3 | 1:A:374:ILE:O | 2.11 | 0.50 |
| 2:B:367:ILE:HG23 | 2:B:367:ILE:O | 2.11 | 0.50 |
| 2:B:3:VAL:HB | 2:B:4:GLN:OE1 | 2.12 | 0.50 |
| 5:E:273:THR:O | 5:E:274:CYS:CB | 2.59 | 0.50 |
| 6:F:541:LEU:HB3 | 6:F:543:GLU:N | 2.26 | 0.50 |
| 8:H:49:CYS:O | 8:H:466:THR:CB | 2.57 | 0.50 |
| 1:I:379:LYS:N | 1:I:379:LYS:HD2 | 2.26 | 0.50 |
| 3:K:170:LYS:C | 3:K:170:LYS:HD3 | 2.32 | 0.50 |
| 3:K:465:ILE:HD12 | 3:K:465:ILE:N | 2.26 | 0.50 |
| 3:K:475:HIS:O | 3:K:478:GLY:O | 2.28 | 0.50 |
| 4:L:198:LYS:HD3 | 4:L:198:LYS:N | 2.27 | 0.50 |
| 5:M:131:ASP:O | 5:M:134:LEU:HB3 | 2.12 | 0.50 |
| 5:M:364:PRO:O | 5:M:365:ARG:CB | 2.59 | 0.50 |
| 6:N:538:ARG:NH1 | 6:N:538:ARG:CG | 2.72 | 0.50 |
| 7:O:171:ILE:O | 7:O:171:ILE:HG22 | 2.12 | 0.50 |
| 1:A:161:LYS:HA | 1:A:164:MET:HG2 | 1.93 | 0.50 |
| 1:A:379:LYS:HD2 | 1:A:379:LYS:N | 2.26 | 0.50 |
| 1:A:147:SER:HB3 | 1:A:418:VAL:O | 2.11 | 0.50 |
| 2:B:292:ASP:HA | 2:B:295:GLU:CD | 2.32 | 0.50 |
| 3:C:475:HIS:O | 3:C:478:GLY:O | 2.28 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:450:ILE:HB | 4:D:451:PRO:HD3 | 1.93 | 0.50 |
| 5:E:210:ASN:N | 5:E:210:ASN:HD22 | 2.08 | 0.50 |
| 5:E:364:PRO:O | 5:E:365:ARG:CB | 2.59 | 0.50 |
| 5:E:171:SER:HA | 5:E:438:ARG:HA | 1.93 | 0.50 |
| 5:E:506:LYS:C | 5:E:507:ILE:HD12 | 2.31 | 0.50 |
| 6:F:440:THR:O | 6:F:444:ILE:HG12 | 2.12 | 0.50 |
| 1:I:159:ILE:HD12 | 1:I:412:THR:HG21 | 1.93 | 0.50 |
| 1:I:147:SER:HB3 | 1:I:418:VAL:O | 2.11 | 0.50 |
| 4:L:430:ARG:O | 4:L:431:SER:C | 2.50 | 0.50 |
| 5:M:55:ARG:NH2 | 5:M:134:LEU:HD13 | 2.26 | 0.50 |
| 6:N:124:ILE:HB | 6:N:444:ILE:HD12 | 1.94 | 0.50 |
| 6:N:167:THR:HA | 6:N:168:GLU:CB | 2.40 | 0.50 |
| 6:N:489:VAL:O | 6:N:489:VAL:HG13 | 2.11 | 0.50 |
| 2:B:271:ASN:ND2 | 2:B:328:THR:OG1 | 2.44 | 0.50 |
| 2:B:46:LEU:HD11 | 2:B:63:ILE:HD12 | 1.93 | 0.50 |
| 2:B:3:VAL:C | 2:B:5:ILE:HG12 | 2.32 | 0.50 |
| 3:C:250:LEU:N | 3:C:250:LEU:HD23 | 2.26 | 0.50 |
| 3:C:465:ILE:N | 3:C:465:ILE:HD12 | 2.26 | 0.50 |
| 6:F:209:PHE:HB2 | 6:F:378:ILE:CB | 2.40 | 0.50 |
| 7:G:459:PHE:HB3 | 7:G:460:ASP:HB3 | 1.93 | 0.50 |
| 7:G:455:GLU:CG | 7:G:461:ALA:HB3 | 2.42 | 0.50 |
| 1:I:129:PHE:HB3 | 1:I:532:LEU:HD21 | 1.93 | 0.50 |
| 2:J:422:ILE:O | 2:J:423:ASP:OD2 | 2.30 | 0.50 |
| 2:J:464:TYR:HA | 2:J:467:ILE:CD1 | 2.42 | 0.50 |
| 4:L:178:VAL:CG1 | 4:L:401:ILE:HD11 | 2.40 | 0.50 |
| 6:N:436:ALA:HA | 6:N:437:LYS:CE | 2.42 | 0.50 |
| 2:B:422:ILE:O | 2:B:423:ASP:OD2 | 2.30 | 0.50 |
| 2:B:507:VAL:HG13 | 3:C:57:LEU:HD12 | 1.94 | 0.50 |
| 3:C:49:LEU:HD21 | 3:C:55:LEU:HD23 | 1.93 | 0.50 |
| 4:D:60:ASP:HB3 | 4:D:63:THR:OG1 | 2.12 | 0.50 |
| 5:E:90:ILE:O | 5:E:94:MET:HG2 | 2.11 | 0.50 |
| 6:F:167:THR:HA | 6:F:168:GLU:CB | 2.40 | 0.50 |
| 6:F:387:ALA:O | 6:F:391:THR:HG23 | 2.12 | 0.50 |
| 6:F:411:ILE:CG2 | 6:F:412:ILE:H | 2.16 | 0.50 |
| 7:G:191:ARG:NH1 | 7:G:192:ASN:HB2 | 2.27 | 0.50 |
| 8:H:31:SER:CB | 8:H:79:HIS:HE1 | 2.25 | 0.50 |
| 8:H:31:SER:O | 8:H:35:ILE:HG12 | 2.11 | 0.50 |
| 8:H:79:HIS:ND1 | 8:H:81:ALA:HB3 | 2.27 | 0.50 |
| 1:I:344:LEU:CD1 | 1:I:345:GLU:H | 2.23 | 0.50 |
| 5:M:535:LYS:O | 5:M:539:LEU:HG | 2.11 | 0.50 |
| 6:N:193:MET:HB3 | 6:N:330:LEU:HD12 | 1.94 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:N:409:LYS:HD3 | 6:N:409:LYS:N | 2.16 | 0.50 |
| 6:N:430:ASN:O | 6:N:433:LYS:CA | 2.60 | 0.50 |
| 1:A:104:ILE:HG12 | 1:A:458:ILE:HD11 | 1.93 | 0.50 |
| 2:B:131:ALA:HB2 | 2:B:415:VAL:CG2 | 2.42 | 0.50 |
| 2:B:231:ILE:HD13 | 2:B:282:ASN:HB2 | 1.92 | 0.50 |
| 2:B:423:ASP:O | 2:B:423:ASP:OD1 | 2.30 | 0.50 |
| 3:C:170:LYS:HD3 | 3:C:170:LYS:C | 2.32 | 0.50 |
| 6:F:436:ALA:HA | 6:F:437:LYS:CE | 2.42 | 0.50 |
| 6:F:489:VAL:O | 6:F:489:VAL:HG13 | 2.11 | 0.50 |
| 7:G:193:ASP:OD1 | 7:G:193:ASP:O | 2.30 | 0.50 |
| 7:G:115:PHE:CD1 | 7:G:437:MET:HB3 | 2.46 | 0.50 |
| 7:G:75:VAL:O | 7:G:81:LYS:HE3 | 2.12 | 0.50 |
| 8:H:259:THR:HG21 | 8:H:263:GLY:HA3 | 1.94 | 0.50 |
| 8:H:29:ILE:O | 8:H:32:ILE:HG22 | 2.11 | 0.50 |
| 2:J:490:SER:HB2 | 2:J:492:LYS:NZ | 2.26 | 0.50 |
| 4:L:115:ILE:HG21 | 4:L:439:ILE:HG13 | 1.94 | 0.50 |
| 4:L:30:SER:O | 4:L:33:ASP:HB2 | 2.11 | 0.50 |
| 6:N:387:ALA:O | 6:N:391:THR:HG23 | 2.12 | 0.50 |
| 7:O:193:ASP:O | 7:O:193:ASP:OD1 | 2.30 | 0.50 |
| 7:O:23:LYS:HA | 7:O:26:ILE:HG22 | 1.93 | 0.50 |
| 2:B:236:THR:HA | 2:B:287:ARG:HD2 | 1.94 | 0.50 |
| 2:B:464:TYR:HA | 2:B:467:ILE:CD1 | 2.42 | 0.50 |
| 4:D:229:LYS:CB | 4:D:232:ALA:HB2 | 2.42 | 0.50 |
| 4:D:430:ARG:O | 4:D:431:SER:C | 2.50 | 0.50 |
| 4:D:418:GLU:HG3 | 4:D:447:LEU:O | 2.11 | 0.50 |
| 5:E:45:GLU:C | 5:E:47:LYS:H | 2.14 | 0.50 |
| 7:G:23:LYS:HA | 7:G:26:ILE:HG22 | 1.93 | 0.50 |
| 7:G:483:PHE:CB | 9:G:601:ADP:N6 | 2.74 | 0.50 |
| 8:H:15:LYS:HE3 | 8:H:16:GLN:N | 2.26 | 0.50 |
| 1:I:92:ARG:HB3 | 5:M:388:THR:HA | 1.93 | 0.50 |
| 2:J:235:ASN:ND2 | 3:K:304:LEU:HD21 | 2.27 | 0.50 |
| 3:K:29:LYS:O | 3:K:33:ASP:HB2 | 2.12 | 0.50 |
| 4:L:195:ARG:O | 4:L:376:SER:HA | 2.12 | 0.50 |
| 5:M:264:SER:O | 5:M:266:GLY:O | 2.30 | 0.50 |
| 5:M:509:ASN:HB3 | 5:M:521:ASP:CB | 2.36 | 0.50 |
| 6:N:195:GLU:OE1 | 6:N:197:MET:HE2 | 2.11 | 0.50 |
| 6:N:232:TYR:HA | 6:N:351:SER:OG | 2.12 | 0.50 |
| 7:O:57:ASN:O | 7:O:58:GLN:NE2 | 2.45 | 0.50 |
| 8:P:83:LYS:O | 8:P:87:MET:HG2 | 2.12 | 0.50 |
| 2:B:164:LYS:O | 2:B:167:SER:N | 2.40 | 0.49 |
| 4:D:198:LYS:N | 4:D:198:LYS:HD3 | 2.27 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:F:406:LEU:O | 6:F:406:LEU:HD23 | 2.12 | 0.49 |
| 7:G:117:GLU:H | 7:G:117:GLU:CD | 2.15 | 0.49 |
| 1:I:77:HIS:CG | 1:I:78:PRO:HD2 | 2.47 | 0.49 |
| 2:J:242:LYS:HE2 | 2:J:247:GLY:N | 2.26 | 0.49 |
| 2:J:34:LYS:O | 2:J:37:LEU:HG | 2.12 | 0.49 |
| 2:J:195:ILE:HG21 | 2:J:381:GLU:HB2 | 1.93 | 0.49 |
| 4:L:221:LYS:HE2 | 4:L:225:GLY:CA | 2.41 | 0.49 |
| 5:M:132:GLN:HA | 5:M:132:GLN:HE21 | 1.77 | 0.49 |
| 7:O:214:PHE:CD1 | 7:O:376:LEU:HB3 | 2.46 | 0.49 |
| 7:O:36:VAL:HG22 | 7:O:83:LEU:HD13 | 1.93 | 0.49 |
| 7:O:75:VAL:O | 7:O:81:LYS:HE3 | 2.12 | 0.49 |
| 8:P:226:MET:HA | 8:P:383:THR:OG1 | 2.11 | 0.49 |
| 1:A:129:PHE:HB3 | 1:A:532:LEU:HD21 | 1.93 | 0.49 |
| 2:B:4:GLN:O | 3:C:72:HIS:CB | 2.60 | 0.49 |
| 2:B:60:GLY:H | 2:B:93:THR:CG2 | 2.25 | 0.49 |
| 3:C:29:LYS:O | 3:C:33:ASP:HB2 | 2.12 | 0.49 |
| 5:E:509:ASN:HB3 | 5:E:521:ASP:CB | 2.36 | 0.49 |
| 6:F:23:VAL:HG22 | 6:F:102:LEU:CD1 | 2.42 | 0.49 |
| 6:F:171:THR:O | 6:F:175:THR:OG1 | 2.24 | 0.49 |
| 6:F:2:SER:C | 6:F:3:LEU:HD22 | 2.32 | 0.49 |
| 7:G:346:LEU:HD23 | 7:G:346:LEU:H | 1.76 | 0.49 |
| 8:H:83:LYS:O | 8:H:87:MET:HG2 | 2.12 | 0.49 |
| 5:M:325:TRP:CG | 5:M:326:GLY:N | 2.80 | 0.49 |
| 6:N:215:LEU:HB3 | 6:N:217:HIS:CD2 | 2.36 | 0.49 |
| 6:N:406:LEU:HD23 | 6:N:406:LEU:O | 2.12 | 0.49 |
| 6:N:491:VAL:HG12 | 6:N:492:ASP:N | 2.27 | 0.49 |
| 7:O:117:GLU:H | 7:O:117:GLU:CD | 2.15 | 0.49 |
| 8:P:259:THR:HG21 | 8:P:263:GLY:HA3 | 1.94 | 0.49 |
| 8:P:72:LEU:HA | 8:P:75:LEU:HB2 | 1.94 | 0.49 |
| 3:C:124:ALA:HB2 | 3:C:438:GLN:HE22 | 1.77 | 0.49 |
| 6:F:43:LEU:CD2 | 6:F:161:LYS:HA | 2.40 | 0.49 |
| 6:F:193:MET:HB3 | 6:F:330:LEU:HD12 | 1.94 | 0.49 |
| 6:F:213:LEU:HD23 | 6:F:377:THR:CG2 | 2.40 | 0.49 |
| 7:G:236:PHE:O | 7:G:351:LEU:HA | 2.12 | 0.49 |
| 8:H:287:MET:O | 8:H:291:ILE:HG12 | 2.12 | 0.49 |
| 8:H:249:VAL:HG13 | 8:H:300:VAL:O | 2.13 | 0.49 |
| 2:J:131:ALA:HB2 | 2:J:415:VAL:CG2 | 2.42 | 0.49 |
| 2:J:236:THR:HA | 2:J:287:ARG:HD2 | 1.94 | 0.49 |
| 2:J:42:MET:HB3 | 6:N:531:ASP:HB2 | 1.95 | 0.49 |
| 3:K:124:ALA:HB2 | 3:K:438:GLN:HE22 | 1.77 | 0.49 |
| 6:N:154:ALA:O | 6:N:157:SER:CB | 2.60 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:N:229:LYS:C | 6:N:231:ALA:H | 2.16 | 0.49 |
| 5:M:364:PRO:HG3 | 6:N:307:ASP:CB | 2.41 | 0.49 |
| 8:P:301:ALA:O | 8:P:323:VAL:HA | 2.11 | 0.49 |
| 1:A:77:HIS:CG | 1:A:78:PRO:HD2 | 2.47 | 0.49 |
| 1:A:8:SER:N | 2:J:21:SER:OG | 2.43 | 0.49 |
| 2:B:160:THR:HG21 | 2:B:390:VAL:HG21 | 1.94 | 0.49 |
| 2:B:195:ILE:HG21 | 2:B:381:GLU:HB2 | 1.93 | 0.49 |
| 6:F:121:GLY:O | 6:F:444:ILE:HD13 | 2.12 | 0.49 |
| 6:F:124:ILE:HB | 6:F:444:ILE:HD12 | 1.94 | 0.49 |
| 6:F:71:PRO:HG2 | 6:F:533:LEU:HD12 | 1.94 | 0.49 |
| 7:G:214:PHE:CD1 | 7:G:376:LEU:HB3 | 2.46 | 0.49 |
| 8:H:301:ALA:O | 8:H:323:VAL:HA | 2.11 | 0.49 |
| 1:I:161:LYS:HA | 1:I:164:MET:HG2 | 1.93 | 0.49 |
| 2:J:170:LYS:NZ | 2:J:170:LYS:HB2 | 2.28 | 0.49 |
| 3:K:16:THR:HA | 3:K:525:ASP:HB3 | 1.95 | 0.49 |
| 4:L:246:PRO:HB2 | 4:L:250:ASN:CG | 2.33 | 0.49 |
| 5:M:273:THR:O | 5:M:274:CYS:CB | 2.59 | 0.49 |
| 7:O:304:THR:HA | 7:O:307:PHE:CE2 | 2.46 | 0.49 |
| 7:O:470:LEU:O | 7:O:473:SER:OG | 2.29 | 0.49 |
| 8:P:249:VAL:HG13 | 8:P:300:VAL:O | 2.12 | 0.49 |
| 2:B:242:LYS:HE3 | 2:B:247:GLY:N | 2.25 | 0.49 |
| 2:B:274:ALA:HB1 | 2:B:329:PHE:HA | 1.94 | 0.49 |
| 2:B:409:MET:HA | 2:B:409:MET:HE1 | 1.93 | 0.49 |
| 3:C:103:ILE:HD12 | 3:C:445:VAL:HG22 | 1.95 | 0.49 |
| 5:E:131:ASP:O | 5:E:134:LEU:HB3 | 2.12 | 0.49 |
| 5:E:350:GLU:C | 5:E:352:GLU:H | 2.11 | 0.49 |
| 5:E:535:LYS:O | 5:E:539:LEU:HG | 2.11 | 0.49 |
| 5:E:84:THR:CG2 | 5:E:86:ASP:H | 2.20 | 0.49 |
| 6:F:280:LEU:N | 6:F:280:LEU:HD23 | 2.27 | 0.49 |
| 6:F:446:ALA:HA | 6:F:449:GLU:HG3 | 1.95 | 0.49 |
| 7:G:36:VAL:HG22 | 7:G:83:LEU:HD13 | 1.93 | 0.49 |
| 2:J:423:ASP:OD1 | 2:J:423:ASP:O | 2.30 | 0.49 |
| 5:M:171:SER:HA | 5:M:438:ARG:HA | 1.93 | 0.49 |
| 6:N:446:ALA:HA | 6:N:449:GLU:HG3 | 1.95 | 0.49 |
| 1:A:433:LEU:O | 1:A:437:ALA:CB | 2.61 | 0.49 |
| 5:E:132:GLN:HE21 | 5:E:132:GLN:HA | 1.77 | 0.49 |
| 6:F:154:ALA:O | 6:F:157:SER:CB | 2.60 | 0.49 |
| 6:F:430:ASN:O | 6:F:433:LYS:CA | 2.60 | 0.49 |
| 7:G:317:ARG:O | 7:G:317:ARG:CD | 2.61 | 0.49 |
| 8:H:250:PHE:CE2 | 8:H:299:ILE:HD12 | 2.45 | 0.49 |
| 8:H:482:HIS:C | 8:H:484:VAL:N | 2.65 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:45:GLY:C | 1:I:166:SER:HB2 | 2.33 | 0.49 |
| 1:I:433:LEU:O | 1:I:437:ALA:CB | 2.61 | 0.49 |
| 1:I:501:GLY:HA3 | 1:I:512:GLU:HG2 | 1.95 | 0.49 |
| 2:J:502:SER:HA | 2:J:505:ALA:HB3 | 1.94 | 0.49 |
| 6:N:2:SER:C | 6:N:3:LEU:HD22 | 2.32 | 0.49 |
| 6:N:458:LEU:HD12 | 6:N:458:LEU:C | 2.33 | 0.49 |
| 7:O:191:ARG:NH1 | 7:O:192:ASN:HB2 | 2.27 | 0.49 |
| 7:O:236:PHE:O | 7:O:351:LEU:HA | 2.12 | 0.49 |
| 8:P:79:HIS:ND1 | 8:P:81:ALA:HB3 | 2.27 | 0.49 |
| 1:A:96:ASP:OD1 | 9:A:601:ADP:O1B | 2.31 | 0.49 |
| 2:B:4:GLN:C | 2:B:5:ILE:CG2 | 2.73 | 0.49 |
| 3:C:229:VAL:HG11 | 3:C:234:MET:HE2 | 1.95 | 0.49 |
| 3:C:430:LYS:O | 3:C:433:GLN:CG | 2.57 | 0.49 |
| 5:E:264:SER:O | 5:E:266:GLY:O | 2.30 | 0.49 |
| 6:F:237:ASN:HA | 6:F:297:ASN:OD1 | 2.13 | 0.49 |
| 6:F:61:VAL:O | 6:F:65:GLU:HB2 | 2.13 | 0.49 |
| 8:H:29:ILE:HG22 | 8:H:30:LYS:N | 2.28 | 0.49 |
| 2:J:183:ARG:O | 2:J:184:LEU:CB | 2.60 | 0.49 |
| 2:J:5:ILE:HD12 | 2:J:7:GLY:H | 1.78 | 0.49 |
| 2:J:72:PRO:HB3 | 3:K:47:MET:HE3 | 1.95 | 0.49 |
| 6:N:23:VAL:HG22 | 6:N:102:LEU:CD1 | 2.42 | 0.49 |
| 8:P:463:LEU:HD11 | 9:P:601:ADP:C8 | 2.48 | 0.49 |
| 4:D:46:LYS:HG3 | 8:H:532:THR:CG2 | 2.40 | 0.49 |
| 5:E:148:ASN:HA | 5:E:151:ASP:HB2 | 1.95 | 0.49 |
| 6:F:232:TYR:HA | 6:F:351:SER:OG | 2.12 | 0.49 |
| 7:G:516:LEU:HD22 | 7:G:517:ILE:CA | 2.42 | 0.49 |
| 2:J:292:ASP:HA | 2:J:295:GLU:CD | 2.32 | 0.49 |
| 2:J:3:VAL:C | 2:J:5:ILE:HG12 | 2.32 | 0.49 |
| 3:K:103:ILE:HD12 | 3:K:445:VAL:HG22 | 1.95 | 0.49 |
| 1:I:12:THR:CG2 | 5:M:97:ASP:H | 2.18 | 0.49 |
| 7:O:455:GLU:CG | 7:O:461:ALA:HB3 | 2.42 | 0.49 |
| 8:P:79:HIS:CE1 | 8:P:81:ALA:HB3 | 2.48 | 0.49 |
| 2:B:183:ARG:O | 2:B:184:LEU:CB | 2.60 | 0.49 |
| 2:B:464:TYR:HA | 2:B:467:ILE:HD11 | 1.94 | 0.49 |
| 4:D:195:ARG:O | 4:D:376:SER:HA | 2.12 | 0.49 |
| 5:E:157:ALA:HA | 5:E:450:MET:HE1 | 1.95 | 0.49 |
| 5:E:558:GLY:HA2 | 6:F:48:ASP:HB2 | 1.94 | 0.49 |
| 6:F:117:ILE:HD12 | 5:M:34:ASP:C | 2.33 | 0.49 |
| 6:F:138:ILE:CG2 | 6:F:138:ILE:O | 2.58 | 0.49 |
| 6:F:199:MET:O | 6:F:381:LYS:HE2 | 2.13 | 0.49 |
| 2:B:32:LEU:HD11 | 6:F:532:GLU:CD | 2.33 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:32:LEU:HG | 6:F:532:GLU:CD | 2.33 | 0.49 |
| 7:G:143:LEU:HD22 | 7:G:411:ALA:HB2 | 1.94 | 0.49 |
| 7:G:44:LEU:C | 7:G:46:PRO:HD2 | 2.33 | 0.49 |
| 7:G:57:ASN:O | 7:G:58:GLN:NE2 | 2.45 | 0.49 |
| 7:G:43:THR:HG21 | 7:G:64:ASN:O | 2.13 | 0.49 |
| 8:H:163:ILE:HG23 | 8:H:179:SER:CB | 2.42 | 0.49 |
| 8:H:356:GLU:HB2 | 8:H:374:GLU:HA | 1.95 | 0.49 |
| 1:I:13:LEU:HD22 | 1:I:14:PHE:H | 1.78 | 0.49 |
| 2:J:160:THR:HG21 | 2:J:390:VAL:HG21 | 1.94 | 0.49 |
| 2:J:427:SER:O | 2:J:430:VAL:HB | 2.12 | 0.49 |
| 4:L:209:MET:HE3 | 4:L:375:VAL:HG11 | 1.95 | 0.49 |
| 4:L:77:MET:HE1 | 7:O:384:GLN:HB2 | 1.94 | 0.49 |
| 6:N:355:TYR:O | 6:N:366:TYR:O | 2.31 | 0.49 |
| 6:N:405:VAL:HG22 | 6:N:509:SER:HB2 | 1.94 | 0.49 |
| 7:O:29:ASN:OD1 | 7:O:79:ALA:HB2 | 2.12 | 0.49 |
| 7:O:317:ARG:CD | 7:O:317:ARG:O | 2.61 | 0.49 |
| 1:A:116:VAL:HG12 | 1:A:120:ILE:HG22 | 1.95 | 0.49 |
| 2:B:170:LYS:HB2 | 2:B:170:LYS:NZ | 2.28 | 0.49 |
| 2:B:233:ILE:O | 2:B:325:VAL:N | 2.46 | 0.49 |
| 2:B:382:ARG:HH11 | 2:B:382:ARG:HG3 | 1.78 | 0.49 |
| 3:C:409:SER:C | 3:C:411:SER:H | 2.17 | 0.49 |
| 4:D:135:LEU:CD1 | 4:D:411:ILE:HD11 | 2.43 | 0.49 |
| 6:F:16:ASP:N | 6:F:16:ASP:OD1 | 2.36 | 0.49 |
| 7:G:127:LYS:C | 7:G:127:LYS:HD3 | 2.34 | 0.49 |
| 7:G:413:GLY:CA | 7:G:491:ASN:HD21 | 2.22 | 0.49 |
| 1:I:132:ALA:HB2 | 1:I:448:ILE:HD13 | 1.94 | 0.49 |
| 2:J:459:LEU:HD13 | 2:J:472:LEU:CD2 | 2.43 | 0.49 |
| 3:K:430:LYS:O | 3:K:433:GLN:CG | 2.57 | 0.49 |
| 5:M:148:ASN:HA | 5:M:151:ASP:HB2 | 1.95 | 0.49 |
| 6:N:121:GLY:O | 6:N:444:ILE:HD13 | 2.12 | 0.49 |
| 7:O:127:LYS:HD3 | 7:O:127:LYS:C | 2.34 | 0.49 |
| 7:O:44:LEU:C | 7:O:46:PRO:HD2 | 2.33 | 0.49 |
| 7:O:44:LEU:HB2 | 7:O:456:ASN:ND2 | 2.28 | 0.49 |
| 8:P:49:CYS:O | 8:P:466:THR:CB | 2.57 | 0.49 |
| 1:A:121:HIS:CE1 | 5:E:68:ARG:HG3 | 2.48 | 0.48 |
| 1:A:132:ALA:HB2 | 1:A:448:ILE:HD13 | 1.94 | 0.48 |
| 1:A:14:PHE:CB | 1:A:15:LEU:HA | 2.43 | 0.48 |
| 4:D:254:VAL:CG2 | 4:D:254:VAL:O | 2.61 | 0.48 |
| 7:G:62:ILE:O | 7:G:63:SER:HB3 | 2.11 | 0.48 |
| 1:I:164:MET:CE | 1:I:169:ILE:HB | 2.43 | 0.48 |
| 2:J:263:LYS:NZ | 3:K:266:GLU:CG | 2.76 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:464:TYR:HA | 2:J:467:ILE:HD11 | 1.94 | 0.48 |
| 2:J:514:ILE:HG22 | 2:J:515:ILE:H | 1.78 | 0.48 |
| 2:J:60:GLY:H | 2:J:93:THR:CG2 | 2.25 | 0.48 |
| 3:K:41:PRO:CA | 3:K:161:THR:HG21 | 2.43 | 0.48 |
| 4:L:135:LEU:CD1 | 4:L:411:ILE:HD11 | 2.43 | 0.48 |
| 4:L:204:ILE:O | 4:L:207:THR:HG23 | 2.13 | 0.48 |
| 4:L:325:SER:O | 4:L:329:GLY:N | 2.46 | 0.48 |
| 5:M:157:ALA:HA | 5:M:450:MET:HE1 | 1.95 | 0.48 |
| 8:P:334:ARG:HD3 | 8:P:380:ARG:HH11 | 1.78 | 0.48 |
| 1:A:10:SER:O | 1:A:11:ASP:O | 2.31 | 0.48 |
| 1:A:45:GLY:C | 1:A:166:SER:HB2 | 2.33 | 0.48 |
| 1:A:164:MET:CE | 1:A:169:ILE:HB | 2.43 | 0.48 |
| 2:B:263:LYS:HZ1 | 3:C:266:GLU:HG2 | 1.78 | 0.48 |
| 2:B:514:ILE:HG22 | 2:B:515:ILE:H | 1.78 | 0.48 |
| 2:B:5:ILE:HD12 | 2:B:7:GLY:H | 1.78 | 0.48 |
| 3:C:16:THR:HA | 3:C:525:ASP:HB3 | 1.95 | 0.48 |
| 3:C:414:PRO:O | 3:C:419:THR:HG23 | 2.14 | 0.48 |
| 5:E:189:GLY:O | 5:E:190:SER:CB | 2.61 | 0.48 |
| 6:F:160:THR:N | 6:F:164:ALA:CB | 2.76 | 0.48 |
| 5:E:547:MET:SD | 6:F:387:ALA:HA | 2.53 | 0.48 |
| 6:F:491:VAL:HG12 | 6:F:492:ASP:N | 2.27 | 0.48 |
| 7:G:107:GLU:HG2 | 7:G:448:VAL:HG21 | 1.95 | 0.48 |
| 7:G:470:LEU:O | 7:G:473:SER:OG | 2.30 | 0.48 |
| 8:H:334:ARG:HD3 | 8:H:380:ARG:HH11 | 1.78 | 0.48 |
| 2:J:274:ALA:HB1 | 2:J:329:PHE:HA | 1.94 | 0.48 |
| 2:J:382:ARG:HG3 | 2:J:382:ARG:HH11 | 1.78 | 0.48 |
| 2:J:463:ILE:CG2 | 2:J:464:TYR:N | 2.76 | 0.48 |
| 5:M:193:VAL:HG12 | 5:M:193:VAL:O | 2.14 | 0.48 |
| 7:O:145:VAL:O | 7:O:408:LEU:CA | 2.58 | 0.48 |
| 8:P:29:ILE:HG22 | 8:P:30:LYS:N | 2.28 | 0.48 |
| 8:P:356:GLU:HB2 | 8:P:374:GLU:HA | 1.95 | 0.48 |
| 1:A:13:LEU:HD22 | 1:A:14:PHE:H | 1.78 | 0.48 |
| 2:B:377:LEU:HD12 | 2:B:377:LEU:H | 1.78 | 0.48 |
| 2:B:57:THR:HG21 | 2:B:382:ARG:NH1 | 2.28 | 0.48 |
| 2:B:459:LEU:HD13 | 2:B:472:LEU:CD2 | 2.43 | 0.48 |
| 6:F:229:LYS:C | 6:F:231:ALA:H | 2.16 | 0.48 |
| 6:F:275:LYS:O | 6:F:276:LYS:C | 2.52 | 0.48 |
| 7:G:29:ASN:OD1 | 7:G:79:ALA:HB2 | 2.12 | 0.48 |
| 7:G:44:LEU:HB2 | 7:G:456:ASN:ND2 | 2.28 | 0.48 |
| 4:D:254:VAL:HG13 | 8:H:264:THR:O | 2.14 | 0.48 |
| 8:H:72:LEU:HA | 8:H:75:LEU:HB2 | 1.94 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:264:ILE:HD12 | 1:I:264:ILE:O | 2.13 | 0.48 |
| 3:K:9:ASN:HD22 | 3:K:10:ALA:N | 2.11 | 0.48 |
| 3:K:409:SER:C | 3:K:411:SER:H | 2.17 | 0.48 |
| 4:L:60:ASP:HB3 | 4:L:63:THR:OG1 | 2.12 | 0.48 |
| 5:M:240:ILE:HG12 | 5:M:244:ILE:HG21 | 1.94 | 0.48 |
| 1:I:540:ARG:HA | 5:M:70:LEU:HD22 | 1.95 | 0.48 |
| 6:N:160:THR:N | 6:N:164:ALA:CB | 2.76 | 0.48 |
| 6:N:199:MET:O | 6:N:381:LYS:HE2 | 2.13 | 0.48 |
| 6:N:433:LYS:O | 6:N:436:ALA:C | 2.52 | 0.48 |
| 8:P:443:GLY:O | 8:P:446:GLN:HG3 | 2.13 | 0.48 |
| 2:B:118:GLN:O | 2:B:121:ILE:HG12 | 2.14 | 0.48 |
| 2:B:427:SER:O | 2:B:430:VAL:HB | 2.12 | 0.48 |
| 2:B:467:ILE:HA | 2:B:468:SER:HA | 1.59 | 0.48 |
| 3:C:9:ASN:HD22 | 3:C:10:ALA:N | 2.11 | 0.48 |
| 4:D:204:ILE:O | 4:D:207:THR:HG23 | 2.13 | 0.48 |
| 4:D:260:MET:O | 4:D:263:ILE:HG22 | 2.13 | 0.48 |
| 4:D:386:ILE:C | 4:D:388:ASP:H | 2.15 | 0.48 |
| 4:D:8:ASN:OD1 | 4:D:8:ASN:O | 2.31 | 0.48 |
| 6:F:405:VAL:HG22 | 6:F:509:SER:HB2 | 1.94 | 0.48 |
| 8:H:348:THR:O | 8:H:352:LEU:HD23 | 2.13 | 0.48 |
| 2:J:442:THR:HG23 | 2:J:452:SER:CB | 2.34 | 0.48 |
| 5:M:32:VAL:CG2 | 5:M:33:LYS:H | 2.15 | 0.48 |
| 5:M:84:THR:CG2 | 5:M:86:ASP:H | 2.20 | 0.48 |
| 6:N:353:LEU:H | 6:N:369:GLU:HB3 | 1.77 | 0.48 |
| 6:N:395:VAL:O | 6:N:399:LEU:HB3 | 2.14 | 0.48 |
| 6:N:83:GLN:CD | 6:N:94:VAL:HG21 | 2.34 | 0.48 |
| 7:O:97:GLY:O | 7:O:101:VAL:HG23 | 2.14 | 0.48 |
| 7:O:217:GLY:HA3 | 7:O:366:GLN:HA | 1.95 | 0.48 |
| 8:P:248:ALA:HB2 | 8:P:352:LEU:HD13 | 1.95 | 0.48 |
| 2:B:502:SER:HA | 2:B:505:ALA:HB3 | 1.94 | 0.48 |
| 3:C:9:ASN:ND2 | 3:C:10:ALA:H | 2.11 | 0.48 |
| 6:F:105:ALA:C | 6:F:107:ARG:N | 2.67 | 0.48 |
| 6:F:355:TYR:O | 6:F:366:TYR:O | 2.31 | 0.48 |
| 7:G:214:PHE:O | 7:G:214:PHE:CG | 2.67 | 0.48 |
| 8:H:31:SER:HB2 | 8:H:79:HIS:HE1 | 1.78 | 0.48 |
| 8:H:85:LEU:HD13 | 8:H:107:ALA:HB1 | 1.95 | 0.48 |
| 1:I:10:SER:O | 1:I:11:ASP:O | 2.31 | 0.48 |
| 1:I:12:THR:CB | 5:M:96:LEU:HA | 2.43 | 0.48 |
| 2:J:250:PHE:HA | 6:N:250:GLY:C | 2.32 | 0.48 |
| 2:J:57:THR:HG21 | 2:J:382:ARG:NH1 | 2.28 | 0.48 |
| 6:N:61:VAL:O | 6:N:65:GLU:HB2 | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:O:516:LEU:HD22 | 7:O:517:ILE:CA | 2.42 | 0.48 |
| 8:P:27:GLN:O | 8:P:31:SER:N | 2.33 | 0.48 |
| 8:P:237:LYS:HB2 | 8:P:314:ASN:CB | 2.31 | 0.48 |
| 2:B:463:ILE:CG2 | 2:B:464:TYR:N | 2.76 | 0.48 |
| 4:D:246:PRO:HB2 | 4:D:250:ASN:CG | 2.33 | 0.48 |
| 4:D:265:LYS:HZ2 | 8:H:343:ARG:HD3 | 1.74 | 0.48 |
| 4:D:523:ASP:O | 7:G:51:ILE:CG2 | 2.53 | 0.48 |
| 6:F:47:VAL:HG12 | 6:F:48:ASP:N | 2.28 | 0.48 |
| 7:G:171:ILE:O | 7:G:171:ILE:HG22 | 2.12 | 0.48 |
| 4:L:291:SER:HA | 4:L:315:ASP:CA | 2.44 | 0.48 |
| 4:L:81:VAL:HG21 | 4:L:514:CYS:SG | 2.54 | 0.48 |
| 6:N:486:THR:O | 6:N:487:ARG:CB | 2.62 | 0.48 |
| 7:O:108:LEU:O | 7:O:108:LEU:HD23 | 2.13 | 0.48 |
| 1:A:494:ARG:CB | 1:A:496:SER:H | 2.21 | 0.48 |
| 4:D:448:GLU:C | 4:D:451:PRO:HD2 | 2.34 | 0.48 |
| 5:E:215:ASP:O | 5:E:216:ARG:CB | 2.62 | 0.48 |
| 5:E:351:LEU:HD22 | 5:E:352:GLU:N | 2.29 | 0.48 |
| 6:F:406:LEU:HD22 | 6:F:407:LYS:HZ1 | 1.78 | 0.48 |
| 6:F:486:THR:O | 6:F:487:ARG:CB | 2.62 | 0.48 |
| 8:H:65:THR:HG22 | 8:H:396:ASP:OD1 | 2.14 | 0.48 |
| 8:H:443:GLY:O | 8:H:446:GLN:HG3 | 2.13 | 0.48 |
| 2:J:206:SER:HB2 | 2:J:368:VAL:HG22 | 1.94 | 0.48 |
| 2:J:314:VAL:HG11 | 3:K:232:PRO:HD3 | 1.95 | 0.48 |
| 2:J:438:ARG:O | 2:J:441:PRO:HG2 | 2.14 | 0.48 |
| 2:J:59:ASP:HB3 | 2:J:62:THR:OG1 | 2.14 | 0.48 |
| 4:L:367:ARG:C | 4:L:369:ASN:N | 2.67 | 0.48 |
| 5:M:215:ASP:O | 5:M:216:ARG:CB | 2.62 | 0.48 |
| 6:N:237:ASN:HA | 6:N:297:ASN:OD1 | 2.13 | 0.48 |
| 6:N:430:ASN:HA | 6:N:433:LYS:HB2 | 1.96 | 0.48 |
| 7:O:500:ALA:O | 7:O:504:ILE:HG13 | 2.14 | 0.48 |
| 4:L:72:HIS:CD2 | 8:P:15:LYS:NZ | 2.82 | 0.48 |
| 8:P:85:LEU:HD13 | 8:P:107:ALA:HB1 | 1.95 | 0.48 |
| 1:A:156:LEU:O | 1:A:156:LEU:HD23 | 2.14 | 0.48 |
| 1:A:92:ARG:HG2 | 5:E:388:THR:CB | 2.43 | 0.48 |
| 6:F:433:LYS:O | 6:F:436:ALA:C | 2.52 | 0.48 |
| 6:F:22:ASN:O | 6:F:72:THR:HG21 | 2.14 | 0.48 |
| 7:G:97:GLY:O | 7:G:101:VAL:HG23 | 2.14 | 0.48 |
| 8:H:310:LEU:HD13 | 8:H:314:ASN:OD1 | 2.14 | 0.48 |
| 5:M:250:SER:HB3 | 5:M:342:ALA:O | 2.14 | 0.48 |
| 6:N:332:THR:HB | 6:N:351:SER:HA | 1.96 | 0.48 |
| 6:N:414:GLY:O | 6:N:415:ALA:CB | 2.62 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:N:429:ALA:O | 6:N:433:LYS:HD3 | 2.14 | 0.48 |
| 6:N:485:GLU:CG | 6:N:489:VAL:HB | 2.44 | 0.48 |
| 7:O:107:GLU:HG2 | 7:O:448:VAL:HG21 | 1.95 | 0.48 |
| 8:P:48:PRO:HB3 | 8:P:172:TYR:CD1 | 2.49 | 0.48 |
| 2:B:263:LYS:NZ | 3:C:266:GLU:CB | 2.77 | 0.48 |
| 3:C:479:ASN:HB3 | 3:C:482:THR:OG1 | 2.14 | 0.48 |
| 5:E:193:VAL:O | 5:E:193:VAL:HG12 | 2.14 | 0.48 |
| 6:F:429:ALA:O | 6:F:433:LYS:HD3 | 2.14 | 0.48 |
| 6:F:458:LEU:HD12 | 6:F:458:LEU:C | 2.33 | 0.48 |
| 7:G:241:ILE:HG12 | 7:G:292:ILE:CG2 | 2.44 | 0.48 |
| 4:D:44:MET:HG3 | 8:H:531:ALA:CB | 2.41 | 0.48 |
| 2:J:285:ILE:HD13 | 2:J:285:ILE:H | 1.78 | 0.48 |
| 2:J:233:ILE:O | 2:J:325:VAL:N | 2.46 | 0.48 |
| 2:J:377:LEU:H | 2:J:377:LEU:HD12 | 1.78 | 0.48 |
| 3:K:268:ASP:O | 3:K:272:ILE:HG12 | 2.14 | 0.48 |
| 4:L:91:ASP:OD1 | 10:L:602:BEF:F1 | 2.22 | 0.48 |
| 5:M:351:LEU:HD22 | 5:M:352:GLU:N | 2.29 | 0.48 |
| 5:M:401:THR:C | 5:M:402:LYS:CG | 2.70 | 0.48 |
| 6:N:2:SER:HA | 6:N:3:LEU:CB | 2.35 | 0.48 |
| 5:M:373:LYS:HE2 | 6:N:311:LYS:HZ3 | 1.79 | 0.48 |
| 7:O:43:THR:HB | 7:O:99:THR:CG2 | 2.39 | 0.48 |
| 8:P:65:THR:HG22 | 8:P:396:ASP:OD1 | 2.14 | 0.48 |
| 1:A:264:ILE:HD12 | 1:A:264:ILE:O | 2.14 | 0.48 |
| 1:A:501:GLY:HA3 | 1:A:512:GLU:HG2 | 1.95 | 0.48 |
| 1:A:94:ILE:HD12 | 1:A:94:ILE:N | 2.29 | 0.48 |
| 3:C:268:ASP:O | 3:C:272:ILE:HG12 | 2.14 | 0.48 |
| 3:C:471:LEU:HG | 3:C:491:ILE:HG13 | 1.96 | 0.48 |
| 5:E:133:ALA:HB2 | 5:E:150:PHE:HE2 | 1.79 | 0.48 |
| 5:E:325:TRP:CG | 5:E:326:GLY:N | 2.80 | 0.48 |
| 6:F:332:THR:HB | 6:F:351:SER:HA | 1.96 | 0.48 |
| 6:F:353:LEU:H | 6:F:369:GLU:HB3 | 1.77 | 0.48 |
| 6:F:83:GLN:CD | 6:F:94:VAL:HG21 | 2.34 | 0.48 |
| 7:G:145:VAL:O | 7:G:408:LEU:CA | 2.58 | 0.48 |
| 7:G:455:GLU:N | 7:G:461:ALA:HB2 | 2.29 | 0.48 |
| 8:H:48:PRO:HB3 | 8:H:172:TYR:CD1 | 2.49 | 0.48 |
| 1:I:116:VAL:HG12 | 1:I:120:ILE:HG22 | 1.95 | 0.48 |
| 1:I:351:GLU:C | 1:I:353:SER:N | 2.66 | 0.48 |
| 4:L:254:VAL:O | 4:L:254:VAL:CG2 | 2.61 | 0.48 |
| 6:N:541:LEU:HB3 | 6:N:543:GLU:N | 2.26 | 0.48 |
| 7:O:174:ASN:ND2 | 7:O:209:MET:SD | 2.80 | 0.48 |
| 8:P:163:ILE:HG23 | 8:P:179:SER:CB | 2.42 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:162:THR:HG21 | 1:A:518:LEU:O | 2.13 | 0.47 |
| 2:B:124:TYR:N | 2:B:124:TYR:HD1 | 2.12 | 0.47 |
| 2:B:282:ASN:ND2 | 2:B:303:ILE:HB | 2.29 | 0.47 |
| 2:B:88:VAL:CG1 | 2:B:393:GLN:HE22 | 2.22 | 0.47 |
| 3:C:39:LEU:CB | 9:C:1101:ADP:O2A | 2.62 | 0.47 |
| 3:C:225:LEU:HD13 | 3:C:320:VAL:HG11 | 1.96 | 0.47 |
| 4:D:81:VAL:HG21 | 4:D:514:CYS:SG | 2.54 | 0.47 |
| 5:E:85:ASN:ND2 | 9:E:601:ADP:O3B | 2.46 | 0.47 |
| 6:F:167:THR:CB | 6:F:169:VAL:N | 2.64 | 0.47 |
| 2:B:32:LEU:CD1 | 6:F:532:GLU:CD | 2.82 | 0.47 |
| 7:G:208:ALA:O | 7:G:211:GLU:HB2 | 2.14 | 0.47 |
| 7:G:500:ALA:O | 7:G:504:ILE:HG13 | 2.14 | 0.47 |
| 8:H:79:HIS:CE1 | 8:H:81:ALA:HB3 | 2.48 | 0.47 |
| 1:I:162:THR:HG21 | 1:I:518:LEU:O | 2.13 | 0.47 |
| 3:K:225:LEU:HD13 | 3:K:320:VAL:HG11 | 1.96 | 0.47 |
| 3:K:471:LEU:HG | 3:K:491:ILE:HG13 | 1.96 | 0.47 |
| 4:L:260:MET:O | 4:L:263:ILE:HG22 | 2.13 | 0.47 |
| 4:L:298:ASN:HB3 | 4:L:299:ASP:CA | 2.43 | 0.47 |
| 4:L:8:ASN:OD1 | 4:L:8:ASN:O | 2.31 | 0.47 |
| 5:M:355:ALA:CB | 6:N:222:PRO:HG2 | 2.43 | 0.47 |
| 6:N:454:ILE:N | 6:N:455:PRO:HD2 | 2.29 | 0.47 |
| 6:N:47:VAL:HG12 | 6:N:48:ASP:N | 2.28 | 0.47 |
| 6:N:71:PRO:HG2 | 6:N:533:LEU:HD12 | 1.94 | 0.47 |
| 7:O:115:PHE:CE1 | 7:O:437:MET:HB3 | 2.49 | 0.47 |
| 7:O:214:PHE:CG | 7:O:214:PHE:O | 2.67 | 0.47 |
| 8:P:310:LEU:HD13 | 8:P:314:ASN:OD1 | 2.14 | 0.47 |
| 8:P:396:ASP:HA | 8:P:399:ARG:HH11 | 1.79 | 0.47 |
| 2:B:242:LYS:HE2 | 2:B:247:GLY:N | 2.26 | 0.47 |
| 4:D:174:ALA:O | 4:D:178:VAL:HG23 | 2.13 | 0.47 |
| 4:D:298:ASN:HB3 | 4:D:299:ASP:CA | 2.43 | 0.47 |
| 5:E:175:LEU:O | 5:E:175:LEU:HD12 | 2.14 | 0.47 |
| 5:E:250:SER:HB3 | 5:E:342:ALA:O | 2.14 | 0.47 |
| 5:E:277:GLU:CB | 5:E:278:PRO:HD2 | 2.44 | 0.47 |
| 5:E:32:VAL:CG2 | 5:E:33:LYS:H | 2.15 | 0.47 |
| 6:F:414:GLY:O | 6:F:415:ALA:CB | 2.62 | 0.47 |
| 7:G:108:LEU:O | 7:G:108:LEU:HD23 | 2.13 | 0.47 |
| 7:G:120:ILE:HG23 | 8:P:472:ASN:ND2 | 2.30 | 0.47 |
| 8:H:167:ILE:HD11 | 8:H:182:VAL:HG21 | 1.96 | 0.47 |
| 8:H:248:ALA:HB2 | 8:H:352:LEU:HD13 | 1.95 | 0.47 |
| 8:H:6:PRO:CG | 4:L:71:LEU:HA | 2.35 | 0.47 |
| 2:J:237:THR:N | 2:J:287:ARG:HD2 | 2.28 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:410:VAL:HB | 2:J:468:SER:OG | 2.13 | 0.47 |
| 3:K:129:LEU:HD23 | 3:K:510:VAL:HG12 | 1.96 | 0.47 |
| 4:L:434:GLY:HA3 | 4:L:436:GLN:OE1 | 2.14 | 0.47 |
| 6:N:86:ILE:HG23 | 6:N:87:THR:HG23 | 1.96 | 0.47 |
| 7:O:241:ILE:HG12 | 7:O:292:ILE:CG2 | 2.44 | 0.47 |
| 8:P:248:ALA:HB2 | 8:P:352:LEU:CD1 | 2.44 | 0.47 |
| 1:A:258:MET:HE2 | 1:A:259:GLY:H | 1.79 | 0.47 |
| 2:B:422:ILE:HG22 | 2:B:424:GLY:H | 1.75 | 0.47 |
| 2:B:59:ASP:HB3 | 2:B:62:THR:OG1 | 2.14 | 0.47 |
| 5:E:428:CYS:O | 5:E:431:ARG:HG3 | 2.15 | 0.47 |
| 1:A:540:ARG:HA | 5:E:70:LEU:HD22 | 1.95 | 0.47 |
| 5:E:74:LEU:HD12 | 5:E:93:GLN:HB3 | 1.96 | 0.47 |
| 8:H:248:ALA:HB2 | 8:H:352:LEU:CD1 | 2.44 | 0.47 |
| 1:I:14:PHE:CB | 1:I:15:LEU:HA | 2.43 | 0.47 |
| 2:J:124:TYR:N | 2:J:124:TYR:CD1 | 2.82 | 0.47 |
| 2:J:319:LEU:HD23 | 2:J:319:LEU:C | 2.35 | 0.47 |
| 3:K:170:LYS:HD3 | 3:K:170:LYS:O | 2.14 | 0.47 |
| 3:K:479:ASN:HB3 | 3:K:482:THR:OG1 | 2.14 | 0.47 |
| 3:K:84:THR:HG21 | 8:P:389:ALA:HA | 1.97 | 0.47 |
| 4:L:350:VAL:HG22 | 4:L:363:VAL:HG13 | 1.97 | 0.47 |
| 6:N:105:ALA:C | 6:N:107:ARG:N | 2.67 | 0.47 |
| 7:O:143:LEU:HD22 | 7:O:411:ALA:HB2 | 1.94 | 0.47 |
| 3:K:117:HIS:HE1 | 8:P:50:GLY:O | 1.97 | 0.47 |
| 4:D:367:ARG:C | 4:D:369:ASN:N | 2.67 | 0.47 |
| 8:H:423:ALA:CA | 9:H:601:ADP:H2' | 2.31 | 0.47 |
| 1:I:221:GLY:HA2 | 1:I:382:SER:CB | 2.42 | 0.47 |
| 1:I:94:ILE:HD12 | 1:I:94:ILE:N | 2.29 | 0.47 |
| 2:J:118:GLN:O | 2:J:121:ILE:HG12 | 2.14 | 0.47 |
| 2:J:263:LYS:HZ1 | 3:K:266:GLU:HG2 | 1.78 | 0.47 |
| 2:J:282:ASN:ND2 | 2:J:303:ILE:HB | 2.29 | 0.47 |
| 2:J:469:THR:CG2 | 2:J:481:ASP:HB2 | 2.44 | 0.47 |
| 2:J:63:ILE:CG2 | 2:J:64:LEU:HG | 2.44 | 0.47 |
| 3:K:112:ILE:HG13 | 3:K:113:GLU:N | 2.29 | 0.47 |
| 3:K:495:VAL:HG23 | 3:K:500:TRP:CH2 | 2.48 | 0.47 |
| 4:L:448:GLU:C | 4:L:451:PRO:HD2 | 2.34 | 0.47 |
| 5:M:175:LEU:HD12 | 5:M:175:LEU:O | 2.14 | 0.47 |
| 6:N:213:LEU:HD23 | 6:N:377:THR:CG2 | 2.40 | 0.47 |
| 9:N:601:ADP:H8 | 9:N:601:ADP:O2' | 1.97 | 0.47 |
| 7:O:43:THR:HG21 | 7:O:64:ASN:O | 2.13 | 0.47 |
| 1:A:419:VAL:CG1 | 1:A:425:VAL:HG21 | 2.44 | 0.47 |
| 2:B:285:ILE:HD13 | 2:B:285:ILE:H | 1.78 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:289:LEU:HD21 | 2:B:304:ASN:OD1 | 2.15 | 0.47 |
| 2:B:410:VAL:HB | 2:B:468:SER:OG | 2.13 | 0.47 |
| 3:C:184:LYS:HA | 3:C:198:ILE:C | 2.35 | 0.47 |
| 3:C:457:ILE:HG22 | 3:C:462:GLY:O | 2.14 | 0.47 |
| 2:B:514:ILE:HG23 | 3:C:47:MET:O | 2.14 | 0.47 |
| 3:C:47:MET:HG2 | 3:C:48:LEU:N | 2.30 | 0.47 |
| 4:D:12:LYS:HZ2 | 7:G:73:LEU:CD2 | 2.28 | 0.47 |
| 5:E:150:PHE:CD1 | 5:E:472:PHE:CE2 | 3.03 | 0.47 |
| 6:F:406:LEU:HB3 | 6:F:407:LYS:HZ2 | 1.80 | 0.47 |
| 6:F:424:ARG:HA | 6:F:424:ARG:NE | 2.12 | 0.47 |
| 7:G:217:GLY:O | 7:G:375:THR:HG22 | 2.15 | 0.47 |
| 7:G:235:LYS:CB | 7:G:353:GLU:HA | 2.44 | 0.47 |
| 4:D:81:VAL:HA | 7:G:382:ALA:HB2 | 1.96 | 0.47 |
| 8:H:164:LYS:HB3 | 8:H:165:PRO:HD3 | 1.96 | 0.47 |
| 8:H:243:LYS:HB3 | 8:H:244:LYS:NZ | 2.29 | 0.47 |
| 2:J:289:LEU:HD21 | 2:J:304:ASN:OD1 | 2.15 | 0.47 |
| 2:J:402:LEU:CD1 | 2:J:483:ARG:HE | 2.24 | 0.47 |
| 3:K:108:ALA:O | 3:K:112:ILE:HG23 | 2.15 | 0.47 |
| 3:K:174:LEU:HG | 3:K:219:VAL:HG22 | 1.96 | 0.47 |
| 3:K:414:PRO:O | 3:K:419:THR:HG23 | 2.14 | 0.47 |
| 4:L:292:ILE:N | 4:L:293:LEU:CA | 2.73 | 0.47 |
| 5:M:133:ALA:HB2 | 5:M:150:PHE:HE2 | 1.79 | 0.47 |
| 5:M:189:GLY:O | 5:M:190:SER:CB | 2.61 | 0.47 |
| 6:N:108:PHE:CE1 | 6:N:118:ILE:HG13 | 2.50 | 0.47 |
| 7:O:452:GLN:HA | 7:O:455:GLU:HB2 | 1.96 | 0.47 |
| 8:P:243:LYS:HB3 | 8:P:244:LYS:NZ | 2.29 | 0.47 |
| 8:P:348:THR:O | 8:P:352:LEU:HD23 | 2.13 | 0.47 |
| 8:P:31:SER:HB2 | 8:P:79:HIS:HE1 | 1.78 | 0.47 |
| 2:B:93:THR:OG1 | 9:B:601:ADP:O2A | 2.31 | 0.47 |
| 1:I:145:SER:O | 1:I:148:VAL:HG23 | 2.15 | 0.47 |
| 5:M:150:PHE:CD1 | 5:M:472:PHE:CE2 | 3.03 | 0.47 |
| 6:N:246:GLU:H | 6:N:246:GLU:CD | 2.18 | 0.47 |
| 6:N:280:LEU:HD23 | 6:N:280:LEU:N | 2.27 | 0.47 |
| 2:B:142:ASN:CB | 2:B:143:SER:HA | 2.18 | 0.47 |
| 3:C:108:ALA:O | 3:C:112:ILE:HG23 | 2.15 | 0.47 |
| 3:C:112:ILE:HG13 | 3:C:113:GLU:N | 2.29 | 0.47 |
| 3:C:174:LEU:HG | 3:C:219:VAL:HG22 | 1.96 | 0.47 |
| 3:C:407:MET:HE1 | 3:C:408:LEU:HD23 | 1.97 | 0.47 |
| 4:D:352:GLU:HA | 4:D:361:VAL:HA | 1.95 | 0.47 |
| 4:D:24:ASN:ND2 | 4:D:524:ILE:HD11 | 2.29 | 0.47 |
| 6:F:246:GLU:H | 6:F:246:GLU:CD | 2.18 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:F:485:GLU:CG | 6:F:489:VAL:HB | 2.44 | 0.47 |
| 7:G:279:PHE:O | 7:G:282:LEU:HD12 | 2.15 | 0.47 |
| 7:G:291:ASN:C | 7:G:312:ILE:HG13 | 2.34 | 0.47 |
| 7:G:292:ILE:N | 7:G:312:ILE:HG13 | 2.30 | 0.47 |
| 7:G:217:GLY:HA3 | 7:G:366:GLN:HA | 1.95 | 0.47 |
| 4:D:521:ILE:CB | 7:G:50:ASP:O | 2.61 | 0.47 |
| 8:H:35:ILE:HD13 | 8:H:82:VAL:HA | 1.95 | 0.47 |
| 8:H:99:GLY:O | 8:H:103:VAL:HG23 | 2.15 | 0.47 |
| 1:I:156:LEU:HD23 | 1:I:156:LEU:O | 2.14 | 0.47 |
| 2:J:463:ILE:HD11 | 2:J:468:SER:OG | 2.15 | 0.47 |
| 2:J:403:GLY:O | 2:J:482:MET:HG3 | 2.14 | 0.47 |
| 2:J:60:GLY:O | 2:J:63:ILE:HG22 | 2.15 | 0.47 |
| 3:K:142:PRO:HG3 | 3:K:411:SER:CA | 2.44 | 0.47 |
| 3:K:175:ALA:O | 3:K:179:VAL:HG23 | 2.14 | 0.47 |
| 3:K:184:LYS:HA | 3:K:198:ILE:C | 2.35 | 0.47 |
| 3:K:25:ILE:HD13 | 3:K:26:THR:N | 2.30 | 0.47 |
| 3:K:457:ILE:HG22 | 3:K:462:GLY:O | 2.14 | 0.47 |
| 6:N:275:LYS:O | 6:N:276:LYS:C | 2.52 | 0.47 |
| 6:N:3:LEU:N | 6:N:3:LEU:HD22 | 2.30 | 0.47 |
| 6:N:22:ASN:O | 6:N:72:THR:HG21 | 2.14 | 0.47 |
| 7:O:51:ILE:HB | 7:O:69:ILE:HD11 | 1.96 | 0.47 |
| 2:B:124:TYR:N | 2:B:124:TYR:CD1 | 2.82 | 0.47 |
| 2:B:463:ILE:HD11 | 2:B:468:SER:OG | 2.15 | 0.47 |
| 3:C:117:HIS:CG | 3:C:118:PRO:HD2 | 2.50 | 0.47 |
| 4:D:350:VAL:HG22 | 4:D:363:VAL:HG13 | 1.97 | 0.47 |
| 5:E:88:ALA:HB1 | 5:E:109:LYS:HZ2 | 1.77 | 0.47 |
| 6:F:3:LEU:N | 6:F:3:LEU:HD22 | 2.30 | 0.47 |
| 6:F:424:ARG:HE | 6:F:424:ARG:CA | 2.17 | 0.47 |
| 6:F:86:ILE:HG23 | 6:F:87:THR:HG23 | 1.96 | 0.47 |
| 7:G:204:ILE:O | 7:G:379:ARG:HD3 | 2.14 | 0.47 |
| 8:H:396:ASP:HA | 8:H:399:ARG:HH11 | 1.79 | 0.47 |
| 1:A:351:GLU:C | 1:A:353:SER:N | 2.66 | 0.47 |
| 2:B:232:LEU:HD22 | 2:B:233:ILE:H | 1.80 | 0.47 |
| 2:B:27:ILE:HG12 | 2:B:27:ILE:O | 2.15 | 0.47 |
| 2:B:328:THR:O | 2:B:329:PHE:CB | 2.62 | 0.47 |
| 3:C:41:PRO:CA | 3:C:161:THR:HG21 | 2.43 | 0.47 |
| 3:C:25:ILE:HD13 | 3:C:26:THR:N | 2.30 | 0.47 |
| 3:C:262:GLU:H | 8:H:266:LEU:CD1 | 2.28 | 0.47 |
| 5:E:176:PHE:O | 5:E:180:LEU:HD23 | 2.15 | 0.47 |
| 5:E:84:THR:CG2 | 5:E:85:ASN:N | 2.78 | 0.47 |
| 7:G:409:ILE:CG2 | 7:G:410:VAL:H | 2.28 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:K:9:ASN:ND2 | 3:K:10:ALA:H | 2.11 | 0.47 |
| 3:K:117:HIS:CG | 3:K:118:PRO:HD2 | 2.50 | 0.47 |
| 5:M:428:CYS:O | 5:M:431:ARG:HG3 | 2.14 | 0.47 |
| 6:N:16:ASP:N | 6:N:16:ASP:OD1 | 2.36 | 0.47 |
| 5:M:547:MET:SD | 6:N:387:ALA:HA | 2.55 | 0.47 |
| 6:N:76:ILE:HG21 | 6:N:95:VAL:HG13 | 1.96 | 0.47 |
| 7:O:217:GLY:HA3 | 7:O:365:PHE:O | 2.15 | 0.47 |
| 7:O:455:GLU:N | 7:O:461:ALA:HB2 | 2.29 | 0.47 |
| 7:O:94:VAL:CG1 | 7:O:95:GLY:H | 2.28 | 0.47 |
| 1:A:12:THR:CB | 5:E:96:LEU:HA | 2.44 | 0.47 |
| 1:A:480:TYR:O | 1:A:483:ALA:CB | 2.63 | 0.47 |
| 2:B:403:GLY:O | 2:B:482:MET:HG3 | 2.14 | 0.47 |
| 3:C:142:PRO:HG3 | 3:C:411:SER:CA | 2.44 | 0.47 |
| 3:C:202:ARG:O | 3:C:204:VAL:O | 2.32 | 0.47 |
| 3:C:348:VAL:HG12 | 3:C:349:GLY:N | 2.30 | 0.47 |
| 4:D:178:VAL:CB | 4:D:401:ILE:HD11 | 2.45 | 0.47 |
| 6:F:430:ASN:HA | 6:F:433:LYS:HB2 | 1.96 | 0.47 |
| 6:F:454:ILE:HB | 6:F:455:PRO:HD3 | 1.97 | 0.47 |
| 2:J:494:LYS:HD2 | 2:J:494:LYS:HA | 1.79 | 0.47 |
| 3:K:246:LEU:O | 3:K:247:ASP:HB3 | 2.15 | 0.47 |
| 2:J:324:GLU:H | 3:K:311:LYS:NZ | 2.12 | 0.47 |
| 3:K:348:VAL:HG12 | 3:K:349:GLY:N | 2.30 | 0.47 |
| 4:L:134:ILE:HD12 | 4:L:421:ILE:HD13 | 1.95 | 0.47 |
| 4:L:174:ALA:O | 4:L:178:VAL:HG23 | 2.13 | 0.47 |
| 4:L:352:GLU:HA | 4:L:361:VAL:HA | 1.95 | 0.47 |
| 4:L:461:ASN:HD22 | 4:L:462:SER:N | 2.13 | 0.47 |
| 4:L:523:ASP:O | 7:O:51:ILE:CG2 | 2.53 | 0.47 |
| 4:L:92:GLY:O | 4:L:96:VAL:HG23 | 2.15 | 0.47 |
| 5:M:277:GLU:CB | 5:M:278:PRO:HD2 | 2.44 | 0.47 |
| 7:O:455:GLU:HG3 | 7:O:461:ALA:HB3 | 1.97 | 0.47 |
| 8:P:35:ILE:HD13 | 8:P:82:VAL:HA | 1.95 | 0.47 |
| 8:P:99:GLY:O | 8:P:103:VAL:HG23 | 2.15 | 0.47 |
| 2:B:319:LEU:C | 2:B:319:LEU:HD23 | 2.35 | 0.47 |
| 2:B:438:ARG:O | 2:B:441:PRO:HG2 | 2.14 | 0.47 |
| 3:C:275:ILE:O | 8:H:274:LEU:HD21 | 2.15 | 0.47 |
| 4:D:292:ILE:N | 4:D:293:LEU:CA | 2.73 | 0.47 |
| 4:D:434:GLY:HA3 | 4:D:436:GLN:OE1 | 2.14 | 0.47 |
| 5:E:240:ILE:HG12 | 5:E:244:ILE:HG21 | 1.94 | 0.47 |
| 5:E:262:GLU:HA | 5:E:263:GLY:HA2 | 1.67 | 0.47 |
| 6:F:141:THR:CB | 6:F:409:LYS:HG3 | 2.45 | 0.47 |
| 2:B:165:ILE:HD13 | 6:F:526:ASN:HB2 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:G:217:GLY:HA3 | 7:G:365:PHE:O | 2.15 | 0.47 |
| 8:H:6:PRO:CB | 8:H:7:GLN:HG3 | 2.38 | 0.47 |
| 1:I:419:VAL:CG1 | 1:I:425:VAL:HG21 | 2.44 | 0.47 |
| 1:I:29:ASN:HD22 | 1:I:538:ILE:HG23 | 1.80 | 0.47 |
| 2:J:263:LYS:HZ1 | 3:K:266:GLU:CG | 2.26 | 0.47 |
| 2:J:477:GLY:O | 2:J:478:THR:CB | 2.62 | 0.47 |
| 5:M:210:ASN:HD22 | 5:M:210:ASN:N | 2.08 | 0.47 |
| 7:O:279:PHE:O | 7:O:282:LEU:HD12 | 2.15 | 0.47 |
| 7:O:291:ASN:C | 7:O:312:ILE:HG13 | 2.34 | 0.47 |
| 7:O:354:GLU:HA | 7:O:363:ASN:HA | 1.97 | 0.47 |
| 1:A:128:GLY:O | 1:A:448:ILE:HD13 | 2.15 | 0.46 |
| 1:A:145:SER:O | 1:A:148:VAL:HG23 | 2.15 | 0.46 |
| 1:A:16:GLY:CA | 1:A:548:ASP:HB3 | 2.44 | 0.46 |
| 4:D:496:HIS:O | 4:D:498:LEU:HD12 | 2.15 | 0.46 |
| 4:D:521:ILE:CD1 | 7:G:62:ILE:HD12 | 2.44 | 0.46 |
| 6:F:395:VAL:O | 6:F:399:LEU:HB3 | 2.14 | 0.46 |
| 7:G:115:PHE:CE1 | 7:G:437:MET:HB3 | 2.49 | 0.46 |
| 7:G:17:THR:HG22 | 7:G:526:ASN:HD22 | 1.80 | 0.46 |
| 7:G:354:GLU:HA | 7:G:363:ASN:HA | 1.97 | 0.46 |
| 8:H:442:PRO:HA | 8:H:446:GLN:HE21 | 1.80 | 0.46 |
| 1:I:480:TYR:O | 1:I:483:ALA:CB | 2.63 | 0.46 |
| 2:J:30:GLY:HA2 | 2:J:33:VAL:HG21 | 1.97 | 0.46 |
| 3:K:202:ARG:O | 3:K:204:VAL:O | 2.32 | 0.46 |
| 5:M:84:THR:CG2 | 5:M:85:ASN:N | 2.78 | 0.46 |
| 7:O:235:LYS:CB | 7:O:353:GLU:HA | 2.44 | 0.46 |
| 7:O:204:ILE:O | 7:O:379:ARG:HD3 | 2.14 | 0.46 |
| 1:A:143:VAL:HG12 | 1:A:419:VAL:HG22 | 1.97 | 0.46 |
| 1:A:16:GLY:HA3 | 1:A:548:ASP:CB | 2.44 | 0.46 |
| 2:B:26:ALA:HB1 | 2:B:77:LEU:HD11 | 1.98 | 0.46 |
| 2:B:444:LEU:HD21 | 9:B:601:ADP:C1' | 2.46 | 0.46 |
| 2:B:513:ASN:O | 2:B:514:ILE:CD1 | 2.46 | 0.46 |
| 3:C:175:ALA:O | 3:C:179:VAL:HG23 | 2.15 | 0.46 |
| 3:C:250:LEU:CG | 3:C:301:VAL:CB | 2.92 | 0.46 |
| 5:E:103:LEU:HA | 5:E:106:GLN:HE21 | 1.81 | 0.46 |
| 5:E:301:TYR:HA | 5:E:304:ASP:OD2 | 2.15 | 0.46 |
| 6:F:332:THR:HB | 6:F:350:PHE:O | 2.15 | 0.46 |
| 6:F:454:ILE:N | 6:F:455:PRO:HD2 | 2.29 | 0.46 |
| 6:F:422:LEU:HD13 | 6:F:517:ILE:HD11 | 1.98 | 0.46 |
| 2:B:42:MET:HE3 | 6:F:529:LEU:O | 2.15 | 0.46 |
| 6:F:76:ILE:HG21 | 6:F:95:VAL:HG13 | 1.96 | 0.46 |
| 7:G:304:THR:HA | 7:G:307:PHE:CE2 | 2.46 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:K:229:VAL:HG12 | 3:K:230:VAL:H | 1.80 | 0.46 |
| 3:K:202:ARG:HH21 | 3:K:323:SER:HB3 | 1.81 | 0.46 |
| 4:L:194:ILE:O | 4:L:194:ILE:HG12 | 2.15 | 0.46 |
| 5:M:176:PHE:O | 5:M:180:LEU:HD23 | 2.15 | 0.46 |
| 6:N:143:LEU:HD13 | 6:N:145:ASN:CG | 2.36 | 0.46 |
| 6:N:143:LEU:HD21 | 6:N:145:ASN:HB3 | 1.97 | 0.46 |
| 6:N:515:ASN:C | 6:N:515:ASN:HD22 | 2.18 | 0.46 |
| 7:O:208:ALA:O | 7:O:211:GLU:HB2 | 2.14 | 0.46 |
| 7:O:60:THR:O | 7:O:60:THR:HG23 | 2.15 | 0.46 |
| 7:O:83:LEU:HD23 | 7:O:86:ILE:CD1 | 2.45 | 0.46 |
| 8:P:167:ILE:HD11 | 8:P:182:VAL:HG21 | 1.96 | 0.46 |
| 2:B:408:GLU:CD | 2:B:440:LEU:HD23 | 2.36 | 0.46 |
| 2:B:469:THR:CG2 | 2:B:481:ASP:HB2 | 2.44 | 0.46 |
| 3:C:170:LYS:HD3 | 3:C:170:LYS:O | 2.14 | 0.46 |
| 4:D:77:MET:HE1 | 7:G:384:GLN:HB2 | 1.97 | 0.46 |
| 6:F:195:GLU:OE1 | 6:F:197:MET:HE2 | 2.15 | 0.46 |
| 6:F:362:GLU:CG | 6:F:364:PHE:CE2 | 2.93 | 0.46 |
| 8:H:184:GLU:O | 8:H:188:HIS:HD2 | 1.97 | 0.46 |
| 2:J:124:TYR:N | 2:J:124:TYR:HD1 | 2.12 | 0.46 |
| 4:L:147:ARG:O | 4:L:151:VAL:HG23 | 2.16 | 0.46 |
| 4:L:178:VAL:CB | 4:L:401:ILE:HD11 | 2.45 | 0.46 |
| 5:M:301:TYR:HA | 5:M:304:ASP:OD2 | 2.15 | 0.46 |
| 6:N:166:LEU:HG | 6:N:167:THR:OG1 | 2.15 | 0.46 |
| 6:N:16:ASP:HA | 6:N:19:LEU:CG | 2.45 | 0.46 |
| 5:M:114:GLU:HB3 | 6:N:201:HIS:CE1 | 2.50 | 0.46 |
| 6:N:427:ARG:HG2 | 6:N:448:ALA:CB | 2.46 | 0.46 |
| 6:N:454:ILE:HB | 6:N:455:PRO:HD3 | 1.97 | 0.46 |
| 7:O:292:ILE:N | 7:O:312:ILE:HG13 | 2.30 | 0.46 |
| 8:P:442:PRO:HA | 8:P:446:GLN:HE21 | 1.80 | 0.46 |
| 2:B:242:LYS:HA | 3:C:269:TRP:HE1 | 1.81 | 0.46 |
| 2:B:360:LYS:HA | 2:B:361:ALA:HA | 1.69 | 0.46 |
| 2:B:477:GLY:O | 2:B:478:THR:CB | 2.62 | 0.46 |
| 2:B:58:ASN:ND2 | 2:B:58:ASN:C | 2.69 | 0.46 |
| 4:D:134:ILE:HD12 | 4:D:421:ILE:HD13 | 1.95 | 0.46 |
| 9:D:601:ADP:C3' | 9:D:601:ADP:C8 | 2.98 | 0.46 |
| 4:D:92:GLY:O | 4:D:96:VAL:HG23 | 2.15 | 0.46 |
| 6:F:143:LEU:HD13 | 6:F:145:ASN:CG | 2.36 | 0.46 |
| 6:F:16:ASP:HA | 6:F:19:LEU:CG | 2.45 | 0.46 |
| 6:F:370:ASN:HD22 | 6:F:370:ASN:N | 2.14 | 0.46 |
| 7:G:144:ALA:HA | 7:G:409:ILE:O | 2.14 | 0.46 |
| 7:G:51:ILE:HB | 7:G:69:ILE:HD11 | 1.96 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:162:SER:O | 2:J:163:SER:CB | 2.64 | 0.46 |
| 2:J:328:THR:O | 2:J:329:PHE:CB | 2.62 | 0.46 |
| 4:L:254:VAL:HG22 | 8:P:264:THR:O | 2.16 | 0.46 |
| 5:M:114:GLU:HG2 | 6:N:201:HIS:ND1 | 2.31 | 0.46 |
| 1:I:92:ARG:HG2 | 5:M:388:THR:CB | 2.46 | 0.46 |
| 2:J:165:ILE:HD13 | 6:N:526:ASN:HB2 | 1.98 | 0.46 |
| 7:O:217:GLY:O | 7:O:375:THR:HG22 | 2.15 | 0.46 |
| 7:O:80:ALA:O | 7:O:84:VAL:HG23 | 2.16 | 0.46 |
| 8:P:164:LYS:HB3 | 8:P:165:PRO:HD3 | 1.96 | 0.46 |
| 8:P:487:PRO:HA | 8:P:488:GLY:HA3 | 1.69 | 0.46 |
| 1:A:351:GLU:C | 1:A:353:SER:H | 2.17 | 0.46 |
| 4:D:234:ILE:HG22 | 4:D:236:LEU:HD22 | 1.97 | 0.46 |
| 4:D:461:ASN:HD22 | 4:D:462:SER:N | 2.13 | 0.46 |
| 7:G:454:CYS:HB3 | 7:G:461:ALA:HA | 1.98 | 0.46 |
| 7:G:83:LEU:HD23 | 7:G:86:ILE:CD1 | 2.45 | 0.46 |
| 7:G:80:ALA:O | 7:G:84:VAL:HG23 | 2.16 | 0.46 |
| 8:H:32:ILE:HD13 | 8:H:32:ILE:O | 2.16 | 0.46 |
| 2:J:164:LYS:O | 2:J:167:SER:N | 2.40 | 0.46 |
| 2:J:331:GLU:HA | 2:J:332:PRO:HD3 | 1.79 | 0.46 |
| 3:K:402:VAL:HG13 | 3:K:502:PRO:CG | 2.45 | 0.46 |
| 3:K:47:MET:HG2 | 3:K:48:LEU:N | 2.30 | 0.46 |
| 3:K:51:PRO:O | 3:K:52:MET:CG | 2.63 | 0.46 |
| 4:L:239:PHE:C | 4:L:290:LYS:HG3 | 2.36 | 0.46 |
| 4:L:284:ASN:O | 4:L:310:ILE:CG2 | 2.63 | 0.46 |
| 5:M:74:LEU:HD12 | 5:M:93:GLN:HB3 | 1.96 | 0.46 |
| 7:O:236:PHE:O | 7:O:239:PRO:CG | 2.64 | 0.46 |
| 7:O:454:CYS:HB3 | 7:O:461:ALA:HA | 1.98 | 0.46 |
| 8:P:184:GLU:O | 8:P:188:HIS:HD2 | 1.97 | 0.46 |
| 8:P:6:PRO:CB | 8:P:7:GLN:CA | 2.93 | 0.46 |
| 1:A:29:ASN:HD22 | 1:A:538:ILE:HG23 | 1.81 | 0.46 |
| 2:B:286:ASN:HD22 | 2:B:287:ARG:N | 2.14 | 0.46 |
| 2:B:224:LYS:O | 2:B:343:ILE:HA | 2.16 | 0.46 |
| 3:C:229:VAL:HG12 | 3:C:230:VAL:H | 1.80 | 0.46 |
| 4:D:291:SER:HA | 4:D:315:ASP:CA | 2.44 | 0.46 |
| 6:F:166:LEU:HG | 6:F:167:THR:OG1 | 2.15 | 0.46 |
| 6:F:343:LEU:HA | 6:F:344:SER:HA | 1.48 | 0.46 |
| 6:F:420:ILE:HB | 6:F:482:ASP:OD1 | 2.16 | 0.46 |
| 2:J:411:MET:CE | 2:J:498:VAL:HG21 | 2.45 | 0.46 |
| 4:L:496:HIS:O | 4:L:498:LEU:HD12 | 2.15 | 0.46 |
| 4:L:77:MET:CE | 7:O:384:GLN:HB2 | 2.45 | 0.46 |
| 2:J:40:LYS:HZ1 | 6:N:117:ILE:HG13 | 1.80 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:N:5:LEU:CA | 6:N:6:LEU:HB2 | 2.35 | 0.46 |
| 7:O:144:ALA:HA | 7:O:409:ILE:O | 2.15 | 0.46 |
| 7:O:17:THR:HG22 | 7:O:526:ASN:HD22 | 1.80 | 0.46 |
| 7:O:200:GLY:O | 7:O:375:THR:HA | 2.16 | 0.46 |
| 2:B:60:GLY:O | 2:B:63:ILE:HG22 | 2.15 | 0.46 |
| 2:B:63:ILE:CG2 | 2:B:64:LEU:HG | 2.44 | 0.46 |
| 3:C:129:LEU:HD23 | 3:C:510:VAL:HG12 | 1.96 | 0.46 |
| 7:G:207:GLY:HA3 | 7:G:379:ARG:HH11 | 1.81 | 0.46 |
| 7:G:491:ASN:OD1 | 7:G:496:VAL:CG2 | 2.64 | 0.46 |
| 7:G:60:THR:HG23 | 7:G:60:THR:O | 2.15 | 0.46 |
| 8:H:94:ILE:H | 8:H:94:ILE:HG13 | 1.50 | 0.46 |
| 2:J:242:LYS:HD3 | 3:K:269:TRP:CZ2 | 2.50 | 0.46 |
| 2:J:4:GLN:C | 2:J:5:ILE:CG2 | 2.73 | 0.46 |
| 4:L:392:ARG:HD3 | 4:L:393:SER:N | 2.31 | 0.46 |
| 6:N:233:VAL:HG13 | 6:N:351:SER:CB | 2.43 | 0.46 |
| 8:P:32:ILE:O | 8:P:32:ILE:HD13 | 2.16 | 0.46 |
| 8:P:457:GLU:C | 8:P:460:PRO:HD2 | 2.36 | 0.46 |
| 4:D:182:SER:HB2 | 4:D:187:LYS:CE | 2.46 | 0.46 |
| 5:E:269:LEU:HD22 | 5:E:269:LEU:N | 2.31 | 0.46 |
| 5:E:84:THR:HG22 | 5:E:85:ASN:N | 2.31 | 0.46 |
| 6:F:233:VAL:HG13 | 6:F:351:SER:CB | 2.43 | 0.46 |
| 6:F:427:ARG:HG2 | 6:F:448:ALA:CB | 2.46 | 0.46 |
| 6:F:458:LEU:HG | 6:F:459:VAL:HG23 | 1.97 | 0.46 |
| 7:G:200:GLY:O | 7:G:375:THR:HA | 2.15 | 0.46 |
| 7:G:296:LYS:HA | 7:G:318:VAL:HG23 | 1.97 | 0.46 |
| 7:G:33:CYS:SG | 7:G:106:GLY:HA2 | 2.56 | 0.46 |
| 8:H:457:GLU:C | 8:H:460:PRO:HD2 | 2.36 | 0.46 |
| 8:H:464:ALA:HB1 | 8:H:474:VAL:HG21 | 1.98 | 0.46 |
| 1:I:351:GLU:C | 1:I:353:SER:H | 2.17 | 0.46 |
| 2:J:408:GLU:CD | 2:J:440:LEU:HD23 | 2.36 | 0.46 |
| 3:K:298:GLU:HA | 3:K:320:VAL:H | 1.81 | 0.46 |
| 3:K:407:MET:HE1 | 3:K:408:LEU:HD23 | 1.97 | 0.46 |
| 4:L:234:ILE:HG22 | 4:L:236:LEU:HD22 | 1.97 | 0.46 |
| 6:N:332:THR:HB | 6:N:350:PHE:O | 2.15 | 0.46 |
| 6:N:122:PHE:HD1 | 6:N:447:PHE:HD1 | 1.63 | 0.46 |
| 6:N:458:LEU:HG | 6:N:459:VAL:HG23 | 1.97 | 0.46 |
| 7:O:234:LYS:HA | 7:O:234:LYS:HD3 | 1.34 | 0.46 |
| 7:O:33:CYS:SG | 7:O:106:GLY:HA2 | 2.56 | 0.46 |
| 7:O:491:ASN:OD1 | 7:O:496:VAL:CG2 | 2.64 | 0.46 |
| 1:A:486:MET:CB | 1:A:487:ALA:HB2 | 2.46 | 0.46 |
| 2:B:162:SER:O | 2:B:163:SER:CB | 2.63 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:246:LEU:O | 3:C:247:ASP:HB3 | 2.15 | 0.46 |
| 4:D:344:LEU:O | 4:D:345:ASP:OD1 | 2.33 | 0.46 |
| 4:D:392:ARG:HD3 | 4:D:393:SER:N | 2.31 | 0.46 |
| 4:D:417:PRO:O | 4:D:421:ILE:HG12 | 2.16 | 0.46 |
| 4:D:469:LEU:C | 4:D:471:SER:H | 2.19 | 0.46 |
| 5:E:239:LEU:HD23 | 5:E:240:ILE:N | 2.31 | 0.46 |
| 6:F:330:LEU:O | 6:F:372:ASP:O | 2.34 | 0.46 |
| 1:I:143:VAL:HG12 | 1:I:419:VAL:HG22 | 1.97 | 0.46 |
| 2:J:242:LYS:HA | 3:K:269:TRP:HE1 | 1.80 | 0.46 |
| 2:J:26:ALA:HB1 | 2:J:77:LEU:HD11 | 1.97 | 0.46 |
| 2:J:295:GLU:HB2 | 6:N:337:GLN:CD | 2.35 | 0.46 |
| 3:K:142:PRO:HB3 | 3:K:410:PRO:O | 2.15 | 0.46 |
| 4:L:144:LEU:HD23 | 4:L:144:LEU:N | 2.31 | 0.46 |
| 5:M:184:ALA:O | 5:M:188:LEU:CB | 2.64 | 0.46 |
| 1:A:210:GLY:O | 1:A:211:LYS:CB | 2.64 | 0.46 |
| 1:A:218:LEU:HD23 | 1:A:385:ILE:HG12 | 1.98 | 0.46 |
| 9:C:1101:ADP:O3' | 9:C:1101:ADP:C8 | 2.69 | 0.46 |
| 3:C:95:THR:HG23 | 9:C:1101:ADP:O1A | 2.15 | 0.46 |
| 4:D:144:LEU:N | 4:D:144:LEU:HD23 | 2.31 | 0.46 |
| 4:D:161:LYS:HD2 | 4:D:161:LYS:HA | 1.66 | 0.46 |
| 4:D:284:ASN:O | 4:D:310:ILE:CG2 | 2.63 | 0.46 |
| 6:F:454:ILE:O | 6:F:457:THR:OG1 | 2.30 | 0.46 |
| 7:G:236:PHE:O | 7:G:239:PRO:CG | 2.64 | 0.46 |
| 7:G:291:ASN:HA | 7:G:312:ILE:HB | 1.97 | 0.46 |
| 8:H:175:GLU:H | 8:H:175:GLU:HG3 | 1.45 | 0.46 |
| 8:H:291:ILE:HD12 | 8:H:347:PRO:HG3 | 1.97 | 0.46 |
| 1:I:224:LEU:CD1 | 1:I:226:CYS:CB | 2.90 | 0.46 |
| 2:J:286:ASN:HD22 | 2:J:287:ARG:N | 2.14 | 0.46 |
| 4:L:241:ILE:N | 4:L:241:ILE:HD12 | 2.30 | 0.46 |
| 4:L:120:ILE:CG1 | 4:L:439:ILE:HG21 | 2.44 | 0.46 |
| 6:N:141:THR:CG2 | 6:N:142:ASN:N | 2.78 | 0.46 |
| 7:O:396:ALA:O | 7:O:397:ILE:C | 2.55 | 0.46 |
| 7:O:418:MET:HE3 | 7:O:447:GLU:HG2 | 1.98 | 0.46 |
| 4:L:9:ALA:CB | 7:O:76:VAL:H | 2.27 | 0.46 |
| 4:D:185:ASN:H | 4:D:187:LYS:N | 2.14 | 0.45 |
| 6:F:243:GLU:OE2 | 6:F:243:GLU:CA | 2.52 | 0.45 |
| 6:F:296:ILE:HD12 | 6:F:328:LEU:HD22 | 1.99 | 0.45 |
| 6:F:540:THR:CB | 6:F:541:LEU:HD22 | 2.44 | 0.45 |
| 6:F:72:THR:O | 6:F:75:LEU:HB3 | 2.16 | 0.45 |
| 7:G:452:GLN:HA | 7:G:455:GLU:HB2 | 1.96 | 0.45 |
| 4:D:521:ILE:CG2 | 7:G:51:ILE:HA | 2.40 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:H:386:LEU:H | 8:H:386:LEU:HD12 | 1.81 | 0.45 |
| 1:I:12:THR:HA | 1:I:13:LEU:HA | 1.69 | 0.45 |
| 1:I:66:GLY:CA | 1:I:99:THR:HG22 | 2.47 | 0.45 |
| 2:J:203:LEU:O | 2:J:204:SER:OG | 2.30 | 0.45 |
| 2:J:219:GLY:HA3 | 2:J:304:ASN:ND2 | 2.31 | 0.45 |
| 2:J:58:ASN:ND2 | 2:J:58:ASN:C | 2.69 | 0.45 |
| 4:L:24:ASN:ND2 | 4:L:524:ILE:HD11 | 2.30 | 0.45 |
| 5:M:103:LEU:HA | 5:M:106:GLN:HE21 | 1.80 | 0.45 |
| 5:M:239:LEU:HD23 | 5:M:240:ILE:N | 2.31 | 0.45 |
| 6:N:153:VAL:CB | 6:N:507:TRP:CB | 2.94 | 0.45 |
| 8:P:169:SER:HB2 | 9:P:601:ADP:O2A | 2.15 | 0.45 |
| 1:A:256:MET:HE3 | 1:A:261:GLN:HA | 1.97 | 0.45 |
| 1:A:420:PRO:O | 1:A:424:CYS:HB3 | 2.16 | 0.45 |
| 2:B:116:HIS:CE1 | 2:B:118:GLN:CB | 2.99 | 0.45 |
| 2:B:116:HIS:HA | 2:B:117:PRO:HD3 | 1.74 | 0.45 |
| 2:B:210:GLU:CB | 2:B:357:SER:O | 2.65 | 0.45 |
| 3:C:335:THR:HB | 8:H:237:LYS:CE | 2.34 | 0.45 |
| 4:D:239:PHE:C | 4:D:290:LYS:HG3 | 2.36 | 0.45 |
| 4:D:325:SER:O | 4:D:329:GLY:N | 2.47 | 0.45 |
| 4:D:418:GLU:HG2 | 4:D:451:PRO:HD3 | 1.98 | 0.45 |
| 4:D:50:THR:HG22 | 4:D:54:GLU:N | 2.31 | 0.45 |
| 4:D:98:ILE:HG12 | 4:D:98:ILE:H | 1.57 | 0.45 |
| 6:F:160:THR:N | 6:F:164:ALA:HB3 | 2.31 | 0.45 |
| 6:F:43:LEU:HD21 | 6:F:161:LYS:CA | 2.42 | 0.45 |
| 1:I:336:THR:HB | 1:I:354:TYR:HD1 | 1.80 | 0.45 |
| 1:I:420:PRO:O | 1:I:424:CYS:HB3 | 2.16 | 0.45 |
| 1:I:433:LEU:O | 1:I:437:ALA:CA | 2.65 | 0.45 |
| 2:J:27:ILE:O | 2:J:27:ILE:HG12 | 2.15 | 0.45 |
| 4:L:182:SER:HB2 | 4:L:187:LYS:CE | 2.46 | 0.45 |
| 4:L:499:GLN:HA | 4:L:500:PRO:HD3 | 1.86 | 0.45 |
| 4:L:50:THR:HG22 | 4:L:54:GLU:N | 2.30 | 0.45 |
| 5:M:396:GLU:HA | 5:M:397:GLN:HA | 1.53 | 0.45 |
| 6:N:296:ILE:HG12 | 6:N:317:LEU:HB2 | 1.98 | 0.45 |
| 6:N:337:GLN:HG2 | 6:N:347:ILE:CD1 | 2.46 | 0.45 |
| 7:O:296:LYS:HA | 7:O:318:VAL:HG23 | 1.97 | 0.45 |
| 7:O:329:ALA:HA | 7:O:371:ALA:HB1 | 1.98 | 0.45 |
| 8:P:426:THR:HG23 | 8:P:427:GLU:N | 2.31 | 0.45 |
| 1:A:69:ILE:O | 1:A:73:LEU:HD13 | 2.15 | 0.45 |
| 2:B:492:LYS:H | 2:B:492:LYS:HZ1 | 1.63 | 0.45 |
| 2:B:411:MET:CE | 2:B:498:VAL:HG21 | 2.46 | 0.45 |
| 3:C:174:LEU:HG | 3:C:219:VAL:CG2 | 2.47 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:142:PRO:HB3 | 3:C:410:PRO:O | 2.15 | 0.45 |
| 4:D:194:ILE:O | 4:D:194:ILE:HG12 | 2.15 | 0.45 |
| 6:F:159:LEU:CA | 6:F:164:ALA:HB2 | 2.41 | 0.45 |
| 6:F:167:THR:CB | 6:F:168:GLU:HB3 | 2.47 | 0.45 |
| 6:F:489:VAL:O | 6:F:490:GLY:C | 2.41 | 0.45 |
| 8:H:426:THR:HG23 | 8:H:427:GLU:N | 2.31 | 0.45 |
| 1:I:210:GLY:O | 1:I:211:LYS:CB | 2.64 | 0.45 |
| 1:I:128:GLY:O | 1:I:448:ILE:HD13 | 2.15 | 0.45 |
| 2:J:293:TYR:O | 2:J:297:LEU:HD23 | 2.17 | 0.45 |
| 3:K:471:LEU:HD12 | 3:K:491:ILE:HG21 | 1.98 | 0.45 |
| 6:N:221:HIS:HB2 | 6:N:224:MET:CG | 2.43 | 0.45 |
| 6:N:420:ILE:HB | 6:N:482:ASP:OD1 | 2.15 | 0.45 |
| 6:N:415:ALA:HA | 9:N:601:ADP:H1' | 1.97 | 0.45 |
| 6:N:79:ALA:HB1 | 6:N:523:ILE:HD11 | 1.98 | 0.45 |
| 8:P:252:CYS:HB2 | 8:P:343:ARG:N | 2.32 | 0.45 |
| 3:C:64:ILE:HG22 | 3:C:65:LEU:N | 2.31 | 0.45 |
| 6:F:122:PHE:HD1 | 6:F:447:PHE:HD1 | 1.63 | 0.45 |
| 1:I:120:ILE:O | 1:I:120:ILE:HD13 | 2.16 | 0.45 |
| 1:I:205:VAL:C | 1:I:206:LEU:HD23 | 2.36 | 0.45 |
| 1:I:419:VAL:HG13 | 1:I:425:VAL:HG21 | 1.98 | 0.45 |
| 1:I:458:ILE:H | 1:I:458:ILE:HD12 | 1.82 | 0.45 |
| 2:J:210:GLU:CB | 2:J:357:SER:O | 2.64 | 0.45 |
| 3:K:230:VAL:HG21 | 3:K:303:ASP:H | 1.80 | 0.45 |
| 3:K:508:GLN:CG | 8:P:215:GLY:HA2 | 2.46 | 0.45 |
| 4:L:30:SER:HA | 4:L:33:ASP:CG | 2.37 | 0.45 |
| 5:M:269:LEU:HD22 | 5:M:269:LEU:N | 2.31 | 0.45 |
| 6:N:221:HIS:CD2 | 6:N:224:MET:SD | 3.09 | 0.45 |
| 7:O:241:ILE:HD12 | 7:O:330:VAL:HG21 | 1.98 | 0.45 |
| 7:O:400:VAL:O | 7:O:404:LEU:HB2 | 2.17 | 0.45 |
| 8:P:386:LEU:H | 8:P:386:LEU:HD12 | 1.81 | 0.45 |
| 1:A:66:GLY:CA | 1:A:99:THR:HG22 | 2.47 | 0.45 |
| 3:C:202:ARG:HH21 | 3:C:323:SER:HB3 | 1.81 | 0.45 |
| 4:D:292:ILE:CG1 | 4:D:293:LEU:HA | 2.47 | 0.45 |
| 5:E:297:LYS:HA | 5:E:297:LYS:HD2 | 1.66 | 0.45 |
| 6:F:337:GLN:HG2 | 6:F:347:ILE:CD1 | 2.46 | 0.45 |
| 7:G:282:LEU:HD23 | 7:G:303:ALA:O | 2.17 | 0.45 |
| 7:G:165:ALA:CB | 7:G:399:ILE:HG21 | 2.46 | 0.45 |
| 8:H:291:ILE:HD12 | 8:H:347:PRO:HG2 | 1.96 | 0.45 |
| 8:H:329:LEU:HD23 | 8:H:329:LEU:O | 2.17 | 0.45 |
| 8:H:101:ASN:N | 9:H:601:ADP:O2B | 2.43 | 0.45 |
| 1:I:86:LEU:HD21 | 1:I:101:VAL:HG12 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:234:ALA:HA | 2:J:325:VAL:HB | 1.99 | 0.45 |
| 2:J:386:ASP:O | 2:J:390:VAL:HG23 | 2.17 | 0.45 |
| 2:J:88:VAL:HG12 | 2:J:89:GLY:N | 2.32 | 0.45 |
| 3:K:64:ILE:HG22 | 3:K:65:LEU:N | 2.32 | 0.45 |
| 4:L:185:ASN:H | 4:L:187:LYS:N | 2.14 | 0.45 |
| 8:P:247:VAL:HG22 | 8:P:248:ALA:N | 2.32 | 0.45 |
| 1:A:205:VAL:C | 1:A:206:LEU:HD23 | 2.36 | 0.45 |
| 1:A:336:THR:HB | 1:A:354:TYR:HD1 | 1.80 | 0.45 |
| 1:A:55:ASP:O | 1:A:57:ILE:N | 2.50 | 0.45 |
| 1:A:86:LEU:HD21 | 1:A:101:VAL:HG12 | 1.99 | 0.45 |
| 3:C:298:GLU:HA | 3:C:320:VAL:H | 1.81 | 0.45 |
| 2:B:4:GLN:CB | 3:C:71:ALA:HB3 | 2.45 | 0.45 |
| 4:D:226:PRO:CG | 4:D:311:MET:HG2 | 2.47 | 0.45 |
| 5:E:189:GLY:O | 5:E:190:SER:HB2 | 2.17 | 0.45 |
| 5:E:439:VAL:HB | 5:E:528:VAL:HG13 | 1.99 | 0.45 |
| 6:F:141:THR:CG2 | 6:F:142:ASN:N | 2.78 | 0.45 |
| 6:F:173:ILE:HD11 | 6:F:209:PHE:N | 2.32 | 0.45 |
| 6:F:238:VAL:HG22 | 6:F:239:SER:N | 2.32 | 0.45 |
| 7:G:317:ARG:HD2 | 7:G:317:ARG:O | 2.16 | 0.45 |
| 8:H:96:MET:CB | 8:H:515:GLU:OE1 | 2.65 | 0.45 |
| 1:I:486:MET:CB | 1:I:487:ALA:HB2 | 2.46 | 0.45 |
| 1:I:69:ILE:O | 1:I:73:LEU:HD13 | 2.16 | 0.45 |
| 2:J:232:LEU:HD22 | 2:J:233:ILE:H | 1.80 | 0.45 |
| 2:J:456:VAL:HG13 | 2:J:457:SER:N | 2.32 | 0.45 |
| 4:L:226:PRO:CG | 4:L:311:MET:HG2 | 2.47 | 0.45 |
| 5:M:439:VAL:HB | 5:M:528:VAL:HG13 | 1.99 | 0.45 |
| 5:M:84:THR:HG22 | 5:M:85:ASN:N | 2.31 | 0.45 |
| 6:N:108:PHE:C | 6:N:108:PHE:CD1 | 2.90 | 0.45 |
| 6:N:238:VAL:HG22 | 6:N:239:SER:N | 2.32 | 0.45 |
| 6:N:399:LEU:HD12 | 6:N:399:LEU:O | 2.17 | 0.45 |
| 7:O:317:ARG:HD2 | 7:O:317:ARG:O | 2.16 | 0.45 |
| 7:O:207:GLY:HA3 | 7:O:379:ARG:HH11 | 1.81 | 0.45 |
| 8:P:464:ALA:HB1 | 8:P:474:VAL:HG21 | 1.98 | 0.45 |
| 8:P:96:MET:CB | 8:P:515:GLU:OE1 | 2.65 | 0.45 |
| 1:A:532:LEU:O | 1:A:536:VAL:HG23 | 2.16 | 0.45 |
| 2:B:30:GLY:HA2 | 2:B:33:VAL:HG21 | 1.97 | 0.45 |
| 2:B:386:ASP:O | 2:B:390:VAL:HG23 | 2.17 | 0.45 |
| 9:C:1101:ADP:O1A | 10:C:1102:BEF:F3 | 2.24 | 0.45 |
| 3:C:230:VAL:HG21 | 3:C:303:ASP:H | 1.80 | 0.45 |
| 3:C:222:GLY:HA3 | 3:C:368:LEU:O | 2.17 | 0.45 |
| 4:D:103:LEU:HD22 | 4:D:515:VAL:HG21 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:F:108:PHE:CE1 | 6:F:118:ILE:HG13 | 2.50 | 0.45 |
| 6:F:296:ILE:HG12 | 6:F:317:LEU:HB2 | 1.98 | 0.45 |
| 1:I:164:MET:HE3 | 1:I:169:ILE:HB | 1.99 | 0.45 |
| 2:J:45:LEU:HB2 | 6:N:533:LEU:HB3 | 1.95 | 0.45 |
| 4:L:299:ASP:OD1 | 4:L:301:ALA:HB3 | 2.16 | 0.45 |
| 4:L:469:LEU:C | 4:L:471:SER:H | 2.19 | 0.45 |
| 9:L:601:ADP:H2' | 9:L:601:ADP:N3 | 2.31 | 0.45 |
| 6:N:173:ILE:HD11 | 6:N:209:PHE:N | 2.32 | 0.45 |
| 6:N:72:THR:O | 6:N:75:LEU:HB3 | 2.16 | 0.45 |
| 7:O:226:TYR:CE1 | 7:O:229:PHE:CB | 3.00 | 0.45 |
| 7:O:291:ASN:HA | 7:O:312:ILE:HB | 1.97 | 0.45 |
| 8:P:63:ILE:HD12 | 8:P:74:GLU:CG | 2.45 | 0.45 |
| 8:P:71:MET:O | 8:P:75:LEU:HG | 2.17 | 0.45 |
| 2:B:219:GLY:HA3 | 2:B:304:ASN:ND2 | 2.31 | 0.45 |
| 2:B:293:TYR:O | 2:B:297:LEU:HD23 | 2.17 | 0.45 |
| 3:C:414:PRO:HG2 | 3:C:481:THR:CG2 | 2.47 | 0.45 |
| 3:C:471:LEU:HD12 | 3:C:491:ILE:HG21 | 1.98 | 0.45 |
| 6:F:207:THR:HB | 6:F:380:ILE:HA | 1.99 | 0.45 |
| 6:F:436:ALA:HA | 6:F:437:LYS:HA | 1.66 | 0.45 |
| 6:F:515:ASN:HD22 | 6:F:515:ASN:C | 2.18 | 0.45 |
| 7:G:249:GLU:O | 7:G:250:LEU:C | 2.55 | 0.45 |
| 8:H:247:VAL:HG22 | 8:H:248:ALA:N | 2.32 | 0.45 |
| 1:I:55:ASP:O | 1:I:57:ILE:N | 2.50 | 0.45 |
| 2:J:469:THR:O | 2:J:470:SER:CB | 2.59 | 0.45 |
| 3:K:10:ALA:HA | 3:K:11:SER:HA | 1.59 | 0.45 |
| 4:L:313:VAL:HG11 | 4:L:361:VAL:HG21 | 1.99 | 0.45 |
| 6:N:491:VAL:HG12 | 6:N:492:ASP:H | 1.82 | 0.45 |
| 6:N:540:THR:CB | 6:N:541:LEU:HD22 | 2.44 | 0.45 |
| 1:A:129:PHE:CD2 | 1:A:129:PHE:N | 2.84 | 0.45 |
| 1:A:25:ILE:HG22 | 1:A:26:ARG:N | 2.32 | 0.45 |
| 2:B:222:GLN:HB3 | 2:B:223:PRO:HD2 | 1.98 | 0.45 |
| 2:B:74:ALA:O | 2:B:78:VAL:HG23 | 2.17 | 0.45 |
| 3:C:219:VAL:HG13 | 3:C:379:ILE:HD12 | 1.99 | 0.45 |
| 5:E:500:SER:O | 5:E:504:LYS:HG2 | 2.17 | 0.45 |
| 6:F:117:ILE:HG12 | 5:M:33:LYS:CE | 2.39 | 0.45 |
| 6:F:92:THR:OG1 | 9:F:601:ADP:PB | 2.74 | 0.45 |
| 7:G:170:LEU:O | 7:G:170:LEU:CD2 | 2.58 | 0.45 |
| 1:I:62:VAL:O | 1:I:397:GLU:HG3 | 2.17 | 0.45 |
| 2:J:88:VAL:CG1 | 2:J:393:GLN:HE22 | 2.22 | 0.45 |
| 2:J:40:LYS:HA | 6:N:116:ARG:HG3 | 1.99 | 0.45 |
| 3:K:229:VAL:HG11 | 3:K:234:MET:HE2 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:M:267:VAL:HG12 | 5:M:268:LYS:N | 2.32 | 0.45 |
| 5:M:456:GLU:HA | 5:M:456:GLU:OE2 | 2.17 | 0.45 |
| 5:M:500:SER:O | 5:M:504:LYS:HG2 | 2.17 | 0.45 |
| 6:N:167:THR:CA | 6:N:168:GLU:CB | 2.95 | 0.45 |
| 6:N:178:VAL:HG21 | 6:N:402:VAL:CG1 | 2.47 | 0.45 |
| 6:N:166:LEU:CD2 | 6:N:205:LYS:HA | 2.47 | 0.45 |
| 6:N:207:THR:HB | 6:N:380:ILE:HA | 1.99 | 0.45 |
| 6:N:296:ILE:HD12 | 6:N:328:LEU:HD22 | 1.99 | 0.45 |
| 6:N:330:LEU:O | 6:N:372:ASP:O | 2.34 | 0.45 |
| 7:O:438:ILE:HD12 | 7:O:438:ILE:N | 2.32 | 0.45 |
| 1:A:120:ILE:HD13 | 1:A:120:ILE:O | 2.16 | 0.45 |
| 2:B:368:VAL:O | 2:B:377:LEU:HD23 | 2.17 | 0.45 |
| 2:B:456:VAL:HG13 | 2:B:457:SER:N | 2.32 | 0.45 |
| 3:C:402:VAL:HG13 | 3:C:502:PRO:CG | 2.45 | 0.45 |
| 5:E:150:PHE:CD1 | 5:E:472:PHE:HE2 | 2.35 | 0.45 |
| 5:E:255:PRO:HG3 | 5:E:336:LEU:CB | 2.47 | 0.45 |
| 5:E:84:THR:HA | 5:E:418:GLU:OE1 | 2.17 | 0.45 |
| 6:F:342:ASP:CG | 6:F:345:PRO:HG2 | 2.38 | 0.45 |
| 6:F:399:LEU:HD12 | 6:F:399:LEU:O | 2.17 | 0.45 |
| 6:F:491:VAL:HG12 | 6:F:492:ASP:H | 1.82 | 0.45 |
| 7:G:159:GLU:O | 7:G:179:VAL:HG11 | 2.17 | 0.45 |
| 8:H:332:LEU:O | 8:H:335:VAL:HB | 2.17 | 0.45 |
| 8:H:335:VAL:HG13 | 8:H:379:SER:CB | 2.46 | 0.45 |
| 8:H:252:CYS:HB2 | 8:H:343:ARG:N | 2.32 | 0.45 |
| 8:H:62:ILE:HD13 | 8:H:63:ILE:N | 2.32 | 0.45 |
| 1:I:129:PHE:N | 1:I:129:PHE:CD2 | 2.84 | 0.45 |
| 1:I:218:LEU:HD23 | 1:I:385:ILE:HG12 | 1.98 | 0.45 |
| 2:J:222:GLN:HB3 | 2:J:223:PRO:HD2 | 1.98 | 0.45 |
| 3:K:222:GLY:HA3 | 3:K:368:LEU:O | 2.17 | 0.45 |
| 4:L:418:GLU:HG2 | 4:L:451:PRO:HD3 | 1.98 | 0.45 |
| 2:J:32:LEU:HD12 | 6:N:532:GLU:OE2 | 2.17 | 0.45 |
| 6:N:539:SER:HB2 | 6:N:542:LYS:HD3 | 1.99 | 0.45 |
| 7:O:204:ILE:HA | 7:O:205:PRO:HD3 | 1.79 | 0.45 |
| 8:P:134:ALA:O | 8:P:138:THR:HG23 | 2.17 | 0.45 |
| 1:A:120:ILE:HG21 | 1:A:125:ILE:CG1 | 2.47 | 0.44 |
| 2:B:203:LEU:O | 2:B:204:SER:OG | 2.30 | 0.44 |
| 2:B:411:MET:HG2 | 2:B:411:MET:H | 1.53 | 0.44 |
| 3:C:495:VAL:HG23 | 3:C:500:TRP:CH2 | 2.49 | 0.44 |
| 4:D:147:ARG:O | 4:D:151:VAL:HG23 | 2.16 | 0.44 |
| 4:D:299:ASP:OD1 | 4:D:301:ALA:HB3 | 2.16 | 0.44 |
| 4:D:238:GLN:HE22 | 4:D:318:ARG:NH1 | 2.15 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:E:184:ALA:O | 5:E:188:LEU:CB | 2.64 | 0.44 |
| 5:E:84:THR:O | 5:E:90:ILE:HD11 | 2.18 | 0.44 |
| 6:F:122:PHE:CD1 | 6:F:447:PHE:HD1 | 2.35 | 0.44 |
| 6:F:231:ALA:O | 6:F:351:SER:OG | 2.22 | 0.44 |
| 6:F:83:GLN:OE1 | 6:F:515:ASN:ND2 | 2.50 | 0.44 |
| 6:F:539:SER:HB2 | 6:F:542:LYS:HD3 | 2.00 | 0.44 |
| 7:G:438:ILE:HD12 | 7:G:438:ILE:N | 2.32 | 0.44 |
| 3:K:250:LEU:CG | 3:K:301:VAL:CB | 2.92 | 0.44 |
| 4:L:181:ILE:HD11 | 4:L:375:VAL:HG23 | 1.98 | 0.44 |
| 6:N:122:PHE:CD1 | 6:N:447:PHE:HD1 | 2.35 | 0.44 |
| 6:N:167:THR:CB | 6:N:168:GLU:HB3 | 2.47 | 0.44 |
| 6:N:422:LEU:HD13 | 6:N:517:ILE:HD11 | 1.98 | 0.44 |
| 7:O:109:MET:SD | 7:O:514:THR:CB | 3.05 | 0.44 |
| 7:O:123:HIS:ND1 | 7:O:123:HIS:N | 2.65 | 0.44 |
| 4:L:524:ILE:CB | 7:O:52:LEU:O | 2.64 | 0.44 |
| 8:P:428:ILE:CD1 | 8:P:478:LEU:HD13 | 2.48 | 0.44 |
| 1:A:221:GLY:HA2 | 1:A:382:SER:CB | 2.42 | 0.44 |
| 1:A:419:VAL:HG13 | 1:A:425:VAL:HG21 | 1.98 | 0.44 |
| 1:A:433:LEU:O | 1:A:437:ALA:CA | 2.64 | 0.44 |
| 2:B:37:LEU:CB | 2:B:444:LEU:HD13 | 2.47 | 0.44 |
| 5:E:271:ILE:CB | 5:E:362:ILE:HA | 2.48 | 0.44 |
| 5:E:387:THR:HA | 5:E:388:THR:HA | 1.61 | 0.44 |
| 6:F:153:VAL:CB | 6:F:507:TRP:CB | 2.94 | 0.44 |
| 6:F:433:LYS:HG3 | 6:F:444:ILE:CG2 | 2.46 | 0.44 |
| 7:G:109:MET:SD | 7:G:514:THR:CB | 3.05 | 0.44 |
| 7:G:241:ILE:HD12 | 7:G:330:VAL:HG21 | 1.98 | 0.44 |
| 8:H:256:ILE:HD13 | 8:H:280:GLU:OE1 | 2.17 | 0.44 |
| 1:I:112:ALA:HB1 | 1:I:539:LEU:HD21 | 1.98 | 0.44 |
| 2:J:370:ARG:O | 2:J:372:ALA:N | 2.50 | 0.44 |
| 3:K:414:PRO:HG2 | 3:K:481:THR:CG2 | 2.47 | 0.44 |
| 4:L:521:ILE:CG2 | 7:O:52:LEU:N | 2.78 | 0.44 |
| 5:M:84:THR:HA | 5:M:418:GLU:OE1 | 2.17 | 0.44 |
| 5:M:73:ILE:O | 5:M:74:LEU:HD22 | 2.17 | 0.44 |
| 6:N:214:VAL:HG22 | 6:N:377:THR:OG1 | 2.18 | 0.44 |
| 6:N:90:GLY:O | 6:N:94:VAL:CG2 | 2.34 | 0.44 |
| 7:O:159:GLU:O | 7:O:179:VAL:HG11 | 2.17 | 0.44 |
| 7:O:241:ILE:HD12 | 7:O:330:VAL:CG2 | 2.48 | 0.44 |
| 8:P:62:ILE:HD13 | 8:P:63:ILE:N | 2.32 | 0.44 |
| 4:D:370:ASN:O | 4:D:373:PRO:HD3 | 2.18 | 0.44 |
| 5:E:267:VAL:HG12 | 5:E:268:LYS:N | 2.32 | 0.44 |
| 5:E:351:LEU:HD22 | 5:E:352:GLU:H | 1.82 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:F:108:PHE:CD1 | 6:F:108:PHE:C | 2.90 | 0.44 |
| 7:G:329:ALA:HA | 7:G:371:ALA:HB1 | 1.98 | 0.44 |
| 7:G:452:GLN:CD | 7:G:452:GLN:H | 2.21 | 0.44 |
| 8:H:428:ILE:CD1 | 8:H:478:LEU:HD13 | 2.48 | 0.44 |
| 2:J:224:LYS:O | 2:J:343:ILE:HA | 2.16 | 0.44 |
| 3:K:457:ILE:HD13 | 3:K:467:LEU:CD1 | 2.19 | 0.44 |
| 5:M:189:GLY:O | 5:M:190:SER:HB2 | 2.17 | 0.44 |
| 5:M:340:LEU:H | 5:M:340:LEU:HD23 | 1.81 | 0.44 |
| 5:M:450:MET:HE3 | 5:M:454:VAL:CG2 | 2.47 | 0.44 |
| 6:N:330:LEU:HB3 | 6:N:375:SER:OG | 2.17 | 0.44 |
| 7:O:244:LEU:HB3 | 7:O:246:VAL:HG22 | 1.99 | 0.44 |
| 1:A:90:GLN:HE21 | 1:A:527:SER:HB3 | 1.83 | 0.44 |
| 2:B:417:THR:HG23 | 2:B:418:GLU:N | 2.33 | 0.44 |
| 2:B:42:MET:HE3 | 2:B:42:MET:HA | 2.00 | 0.44 |
| 4:D:12:LYS:HZ2 | 7:G:73:LEU:HD22 | 1.82 | 0.44 |
| 4:D:209:MET:HE3 | 4:D:375:VAL:HG11 | 2.00 | 0.44 |
| 4:D:313:VAL:HG11 | 4:D:361:VAL:HG21 | 1.99 | 0.44 |
| 5:E:340:LEU:HD23 | 5:E:340:LEU:H | 1.81 | 0.44 |
| 6:F:101:LEU:HD23 | 6:F:101:LEU:O | 2.17 | 0.44 |
| 8:H:134:ALA:O | 8:H:138:THR:HG23 | 2.17 | 0.44 |
| 3:C:515:GLU:CD | 8:H:389:ALA:HB3 | 2.38 | 0.44 |
| 1:I:54:VAL:HG12 | 1:I:56:ASP:N | 2.29 | 0.44 |
| 1:I:91:ASP:HA | 1:I:95:GLY:HA2 | 2.00 | 0.44 |
| 4:L:417:PRO:O | 4:L:421:ILE:HG12 | 2.16 | 0.44 |
| 6:N:101:LEU:HD23 | 6:N:101:LEU:O | 2.17 | 0.44 |
| 5:E:37:ASN:HB2 | 6:N:114:HIS:HA | 2.00 | 0.44 |
| 6:N:159:LEU:CA | 6:N:164:ALA:HB2 | 2.41 | 0.44 |
| 8:P:101:ASN:N | 8:P:101:ASN:HD22 | 2.16 | 0.44 |
| 8:P:332:LEU:O | 8:P:335:VAL:HB | 2.17 | 0.44 |
| 8:P:209:VAL:CG2 | 8:P:386:LEU:HD11 | 2.35 | 0.44 |
| 1:A:120:ILE:CG2 | 1:A:121:HIS:N | 2.81 | 0.44 |
| 1:A:62:VAL:O | 1:A:397:GLU:HG3 | 2.17 | 0.44 |
| 3:C:463:ASP:O | 3:C:467:LEU:HB2 | 2.18 | 0.44 |
| 4:D:181:ILE:HD11 | 4:D:375:VAL:HG23 | 1.98 | 0.44 |
| 5:E:276:PHE:HB3 | 5:E:327:PHE:HA | 2.00 | 0.44 |
| 5:E:456:GLU:HA | 5:E:456:GLU:OE2 | 2.17 | 0.44 |
| 6:F:114:HIS:CD2 | 5:M:37:ASN:HD22 | 2.35 | 0.44 |
| 6:F:36:ASN:HB3 | 6:F:57:LYS:HZ3 | 0.68 | 0.44 |
| 6:F:330:LEU:HB3 | 6:F:375:SER:OG | 2.17 | 0.44 |
| 6:F:89:ASP:OD1 | 9:F:601:ADP:O1B | 2.35 | 0.44 |
| 7:G:226:TYR:CE1 | 7:G:229:PHE:CB | 3.00 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:G:241:ILE:HD12 | 7:G:330:VAL:CG2 | 2.48 | 0.44 |
| 7:G:244:LEU:HB3 | 7:G:246:VAL:HG22 | 1.99 | 0.44 |
| 8:H:424:GLY:O | 8:H:428:ILE:HG13 | 2.18 | 0.44 |
| 8:H:6:PRO:CB | 8:H:7:GLN:CA | 2.93 | 0.44 |
| 1:I:183:ALA:CB | 1:I:383:SER:HB2 | 2.47 | 0.44 |
| 2:J:243:VAL:HG12 | 2:J:245:ILE:N | 2.29 | 0.44 |
| 2:J:74:ALA:O | 2:J:78:VAL:HG23 | 2.17 | 0.44 |
| 4:L:219:ALA:HB1 | 4:L:221:LYS:HZ3 | 1.83 | 0.44 |
| 4:L:238:GLN:HE22 | 4:L:318:ARG:NH1 | 2.15 | 0.44 |
| 4:L:370:ASN:O | 4:L:373:PRO:HD3 | 2.18 | 0.44 |
| 4:L:134:ILE:HB | 4:L:421:ILE:CD1 | 2.48 | 0.44 |
| 5:M:340:LEU:HA | 5:M:341:PRO:HD3 | 1.83 | 0.44 |
| 5:M:373:LYS:HE2 | 6:N:311:LYS:NZ | 2.31 | 0.44 |
| 6:N:141:THR:CB | 6:N:409:LYS:HG3 | 2.45 | 0.44 |
| 6:N:503:ILE:O | 6:N:503:ILE:HG22 | 2.18 | 0.44 |
| 7:O:170:LEU:CD2 | 7:O:170:LEU:O | 2.58 | 0.44 |
| 7:O:186:VAL:HG21 | 7:O:400:VAL:HG22 | 1.98 | 0.44 |
| 8:P:155:ASP:HB3 | 8:P:156:LYS:H | 1.48 | 0.44 |
| 8:P:256:ILE:HD13 | 8:P:280:GLU:OE1 | 2.17 | 0.44 |
| 8:P:329:LEU:HD23 | 8:P:329:LEU:O | 2.17 | 0.44 |
| 8:P:113:VAL:CG1 | 8:P:451:GLN:HG3 | 2.37 | 0.44 |
| 1:A:112:ALA:HB1 | 1:A:539:LEU:HD21 | 1.98 | 0.44 |
| 1:A:17:GLY:HA2 | 1:A:546:THR:O | 2.18 | 0.44 |
| 2:B:186:GLY:HA2 | 2:B:187:SER:HA | 1.47 | 0.44 |
| 2:B:36:THR:HG22 | 2:B:42:MET:O | 2.18 | 0.44 |
| 2:B:389:SER:O | 2:B:393:GLN:HG3 | 2.17 | 0.44 |
| 4:D:7:SER:HA | 7:G:35:ALA:HB1 | 2.00 | 0.44 |
| 5:E:429:VAL:O | 5:E:432:ASN:HB2 | 2.18 | 0.44 |
| 6:F:166:LEU:CD2 | 6:F:205:LYS:HA | 2.47 | 0.44 |
| 4:D:273:ASN:ND2 | 7:G:268:GLN:HE22 | 2.15 | 0.44 |
| 8:H:113:VAL:CG1 | 8:H:451:GLN:HG3 | 2.37 | 0.44 |
| 1:I:120:ILE:CG2 | 1:I:121:HIS:N | 2.81 | 0.44 |
| 1:I:90:GLN:HE21 | 1:I:527:SER:HB3 | 1.83 | 0.44 |
| 1:I:532:LEU:O | 1:I:536:VAL:HG23 | 2.16 | 0.44 |
| 1:I:538:ILE:HA | 1:I:541:ILE:HD12 | 2.00 | 0.44 |
| 1:I:17:GLY:HA2 | 1:I:546:THR:O | 2.18 | 0.44 |
| 1:I:16:GLY:CA | 1:I:548:ASP:HB3 | 2.44 | 0.44 |
| 2:J:8:ASP:OD1 | 2:J:8:ASP:N | 2.51 | 0.44 |
| 3:K:219:VAL:HG13 | 3:K:379:ILE:HD12 | 1.99 | 0.44 |
| 5:M:314:LYS:HZ1 | 5:M:338:ASN:HA | 1.82 | 0.44 |
| 6:N:209:PHE:CE2 | 6:N:376:CYS:SG | 2.97 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:250:PHE:CB | 6:N:250:GLY:O | 2.65 | 0.44 |
| 6:N:430:ASN:CA | 6:N:433:LYS:HB2 | 2.48 | 0.44 |
| 7:O:454:CYS:HB2 | 7:O:461:ALA:HB1 | 1.98 | 0.44 |
| 1:A:120:ILE:HG21 | 1:A:125:ILE:HG12 | 2.00 | 0.44 |
| 2:B:482:MET:SD | 2:B:487:ILE:HB | 2.58 | 0.44 |
| 3:C:114:LYS:CA | 3:C:115:ASN:CB | 2.94 | 0.44 |
| 3:C:306:GLN:C | 3:C:310:LEU:HG | 2.37 | 0.44 |
| 5:E:535:LYS:C | 5:E:535:LYS:HD2 | 2.38 | 0.44 |
| 6:F:79:ALA:HB1 | 6:F:523:ILE:HD11 | 1.98 | 0.44 |
| 7:G:396:ALA:O | 7:G:397:ILE:C | 2.55 | 0.44 |
| 1:I:120:ILE:HG21 | 1:I:125:ILE:CG1 | 2.48 | 0.44 |
| 1:I:419:VAL:HA | 1:I:420:PRO:HD3 | 1.86 | 0.44 |
| 2:J:231:ILE:HG12 | 2:J:231:ILE:H | 1.60 | 0.44 |
| 5:M:351:LEU:HD22 | 5:M:352:GLU:H | 1.83 | 0.44 |
| 6:N:195:GLU:HG2 | 6:N:197:MET:CE | 2.48 | 0.44 |
| 6:N:83:GLN:OE1 | 6:N:515:ASN:ND2 | 2.51 | 0.44 |
| 8:P:15:LYS:HG3 | 8:P:16:GLN:H | 1.83 | 0.44 |
| 1:A:350:PHE:HE2 | 1:A:354:TYR:CB | 2.16 | 0.44 |
| 1:A:458:ILE:H | 1:A:458:ILE:HD12 | 1.82 | 0.44 |
| 3:C:28:ALA:HB2 | 3:C:74:ALA:O | 2.18 | 0.44 |
| 4:D:234:ILE:HB | 4:D:345:ASP:HB2 | 2.00 | 0.44 |
| 4:D:134:ILE:HB | 4:D:421:ILE:CD1 | 2.48 | 0.44 |
| 6:F:174:VAL:O | 6:F:178:VAL:HG23 | 2.18 | 0.44 |
| 7:G:123:HIS:N | 7:G:123:HIS:ND1 | 2.65 | 0.44 |
| 8:H:243:LYS:HA | 8:H:243:LYS:HD3 | 1.87 | 0.44 |
| 8:H:393:ASN:O | 8:H:397:ILE:HG13 | 2.18 | 0.44 |
| 5:E:492:ILE:CD1 | 2:J:115:ILE:HG12 | 2.45 | 0.44 |
| 2:J:37:LEU:CB | 2:J:444:LEU:HD13 | 2.47 | 0.44 |
| 2:J:482:MET:SD | 2:J:487:ILE:HB | 2.57 | 0.44 |
| 2:J:92:THR:HA | 2:J:95:VAL:HG23 | 2.00 | 0.44 |
| 5:M:255:PRO:HG3 | 5:M:336:LEU:CB | 2.47 | 0.44 |
| 6:N:124:ILE:HB | 6:N:444:ILE:CD1 | 2.48 | 0.44 |
| 6:N:370:ASN:N | 6:N:370:ASN:HD22 | 2.14 | 0.44 |
| 6:N:422:LEU:O | 6:N:426:LEU:HB2 | 2.17 | 0.44 |
| 7:O:162:ALA:CB | 7:O:179:VAL:HG13 | 2.47 | 0.44 |
| 7:O:282:LEU:HD23 | 7:O:303:ALA:O | 2.17 | 0.44 |
| 1:A:129:PHE:CB | 1:A:532:LEU:HD21 | 2.48 | 0.44 |
| 1:A:185:LEU:HD23 | 1:A:185:LEU:HA | 1.85 | 0.44 |
| 1:A:267:PRO:CA | 1:A:268:GLU:CB | 2.95 | 0.44 |
| 1:A:143:VAL:HG11 | 1:A:425:VAL:HG22 | 1.99 | 0.44 |
| 2:B:231:ILE:HG22 | 2:B:232:LEU:H | 1.83 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:237:THR:N | 2:B:287:ARG:HD2 | 2.28 | 0.44 |
| 2:B:234:ALA:HA | 2:B:325:VAL:HB | 1.99 | 0.44 |
| 2:B:459:LEU:HD13 | 2:B:472:LEU:HD23 | 2.00 | 0.44 |
| 4:D:485:ARG:H | 4:D:485:ARG:CD | 2.27 | 0.44 |
| 5:E:107:LEU:CD2 | 5:E:544:LEU:HG | 2.35 | 0.44 |
| 6:F:167:THR:CA | 6:F:168:GLU:CB | 2.95 | 0.44 |
| 6:F:178:VAL:HG21 | 6:F:402:VAL:CG1 | 2.47 | 0.44 |
| 6:F:190:ASP:O | 6:F:193:MET:HG2 | 2.18 | 0.44 |
| 6:F:238:VAL:HG22 | 6:F:239:SER:H | 1.83 | 0.44 |
| 6:F:451:LEU:O | 6:F:455:PRO:CG | 2.66 | 0.44 |
| 7:G:400:VAL:O | 7:G:404:LEU:HB2 | 2.17 | 0.44 |
| 1:I:16:GLY:HA3 | 1:I:548:ASP:CB | 2.45 | 0.44 |
| 1:I:267:PRO:CA | 1:I:268:GLU:CB | 2.95 | 0.44 |
| 2:J:100:ALA:O | 2:J:104:ARG:HG3 | 2.18 | 0.44 |
| 2:J:389:SER:O | 2:J:393:GLN:HG3 | 2.17 | 0.44 |
| 2:J:401:VAL:HG22 | 2:J:402:LEU:N | 2.33 | 0.44 |
| 3:K:350:THR:HG22 | 3:K:350:THR:O | 2.18 | 0.44 |
| 3:K:483:GLY:O | 3:K:491:ILE:HB | 2.18 | 0.44 |
| 3:K:50:ASP:OD1 | 3:K:54:GLY:HA3 | 2.18 | 0.44 |
| 4:L:379:ILE:HD12 | 4:L:379:ILE:N | 2.33 | 0.44 |
| 5:M:150:PHE:CD1 | 5:M:472:PHE:HE2 | 2.35 | 0.44 |
| 6:N:143:LEU:CD1 | 6:N:145:ASN:CB | 2.96 | 0.44 |
| 6:N:280:LEU:CD1 | 6:N:343:LEU:HD11 | 2.48 | 0.44 |
| 7:O:382:ALA:O | 7:O:386:ILE:HG13 | 2.18 | 0.44 |
| 7:O:454:CYS:CB | 7:O:461:ALA:HA | 2.48 | 0.44 |
| 2:B:100:ALA:O | 2:B:104:ARG:HG3 | 2.18 | 0.43 |
| 2:B:102:LEU:HD23 | 2:B:102:LEU:C | 2.39 | 0.43 |
| 3:C:467:LEU:HD21 | 3:C:491:ILE:CG2 | 2.46 | 0.43 |
| 3:C:523:VAL:HG22 | 8:H:54:ILE:CD1 | 2.48 | 0.43 |
| 4:D:125:GLN:HB2 | 7:G:173:ASN:ND2 | 2.32 | 0.43 |
| 5:E:142:HIS:CD2 | 5:E:144:ILE:HB | 2.53 | 0.43 |
| 5:E:314:LYS:HZ1 | 5:E:338:ASN:HA | 1.83 | 0.43 |
| 5:E:346:VAL:O | 5:E:347:GLY:C | 2.57 | 0.43 |
| 6:F:105:ALA:HA | 6:F:108:PHE:CE2 | 2.54 | 0.43 |
| 6:F:195:GLU:OE1 | 6:F:197:MET:CE | 2.65 | 0.43 |
| 6:F:422:LEU:O | 6:F:426:LEU:HB2 | 2.17 | 0.43 |
| 7:G:303:ALA:O | 7:G:307:PHE:CD2 | 2.70 | 0.43 |
| 7:G:454:CYS:HB2 | 7:G:461:ALA:HB1 | 1.98 | 0.43 |
| 7:G:62:ILE:O | 7:G:62:ILE:HG23 | 2.17 | 0.43 |
| 8:H:71:MET:O | 8:H:75:LEU:HG | 2.17 | 0.43 |
| 1:I:120:ILE:HG21 | 1:I:125:ILE:HG12 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:143:VAL:HG11 | 1:I:425:VAL:HG22 | 1.99 | 0.43 |
| 3:K:174:LEU:HG | 3:K:219:VAL:CG2 | 2.47 | 0.43 |
| 3:K:35:ILE:C | 3:K:37:THR:H | 2.21 | 0.43 |
| 3:K:28:ALA:HB2 | 3:K:74:ALA:O | 2.18 | 0.43 |
| 5:M:132:GLN:HA | 5:M:132:GLN:NE2 | 2.32 | 0.43 |
| 6:N:342:ASP:CG | 6:N:345:PRO:HG2 | 2.38 | 0.43 |
| 7:O:249:GLU:O | 7:O:250:LEU:C | 2.55 | 0.43 |
| 7:O:62:ILE:O | 7:O:62:ILE:HG23 | 2.17 | 0.43 |
| 8:P:291:ILE:HD12 | 8:P:347:PRO:HG2 | 1.96 | 0.43 |
| 8:P:6:PRO:CB | 8:P:7:GLN:HG3 | 2.38 | 0.43 |
| 2:B:370:ARG:O | 2:B:372:ALA:N | 2.50 | 0.43 |
| 2:B:88:VAL:HG12 | 2:B:89:GLY:N | 2.32 | 0.43 |
| 3:C:219:VAL:O | 3:C:219:VAL:HG12 | 2.18 | 0.43 |
| 3:C:35:ILE:C | 3:C:37:THR:H | 2.22 | 0.43 |
| 3:C:441:PRO:O | 3:C:444:ALA:HB3 | 2.18 | 0.43 |
| 3:C:51:PRO:O | 3:C:52:MET:CG | 2.63 | 0.43 |
| 5:E:396:GLU:HA | 5:E:397:GLN:HA | 1.53 | 0.43 |
| 5:E:450:MET:HE3 | 5:E:454:VAL:CG2 | 2.47 | 0.43 |
| 1:A:12:THR:CG2 | 5:E:97:ASP:H | 2.24 | 0.43 |
| 6:F:538:ARG:CG | 6:F:538:ARG:NH1 | 2.72 | 0.43 |
| 7:G:30:ILE:O | 7:G:33:CYS:HB3 | 2.19 | 0.43 |
| 7:G:346:LEU:HD23 | 7:G:346:LEU:N | 2.33 | 0.43 |
| 8:H:15:LYS:HG3 | 8:H:16:GLN:H | 1.83 | 0.43 |
| 1:I:25:ILE:HG22 | 1:I:26:ARG:N | 2.32 | 0.43 |
| 3:K:114:LYS:CA | 3:K:115:ASN:CB | 2.94 | 0.43 |
| 3:K:467:LEU:HD21 | 3:K:491:ILE:CG2 | 2.46 | 0.43 |
| 3:K:48:LEU:HD21 | 3:K:64:ILE:HD13 | 1.99 | 0.43 |
| 4:L:236:LEU:O | 4:L:332:PRO:HA | 2.18 | 0.43 |
| 4:L:94:THR:HG23 | 9:L:601:ADP:O3B | 2.18 | 0.43 |
| 5:M:276:PHE:HB3 | 5:M:327:PHE:HA | 2.00 | 0.43 |
| 9:M:601:ADP:C4' | 9:M:601:ADP:C8 | 3.01 | 0.43 |
| 6:N:190:ASP:O | 6:N:193:MET:HG2 | 2.18 | 0.43 |
| 6:N:234:LEU:HD12 | 6:N:280:LEU:HD11 | 2.00 | 0.43 |
| 7:O:492:PHE:CB | 7:O:497:TRP:HZ2 | 2.31 | 0.43 |
| 1:A:532:LEU:HD22 | 1:A:536:VAL:CG2 | 2.48 | 0.43 |
| 9:B:601:ADP:O1A | 9:B:601:ADP:O3' | 2.29 | 0.43 |
| 3:C:10:ALA:HA | 3:C:11:SER:HA | 1.59 | 0.43 |
| 3:C:162:LYS:C | 3:C:164:VAL:H | 2.22 | 0.43 |
| 3:C:318:ARG:O | 3:C:319:ARG:C | 2.56 | 0.43 |
| 3:C:457:ILE:HD13 | 3:C:467:LEU:CD1 | 2.19 | 0.43 |
| 3:C:48:LEU:HD21 | 3:C:64:ILE:HD13 | 1.99 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:508:GLN:CG | 8:H:215:GLY:HA2 | 2.46 | 0.43 |
| 4:D:146:ASP:HB2 | 4:D:149:GLN:HB2 | 2.00 | 0.43 |
| 4:D:184:GLU:HA | 4:D:187:LYS:HG2 | 2.00 | 0.43 |
| 6:F:147:ARG:HH22 | 6:F:409:LYS:HA | 1.84 | 0.43 |
| 6:F:280:LEU:CD1 | 6:F:343:LEU:HD11 | 2.48 | 0.43 |
| 7:G:448:VAL:HA | 7:G:451:ARG:HB2 | 2.00 | 0.43 |
| 1:I:494:ARG:CB | 1:I:496:SER:H | 2.21 | 0.43 |
| 2:J:146:LYS:HD3 | 2:J:146:LYS:N | 2.33 | 0.43 |
| 2:J:36:THR:HG22 | 2:J:42:MET:O | 2.18 | 0.43 |
| 3:K:209:ILE:HG23 | 3:K:382:ARG:HA | 1.99 | 0.43 |
| 3:K:463:ASP:O | 3:K:467:LEU:HB2 | 2.18 | 0.43 |
| 4:L:517:SER:O | 4:L:521:ILE:HG13 | 2.19 | 0.43 |
| 5:M:346:VAL:O | 5:M:347:GLY:C | 2.57 | 0.43 |
| 6:N:105:ALA:HA | 6:N:108:PHE:CE2 | 2.54 | 0.43 |
| 6:N:11:GLU:OE2 | 6:N:11:GLU:N | 2.52 | 0.43 |
| 6:N:362:GLU:CG | 6:N:364:PHE:CE2 | 2.93 | 0.43 |
| 6:N:83:GLN:HB2 | 6:N:91:THR:HG22 | 2.00 | 0.43 |
| 7:O:165:ALA:CB | 7:O:399:ILE:HG21 | 2.46 | 0.43 |
| 7:O:409:ILE:CG2 | 7:O:410:VAL:H | 2.28 | 0.43 |
| 7:O:452:GLN:CD | 7:O:452:GLN:H | 2.21 | 0.43 |
| 8:P:250:PHE:N | 8:P:250:PHE:CD2 | 2.86 | 0.43 |
| 8:P:311:HIS:CG | 8:P:312:TYR:N | 2.86 | 0.43 |
| 8:P:338:ALA:N | 8:P:353:GLY:HA3 | 2.33 | 0.43 |
| 8:P:393:ASN:O | 8:P:397:ILE:HG13 | 2.18 | 0.43 |
| 1:A:118:ASN:O | 1:A:119:LYS:CG | 2.65 | 0.43 |
| 1:A:538:ILE:HA | 1:A:541:ILE:HD12 | 2.00 | 0.43 |
| 2:B:146:LYS:HD3 | 2:B:146:LYS:N | 2.33 | 0.43 |
| 2:B:5:ILE:O | 3:C:70:VAL:HA | 2.18 | 0.43 |
| 3:C:129:LEU:HD21 | 3:C:511:LYS:HA | 2.00 | 0.43 |
| 4:D:242:SER:HB3 | 4:D:298:ASN:HB2 | 2.00 | 0.43 |
| 4:D:518:ILE:HA | 4:D:521:ILE:HD12 | 2.01 | 0.43 |
| 6:F:171:THR:CB | 6:F:172:PRO:HD3 | 2.48 | 0.43 |
| 6:F:209:PHE:HZ | 6:F:211:LYS:HD2 | 1.83 | 0.43 |
| 6:F:214:VAL:HG22 | 6:F:377:THR:OG1 | 2.18 | 0.43 |
| 7:G:454:CYS:CB | 7:G:461:ALA:HA | 2.48 | 0.43 |
| 7:G:492:PHE:CB | 7:G:497:TRP:HZ2 | 2.31 | 0.43 |
| 7:G:82:THR:HG21 | 7:G:517:ILE:HD11 | 1.99 | 0.43 |
| 8:H:311:HIS:CG | 8:H:312:TYR:N | 2.86 | 0.43 |
| 1:I:351:GLU:OE2 | 1:I:351:GLU:N | 2.51 | 0.43 |
| 3:K:310:LEU:HD21 | 3:K:316:VAL:HG22 | 1.99 | 0.43 |
| 3:K:318:ARG:O | 3:K:319:ARG:C | 2.56 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:L:161:LYS:HD2 | 4:L:161:LYS:HA | 1.66 | 0.43 |
| 5:M:142:HIS:CD2 | 5:M:144:ILE:HB | 2.53 | 0.43 |
| 5:M:271:ILE:CB | 5:M:362:ILE:HA | 2.48 | 0.43 |
| 6:N:171:THR:CB | 6:N:172:PRO:HD3 | 2.48 | 0.43 |
| 6:N:195:GLU:OE1 | 6:N:197:MET:CE | 2.65 | 0.43 |
| 6:N:195:GLU:CD | 6:N:197:MET:SD | 2.97 | 0.43 |
| 6:N:221:HIS:HA | 6:N:222:PRO:HD3 | 1.92 | 0.43 |
| 6:N:185:GLN:HB3 | 6:N:407:LYS:HD3 | 2.00 | 0.43 |
| 2:J:32:LEU:HG | 6:N:532:GLU:CD | 2.37 | 0.43 |
| 4:L:72:HIS:CD2 | 8:P:15:LYS:HZ2 | 2.37 | 0.43 |
| 8:P:467:ALA:HB2 | 8:P:493:ASP:CB | 2.49 | 0.43 |
| 1:A:177:SER:O | 1:A:181:VAL:HG23 | 2.19 | 0.43 |
| 2:B:169:ASP:HB2 | 2:B:172:HIS:HB2 | 2.00 | 0.43 |
| 2:B:226:ILE:HG13 | 2:B:282:ASN:OD1 | 2.18 | 0.43 |
| 3:C:152:LYS:HG2 | 3:C:176:LEU:HG | 2.01 | 0.43 |
| 3:C:61:GLY:CA | 3:C:94:THR:HG22 | 2.49 | 0.43 |
| 4:D:248:THR:O | 4:D:250:ASN:OD1 | 2.37 | 0.43 |
| 4:D:30:SER:HA | 4:D:33:ASP:CG | 2.37 | 0.43 |
| 4:D:461:ASN:CB | 4:D:464:LYS:HG2 | 2.47 | 0.43 |
| 4:D:66:LYS:HA | 4:D:66:LYS:HD2 | 1.62 | 0.43 |
| 5:E:373:LYS:HE2 | 6:F:311:LYS:HZ3 | 1.83 | 0.43 |
| 6:F:324:ASN:HA | 6:F:327:ARG:HB2 | 2.00 | 0.43 |
| 8:H:250:PHE:N | 8:H:250:PHE:CD2 | 2.86 | 0.43 |
| 8:H:333:CYS:SG | 8:H:339:THR:HA | 2.59 | 0.43 |
| 8:H:464:ALA:HB2 | 8:H:474:VAL:HG11 | 2.00 | 0.43 |
| 1:I:187:VAL:CG1 | 1:I:382:SER:H | 2.31 | 0.43 |
| 1:I:460:LYS:O | 1:I:464:VAL:HG23 | 2.18 | 0.43 |
| 1:I:73:LEU:O | 1:I:74:ASP:OD1 | 2.36 | 0.43 |
| 1:I:86:LEU:C | 1:I:86:LEU:HD23 | 2.39 | 0.43 |
| 2:J:102:LEU:HD23 | 2:J:102:LEU:C | 2.39 | 0.43 |
| 2:J:422:ILE:CB | 2:J:427:SER:CB | 2.79 | 0.43 |
| 2:J:459:LEU:HD13 | 2:J:472:LEU:HD23 | 2.00 | 0.43 |
| 2:J:515:ILE:O | 3:K:48:LEU:HA | 2.19 | 0.43 |
| 3:K:9:ASN:HB2 | 8:P:78:VAL:HG13 | 2.00 | 0.43 |
| 4:L:22:LYS:O | 4:L:26:ILE:HG13 | 2.19 | 0.43 |
| 5:M:73:ILE:HG12 | 5:M:83:ILE:CG1 | 2.44 | 0.43 |
| 7:O:130:ARG:HE | 7:O:130:ARG:HA | 1.84 | 0.43 |
| 7:O:452:GLN:O | 7:O:456:ASN:N | 2.49 | 0.43 |
| 1:I:54:VAL:HB | 7:O:525:THR:HA | 2.00 | 0.43 |
| 7:O:51:ILE:HD12 | 7:O:69:ILE:HD11 | 2.01 | 0.43 |
| 1:A:224:LEU:CD1 | 1:A:226:CYS:CB | 2.90 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:187:VAL:CG1 | 1:A:382:SER:H | 2.30 | 0.43 |
| 1:A:460:LYS:O | 1:A:464:VAL:HG23 | 2.18 | 0.43 |
| 1:A:54:VAL:HG12 | 1:A:56:ASP:N | 2.30 | 0.43 |
| 2:B:401:VAL:HG22 | 2:B:402:LEU:N | 2.33 | 0.43 |
| 2:B:45:LEU:HD12 | 6:F:533:LEU:HD13 | 2.00 | 0.43 |
| 3:C:229:VAL:HG11 | 3:C:234:MET:CE | 2.49 | 0.43 |
| 3:C:209:ILE:HG23 | 3:C:382:ARG:HA | 2.00 | 0.43 |
| 5:E:127:SER:O | 5:E:128:ALA:C | 2.57 | 0.43 |
| 5:E:33:LYS:O | 5:E:33:LYS:HG2 | 2.19 | 0.43 |
| 5:E:73:ILE:O | 5:E:74:LEU:HD22 | 2.18 | 0.43 |
| 6:F:114:HIS:ND1 | 6:F:115:PRO:HD2 | 2.34 | 0.43 |
| 6:F:221:HIS:CD2 | 6:F:224:MET:SD | 3.09 | 0.43 |
| 6:F:430:ASN:C | 6:F:432:ASN:H | 2.22 | 0.43 |
| 7:G:130:ARG:HA | 7:G:130:ARG:HE | 1.84 | 0.43 |
| 7:G:166:MET:O | 7:G:171:ILE:HB | 2.18 | 0.43 |
| 7:G:162:ALA:CB | 7:G:179:VAL:HG13 | 2.47 | 0.43 |
| 7:G:382:ALA:O | 7:G:386:ILE:HG13 | 2.18 | 0.43 |
| 8:H:155:ASP:HB3 | 8:H:156:LYS:H | 1.48 | 0.43 |
| 2:J:329:PHE:CD2 | 2:J:329:PHE:O | 2.53 | 0.43 |
| 3:K:152:LYS:HG2 | 3:K:176:LEU:HG | 2.01 | 0.43 |
| 4:L:146:ASP:HB2 | 4:L:149:GLN:HB2 | 2.01 | 0.43 |
| 5:M:262:GLU:HA | 5:M:263:GLY:HA2 | 1.67 | 0.43 |
| 5:M:431:ARG:HA | 5:M:434:VAL:HG12 | 2.01 | 0.43 |
| 6:N:527:LEU:HD23 | 6:N:527:LEU:HA | 1.71 | 0.43 |
| 7:O:83:LEU:HA | 7:O:86:ILE:HD11 | 2.01 | 0.43 |
| 8:P:333:CYS:SG | 8:P:339:THR:HA | 2.59 | 0.43 |
| 8:P:420:LEU:HD23 | 8:P:421:PRO:HD2 | 2.01 | 0.43 |
| 8:P:424:GLY:O | 8:P:428:ILE:HG13 | 2.18 | 0.43 |
| 8:P:35:ILE:HG23 | 8:P:85:LEU:HD12 | 2.01 | 0.43 |
| 1:A:350:PHE:O | 1:A:351:GLU:OE2 | 2.36 | 0.43 |
| 1:A:396:ASP:O | 1:A:399:GLU:HB3 | 2.19 | 0.43 |
| 1:A:434:ASP:O | 1:A:438:THR:HG23 | 2.19 | 0.43 |
| 1:A:86:LEU:C | 1:A:86:LEU:HD23 | 2.39 | 0.43 |
| 1:A:90:GLN:HG3 | 1:A:101:VAL:CG2 | 2.19 | 0.43 |
| 2:B:490:SER:HB2 | 2:B:492:LYS:CE | 2.49 | 0.43 |
| 2:B:8:ASP:N | 2:B:8:ASP:OD1 | 2.51 | 0.43 |
| 3:C:174:LEU:HD21 | 3:C:379:ILE:HG21 | 2.01 | 0.43 |
| 4:D:461:ASN:HB3 | 4:D:464:LYS:CG | 2.48 | 0.43 |
| 6:F:390:GLN:HE21 | 6:F:390:GLN:HA | 1.84 | 0.43 |
| 6:F:419:TYR:O | 6:F:422:LEU:HB2 | 2.19 | 0.43 |
| 7:G:516:LEU:CD2 | 7:G:517:ILE:N | 2.68 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:H:101:ASN:HD22 | 8:H:101:ASN:N | 2.16 | 0.43 |
| 3:C:341:GLU:OE2 | 8:H:281:GLU:OE2 | 2.37 | 0.43 |
| 8:H:467:ALA:HB2 | 8:H:493:ASP:CB | 2.49 | 0.43 |
| 8:H:523:THR:HA | 8:H:526:PHE:HD2 | 1.83 | 0.43 |
| 2:J:417:THR:HG23 | 2:J:418:GLU:N | 2.33 | 0.43 |
| 3:K:306:GLN:C | 3:K:310:LEU:HG | 2.37 | 0.43 |
| 4:L:58:SER:HA | 4:L:392:ARG:HH12 | 1.84 | 0.43 |
| 4:L:469:LEU:HA | 4:L:469:LEU:HD23 | 1.87 | 0.43 |
| 5:M:429:VAL:O | 5:M:432:ASN:HB2 | 2.18 | 0.43 |
| 7:O:132:ALA:HB2 | 7:O:439:ILE:HD13 | 2.01 | 0.43 |
| 7:O:139:LYS:CB | 7:O:420:VAL:HG12 | 2.49 | 0.43 |
| 7:O:55:THR:HG21 | 7:O:72:LEU:HD23 | 2.01 | 0.43 |
| 1:A:431:ILE:HG21 | 1:A:482:ALA:HA | 2.01 | 0.43 |
| 1:A:66:GLY:HA3 | 1:A:99:THR:HG22 | 2.01 | 0.43 |
| 2:B:243:VAL:HG12 | 2:B:245:ILE:N | 2.29 | 0.43 |
| 2:B:326:VAL:HG13 | 3:C:304:LEU:CD2 | 2.48 | 0.43 |
| 3:C:310:LEU:HD21 | 3:C:316:VAL:HG22 | 1.99 | 0.43 |
| 4:D:58:SER:HA | 4:D:392:ARG:HH12 | 1.84 | 0.43 |
| 4:D:55:ILE:HD12 | 8:H:80:PRO:HB3 | 2.01 | 0.43 |
| 6:F:195:GLU:HG2 | 6:F:197:MET:CE | 2.48 | 0.43 |
| 5:E:364:PRO:HG3 | 6:F:307:ASP:CB | 2.49 | 0.43 |
| 6:F:420:ILE:CG2 | 6:F:482:ASP:CG | 2.86 | 0.43 |
| 7:G:234:LYS:HA | 7:G:234:LYS:HD3 | 1.34 | 0.43 |
| 8:H:335:VAL:HG23 | 8:H:381:THR:OG1 | 2.19 | 0.43 |
| 1:I:129:PHE:CB | 1:I:532:LEU:HD21 | 2.48 | 0.43 |
| 1:I:187:VAL:O | 1:I:381:SER:CA | 2.67 | 0.43 |
| 1:I:256:MET:HE3 | 1:I:260:VAL:O | 2.19 | 0.43 |
| 1:I:267:PRO:HB2 | 1:I:269:GLN:CB | 2.49 | 0.43 |
| 2:J:350:GLU:HG2 | 2:J:350:GLU:H | 1.37 | 0.43 |
| 2:J:60:GLY:H | 2:J:93:THR:HG22 | 1.83 | 0.43 |
| 5:M:87:GLY:HA3 | 5:M:120:THR:HG22 | 2.01 | 0.43 |
| 5:M:33:LYS:O | 5:M:33:LYS:HG2 | 2.19 | 0.43 |
| 5:M:447:GLU:HG2 | 5:M:479:ILE:HB | 2.01 | 0.43 |
| 6:N:114:HIS:ND1 | 6:N:115:PRO:HD2 | 2.34 | 0.43 |
| 6:N:160:THR:N | 6:N:164:ALA:HB3 | 2.31 | 0.43 |
| 6:N:32:VAL:HA | 6:N:44:LYS:HZ2 | 1.84 | 0.43 |
| 7:O:101:VAL:HG22 | 7:O:506:ALA:HA | 2.01 | 0.43 |
| 4:L:523:ASP:C | 7:O:51:ILE:HG23 | 2.37 | 0.43 |
| 8:P:335:VAL:HG23 | 8:P:381:THR:OG1 | 2.19 | 0.43 |
| 1:A:129:PHE:HD2 | 1:A:129:PHE:N | 2.17 | 0.43 |
| 1:A:345:GLU:HA | 1:A:346:GLY:HA2 | 1.67 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:351:GLU:N | 1:A:351:GLU:OE2 | 2.52 | 0.43 |
| 2:B:92:THR:HA | 2:B:95:VAL:HG23 | 2.00 | 0.43 |
| 3:C:108:ALA:N | 3:C:109:PRO:CD | 2.81 | 0.43 |
| 3:C:35:ILE:CD1 | 3:C:65:LEU:HG | 2.47 | 0.43 |
| 4:D:22:LYS:O | 4:D:26:ILE:HG13 | 2.19 | 0.43 |
| 4:D:325:SER:HB3 | 4:D:332:PRO:CG | 2.49 | 0.43 |
| 4:D:134:ILE:HB | 4:D:421:ILE:HD13 | 2.01 | 0.43 |
| 5:E:87:GLY:HA3 | 5:E:120:THR:HG22 | 2.01 | 0.43 |
| 5:E:245:LEU:HD22 | 5:E:245:LEU:HA | 1.80 | 0.43 |
| 5:E:447:GLU:HG2 | 5:E:479:ILE:HB | 2.01 | 0.43 |
| 6:F:234:LEU:HD12 | 6:F:280:LEU:HD11 | 2.00 | 0.43 |
| 6:F:185:GLN:HB3 | 6:F:407:LYS:HD3 | 2.00 | 0.43 |
| 6:F:429:ALA:O | 6:F:432:ASN:HB2 | 2.19 | 0.43 |
| 6:F:433:LYS:HB3 | 6:F:444:ILE:HG13 | 2.00 | 0.43 |
| 6:F:503:ILE:O | 6:F:503:ILE:HG22 | 2.18 | 0.43 |
| 6:F:81:ALA:O | 6:F:82:ALA:C | 2.57 | 0.43 |
| 6:F:83:GLN:HB2 | 6:F:91:THR:HG22 | 2.00 | 0.43 |
| 7:G:113:LYS:O | 7:G:116:LEU:HB2 | 2.19 | 0.43 |
| 7:G:17:THR:HG21 | 7:G:525:THR:O | 2.19 | 0.43 |
| 7:G:51:ILE:HD12 | 7:G:69:ILE:HD11 | 2.01 | 0.43 |
| 7:G:55:THR:HG21 | 7:G:72:LEU:HD23 | 2.01 | 0.43 |
| 1:I:177:SER:O | 1:I:181:VAL:HG23 | 2.19 | 0.43 |
| 2:J:243:VAL:CG1 | 2:J:245:ILE:HG13 | 2.49 | 0.43 |
| 2:J:58:ASN:HD21 | 2:J:93:THR:HG21 | 1.84 | 0.43 |
| 3:K:219:VAL:O | 3:K:219:VAL:HG12 | 2.18 | 0.43 |
| 3:K:282:LEU:O | 3:K:286:GLN:HG3 | 2.19 | 0.43 |
| 4:L:103:LEU:HD22 | 4:L:515:VAL:HG21 | 1.99 | 0.43 |
| 4:L:461:ASN:HB3 | 4:L:464:LYS:CG | 2.48 | 0.43 |
| 5:M:483:LEU:HD21 | 9:M:601:ADP:H1' | 2.00 | 0.43 |
| 5:M:84:THR:O | 5:M:90:ILE:HD11 | 2.18 | 0.43 |
| 6:N:113:VAL:CB | 6:N:118:ILE:HD11 | 2.47 | 0.43 |
| 6:N:324:ASN:HA | 6:N:327:ARG:HB2 | 2.00 | 0.43 |
| 6:N:451:LEU:O | 6:N:455:PRO:CG | 2.66 | 0.43 |
| 6:N:81:ALA:O | 6:N:82:ALA:C | 2.57 | 0.43 |
| 7:O:82:THR:HG21 | 7:O:517:ILE:HD11 | 1.99 | 0.43 |
| 8:P:482:HIS:C | 8:P:484:VAL:N | 2.65 | 0.43 |
| 2:B:308:HIS:CE1 | 2:B:313:GLY:HA3 | 2.54 | 0.43 |
| 3:C:350:THR:HG22 | 3:C:350:THR:O | 2.18 | 0.43 |
| 3:C:483:GLY:O | 3:C:491:ILE:HB | 2.18 | 0.43 |
| 3:C:50:ASP:OD1 | 3:C:54:GLY:HA3 | 2.18 | 0.43 |
| 4:D:241:ILE:HD12 | 4:D:241:ILE:N | 2.30 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:253:ILE:HG12 | 4:D:253:ILE:H | 1.64 | 0.43 |
| 4:D:328:LEU:O | 4:D:345:ASP:CG | 2.57 | 0.43 |
| 6:F:221:HIS:HB2 | 6:F:224:MET:CG | 2.43 | 0.43 |
| 6:F:28:GLY:C | 6:F:30:GLN:H | 2.22 | 0.43 |
| 2:B:32:LEU:HD11 | 6:F:532:GLU:OE2 | 2.17 | 0.43 |
| 6:F:5:LEU:HB3 | 6:F:6:LEU:C | 2.39 | 0.43 |
| 8:H:420:LEU:HD23 | 8:H:421:PRO:HD2 | 2.01 | 0.43 |
| 8:H:77:ILE:H | 8:H:77:ILE:CD1 | 2.26 | 0.43 |
| 1:I:281:VAL:O | 1:I:285:VAL:HG23 | 2.19 | 0.43 |
| 1:I:434:ASP:O | 1:I:438:THR:HG23 | 2.19 | 0.43 |
| 2:J:165:ILE:HG12 | 6:N:529:LEU:CD1 | 2.43 | 0.43 |
| 2:J:169:ASP:HB2 | 2:J:172:HIS:HB2 | 2.00 | 0.43 |
| 2:J:294:PRO:HA | 2:J:297:LEU:HB2 | 2.00 | 0.43 |
| 2:J:440:LEU:N | 2:J:441:PRO:HD2 | 2.33 | 0.43 |
| 2:J:467:ILE:HA | 2:J:468:SER:HA | 1.59 | 0.43 |
| 2:J:47:GLN:HE22 | 2:J:53:THR:N | 2.17 | 0.43 |
| 3:K:441:PRO:O | 3:K:444:ALA:HB3 | 2.18 | 0.43 |
| 4:L:184:GLU:HA | 4:L:187:LYS:HG2 | 2.00 | 0.43 |
| 4:L:221:LYS:HE3 | 4:L:306:SER:CB | 2.49 | 0.43 |
| 4:L:226:PRO:HD2 | 4:L:311:MET:HG2 | 2.01 | 0.43 |
| 4:L:389:GLU:O | 4:L:392:ARG:HD3 | 2.19 | 0.43 |
| 4:L:423:ARG:O | 4:L:427:LYS:HG2 | 2.19 | 0.43 |
| 5:M:310:ILE:HG23 | 5:M:335:LEU:HD23 | 2.01 | 0.43 |
| 6:N:151:LEU:O | 6:N:171:THR:HG21 | 2.19 | 0.43 |
| 6:N:174:VAL:O | 6:N:178:VAL:HG23 | 2.18 | 0.43 |
| 6:N:420:ILE:O | 6:N:424:ARG:N | 2.40 | 0.43 |
| 6:N:426:LEU:HD22 | 6:N:426:LEU:HA | 1.86 | 0.43 |
| 7:O:17:THR:HG21 | 7:O:525:THR:O | 2.19 | 0.43 |
| 8:P:464:ALA:HB2 | 8:P:474:VAL:HG11 | 2.00 | 0.43 |
| 2:B:294:PRO:HA | 2:B:297:LEU:HB2 | 2.00 | 0.42 |
| 2:B:319:LEU:O | 2:B:319:LEU:HD23 | 2.19 | 0.42 |
| 2:B:440:LEU:N | 2:B:441:PRO:HD2 | 2.33 | 0.42 |
| 3:C:282:LEU:O | 3:C:286:GLN:HG3 | 2.19 | 0.42 |
| 5:E:132:GLN:NE2 | 5:E:132:GLN:HA | 2.33 | 0.42 |
| 5:E:431:ARG:HA | 5:E:434:VAL:HG12 | 2.00 | 0.42 |
| 1:A:546:THR:HA | 5:E:75:ILE:HB | 2.01 | 0.42 |
| 6:F:143:LEU:CD1 | 6:F:145:ASN:CB | 2.96 | 0.42 |
| 7:G:101:VAL:HG22 | 7:G:506:ALA:HA | 2.01 | 0.42 |
| 7:G:282:LEU:HD12 | 7:G:283:ARG:N | 2.34 | 0.42 |
| 7:G:178:PHE:CZ | 7:G:389:VAL:HG13 | 2.53 | 0.42 |
| 8:H:302:GLY:HA2 | 8:H:324:PRO:HD2 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:H:35:ILE:HG23 | 8:H:85:LEU:HD12 | 2.01 | 0.42 |
| 1:I:543:THR:O | 5:M:72:LYS:HB3 | 2.19 | 0.42 |
| 2:J:218:PHE:HA | 2:J:304:ASN:O | 2.19 | 0.42 |
| 2:J:319:LEU:HD23 | 2:J:319:LEU:O | 2.19 | 0.42 |
| 3:K:162:LYS:C | 3:K:164:VAL:H | 2.22 | 0.42 |
| 3:K:237:HIS:C | 3:K:238:ILE:HG13 | 2.40 | 0.42 |
| 4:L:138:MET:HE1 | 4:L:416:ALA:HB1 | 2.01 | 0.42 |
| 4:L:134:ILE:HB | 4:L:421:ILE:HD13 | 2.01 | 0.42 |
| 4:L:77:MET:O | 4:L:81:VAL:HG23 | 2.18 | 0.42 |
| 5:M:477:ASP:O | 5:M:480:PRO:HD2 | 2.19 | 0.42 |
| 6:N:147:ARG:HH22 | 6:N:409:LYS:HA | 1.84 | 0.42 |
| 6:N:92:THR:OG1 | 9:N:601:ADP:O2B | 2.35 | 0.42 |
| 7:O:236:PHE:O | 7:O:239:PRO:HG3 | 2.19 | 0.42 |
| 8:P:318:ILE:HG22 | 8:P:319:LEU:O | 2.19 | 0.42 |
| 8:P:137:PHE:HE2 | 8:P:434:ILE:HA | 1.84 | 0.42 |
| 2:B:494:LYS:HD2 | 2:B:494:LYS:HA | 1.79 | 0.42 |
| 4:D:200:VAL:HA | 4:D:381:GLY:O | 2.18 | 0.42 |
| 4:D:236:LEU:O | 4:D:332:PRO:HA | 2.18 | 0.42 |
| 4:D:423:ARG:O | 4:D:427:LYS:HG2 | 2.19 | 0.42 |
| 4:D:436:GLN:CD | 4:D:436:GLN:H | 2.22 | 0.42 |
| 4:D:517:SER:O | 4:D:521:ILE:HG13 | 2.19 | 0.42 |
| 5:E:263:GLY:HA3 | 5:E:380:ILE:O | 2.19 | 0.42 |
| 5:E:466:GLN:HG3 | 5:E:467:TYR:CD2 | 2.54 | 0.42 |
| 5:E:485:GLU:HB2 | 5:E:491:PRO:HG3 | 2.01 | 0.42 |
| 6:F:143:LEU:HD21 | 6:F:145:ASN:HB3 | 1.97 | 0.42 |
| 6:F:430:ASN:CA | 6:F:433:LYS:HB2 | 2.48 | 0.42 |
| 7:G:117:GLU:CD | 7:G:117:GLU:N | 2.73 | 0.42 |
| 1:I:66:GLY:HA3 | 1:I:99:THR:HG22 | 2.01 | 0.42 |
| 2:J:120:ILE:HG23 | 2:J:124:TYR:CE1 | 2.54 | 0.42 |
| 2:J:287:ARG:H | 2:J:287:ARG:HG2 | 1.58 | 0.42 |
| 4:L:200:VAL:HA | 4:L:381:GLY:O | 2.18 | 0.42 |
| 4:L:436:GLN:CD | 4:L:436:GLN:H | 2.22 | 0.42 |
| 4:L:518:ILE:HA | 4:L:521:ILE:HD12 | 2.01 | 0.42 |
| 5:M:127:SER:O | 5:M:128:ALA:C | 2.57 | 0.42 |
| 6:N:16:ASP:O | 6:N:20:LYS:N | 2.46 | 0.42 |
| 6:N:233:VAL:HG12 | 6:N:294:VAL:CG2 | 2.49 | 0.42 |
| 6:N:352:GLY:C | 6:N:367:VAL:HG12 | 2.40 | 0.42 |
| 6:N:352:GLY:CA | 6:N:369:GLU:C | 2.48 | 0.42 |
| 6:N:419:TYR:O | 6:N:422:LEU:HB2 | 2.19 | 0.42 |
| 7:O:36:VAL:CG2 | 7:O:37:GLN:N | 2.83 | 0.42 |
| 7:O:178:PHE:CZ | 7:O:389:VAL:HG13 | 2.53 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:P:48:PRO:HG3 | 8:P:169:SER:HA | 2.02 | 0.42 |
| 1:A:17:GLY:HA2 | 1:A:547:VAL:HA | 2.01 | 0.42 |
| 1:A:482:ALA:O | 1:A:485:GLN:O | 2.37 | 0.42 |
| 2:B:236:THR:HA | 2:B:287:ARG:CD | 2.50 | 0.42 |
| 3:C:228:ASP:OD2 | 3:C:229:VAL:N | 2.53 | 0.42 |
| 3:C:291:ARG:N | 3:C:292:PRO:CD | 2.80 | 0.42 |
| 4:D:232:ALA:O | 4:D:234:ILE:HD12 | 2.19 | 0.42 |
| 4:D:254:VAL:HG22 | 8:H:265:VAL:CA | 2.34 | 0.42 |
| 5:E:273:THR:HG21 | 5:E:364:PRO:CA | 2.47 | 0.42 |
| 6:F:195:GLU:CD | 6:F:197:MET:SD | 2.97 | 0.42 |
| 6:F:527:LEU:HA | 6:F:527:LEU:HD23 | 1.71 | 0.42 |
| 7:G:236:PHE:O | 7:G:239:PRO:HD3 | 2.19 | 0.42 |
| 7:G:236:PHE:O | 7:G:239:PRO:HG3 | 2.19 | 0.42 |
| 4:D:72:HIS:CD2 | 8:H:15:LYS:NZ | 2.87 | 0.42 |
| 8:H:338:ALA:N | 8:H:353:GLY:HA3 | 2.33 | 0.42 |
| 8:H:35:ILE:CD1 | 8:H:82:VAL:HA | 2.49 | 0.42 |
| 1:I:363:GLN:HE21 | 1:I:363:GLN:HB2 | 1.66 | 0.42 |
| 2:J:226:ILE:HG13 | 2:J:282:ASN:OD1 | 2.18 | 0.42 |
| 2:J:490:SER:HB2 | 2:J:492:LYS:CE | 2.49 | 0.42 |
| 2:J:513:ASN:O | 2:J:514:ILE:CD1 | 2.46 | 0.42 |
| 3:K:61:GLY:CA | 3:K:94:THR:HG22 | 2.49 | 0.42 |
| 5:M:297:LYS:HD2 | 5:M:297:LYS:HA | 1.66 | 0.42 |
| 5:M:320:VAL:HG22 | 5:M:341:PRO:CD | 2.40 | 0.42 |
| 5:M:477:ASP:C | 5:M:480:PRO:HD2 | 2.39 | 0.42 |
| 6:N:430:ASN:C | 6:N:432:ASN:H | 2.22 | 0.42 |
| 7:O:346:LEU:HD23 | 7:O:346:LEU:N | 2.33 | 0.42 |
| 7:O:86:ILE:HG13 | 7:O:86:ILE:H | 1.58 | 0.42 |
| 8:P:177:ILE:O | 8:P:181:LEU:HD12 | 2.19 | 0.42 |
| 8:P:486:GLU:N | 8:P:487:PRO:HA | 2.34 | 0.42 |
| 8:P:35:ILE:HD13 | 8:P:82:VAL:HG22 | 2.00 | 0.42 |
| 1:A:178:ASN:HD21 | 1:A:182:ASP:CG | 2.23 | 0.42 |
| 1:A:281:VAL:O | 1:A:285:VAL:HG23 | 2.19 | 0.42 |
| 1:A:301:GLY:HA2 | 1:A:320:ARG:H | 1.84 | 0.42 |
| 1:A:183:ALA:CB | 1:A:383:SER:HB2 | 2.47 | 0.42 |
| 2:B:218:PHE:HA | 2:B:304:ASN:O | 2.19 | 0.42 |
| 2:B:326:VAL:HG11 | 3:C:304:LEU:HD13 | 2.01 | 0.42 |
| 2:B:372:ALA:HA | 6:F:519:GLY:HA2 | 2.01 | 0.42 |
| 4:D:77:MET:O | 4:D:81:VAL:HG23 | 2.18 | 0.42 |
| 5:E:477:ASP:C | 5:E:480:PRO:HD2 | 2.39 | 0.42 |
| 6:F:136:PHE:O | 6:F:138:ILE:HG13 | 2.19 | 0.42 |
| 6:F:209:PHE:CE2 | 6:F:376:CYS:SG | 2.97 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:F:433:LYS:CG | 6:F:444:ILE:HG13 | 2.48 | 0.42 |
| 6:F:485:GLU:O | 6:F:488:TYR:N | 2.53 | 0.42 |
| 6:F:6:LEU:HD12 | 6:F:7:ASN:H | 1.85 | 0.42 |
| 8:H:306:GLY:O | 8:H:310:LEU:HB2 | 2.20 | 0.42 |
| 8:H:137:PHE:HE2 | 8:H:434:ILE:HA | 1.84 | 0.42 |
| 1:I:17:GLY:HA2 | 1:I:547:VAL:HA | 2.01 | 0.42 |
| 1:I:296:VAL:O | 1:I:297:LEU:HD23 | 2.19 | 0.42 |
| 1:I:301:GLY:HA2 | 1:I:320:ARG:H | 1.84 | 0.42 |
| 1:I:133:LEU:HG | 1:I:532:LEU:HD12 | 2.01 | 0.42 |
| 2:J:3:VAL:HB | 2:J:4:GLN:CD | 2.40 | 0.42 |
| 2:J:76:VAL:O | 2:J:79:ASN:HB2 | 2.20 | 0.42 |
| 3:K:228:ASP:OD2 | 3:K:229:VAL:N | 2.52 | 0.42 |
| 3:K:229:VAL:HG11 | 3:K:234:MET:CE | 2.49 | 0.42 |
| 3:K:320:VAL:HG12 | 3:K:324:ASP:HB3 | 2.01 | 0.42 |
| 4:L:242:SER:HB3 | 4:L:298:ASN:HB2 | 2.00 | 0.42 |
| 4:L:248:THR:O | 4:L:250:ASN:OD1 | 2.37 | 0.42 |
| 4:L:325:SER:HB3 | 4:L:332:PRO:CG | 2.49 | 0.42 |
| 4:L:94:THR:O | 4:L:96:VAL:N | 2.52 | 0.42 |
| 5:M:535:LYS:HD2 | 5:M:535:LYS:C | 2.38 | 0.42 |
| 6:N:238:VAL:HG22 | 6:N:239:SER:H | 1.83 | 0.42 |
| 6:N:433:LYS:HB3 | 6:N:444:ILE:HG13 | 2.00 | 0.42 |
| 7:O:448:VAL:HA | 7:O:451:ARG:HB2 | 2.00 | 0.42 |
| 8:P:296:VAL:HG11 | 8:P:299:ILE:HD11 | 2.01 | 0.42 |
| 8:P:335:VAL:HG13 | 8:P:379:SER:CB | 2.46 | 0.42 |
| 1:A:187:VAL:O | 1:A:381:SER:CA | 2.67 | 0.42 |
| 1:A:296:VAL:O | 1:A:297:LEU:HD23 | 2.19 | 0.42 |
| 2:B:415:VAL:HB | 2:B:434:ALA:HB2 | 2.02 | 0.42 |
| 2:B:159:THR:CG2 | 2:B:487:ILE:HA | 2.50 | 0.42 |
| 3:C:243:VAL:O | 3:C:348:VAL:HG13 | 2.19 | 0.42 |
| 3:C:298:GLU:HG3 | 3:C:325:ASN:HD22 | 1.84 | 0.42 |
| 3:C:332:THR:HB | 3:C:349:GLY:CA | 2.49 | 0.42 |
| 3:C:415:GLY:HA3 | 3:C:501:GLU:OE1 | 2.20 | 0.42 |
| 4:D:389:GLU:O | 4:D:392:ARG:HD3 | 2.19 | 0.42 |
| 5:E:269:LEU:HD22 | 5:E:269:LEU:H | 1.84 | 0.42 |
| 5:E:350:GLU:O | 5:E:353:HIS:N | 2.52 | 0.42 |
| 5:E:445:ALA:CB | 5:E:510:ILE:O | 2.67 | 0.42 |
| 6:F:124:ILE:HB | 6:F:444:ILE:CD1 | 2.48 | 0.42 |
| 6:F:147:ARG:HG3 | 6:F:147:ARG:O | 2.20 | 0.42 |
| 1:I:178:ASN:HD21 | 1:I:182:ASP:CG | 2.23 | 0.42 |
| 1:I:476:LYS:C | 1:I:509:ILE:HD11 | 2.40 | 0.42 |
| 1:I:431:ILE:HG21 | 1:I:482:ALA:HA | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:532:LEU:HD22 | 1:I:536:VAL:CG2 | 2.48 | 0.42 |
| 2:J:132:LEU:HD21 | 2:J:495:ARG:CG | 2.43 | 0.42 |
| 2:J:213:ILE:HG23 | 2:J:354:LEU:HD21 | 2.02 | 0.42 |
| 2:J:404:GLY:HA2 | 9:J:601:ADP:N3 | 2.34 | 0.42 |
| 3:K:243:VAL:O | 3:K:348:VAL:HG13 | 2.19 | 0.42 |
| 3:K:286:GLN:OE1 | 3:K:340:VAL:HG22 | 2.19 | 0.42 |
| 3:K:129:LEU:HD21 | 3:K:511:LYS:HA | 2.00 | 0.42 |
| 4:L:439:ILE:O | 4:L:439:ILE:HG22 | 2.19 | 0.42 |
| 6:N:147:ARG:O | 6:N:147:ARG:HG3 | 2.20 | 0.42 |
| 6:N:171:THR:N | 6:N:172:PRO:HD2 | 2.33 | 0.42 |
| 6:N:5:LEU:HB3 | 6:N:6:LEU:C | 2.39 | 0.42 |
| 7:O:41:LYS:N | 7:O:42:PRO:HD2 | 2.34 | 0.42 |
| 7:O:455:GLU:CG | 7:O:461:ALA:HB2 | 2.49 | 0.42 |
| 8:P:269:ASN:O | 8:P:272:GLU:HB2 | 2.19 | 0.42 |
| 8:P:77:ILE:H | 8:P:77:ILE:CD1 | 2.26 | 0.42 |
| 1:A:550:GLU:HA | 1:A:551:PRO:HD3 | 1.88 | 0.42 |
| 3:C:140:SER:HB2 | 3:C:411:SER:HB2 | 2.02 | 0.42 |
| 3:C:47:MET:CE | 3:C:49:LEU:HD21 | 2.49 | 0.42 |
| 4:D:94:THR:O | 4:D:96:VAL:N | 2.52 | 0.42 |
| 5:E:476:LEU:HD13 | 5:E:476:LEU:HA | 1.89 | 0.42 |
| 6:F:11:GLU:OE2 | 6:F:11:GLU:N | 2.52 | 0.42 |
| 6:F:230:ASN:N | 6:F:353:LEU:HD23 | 2.35 | 0.42 |
| 7:G:83:LEU:HA | 7:G:86:ILE:HD11 | 2.01 | 0.42 |
| 8:H:177:ILE:O | 8:H:181:LEU:HD12 | 2.20 | 0.42 |
| 8:H:296:VAL:HG11 | 8:H:299:ILE:HD11 | 2.01 | 0.42 |
| 8:H:318:ILE:HG22 | 8:H:319:LEU:O | 2.19 | 0.42 |
| 1:I:115:LEU:HD23 | 1:I:115:LEU:HA | 1.80 | 0.42 |
| 1:I:351:GLU:H | 1:I:354:TYR:HD2 | 1.68 | 0.42 |
| 2:J:116:HIS:CE1 | 2:J:118:GLN:CB | 2.99 | 0.42 |
| 2:J:231:ILE:HG22 | 2:J:232:LEU:H | 1.83 | 0.42 |
| 2:J:415:VAL:HB | 2:J:434:ALA:HB2 | 2.02 | 0.42 |
| 4:L:178:VAL:HG11 | 4:L:401:ILE:CD1 | 2.48 | 0.42 |
| 4:L:234:ILE:N | 4:L:234:ILE:HD12 | 2.35 | 0.42 |
| 5:M:263:GLY:HA3 | 5:M:380:ILE:O | 2.20 | 0.42 |
| 5:M:269:LEU:HD22 | 5:M:269:LEU:H | 1.85 | 0.42 |
| 5:M:280:LYS:HA | 5:M:281:PRO:HD3 | 1.80 | 0.42 |
| 5:M:445:ALA:CB | 5:M:510:ILE:O | 2.67 | 0.42 |
| 5:M:466:GLN:HG3 | 5:M:467:TYR:CD2 | 2.54 | 0.42 |
| 6:N:6:LEU:HD13 | 6:N:7:ASN:H | 1.85 | 0.42 |
| 7:O:113:LYS:O | 7:O:116:LEU:HB2 | 2.19 | 0.42 |
| 7:O:117:GLU:CD | 7:O:117:GLU:N | 2.73 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:O:282:LEU:HD12 | 7:O:283:ARG:N | 2.34 | 0.42 |
| 4:L:521:ILE:HD13 | 7:O:52:LEU:HB2 | 2.00 | 0.42 |
| 8:P:163:ILE:HD11 | 8:P:404:GLY:CA | 2.50 | 0.42 |
| 3:K:9:ASN:HB2 | 8:P:78:VAL:CG1 | 2.50 | 0.42 |
| 8:P:94:ILE:H | 8:P:94:ILE:HG13 | 1.50 | 0.42 |
| 1:A:12:THR:HA | 1:A:13:LEU:HA | 1.69 | 0.42 |
| 2:B:3:VAL:HB | 2:B:4:GLN:CD | 2.40 | 0.42 |
| 2:B:60:GLY:H | 2:B:93:THR:HG22 | 1.84 | 0.42 |
| 3:C:104:LEU:CD2 | 3:C:517:ALA:HA | 2.49 | 0.42 |
| 3:C:320:VAL:HG12 | 3:C:324:ASP:HB3 | 2.02 | 0.42 |
| 3:C:34:VAL:HG12 | 3:C:35:ILE:N | 2.35 | 0.42 |
| 4:D:221:LYS:HE2 | 4:D:221:LYS:HB2 | 1.94 | 0.42 |
| 4:D:221:LYS:HE3 | 4:D:306:SER:CB | 2.49 | 0.42 |
| 4:D:138:MET:HE1 | 4:D:416:ALA:HB1 | 2.01 | 0.42 |
| 4:D:499:GLN:HA | 4:D:500:PRO:HD3 | 1.86 | 0.42 |
| 5:E:116:GLY:HA3 | 5:E:428:CYS:CB | 2.50 | 0.42 |
| 6:F:456:LYS:O | 6:F:460:LYS:N | 2.53 | 0.42 |
| 2:B:49:ALA:HB2 | 6:F:536:ALA:O | 2.20 | 0.42 |
| 6:F:53:ILE:CG1 | 6:F:53:ILE:O | 2.68 | 0.42 |
| 7:G:450:PRO:O | 7:G:453:LEU:HB2 | 2.20 | 0.42 |
| 8:H:24:ALA:HB2 | 8:H:531:ALA:O | 2.20 | 0.42 |
| 1:I:129:PHE:N | 1:I:129:PHE:HD2 | 2.17 | 0.42 |
| 2:J:232:LEU:CD1 | 2:J:234:ALA:HB2 | 2.50 | 0.42 |
| 2:J:27:ILE:HG21 | 2:J:104:ARG:HD2 | 2.02 | 0.42 |
| 2:J:236:THR:HA | 2:J:287:ARG:CD | 2.50 | 0.42 |
| 2:J:511:VAL:O | 2:J:513:ASN:N | 2.49 | 0.42 |
| 3:K:104:LEU:CD2 | 3:K:517:ALA:HA | 2.49 | 0.42 |
| 3:K:207:GLU:HB2 | 3:K:380:MET:HA | 2.02 | 0.42 |
| 3:K:47:MET:CE | 3:K:49:LEU:HD21 | 2.49 | 0.42 |
| 5:M:362:ILE:N | 5:M:362:ILE:HD12 | 2.34 | 0.42 |
| 6:N:56:THR:HB | 6:N:390:GLN:HE22 | 1.79 | 0.42 |
| 7:O:30:ILE:O | 7:O:33:CYS:HB3 | 2.19 | 0.42 |
| 8:P:291:ILE:HD12 | 8:P:347:PRO:HG3 | 1.97 | 0.42 |
| 8:P:420:LEU:HD23 | 8:P:421:PRO:CD | 2.50 | 0.42 |
| 8:P:459:VAL:O | 8:P:462:THR:HG22 | 2.20 | 0.42 |
| 1:A:143:VAL:CG1 | 1:A:420:PRO:HD2 | 2.50 | 0.42 |
| 1:A:335:ALA:HB2 | 1:A:356:GLY:CA | 2.49 | 0.42 |
| 1:A:91:ASP:HA | 1:A:95:GLY:HA2 | 2.00 | 0.42 |
| 2:B:120:ILE:HG23 | 2:B:124:TYR:CE1 | 2.54 | 0.42 |
| 2:B:243:VAL:CG1 | 2:B:245:ILE:HG13 | 2.49 | 0.42 |
| 3:C:182:VAL:HG23 | 3:C:184:LYS:HG3 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:207:GLU:HB2 | 3:C:380:MET:HA | 2.02 | 0.42 |
| 3:C:286:GLN:OE1 | 3:C:340:VAL:HG22 | 2.19 | 0.42 |
| 2:B:507:VAL:HG21 | 3:C:388:ILE:HG12 | 2.01 | 0.42 |
| 4:D:439:ILE:HG22 | 4:D:439:ILE:O | 2.19 | 0.42 |
| 4:D:99:LEU:HA | 4:D:449:VAL:HG11 | 2.02 | 0.42 |
| 4:D:81:VAL:HG22 | 7:G:382:ALA:CB | 2.49 | 0.42 |
| 6:F:117:ILE:HD12 | 5:M:34:ASP:CA | 2.31 | 0.42 |
| 8:H:420:LEU:HD23 | 8:H:421:PRO:CD | 2.50 | 0.42 |
| 8:H:35:ILE:HD13 | 8:H:82:VAL:HG22 | 2.00 | 0.42 |
| 1:I:396:ASP:O | 1:I:399:GLU:HB3 | 2.19 | 0.42 |
| 2:J:161:LEU:HD22 | 2:J:166:LEU:HD11 | 2.01 | 0.42 |
| 2:J:424:GLY:O | 2:J:427:SER:OG | 2.33 | 0.42 |
| 3:K:456:LEU:HA | 3:K:456:LEU:HD22 | 1.79 | 0.42 |
| 5:M:170:ALA:N | 5:M:523:LYS:HZ1 | 2.18 | 0.42 |
| 6:N:422:LEU:CD1 | 6:N:517:ILE:HD11 | 2.50 | 0.42 |
| 7:O:507:LEU:C | 7:O:507:LEU:HD13 | 2.40 | 0.42 |
| 8:P:302:GLY:HA2 | 8:P:324:PRO:HD2 | 2.01 | 0.42 |
| 8:P:523:THR:HA | 8:P:526:PHE:HD2 | 1.83 | 0.42 |
| 3:K:527:VAL:HG11 | 8:P:75:LEU:HD21 | 2.02 | 0.42 |
| 2:B:155:HIS:O | 2:B:159:THR:HG23 | 2.20 | 0.42 |
| 3:C:237:HIS:C | 3:C:238:ILE:HG13 | 2.39 | 0.42 |
| 3:C:241:PRO:O | 3:C:350:THR:HA | 2.20 | 0.42 |
| 3:C:103:ILE:CG2 | 3:C:517:ALA:HB1 | 2.50 | 0.42 |
| 4:D:226:PRO:HD2 | 4:D:311:MET:HG2 | 2.01 | 0.42 |
| 4:D:60:ASP:N | 4:D:392:ARG:NH2 | 2.68 | 0.42 |
| 5:E:477:ASP:O | 5:E:480:PRO:HD2 | 2.19 | 0.42 |
| 6:F:171:THR:N | 6:F:172:PRO:HD2 | 2.33 | 0.42 |
| 6:F:356:GLN:HA | 6:F:365:THR:HA | 2.02 | 0.42 |
| 7:G:109:MET:SD | 7:G:514:THR:HG21 | 2.59 | 0.42 |
| 7:G:132:ALA:HB2 | 7:G:439:ILE:HD13 | 2.01 | 0.42 |
| 1:A:256:MET:H | 7:G:255:ASP:CB | 2.32 | 0.42 |
| 7:G:455:GLU:CG | 7:G:461:ALA:HB2 | 2.49 | 0.42 |
| 4:D:9:ALA:HB1 | 7:G:76:VAL:H | 1.85 | 0.42 |
| 1:I:335:ALA:HB2 | 1:I:356:GLY:CA | 2.50 | 0.42 |
| 1:I:54:VAL:C | 1:I:56:ASP:H | 2.23 | 0.42 |
| 2:J:308:HIS:CE1 | 2:J:313:GLY:HA3 | 2.54 | 0.42 |
| 2:J:424:GLY:H | 2:J:427:SER:HB3 | 1.85 | 0.42 |
| 2:J:459:LEU:HD11 | 2:J:471:GLY:C | 2.40 | 0.42 |
| 4:L:113:LYS:HB2 | 4:L:113:LYS:HE3 | 1.86 | 0.42 |
| 4:L:60:ASP:N | 4:L:392:ARG:NH2 | 2.68 | 0.42 |
| 5:M:268:LYS:O | 5:M:319:ASP:N | 2.53 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:M:350:GLU:O | 5:M:353:HIS:N | 2.52 | 0.42 |
| 6:N:243:GLU:CA | 6:N:243:GLU:OE2 | 2.52 | 0.42 |
| 6:N:356:GLN:HA | 6:N:365:THR:HA | 2.02 | 0.42 |
| 7:O:104:LEU:O | 7:O:108:LEU:HB2 | 2.20 | 0.42 |
| 7:O:409:ILE:CG2 | 7:O:410:VAL:N | 2.82 | 0.42 |
| 8:P:256:ILE:HD11 | 8:P:308:LEU:HD13 | 2.02 | 0.42 |
| 1:A:118:ASN:C | 1:A:119:LYS:CD | 2.88 | 0.42 |
| 1:A:543:THR:O | 5:E:72:LYS:HB3 | 2.20 | 0.42 |
| 1:A:73:LEU:O | 1:A:74:ASP:OD1 | 2.36 | 0.42 |
| 2:B:232:LEU:CD1 | 2:B:234:ALA:HB2 | 2.50 | 0.42 |
| 2:B:422:ILE:HG22 | 2:B:424:GLY:CA | 2.50 | 0.42 |
| 2:B:459:LEU:HD11 | 2:B:471:GLY:C | 2.40 | 0.42 |
| 2:B:459:LEU:CD1 | 2:B:471:GLY:O | 2.68 | 0.42 |
| 2:B:47:GLN:HE22 | 2:B:53:THR:N | 2.17 | 0.42 |
| 5:E:362:ILE:N | 5:E:362:ILE:HD12 | 2.34 | 0.42 |
| 6:F:133:LEU:HD12 | 6:F:422:LEU:HD11 | 2.02 | 0.42 |
| 6:F:309:PHE:HB3 | 6:F:314:ILE:O | 2.20 | 0.42 |
| 6:F:332:THR:O | 6:F:333:GLY:C | 2.58 | 0.42 |
| 6:F:422:LEU:CD1 | 6:F:517:ILE:HD11 | 2.50 | 0.42 |
| 6:F:68:ILE:HD13 | 6:F:74:VAL:HG13 | 2.02 | 0.42 |
| 7:G:139:LYS:CB | 7:G:420:VAL:HG12 | 2.49 | 0.42 |
| 7:G:83:LEU:HA | 7:G:86:ILE:CD1 | 2.50 | 0.42 |
| 8:H:256:ILE:HD11 | 8:H:308:LEU:HD13 | 2.02 | 0.42 |
| 8:H:48:PRO:HG3 | 8:H:169:SER:HA | 2.01 | 0.42 |
| 1:I:250:ASN:HD21 | 1:I:252:GLN:HG2 | 1.85 | 0.42 |
| 1:I:350:PHE:O | 1:I:351:GLU:OE2 | 2.36 | 0.42 |
| 1:I:549:PRO:HA | 5:M:77:PRO:O | 2.20 | 0.42 |
| 2:J:245:ILE:O | 2:J:246:PHE:HB3 | 2.19 | 0.42 |
| 2:J:57:THR:HG21 | 2:J:382:ARG:CD | 2.46 | 0.42 |
| 3:K:85:GLN:NE2 | 3:K:508:GLN:OE1 | 2.53 | 0.42 |
| 4:L:232:ALA:O | 4:L:234:ILE:HD12 | 2.19 | 0.42 |
| 4:L:226:PRO:CD | 4:L:311:MET:HG2 | 2.50 | 0.42 |
| 4:L:485:ARG:CD | 4:L:485:ARG:H | 2.27 | 0.42 |
| 5:M:273:THR:HG21 | 5:M:364:PRO:CA | 2.47 | 0.42 |
| 5:M:332:ASN:HA | 5:M:335:LEU:HD12 | 2.02 | 0.42 |
| 6:N:309:PHE:HB3 | 6:N:314:ILE:O | 2.20 | 0.42 |
| 6:N:230:ASN:N | 6:N:353:LEU:HD23 | 2.35 | 0.42 |
| 6:N:53:ILE:O | 6:N:53:ILE:CG1 | 2.68 | 0.42 |
| 7:O:166:MET:O | 7:O:171:ILE:HB | 2.18 | 0.42 |
| 7:O:182:CYS:SG | 7:O:183:VAL:N | 2.93 | 0.42 |
| 1:A:219:VAL:HG12 | 1:A:221:GLY:N | 2.34 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:267:PRO:HB2 | 1:A:269:GLN:CB | 2.49 | 0.41 |
| 1:A:54:VAL:C | 1:A:56:ASP:H | 2.23 | 0.41 |
| 2:B:162:SER:O | 2:B:163:SER:OG | 2.30 | 0.41 |
| 2:B:197:LYS:C | 2:B:198:ILE:HD12 | 2.41 | 0.41 |
| 2:B:15:ALA:O | 2:B:19:ARG:HG2 | 2.20 | 0.41 |
| 2:B:58:ASN:HD21 | 2:B:93:THR:HG21 | 1.84 | 0.41 |
| 3:C:303:ASP:HB3 | 3:C:304:LEU:H | 1.46 | 0.41 |
| 4:D:234:ILE:N | 4:D:234:ILE:HD12 | 2.35 | 0.41 |
| 4:D:379:ILE:N | 4:D:379:ILE:HD12 | 2.33 | 0.41 |
| 7:G:507:LEU:HD13 | 7:G:507:LEU:C | 2.40 | 0.41 |
| 8:H:186:VAL:HA | 8:H:207:ILE:HD11 | 2.02 | 0.41 |
| 1:I:143:VAL:CG1 | 1:I:420:PRO:HD2 | 2.50 | 0.41 |
| 1:I:219:VAL:HG12 | 1:I:221:GLY:N | 2.35 | 0.41 |
| 2:J:474:LEU:HG | 9:J:601:ADP:C2 | 2.55 | 0.41 |
| 3:K:298:GLU:HG3 | 3:K:325:ASN:HD22 | 1.84 | 0.41 |
| 4:L:265:LYS:NZ | 8:P:343:ARG:HD3 | 2.36 | 0.41 |
| 6:N:433:LYS:HG3 | 6:N:444:ILE:CG2 | 2.46 | 0.41 |
| 6:N:434:LEU:HD23 | 6:N:441:LYS:CB | 2.40 | 0.41 |
| 7:O:145:VAL:O | 7:O:409:ILE:N | 2.52 | 0.41 |
| 7:O:450:PRO:O | 7:O:453:LEU:HB2 | 2.20 | 0.41 |
| 8:P:163:ILE:HG12 | 8:P:182:VAL:HG11 | 2.01 | 0.41 |
| 1:A:476:LYS:C | 1:A:509:ILE:HD11 | 2.40 | 0.41 |
| 2:B:424:GLY:H | 2:B:427:SER:HB3 | 1.85 | 0.41 |
| 2:B:72:PRO:CG | 3:C:47:MET:HE1 | 2.50 | 0.41 |
| 4:D:65:LEU:HA | 4:D:65:LEU:HD23 | 1.84 | 0.41 |
| 5:E:268:LYS:O | 5:E:319:ASP:N | 2.53 | 0.41 |
| 5:E:38:LYS:HA | 5:E:38:LYS:HD2 | 1.70 | 0.41 |
| 5:E:81:ILE:N | 5:E:81:ILE:HD12 | 2.35 | 0.41 |
| 6:F:533:LEU:HD23 | 6:F:533:LEU:N | 2.35 | 0.41 |
| 6:F:63:LEU:HD11 | 6:F:95:VAL:HG21 | 2.03 | 0.41 |
| 7:G:104:LEU:O | 7:G:108:LEU:HB2 | 2.20 | 0.41 |
| 7:G:182:CYS:SG | 7:G:183:VAL:N | 2.93 | 0.41 |
| 7:G:23:LYS:O | 7:G:26:ILE:HG22 | 2.20 | 0.41 |
| 7:G:396:ALA:O | 7:G:400:VAL:HG13 | 2.20 | 0.41 |
| 7:G:528:GLY:HA3 | 7:G:529:SER:C | 2.41 | 0.41 |
| 8:H:32:ILE:HD11 | 8:H:111:LEU:C | 2.41 | 0.41 |
| 1:I:482:ALA:O | 1:I:485:GLN:O | 2.37 | 0.41 |
| 2:J:105:GLU:O | 2:J:109:LEU:HD23 | 2.21 | 0.41 |
| 2:J:38:GLY:HA3 | 2:J:474:LEU:HD12 | 2.02 | 0.41 |
| 3:K:355:PHE:HE2 | 3:K:366:SER:HB3 | 1.84 | 0.41 |
| 3:K:174:LEU:HD21 | 3:K:379:ILE:HG21 | 2.01 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:M:418:GLU:OE2 | 5:M:418:GLU:HA | 2.20 | 0.41 |
| 5:M:81:ILE:HD12 | 5:M:81:ILE:N | 2.35 | 0.41 |
| 6:N:196:ILE:HG22 | 6:N:378:ILE:HG23 | 2.02 | 0.41 |
| 6:N:429:ALA:O | 6:N:432:ASN:HB2 | 2.19 | 0.41 |
| 6:N:456:LYS:O | 6:N:460:LYS:N | 2.53 | 0.41 |
| 6:N:485:GLU:O | 6:N:488:TYR:N | 2.53 | 0.41 |
| 7:O:109:MET:SD | 7:O:514:THR:HG21 | 2.59 | 0.41 |
| 1:A:273:ILE:HG21 | 5:E:295:TYR:CE2 | 2.54 | 0.41 |
| 1:A:351:GLU:H | 1:A:354:TYR:HD2 | 1.68 | 0.41 |
| 1:A:498:ARG:O | 1:A:499:ASN:HB3 | 2.20 | 0.41 |
| 2:B:27:ILE:HG21 | 2:B:104:ARG:HD2 | 2.02 | 0.41 |
| 2:B:320:VAL:HG21 | 2:B:337:LEU:CA | 2.51 | 0.41 |
| 2:B:492:LYS:O | 2:B:495:ARG:HB3 | 2.20 | 0.41 |
| 2:B:57:THR:HG21 | 2:B:382:ARG:CD | 2.46 | 0.41 |
| 3:C:229:VAL:CG1 | 3:C:230:VAL:N | 2.84 | 0.41 |
| 4:D:411:ILE:O | 4:D:498:LEU:HB3 | 2.21 | 0.41 |
| 4:D:521:ILE:HG23 | 7:G:50:ASP:C | 2.40 | 0.41 |
| 5:E:167:ASP:HB3 | 5:E:168:ILE:H | 1.58 | 0.41 |
| 5:E:73:ILE:HG12 | 5:E:83:ILE:CG1 | 2.44 | 0.41 |
| 6:F:221:HIS:HA | 6:F:222:PRO:HD3 | 1.92 | 0.41 |
| 6:F:524:ALA:O | 6:F:528:LEU:HG | 2.21 | 0.41 |
| 8:H:269:ASN:O | 8:H:272:GLU:HB2 | 2.19 | 0.41 |
| 8:H:54:ILE:CG2 | 8:H:55:ILE:N | 2.83 | 0.41 |
| 2:J:160:THR:HG21 | 2:J:390:VAL:HG11 | 2.01 | 0.41 |
| 2:J:197:LYS:C | 2:J:198:ILE:HD12 | 2.41 | 0.41 |
| 2:J:422:ILE:HG22 | 2:J:424:GLY:CA | 2.50 | 0.41 |
| 2:J:45:LEU:HD23 | 2:J:56:VAL:HG13 | 2.02 | 0.41 |
| 2:J:474:LEU:HD23 | 2:J:474:LEU:N | 2.35 | 0.41 |
| 2:J:159:THR:CG2 | 2:J:487:ILE:HA | 2.49 | 0.41 |
| 2:J:492:LYS:H | 2:J:492:LYS:HZ3 | 1.65 | 0.41 |
| 2:J:492:LYS:O | 2:J:495:ARG:HB3 | 2.21 | 0.41 |
| 3:K:140:SER:HB2 | 3:K:411:SER:HB2 | 2.02 | 0.41 |
| 2:J:263:LYS:NZ | 3:K:266:GLU:HG2 | 2.35 | 0.41 |
| 3:K:244:VAL:HG22 | 3:K:348:VAL:HG22 | 2.03 | 0.41 |
| 3:K:415:GLY:HA3 | 3:K:501:GLU:OE1 | 2.20 | 0.41 |
| 3:K:103:ILE:CG2 | 3:K:517:ALA:HB1 | 2.50 | 0.41 |
| 4:L:263:ILE:C | 4:L:265:LYS:H | 2.23 | 0.41 |
| 5:M:423:LEU:C | 5:M:425:ASP:N | 2.73 | 0.41 |
| 5:M:485:GLU:HB2 | 5:M:491:PRO:HG3 | 2.01 | 0.41 |
| 6:N:133:LEU:HD12 | 6:N:422:LEU:HD11 | 2.02 | 0.41 |
| 6:N:539:SER:O | 6:N:540:THR:C | 2.58 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:O:236:PHE:O | 7:O:239:PRO:HD3 | 2.19 | 0.41 |
| 7:O:23:LYS:O | 7:O:26:ILE:HG22 | 2.20 | 0.41 |
| 7:O:303:ALA:O | 7:O:307:PHE:CD2 | 2.70 | 0.41 |
| 8:P:24:ALA:HB2 | 8:P:531:ALA:O | 2.20 | 0.41 |
| 8:P:62:ILE:HG23 | 8:P:392:ASN:OD1 | 2.20 | 0.41 |
| 8:P:92:GLN:HB3 | 8:P:92:GLN:HE21 | 1.63 | 0.41 |
| 2:B:161:LEU:HD22 | 2:B:166:LEU:HD11 | 2.01 | 0.41 |
| 2:B:246:PHE:CD1 | 2:B:247:GLY:N | 2.89 | 0.41 |
| 2:B:326:VAL:O | 2:B:327:SER:HB3 | 2.21 | 0.41 |
| 2:B:127:ALA:HB1 | 2:B:430:VAL:HG13 | 2.02 | 0.41 |
| 2:B:76:VAL:O | 2:B:79:ASN:HB2 | 2.20 | 0.41 |
| 3:C:230:VAL:O | 3:C:231:HIS:CG | 2.74 | 0.41 |
| 5:E:99:GLU:O | 5:E:102:LYS:HB2 | 2.20 | 0.41 |
| 1:A:541:ILE:HD11 | 5:E:83:ILE:HD13 | 2.02 | 0.41 |
| 6:F:137:LYS:O | 6:F:138:ILE:CB | 2.68 | 0.41 |
| 8:H:146:VAL:HG22 | 8:H:147:VAL:N | 2.35 | 0.41 |
| 1:I:345:GLU:HA | 1:I:346:GLY:HA2 | 1.67 | 0.41 |
| 2:J:162:SER:O | 2:J:163:SER:OG | 2.30 | 0.41 |
| 2:J:246:PHE:CD1 | 2:J:247:GLY:N | 2.89 | 0.41 |
| 2:J:466:GLY:C | 2:J:467:ILE:HG13 | 2.41 | 0.41 |
| 5:M:99:GLU:O | 5:M:102:LYS:HB2 | 2.20 | 0.41 |
| 5:M:451:SER:O | 5:M:455:SER:HB2 | 2.20 | 0.41 |
| 5:M:86:ASP:O | 5:M:90:ILE:HG13 | 2.20 | 0.41 |
| 6:N:136:PHE:O | 6:N:138:ILE:HG13 | 2.19 | 0.41 |
| 6:N:167:THR:CB | 6:N:169:VAL:N | 2.64 | 0.41 |
| 6:N:181:VAL:O | 6:N:184:ALA:HB3 | 2.20 | 0.41 |
| 6:N:28:GLY:C | 6:N:30:GLN:H | 2.22 | 0.41 |
| 6:N:415:ALA:HB2 | 6:N:506:ILE:HD13 | 2.03 | 0.41 |
| 6:N:89:ASP:OD1 | 9:N:601:ADP:O3B | 2.38 | 0.41 |
| 6:N:89:ASP:OD1 | 6:N:90:GLY:N | 2.43 | 0.41 |
| 8:P:213:MET:CE | 8:P:391:GLN:HG3 | 2.51 | 0.41 |
| 8:P:35:ILE:CD1 | 8:P:82:VAL:HA | 2.50 | 0.41 |
| 1:A:156:LEU:HD21 | 1:A:409:VAL:HG13 | 2.02 | 0.41 |
| 1:A:94:ILE:HG22 | 1:A:95:GLY:N | 2.36 | 0.41 |
| 2:B:45:LEU:HB2 | 6:F:533:LEU:HB2 | 2.03 | 0.41 |
| 4:D:305:LEU:HD23 | 4:D:305:LEU:C | 2.41 | 0.41 |
| 5:E:310:ILE:HG23 | 5:E:335:LEU:HD23 | 2.01 | 0.41 |
| 5:E:352:GLU:H | 5:E:352:GLU:HG3 | 1.59 | 0.41 |
| 5:E:412:ASN:C | 5:E:414:MET:H | 2.24 | 0.41 |
| 6:F:171:THR:O | 6:F:175:THR:N | 2.45 | 0.41 |
| 6:F:178:VAL:HG11 | 6:F:402:VAL:HG12 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:F:212:GLY:HA2 | 6:F:370:ASN:OD1 | 2.21 | 0.41 |
| 6:F:466:PRO:O | 6:F:468:ASP:N | 2.54 | 0.41 |
| 7:G:452:GLN:O | 7:G:456:ASN:N | 2.49 | 0.41 |
| 8:H:163:ILE:HG12 | 8:H:182:VAL:HG11 | 2.01 | 0.41 |
| 8:H:213:MET:CE | 8:H:391:GLN:HG3 | 2.51 | 0.41 |
| 2:J:217:LYS:HE2 | 2:J:217:LYS:HB3 | 1.75 | 0.41 |
| 2:J:242:LYS:HD2 | 2:J:243:VAL:N | 2.35 | 0.41 |
| 3:K:182:VAL:HG23 | 3:K:184:LYS:HG3 | 2.02 | 0.41 |
| 5:M:120:THR:O | 5:M:124:VAL:HG23 | 2.20 | 0.41 |
| 5:M:116:GLY:HA3 | 5:M:428:CYS:CB | 2.50 | 0.41 |
| 6:N:182:TYR:C | 6:N:184:ALA:N | 2.73 | 0.41 |
| 6:N:390:GLN:HA | 6:N:390:GLN:HE21 | 1.84 | 0.41 |
| 6:N:154:ALA:HB3 | 6:N:402:VAL:CG2 | 2.47 | 0.41 |
| 8:P:32:ILE:HD11 | 8:P:111:LEU:C | 2.41 | 0.41 |
| 2:B:105:GLU:O | 2:B:109:LEU:HD23 | 2.21 | 0.41 |
| 2:B:57:THR:HB | 2:B:379:GLU:HG3 | 2.03 | 0.41 |
| 2:B:459:LEU:HD22 | 2:B:472:LEU:CD1 | 2.51 | 0.41 |
| 2:B:45:LEU:HD23 | 2:B:56:VAL:HG13 | 2.02 | 0.41 |
| 3:C:184:LYS:HA | 3:C:198:ILE:CA | 2.51 | 0.41 |
| 3:C:355:PHE:HE2 | 3:C:366:SER:HB3 | 1.84 | 0.41 |
| 4:D:183:ASP:O | 4:D:187:LYS:HA | 2.21 | 0.41 |
| 4:D:273:ASN:HD22 | 7:G:268:GLN:NE2 | 2.17 | 0.41 |
| 5:E:250:SER:O | 5:E:251:HIS:O | 2.38 | 0.41 |
| 5:E:423:LEU:C | 5:E:425:ASP:N | 2.73 | 0.41 |
| 5:E:497:THR:O | 5:E:501:LYS:HG2 | 2.20 | 0.41 |
| 6:F:488:TYR:O | 6:F:489:VAL:CG1 | 2.69 | 0.41 |
| 7:G:28:SER:HA | 7:G:31:ASN:OD1 | 2.21 | 0.41 |
| 8:H:63:ILE:HD12 | 8:H:74:GLU:CG | 2.45 | 0.41 |
| 2:J:116:HIS:HA | 2:J:117:PRO:HD3 | 1.74 | 0.41 |
| 2:J:155:HIS:O | 2:J:159:THR:HG23 | 2.20 | 0.41 |
| 2:J:196:ILE:N | 2:J:196:ILE:HD12 | 2.36 | 0.41 |
| 2:J:459:LEU:CD1 | 2:J:471:GLY:O | 2.68 | 0.41 |
| 3:K:184:LYS:HA | 3:K:198:ILE:CA | 2.51 | 0.41 |
| 4:L:183:ASP:O | 4:L:187:LYS:HA | 2.21 | 0.41 |
| 4:L:198:LYS:H | 4:L:198:LYS:CD | 2.33 | 0.41 |
| 4:L:305:LEU:HD23 | 4:L:305:LEU:C | 2.41 | 0.41 |
| 4:L:461:ASN:HD22 | 4:L:462:SER:H | 1.68 | 0.41 |
| 4:L:85:GLN:O | 4:L:89:ALA:HB3 | 2.21 | 0.41 |
| 5:M:38:LYS:HD2 | 5:M:38:LYS:HA | 1.70 | 0.41 |
| 6:N:137:LYS:O | 6:N:138:ILE:CB | 2.69 | 0.41 |
| 7:O:33:CYS:HA | 7:O:83:LEU:CD1 | 2.51 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:O:488:ILE:H | 7:O:488:ILE:CD1 | 2.21 | 0.41 |
| 8:P:455:ALA:O | 8:P:458:VAL:HG23 | 2.21 | 0.41 |
| 1:A:233:MET:HE1 | 1:A:317:GLY:N | 2.35 | 0.41 |
| 1:A:344:LEU:HD12 | 1:A:345:GLU:H | 1.85 | 0.41 |
| 2:B:160:THR:HG21 | 2:B:390:VAL:HG11 | 2.01 | 0.41 |
| 2:B:213:ILE:HG23 | 2:B:354:LEU:HD21 | 2.01 | 0.41 |
| 2:B:88:VAL:HG12 | 2:B:90:ASP:H | 1.85 | 0.41 |
| 3:C:244:VAL:HG22 | 3:C:348:VAL:HG22 | 2.03 | 0.41 |
| 5:E:158:ILE:CB | 5:E:539:LEU:HD21 | 2.51 | 0.41 |
| 5:E:338:ASN:HB2 | 5:E:340:LEU:HD22 | 2.02 | 0.41 |
| 5:E:418:GLU:HA | 5:E:418:GLU:OE2 | 2.20 | 0.41 |
| 6:F:105:ALA:O | 6:F:107:ARG:N | 2.54 | 0.41 |
| 6:F:233:VAL:HG12 | 6:F:294:VAL:CG2 | 2.49 | 0.41 |
| 6:F:497:ASP:CG | 6:F:498:SER:N | 2.74 | 0.41 |
| 7:G:356:GLN:HG2 | 7:G:361:ARG:HD3 | 2.03 | 0.41 |
| 7:G:36:VAL:CG2 | 7:G:37:GLN:N | 2.83 | 0.41 |
| 7:G:41:LYS:N | 7:G:42:PRO:HD2 | 2.34 | 0.41 |
| 7:G:449:ILE:CB | 7:G:450:PRO:HD3 | 2.50 | 0.41 |
| 8:H:251:THR:O | 8:H:252:CYS:C | 2.59 | 0.41 |
| 8:H:459:VAL:HB | 8:H:460:PRO:HD3 | 2.02 | 0.41 |
| 8:H:487:PRO:HA | 8:H:488:GLY:HA3 | 1.69 | 0.41 |
| 8:H:62:ILE:HG23 | 8:H:392:ASN:OD1 | 2.20 | 0.41 |
| 8:H:92:GLN:HE21 | 8:H:92:GLN:HB3 | 1.63 | 0.41 |
| 1:I:498:ARG:O | 1:I:499:ASN:HB3 | 2.20 | 0.41 |
| 2:J:109:LEU:C | 2:J:111:ASP:H | 2.24 | 0.41 |
| 3:K:230:VAL:O | 3:K:231:HIS:CG | 2.74 | 0.41 |
| 4:L:464:LYS:O | 4:L:468:GLU:HG3 | 2.20 | 0.41 |
| 5:M:107:LEU:CD2 | 5:M:544:LEU:HG | 2.34 | 0.41 |
| 5:M:84:THR:HG21 | 5:M:421:ARG:HD3 | 2.03 | 0.41 |
| 6:N:207:THR:O | 6:N:208:THR:HG23 | 2.21 | 0.41 |
| 6:N:420:ILE:CG2 | 6:N:482:ASP:CG | 2.86 | 0.41 |
| 6:N:447:PHE:CE1 | 6:N:521:THR:HG22 | 2.56 | 0.41 |
| 6:N:63:LEU:HD11 | 6:N:95:VAL:HG21 | 2.02 | 0.41 |
| 7:O:356:GLN:HG2 | 7:O:361:ARG:HD3 | 2.03 | 0.41 |
| 1:A:133:LEU:HG | 1:A:532:LEU:HD12 | 2.02 | 0.41 |
| 2:B:242:LYS:HD2 | 2:B:243:VAL:N | 2.35 | 0.41 |
| 3:C:129:LEU:HD13 | 3:C:130:THR:N | 2.36 | 0.41 |
| 3:C:85:GLN:NE2 | 3:C:508:GLN:OE1 | 2.53 | 0.41 |
| 4:D:72:HIS:HA | 4:D:73:PRO:HD3 | 1.96 | 0.41 |
| 6:F:141:THR:HG23 | 6:F:142:ASN:N | 2.36 | 0.41 |
| 5:E:557:SER:OG | 6:F:67:GLN:N | 2.53 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:G:182:CYS:O | 7:G:186:VAL:HG23 | 2.21 | 0.41 |
| 7:G:399:ILE:O | 7:G:399:ILE:HD13 | 2.21 | 0.41 |
| 8:H:486:GLU:N | 8:H:487:PRO:HA | 2.34 | 0.41 |
| 2:J:422:ILE:HA | 2:J:422:ILE:HD13 | 1.93 | 0.41 |
| 3:K:321:LYS:O | 3:K:324:ASP:HB2 | 2.21 | 0.41 |
| 4:L:185:ASN:CB | 4:L:186:SER:CB | 2.92 | 0.41 |
| 4:L:66:LYS:HA | 4:L:66:LYS:HD2 | 1.62 | 0.41 |
| 5:M:497:THR:O | 5:M:501:LYS:HG2 | 2.20 | 0.41 |
| 6:N:212:GLY:HA2 | 6:N:370:ASN:OD1 | 2.21 | 0.41 |
| 6:N:524:ALA:O | 6:N:528:LEU:HG | 2.21 | 0.41 |
| 6:N:533:LEU:HD23 | 6:N:533:LEU:N | 2.35 | 0.41 |
| 6:N:6:LEU:HD12 | 6:N:7:ASN:H | 1.85 | 0.41 |
| 8:P:386:LEU:N | 8:P:386:LEU:HD12 | 2.36 | 0.41 |
| 1:A:209:HIS:HE1 | 7:G:89:ALA:CB | 2.34 | 0.41 |
| 1:A:250:ASN:HD21 | 1:A:252:GLN:HG2 | 1.85 | 0.41 |
| 2:B:142:ASN:CB | 2:B:143:SER:CA | 2.95 | 0.41 |
| 2:B:397:GLU:HG2 | 2:B:492:LYS:HZ3 | 1.86 | 0.41 |
| 2:B:5:ILE:CD1 | 2:B:7:GLY:H | 2.34 | 0.41 |
| 4:D:108:GLU:O | 4:D:112:ASN:N | 2.50 | 0.41 |
| 4:D:48:ILE:CD1 | 8:H:534:ALA:HB3 | 2.51 | 0.41 |
| 5:E:250:SER:O | 5:E:251:HIS:CG | 2.74 | 0.41 |
| 5:E:412:ASN:O | 5:E:413:LYS:CB | 2.69 | 0.41 |
| 6:F:151:LEU:O | 6:F:171:THR:HG21 | 2.19 | 0.41 |
| 6:F:152:GLN:HG2 | 6:F:153:VAL:N | 2.32 | 0.41 |
| 6:F:207:THR:O | 6:F:208:THR:HG23 | 2.21 | 0.41 |
| 8:H:163:ILE:HD11 | 8:H:404:GLY:CA | 2.50 | 0.41 |
| 8:H:38:LEU:HD23 | 8:H:38:LEU:HA | 1.92 | 0.41 |
| 8:H:75:LEU:HA | 8:H:75:LEU:HD23 | 1.93 | 0.41 |
| 1:I:118:ASN:O | 1:I:119:LYS:CG | 2.65 | 0.41 |
| 1:I:51:LYS:O | 1:I:62:VAL:HA | 2.20 | 0.41 |
| 2:J:14:ARG:O | 2:J:15:ALA:HB3 | 2.21 | 0.41 |
| 2:J:320:VAL:HG21 | 2:J:337:LEU:CA | 2.51 | 0.41 |
| 2:J:45:LEU:HD12 | 6:N:533:LEU:HB3 | 2.02 | 0.41 |
| 2:J:5:ILE:CD1 | 2:J:7:GLY:H | 2.34 | 0.41 |
| 3:K:223:VAL:HG11 | 3:K:328:ILE:HG12 | 2.03 | 0.41 |
| 3:K:241:PRO:O | 3:K:350:THR:HA | 2.20 | 0.41 |
| 4:L:99:LEU:HA | 4:L:449:VAL:HG11 | 2.02 | 0.41 |
| 5:M:158:ILE:CB | 5:M:539:LEU:HD21 | 2.51 | 0.41 |
| 6:N:466:PRO:O | 6:N:468:ASP:N | 2.54 | 0.41 |
| 6:N:488:TYR:O | 6:N:489:VAL:CG1 | 2.69 | 0.41 |
| 6:N:75:LEU:HD23 | 6:N:76:ILE:N | 2.36 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:O:182:CYS:O | 7:O:186:VAL:HG23 | 2.21 | 0.41 |
| 8:P:306:GLY:O | 8:P:310:LEU:HB2 | 2.20 | 0.41 |
| 1:A:51:LYS:O | 1:A:62:VAL:HA | 2.20 | 0.41 |
| 4:D:385:MET:HA | 4:D:388:ASP:OD2 | 2.21 | 0.41 |
| 5:E:225:LYS:HG3 | 5:E:225:LYS:O | 2.21 | 0.41 |
| 6:F:16:ASP:O | 6:F:20:LYS:N | 2.46 | 0.41 |
| 6:F:181:VAL:O | 6:F:184:ALA:HB3 | 2.20 | 0.41 |
| 6:F:182:TYR:C | 6:F:184:ALA:N | 2.73 | 0.41 |
| 6:F:16:ASP:HA | 6:F:19:LEU:HB2 | 2.02 | 0.41 |
| 6:F:447:PHE:CE1 | 6:F:521:THR:HG22 | 2.56 | 0.41 |
| 8:H:146:VAL:HG22 | 8:H:148:GLY:H | 1.86 | 0.41 |
| 1:I:344:LEU:HD12 | 1:I:345:GLU:H | 1.85 | 0.41 |
| 2:J:326:VAL:O | 2:J:327:SER:HB3 | 2.21 | 0.41 |
| 2:J:127:ALA:HB1 | 2:J:430:VAL:HG13 | 2.02 | 0.41 |
| 4:L:157:SER:C | 4:L:159:SER:H | 2.24 | 0.41 |
| 4:L:454:LEU:CD1 | 9:L:601:ADP:H8 | 2.34 | 0.41 |
| 4:L:35:ILE:HG22 | 4:L:98:ILE:HD11 | 2.03 | 0.41 |
| 5:M:338:ASN:HB2 | 5:M:340:LEU:HD22 | 2.02 | 0.41 |
| 5:M:472:PHE:HZ | 5:M:542:THR:HG22 | 1.86 | 0.41 |
| 6:N:105:ALA:O | 6:N:108:PHE:CD2 | 2.74 | 0.41 |
| 6:N:331:VAL:O | 6:N:332:THR:CB | 2.68 | 0.41 |
| 6:N:444:ILE:HG12 | 6:N:444:ILE:H | 1.66 | 0.41 |
| 6:N:56:THR:HB | 6:N:390:GLN:CD | 2.42 | 0.41 |
| 7:O:396:ALA:O | 7:O:400:VAL:HG13 | 2.20 | 0.41 |
| 7:O:399:ILE:HD13 | 7:O:399:ILE:O | 2.21 | 0.41 |
| 8:P:48:PRO:CA | 8:P:169:SER:O | 2.68 | 0.41 |
| 8:P:253:PRO:HA | 8:P:303:ALA:O | 2.21 | 0.41 |
| 8:P:267:LEU:HD23 | 8:P:267:LEU:N | 2.36 | 0.41 |
| 8:P:8:ASN:HA | 8:P:9:PRO:HD3 | 1.90 | 0.41 |
| 1:A:397:GLU:HA | 1:A:400:ARG:HH11 | 1.86 | 0.41 |
| 2:B:245:ILE:O | 2:B:246:PHE:HB3 | 2.19 | 0.41 |
| 3:C:240:ASN:HA | 3:C:352:CYS:O | 2.21 | 0.41 |
| 4:D:123:SER:OG | 4:D:440:TRP:HA | 2.21 | 0.41 |
| 4:D:226:PRO:CD | 4:D:311:MET:HG2 | 2.50 | 0.41 |
| 5:E:120:THR:O | 5:E:124:VAL:HG23 | 2.20 | 0.41 |
| 5:E:451:SER:O | 5:E:455:SER:HB2 | 2.20 | 0.41 |
| 6:F:113:VAL:CB | 6:F:118:ILE:HD11 | 2.47 | 0.41 |
| 6:F:23:VAL:O | 6:F:25:SER:N | 2.54 | 0.41 |
| 6:F:331:VAL:O | 6:F:332:THR:CB | 2.68 | 0.41 |
| 6:F:352:GLY:C | 6:F:367:VAL:HG12 | 2.40 | 0.41 |
| 7:G:145:VAL:O | 7:G:409:ILE:N | 2.52 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:G:214:PHE:O | 7:G:214:PHE:CD2 | 2.74 | 0.41 |
| 7:G:43:THR:HG23 | 7:G:64:ASN:HB3 | 2.00 | 0.41 |
| 8:H:48:PRO:CA | 8:H:169:SER:O | 2.68 | 0.41 |
| 8:H:253:PRO:HA | 8:H:303:ALA:O | 2.21 | 0.41 |
| 8:H:386:LEU:N | 8:H:386:LEU:HD12 | 2.36 | 0.41 |
| 8:H:414:PRO:HA | 8:H:415:SER:HA | 1.60 | 0.41 |
| 8:H:437:TYR:C | 8:H:437:TYR:CD2 | 2.95 | 0.41 |
| 8:H:459:VAL:O | 8:H:462:THR:HG22 | 2.20 | 0.41 |
| 1:I:191:ASN:HA | 1:I:195:GLU:O | 2.21 | 0.41 |
| 1:I:203:VAL:O | 1:I:205:VAL:HG23 | 2.21 | 0.41 |
| 1:I:94:ILE:HG22 | 1:I:95:GLY:N | 2.36 | 0.41 |
| 2:J:186:GLY:HA2 | 2:J:187:SER:HA | 1.47 | 0.41 |
| 2:J:242:LYS:HB2 | 3:K:269:TRP:CZ2 | 2.45 | 0.41 |
| 2:J:459:LEU:HD22 | 2:J:472:LEU:CD1 | 2.51 | 0.41 |
| 3:K:129:LEU:HD13 | 3:K:130:THR:N | 2.36 | 0.41 |
| 3:K:240:ASN:HA | 3:K:352:CYS:O | 2.21 | 0.41 |
| 3:K:238:ILE:O | 3:K:241:PRO:HG3 | 2.21 | 0.41 |
| 4:L:219:ALA:HB1 | 4:L:221:LYS:HZ1 | 1.85 | 0.41 |
| 5:M:355:ALA:HB2 | 5:M:362:ILE:CD1 | 2.51 | 0.41 |
| 6:N:105:ALA:O | 6:N:107:ARG:N | 2.54 | 0.41 |
| 6:N:178:VAL:HG11 | 6:N:402:VAL:HG12 | 2.03 | 0.41 |
| 6:N:332:THR:O | 6:N:333:GLY:C | 2.58 | 0.41 |
| 6:N:539:SER:HB2 | 6:N:542:LYS:CG | 2.51 | 0.41 |
| 7:O:191:ARG:C | 7:O:191:ARG:NE | 2.75 | 0.41 |
| 7:O:214:PHE:CD2 | 7:O:214:PHE:O | 2.74 | 0.41 |
| 7:O:516:LEU:HD11 | 7:O:517:ILE:CG1 | 2.48 | 0.41 |
| 7:O:83:LEU:HA | 7:O:86:ILE:CD1 | 2.50 | 0.41 |
| 8:P:141:GLU:O | 8:P:145:MET:HG2 | 2.21 | 0.41 |
| 8:P:146:VAL:HG22 | 8:P:148:GLY:N | 2.36 | 0.41 |
| 8:P:54:ILE:CG2 | 8:P:55:ILE:N | 2.83 | 0.41 |
| 1:A:431:ILE:CG2 | 1:A:432:TYR:N | 2.84 | 0.40 |
| 2:B:109:LEU:C | 2:B:111:ASP:H | 2.24 | 0.40 |
| 3:C:306:GLN:O | 3:C:307:HIS:C | 2.59 | 0.40 |
| 4:D:292:ILE:HG13 | 4:D:294:ARG:N | 2.36 | 0.40 |
| 4:D:425:LEU:HD12 | 4:D:444:ALA:HA | 2.03 | 0.40 |
| 6:F:105:ALA:O | 6:F:108:PHE:CD2 | 2.74 | 0.40 |
| 6:F:420:ILE:HG22 | 6:F:482:ASP:CG | 2.41 | 0.40 |
| 6:F:6:LEU:HD13 | 6:F:7:ASN:H | 1.85 | 0.40 |
| 7:G:33:CYS:HA | 7:G:83:LEU:CD1 | 2.51 | 0.40 |
| 1:I:431:ILE:CG2 | 1:I:432:TYR:N | 2.84 | 0.40 |
| 2:J:88:VAL:HG12 | 2:J:90:ASP:H | 1.86 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:K:245:LEU:HA | 3:K:296:ILE:O | 2.21 | 0.40 |
| 4:L:425:LEU:HD12 | 4:L:444:ALA:HA | 2.03 | 0.40 |
| 4:L:411:ILE:O | 4:L:498:LEU:HB3 | 2.21 | 0.40 |
| 5:M:250:SER:O | 5:M:251:HIS:O | 2.38 | 0.40 |
| 5:M:71:ASP:OD2 | 5:M:85:ASN:HB2 | 2.21 | 0.40 |
| 6:N:68:ILE:HD13 | 6:N:74:VAL:HG13 | 2.02 | 0.40 |
| 7:O:28:SER:HA | 7:O:31:ASN:OD1 | 2.21 | 0.40 |
| 8:P:122:LEU:HD23 | 8:P:126:GLU:OE1 | 2.21 | 0.40 |
| 8:P:146:VAL:HG22 | 8:P:147:VAL:N | 2.35 | 0.40 |
| 8:P:186:VAL:HA | 8:P:207:ILE:HD11 | 2.02 | 0.40 |
| 8:P:459:VAL:HB | 8:P:460:PRO:HD3 | 2.02 | 0.40 |
| 1:A:115:LEU:HD23 | 1:A:115:LEU:HA | 1.80 | 0.40 |
| 1:A:191:ASN:HA | 1:A:195:GLU:O | 2.21 | 0.40 |
| 1:A:198:TYR:CE2 | 1:A:413:LEU:CB | 3.05 | 0.40 |
| 2:B:317:LEU:O | 2:B:321:THR:N | 2.50 | 0.40 |
| 4:D:94:THR:C | 4:D:96:VAL:H | 2.25 | 0.40 |
| 5:E:115:ILE:CB | 5:E:432:ASN:HD21 | 2.35 | 0.40 |
| 5:E:332:ASN:HA | 5:E:335:LEU:HD12 | 2.02 | 0.40 |
| 5:E:355:ALA:HB2 | 5:E:362:ILE:CD1 | 2.51 | 0.40 |
| 5:E:35:GLN:CD | 5:E:36:GLY:CA | 2.86 | 0.40 |
| 6:F:158:LEU:CG | 6:F:158:LEU:O | 2.69 | 0.40 |
| 6:F:459:VAL:O | 6:F:463:GLY:N | 2.54 | 0.40 |
| 6:F:56:THR:HB | 6:F:390:GLN:CD | 2.42 | 0.40 |
| 6:F:56:THR:HB | 6:F:390:GLN:HE22 | 1.79 | 0.40 |
| 6:F:75:LEU:HD23 | 6:F:76:ILE:N | 2.36 | 0.40 |
| 7:G:129:TYR:O | 7:G:132:ALA:HB3 | 2.21 | 0.40 |
| 7:G:94:VAL:CG1 | 7:G:95:GLY:H | 2.28 | 0.40 |
| 1:I:397:GLU:HA | 1:I:400:ARG:HH11 | 1.86 | 0.40 |
| 2:J:15:ALA:O | 2:J:19:ARG:HG2 | 2.21 | 0.40 |
| 2:J:372:ALA:HA | 6:N:519:GLY:HA2 | 2.02 | 0.40 |
| 2:J:140:VAL:HG23 | 2:J:483:ARG:NH2 | 2.36 | 0.40 |
| 4:L:123:SER:OG | 4:L:440:TRP:HA | 2.21 | 0.40 |
| 4:L:292:ILE:HG13 | 4:L:294:ARG:N | 2.36 | 0.40 |
| 4:L:454:LEU:HD13 | 9:L:601:ADP:H8 | 1.86 | 0.40 |
| 4:L:94:THR:C | 4:L:96:VAL:H | 2.25 | 0.40 |
| 5:M:338:ASN:HD22 | 5:M:338:ASN:N | 2.16 | 0.40 |
| 6:N:158:LEU:O | 6:N:158:LEU:CG | 2.69 | 0.40 |
| 6:N:411:ILE:CG2 | 6:N:412:ILE:N | 2.75 | 0.40 |
| 7:O:528:GLY:HA3 | 7:O:529:SER:C | 2.41 | 0.40 |
| 8:P:437:TYR:CD2 | 8:P:437:TYR:C | 2.95 | 0.40 |
| 1:A:555:ASP:HA | 1:A:556:PRO:HD3 | 1.90 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:164:LYS:O | 2:B:166:LEU:HD23 | 2.22 | 0.40 |
| 2:B:474:LEU:N | 2:B:474:LEU:HD23 | 2.35 | 0.40 |
| 3:C:56:VAL:CA | 3:C:57:LEU:HD23 | 2.50 | 0.40 |
| 4:D:135:LEU:HD22 | 4:D:135:LEU:HA | 1.87 | 0.40 |
| 4:D:120:ILE:CG1 | 4:D:439:ILE:HG21 | 2.43 | 0.40 |
| 4:D:47:MET:O | 8:H:534:ALA:N | 2.53 | 0.40 |
| 5:E:88:ALA:CB | 5:E:109:LYS:HZ1 | 2.32 | 0.40 |
| 5:E:261:LYS:O | 5:E:341:PRO:HG3 | 2.21 | 0.40 |
| 5:E:170:ALA:N | 5:E:523:LYS:HZ1 | 2.19 | 0.40 |
| 5:E:557:SER:CB | 6:F:66:MET:HA | 2.52 | 0.40 |
| 5:E:86:ASP:O | 5:E:90:ILE:HG13 | 2.20 | 0.40 |
| 6:F:146:ASP:O | 6:F:147:ARG:C | 2.59 | 0.40 |
| 6:F:196:ILE:HG22 | 6:F:378:ILE:HG23 | 2.02 | 0.40 |
| 6:F:198:GLN:HE21 | 6:F:198:GLN:H | 1.66 | 0.40 |
| 8:H:141:GLU:O | 8:H:145:MET:HG2 | 2.21 | 0.40 |
| 8:H:209:VAL:CG2 | 8:H:386:LEU:HD11 | 2.36 | 0.40 |
| 8:H:49:CYS:O | 8:H:466:THR:CG2 | 2.69 | 0.40 |
| 1:I:198:TYR:CE2 | 1:I:413:LEU:CB | 3.05 | 0.40 |
| 1:I:156:LEU:HD21 | 1:I:409:VAL:HG13 | 2.02 | 0.40 |
| 2:J:24:VAL:HA | 2:J:27:ILE:CG2 | 2.51 | 0.40 |
| 2:J:181:ILE:HG21 | 2:J:391:LEU:O | 2.21 | 0.40 |
| 2:J:61:ALA:HB2 | 2:J:85:ASP:HB2 | 2.02 | 0.40 |
| 4:L:72:HIS:HA | 4:L:73:PRO:HD3 | 1.96 | 0.40 |
| 4:L:65:LEU:HB3 | 4:L:79:VAL:HG13 | 2.04 | 0.40 |
| 5:M:162:GLU:OE2 | 5:M:162:GLU:N | 2.55 | 0.40 |
| 5:M:276:PHE:HZ | 5:M:310:ILE:HG12 | 1.86 | 0.40 |
| 5:M:261:LYS:O | 5:M:341:PRO:HG3 | 2.21 | 0.40 |
| 5:M:387:THR:HA | 5:M:388:THR:HA | 1.61 | 0.40 |
| 6:N:342:ASP:O | 6:N:343:LEU:C | 2.59 | 0.40 |
| 6:N:370:ASN:N | 6:N:370:ASN:ND2 | 2.70 | 0.40 |
| 8:P:146:VAL:HG22 | 8:P:148:GLY:H | 1.86 | 0.40 |
| 8:P:251:THR:O | 8:P:252:CYS:C | 2.59 | 0.40 |
| 8:P:75:LEU:HD23 | 8:P:75:LEU:HA | 1.94 | 0.40 |
| 2:B:140:VAL:HG23 | 2:B:483:ARG:NH2 | 2.36 | 0.40 |
| 2:B:14:ARG:O | 2:B:15:ALA:HB3 | 2.21 | 0.40 |
| 2:B:196:ILE:HD12 | 2:B:196:ILE:N | 2.36 | 0.40 |
| 2:B:354:LEU:HD13 | 2:B:356:PHE:CE2 | 2.56 | 0.40 |
| 2:B:88:VAL:HG11 | 2:B:493:LEU:HB2 | 2.04 | 0.40 |
| 3:C:113:GLU:OE1 | 1:I:460:LYS:NZ | 2.47 | 0.40 |
| 3:C:245:LEU:HA | 3:C:296:ILE:O | 2.21 | 0.40 |
| 3:C:41:PRO:HD3 | 9:C:1101:ADP:N3 | 2.36 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:292:ILE:HG13 | 4:D:293:LEU:C | 2.42 | 0.40 |
| 5:E:107:LEU:O | 5:E:107:LEU:HD12 | 2.21 | 0.40 |
| 5:E:245:LEU:CD1 | 5:E:247:LYS:H | 2.25 | 0.40 |
| 5:E:297:LYS:HB3 | 6:F:256:ALA:CB | 2.52 | 0.40 |
| 5:E:276:PHE:HZ | 5:E:310:ILE:HG12 | 1.86 | 0.40 |
| 5:E:428:CYS:HA | 5:E:431:ARG:CG | 2.52 | 0.40 |
| 6:F:118:ILE:HG22 | 6:F:122:PHE:CD2 | 2.57 | 0.40 |
| 2:B:295:GLU:CB | 6:F:337:GLN:NE2 | 2.79 | 0.40 |
| 7:G:191:ARG:NE | 7:G:191:ARG:C | 2.75 | 0.40 |
| 7:G:413:GLY:HA2 | 9:G:601:ADP:C2 | 2.57 | 0.40 |
| 8:H:122:LEU:HD23 | 8:H:126:GLU:OE1 | 2.22 | 0.40 |
| 8:H:111:LEU:HD21 | 8:H:524:LYS:HA | 2.04 | 0.40 |
| 8:H:5:LEU:HA | 8:H:6:PRO:HD3 | 1.87 | 0.40 |
| 2:J:201:GLY:O | 2:J:202:LYS:CB | 2.69 | 0.40 |
| 2:J:360:LYS:HA | 2:J:361:ALA:HA | 1.70 | 0.40 |
| 3:K:112:ILE:C | 3:K:114:LYS:N | 2.74 | 0.40 |
| 4:L:292:ILE:CG1 | 4:L:293:LEU:HA | 2.47 | 0.40 |
| 4:L:86:ASP:HB2 | 4:L:93:THR:HG22 | 2.03 | 0.40 |
| 5:M:412:ASN:O | 5:M:413:LYS:CB | 2.69 | 0.40 |
| 6:N:16:ASP:HA | 6:N:19:LEU:HB2 | 2.02 | 0.40 |
| 7:O:129:TYR:O | 7:O:132:ALA:HB3 | 2.21 | 0.40 |
| 7:O:449:ILE:CB | 7:O:450:PRO:HD3 | 2.50 | 0.40 |
| 7:O:478:TRP:O | 7:O:479:TYR:CB | 2.69 | 0.40 |
| 8:P:414:PRO:HA | 8:P:415:SER:HA | 1.60 | 0.40 |
| 1:A:307:LEU:O | 1:A:311:VAL:N | 2.53 | 0.40 |
| 2:B:201:GLY:O | 2:B:202:LYS:CB | 2.69 | 0.40 |
| 2:B:354:LEU:HD13 | 2:B:356:PHE:HE2 | 1.87 | 0.40 |
| 3:C:112:ILE:C | 3:C:114:LYS:N | 2.74 | 0.40 |
| 3:C:210:PRO:HB2 | 3:C:211:GLY:H | 1.63 | 0.40 |
| 3:C:413:SER:HA | 3:C:414:PRO:HD3 | 1.90 | 0.40 |
| 4:D:157:SER:C | 4:D:159:SER:H | 2.24 | 0.40 |
| 4:D:263:ILE:C | 4:D:265:LYS:H | 2.23 | 0.40 |
| 5:E:237:SER:HB3 | 5:E:408:VAL:HA | 2.04 | 0.40 |
| 5:E:472:PHE:HZ | 5:E:542:THR:HG22 | 1.86 | 0.40 |
| 6:F:331:VAL:HG23 | 6:F:375:SER:OG | 2.21 | 0.40 |
| 6:F:342:ASP:O | 6:F:343:LEU:C | 2.59 | 0.40 |
| 7:G:204:ILE:HA | 7:G:205:PRO:HD3 | 1.79 | 0.40 |
| 8:H:208:ARG:O | 8:H:383:THR:HA | 2.22 | 0.40 |
| 1:I:303:ASP:OD1 | 1:I:304:ASP:N | 2.55 | 0.40 |
| 2:J:164:LYS:O | 2:J:166:LEU:HD23 | 2.22 | 0.40 |
| 2:J:320:VAL:HB | 2:J:338:GLY:H | 1.87 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 2:J:402:LEU:CD2 | 2:J:483:ARG:HG3 | 2.46 | 0.40 |
| 3:K:34:VAL:HG12 | 3:K:35:ILE:N | 2.35 | 0.40 |
| 4:L:116:HIS:HA | 4:L:117:PRO:HD3 | 1.99 | 0.40 |
| 4:L:20:VAL:HG21 | 4:L:522:ASP:O | 2.22 | 0.40 |
| 4:L:65:LEU:HA | 4:L:65:LEU:HD23 | 1.83 | 0.40 |
| 5:M:412:ASN:C | 5:M:414:MET:H | 2.24 | 0.40 |
| 6:N:331:VAL:HG23 | 6:N:375:SER:OG | 2.21 | 0.40 |
| 7:O:94:VAL:CG1 | 7:O:95:GLY:N | 2.83 | 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 X-ray entries followed by that with respect to entries of similar resolution.

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 | 538/559 (96%) | 441 (82%) | 78 (14%) | 19 (4%) | 3 | 31 |
| 1 | I | 538/559 (96%) | 441 (82%) | 78 (14%) | 19 (4%) | 3 | 31 |
| 1 | a | 538/559 (96%) | 441 (82%) | 78 (14%) | 19 (4%) | 3 | 31 |
| 1 | i | 538/559 (96%) | 441 (82%) | 78 (14%) | 19 (4%) | 3 | 31 |
| 2 | B | 509/527 (97%) | 417 (82%) | 67 (13%) | 25 (5%) | 2 | 24 |
| 2 | J | 509/527 (97%) | 417 (82%) | 67 (13%) | 25 (5%) | 2 | 24 |
| 2 | b | 509/527 (97%) | 417 (82%) | 68 (13%) | 24 (5%) | 2 | 24 |
| 2 | j | 509/527 (97%) | 417 (82%) | 67 (13%) | 25 (5%) | 2 | 24 |
| 3 | C | 508/590 (86%) | 420 (83%) | 68 (13%) | 20 (4%) | 3 | 28 |
| 3 | K | 508/590 (86%) | 421 (83%) | 67 (13%) | 20 (4%) | 3 | 28 |
| 3 | c | 508/590 (86%) | 419 (82%) | 70 (14%) | 19 (4%) | 3 | 29 |
| 3 | k | 508/590 (86%) | 420 (83%) | 68 (13%) | 20 (4%) | 3 | 28 |
| 4 | D | 520/528 (98%) | 429 (82%) | 79 (15%) | 12 (2%) | 6 | 38 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|------------|----------|-------------|----|
| 4 | L | 520/528 (98%) | 429 (82%) | 79 (15%) | 12 (2%) | 6 | 38 |
| 4 | d | 520/528 (98%) | 429 (82%) | 79 (15%) | 12 (2%) | 6 | 38 |
| 4 | l | 520/528 (98%) | 429 (82%) | 79 (15%) | 12 (2%) | 6 | 38 |
| 5 | E | 521/562 (93%) | 443 (85%) | 59 (11%) | 19 (4%) | 3 | 30 |
| 5 | M | 521/562 (93%) | 443 (85%) | 59 (11%) | 19 (4%) | 3 | 30 |
| 5 | e | 521/562 (93%) | 442 (85%) | 60 (12%) | 19 (4%) | 3 | 30 |
| 5 | m | 521/562 (93%) | 443 (85%) | 59 (11%) | 19 (4%) | 3 | 30 |
| 6 | F | 529/546 (97%) | 429 (81%) | 82 (16%) | 18 (3%) | 3 | 31 |
| 6 | N | 529/546 (97%) | 429 (81%) | 82 (16%) | 18 (3%) | 3 | 31 |
| 6 | f | 529/546 (97%) | 429 (81%) | 82 (16%) | 18 (3%) | 3 | 31 |
| 6 | n | 529/546 (97%) | 429 (81%) | 82 (16%) | 18 (3%) | 3 | 31 |
| 7 | G | 505/550 (92%) | 424 (84%) | 60 (12%) | 21 (4%) | 3 | 26 |
| 7 | O | 505/550 (92%) | 424 (84%) | 60 (12%) | 21 (4%) | 3 | 26 |
| 7 | g | 505/550 (92%) | 424 (84%) | 60 (12%) | 21 (4%) | 3 | 26 |
| 7 | o | 505/550 (92%) | 424 (84%) | 60 (12%) | 21 (4%) | 3 | 26 |
| 8 | H | 521/568 (92%) | 439 (84%) | 58 (11%) | 24 (5%) | 2 | 24 |
| 8 | P | 521/568 (92%) | 439 (84%) | 58 (11%) | 24 (5%) | 2 | 24 |
| 8 | h | 521/568 (92%) | 439 (84%) | 58 (11%) | 24 (5%) | 2 | 24 |
| 8 | p | 521/568 (92%) | 439 (84%) | 58 (11%) | 24 (5%) | 2 | 24 |
| All | All | 16604/17720 (94%) | 13767 (83%) | 2207 (13%) | 630 (4%) | 3 | 29 |

All (630) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 5 | ILE |
| 2 | B | 165 | ILE |
| 2 | B | 184 | LEU |
| 2 | B | 185 | LYS |
| 2 | B | 307 | GLU |
| 2 | B | 370 | ARG |
| 2 | B | 470 | SER |
| 3 | C | 16 | THR |
| 3 | C | 210 | PRO |
| 3 | C | 252 | TYR |
| 3 | C | 303 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | D | 205 | ASP |
| 4 | D | 427 | LYS |
| 5 | E | 167 | ASP |
| 5 | E | 351 | LEU |
| 5 | E | 369 | LEU |
| 6 | F | 160 | THR |
| 6 | F | 353 | LEU |
| 6 | F | 460 | LYS |
| 6 | F | 489 | VAL |
| 6 | F | 490 | GLY |
| 7 | G | 46 | PRO |
| 7 | G | 190 | ASP |
| 7 | G | 213 | LEU |
| 7 | G | 487 | ASN |
| 7 | G | 495 | PHE |
| 8 | H | 147 | VAL |
| 8 | H | 483 | ASN |
| 8 | H | 490 | VAL |
| 2 | J | 5 | ILE |
| 2 | J | 165 | ILE |
| 2 | J | 184 | LEU |
| 2 | J | 185 | LYS |
| 2 | J | 307 | GLU |
| 2 | J | 370 | ARG |
| 2 | J | 470 | SER |
| 3 | K | 16 | THR |
| 3 | K | 210 | PRO |
| 3 | K | 252 | TYR |
| 3 | K | 303 | ASP |
| 4 | L | 205 | ASP |
| 4 | L | 427 | LYS |
| 5 | M | 167 | ASP |
| 5 | M | 351 | LEU |
| 5 | M | 369 | LEU |
| 6 | N | 160 | THR |
| 6 | N | 353 | LEU |
| 6 | N | 460 | LYS |
| 6 | N | 489 | VAL |
| 6 | N | 490 | GLY |
| 7 | O | 46 | PRO |
| 7 | O | 190 | ASP |
| 7 | O | 213 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 7 | O | 487 | ASN |
| 7 | O | 495 | PHE |
| 8 | P | 147 | VAL |
| 8 | P | 483 | ASN |
| 8 | P | 490 | VAL |
| 2 | b | 1005 | ILE |
| 2 | b | 1165 | ILE |
| 2 | b | 1184 | LEU |
| 2 | b | 1185 | LYS |
| 2 | b | 1307 | GLU |
| 2 | b | 1370 | ARG |
| 2 | b | 1470 | SER |
| 3 | c | 1016 | THR |
| 3 | c | 1210 | PRO |
| 3 | c | 1252 | TYR |
| 3 | c | 1303 | ASP |
| 4 | d | 1205 | ASP |
| 4 | d | 1427 | LYS |
| 5 | e | 1167 | ASP |
| 5 | e | 1351 | LEU |
| 5 | e | 1369 | LEU |
| 6 | f | 1160 | THR |
| 6 | f | 1353 | LEU |
| 6 | f | 1460 | LYS |
| 6 | f | 1489 | VAL |
| 6 | f | 1490 | GLY |
| 7 | g | 1046 | PRO |
| 7 | g | 1190 | ASP |
| 7 | g | 1213 | LEU |
| 7 | g | 1487 | ASN |
| 7 | g | 1495 | PHE |
| 8 | h | 1006 | PRO |
| 8 | h | 1147 | VAL |
| 8 | h | 1483 | ASN |
| 8 | h | 1490 | VAL |
| 2 | j | 1005 | ILE |
| 2 | j | 1165 | ILE |
| 2 | j | 1184 | LEU |
| 2 | j | 1185 | LYS |
| 2 | j | 1307 | GLU |
| 2 | j | 1370 | ARG |
| 2 | j | 1470 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | k | 1016 | THR |
| 3 | k | 1210 | PRO |
| 3 | k | 1252 | TYR |
| 3 | k | 1303 | ASP |
| 4 | l | 1205 | ASP |
| 4 | l | 1427 | LYS |
| 5 | m | 1167 | ASP |
| 5 | m | 1351 | LEU |
| 5 | m | 1369 | LEU |
| 6 | n | 1160 | THR |
| 6 | n | 1353 | LEU |
| 6 | n | 1460 | LYS |
| 6 | n | 1489 | VAL |
| 6 | n | 1490 | GLY |
| 7 | o | 1046 | PRO |
| 7 | o | 1190 | ASP |
| 7 | o | 1213 | LEU |
| 7 | o | 1487 | ASN |
| 7 | o | 1495 | PHE |
| 8 | p | 1147 | VAL |
| 8 | p | 1483 | ASN |
| 8 | p | 1490 | VAL |
| 1 | A | 11 | ASP |
| 1 | A | 56 | ASP |
| 1 | A | 94 | ILE |
| 1 | A | 265 | ASP |
| 1 | A | 508 | LYS |
| 2 | B | 35 | SER |
| 2 | B | 50 | SER |
| 2 | B | 142 | ASN |
| 2 | B | 220 | ASN |
| 2 | B | 323 | GLY |
| 2 | B | 371 | GLY |
| 3 | C | 19 | GLN |
| 3 | C | 36 | ARG |
| 3 | C | 144 | ASP |
| 3 | C | 258 | GLN |
| 3 | C | 321 | LYS |
| 3 | C | 454 | ARG |
| 4 | D | 188 | ASN |
| 4 | D | 485 | ARG |
| 5 | E | 251 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | E | 347 | GLY |
| 5 | E | 402 | LYS |
| 5 | E | 438 | ARG |
| 6 | F | 138 | ILE |
| 6 | F | 298 | GLN |
| 6 | F | 333 | GLY |
| 6 | F | 467 | LEU |
| 6 | F | 486 | THR |
| 7 | G | 45 | GLY |
| 7 | G | 224 | PHE |
| 7 | G | 256 | ASN |
| 7 | G | 478 | TRP |
| 7 | G | 502 | VAL |
| 1 | I | 11 | ASP |
| 1 | I | 56 | ASP |
| 1 | I | 94 | ILE |
| 1 | I | 265 | ASP |
| 1 | I | 508 | LYS |
| 2 | J | 35 | SER |
| 2 | J | 50 | SER |
| 2 | J | 142 | ASN |
| 2 | J | 220 | ASN |
| 2 | J | 323 | GLY |
| 2 | J | 371 | GLY |
| 3 | K | 19 | GLN |
| 3 | K | 36 | ARG |
| 3 | K | 144 | ASP |
| 3 | K | 258 | GLN |
| 3 | K | 321 | LYS |
| 3 | K | 454 | ARG |
| 4 | L | 188 | ASN |
| 4 | L | 485 | ARG |
| 5 | M | 251 | HIS |
| 5 | M | 347 | GLY |
| 5 | M | 402 | LYS |
| 5 | M | 438 | ARG |
| 6 | N | 138 | ILE |
| 6 | N | 298 | GLN |
| 6 | N | 333 | GLY |
| 6 | N | 467 | LEU |
| 6 | N | 486 | THR |
| 7 | O | 45 | GLY |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 7 | O | 224 | PHE |
| 7 | O | 256 | ASN |
| 7 | O | 478 | TRP |
| 7 | O | 502 | VAL |
| 1 | a | 1011 | ASP |
| 1 | a | 1056 | ASP |
| 1 | a | 1094 | ILE |
| 1 | a | 1265 | ASP |
| 1 | a | 1508 | LYS |
| 2 | b | 1035 | SER |
| 2 | b | 1050 | SER |
| 2 | b | 1142 | ASN |
| 2 | b | 1220 | ASN |
| 2 | b | 1323 | GLY |
| 2 | b | 1371 | GLY |
| 3 | c | 1019 | GLN |
| 3 | c | 1036 | ARG |
| 3 | c | 1144 | ASP |
| 3 | c | 1258 | GLN |
| 3 | c | 1321 | LYS |
| 3 | c | 1454 | ARG |
| 4 | d | 1188 | ASN |
| 4 | d | 1485 | ARG |
| 5 | e | 1251 | HIS |
| 5 | e | 1347 | GLY |
| 5 | e | 1402 | LYS |
| 5 | e | 1438 | ARG |
| 6 | f | 1138 | ILE |
| 6 | f | 1298 | GLN |
| 6 | f | 1333 | GLY |
| 6 | f | 1467 | LEU |
| 6 | f | 1486 | THR |
| 7 | g | 1045 | GLY |
| 7 | g | 1224 | PHE |
| 7 | g | 1256 | ASN |
| 7 | g | 1478 | TRP |
| 7 | g | 1502 | VAL |
| 1 | i | 1011 | ASP |
| 1 | i | 1056 | ASP |
| 1 | i | 1094 | ILE |
| 1 | i | 1265 | ASP |
| 1 | i | 1508 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | j | 1035 | SER |
| 2 | j | 1050 | SER |
| 2 | j | 1142 | ASN |
| 2 | j | 1220 | ASN |
| 2 | j | 1323 | GLY |
| 2 | j | 1371 | GLY |
| 3 | k | 1019 | GLN |
| 3 | k | 1036 | ARG |
| 3 | k | 1144 | ASP |
| 3 | k | 1258 | GLN |
| 3 | k | 1321 | LYS |
| 3 | k | 1454 | ARG |
| 4 | l | 1188 | ASN |
| 4 | l | 1485 | ARG |
| 5 | m | 1251 | HIS |
| 5 | m | 1347 | GLY |
| 5 | m | 1402 | LYS |
| 5 | m | 1438 | ARG |
| 6 | n | 1138 | ILE |
| 6 | n | 1298 | GLN |
| 6 | n | 1333 | GLY |
| 6 | n | 1467 | LEU |
| 6 | n | 1486 | THR |
| 7 | o | 1045 | GLY |
| 7 | o | 1224 | PHE |
| 7 | o | 1256 | ASN |
| 7 | o | 1478 | TRP |
| 7 | o | 1502 | VAL |
| 1 | A | 335 | ALA |
| 1 | A | 337 | LEU |
| 2 | B | 15 | ALA |
| 2 | B | 301 | LEU |
| 2 | B | 467 | ILE |
| 2 | B | 478 | THR |
| 3 | C | 52 | MET |
| 3 | C | 256 | GLU |
| 3 | C | 460 | ALA |
| 3 | C | 490 | LYS |
| 4 | D | 17 | PRO |
| 4 | D | 143 | SER |
| 4 | D | 474 | GLU |
| 5 | E | 36 | GLY |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | E | 190 | SER |
| 6 | F | 204 | PRO |
| 7 | G | 63 | SER |
| 7 | G | 250 | LEU |
| 7 | G | 362 | TYR |
| 8 | H | 6 | PRO |
| 8 | H | 13 | LEU |
| 8 | H | 48 | PRO |
| 8 | H | 146 | VAL |
| 8 | H | 150 | ILE |
| 8 | H | 178 | LEU |
| 8 | H | 343 | ARG |
| 8 | H | 378 | ILE |
| 8 | H | 458 | VAL |
| 8 | H | 460 | PRO |
| 8 | H | 486 | GLU |
| 1 | I | 335 | ALA |
| 1 | I | 337 | LEU |
| 2 | J | 15 | ALA |
| 2 | J | 301 | LEU |
| 2 | J | 467 | ILE |
| 2 | J | 478 | THR |
| 3 | K | 52 | MET |
| 3 | K | 256 | GLU |
| 3 | K | 460 | ALA |
| 3 | K | 490 | LYS |
| 4 | L | 17 | PRO |
| 4 | L | 143 | SER |
| 4 | L | 474 | GLU |
| 5 | M | 36 | GLY |
| 5 | M | 190 | SER |
| 6 | N | 204 | PRO |
| 7 | O | 63 | SER |
| 7 | O | 250 | LEU |
| 7 | O | 362 | TYR |
| 8 | P | 6 | PRO |
| 8 | P | 13 | LEU |
| 8 | P | 48 | PRO |
| 8 | P | 146 | VAL |
| 8 | P | 150 | ILE |
| 8 | P | 178 | LEU |
| 8 | P | 343 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 8 | P | 378 | ILE |
| 8 | P | 458 | VAL |
| 8 | P | 460 | PRO |
| 8 | P | 486 | GLU |
| 1 | a | 1335 | ALA |
| 1 | a | 1337 | LEU |
| 2 | b | 1015 | ALA |
| 2 | b | 1301 | LEU |
| 2 | b | 1467 | ILE |
| 2 | b | 1478 | THR |
| 3 | c | 1052 | MET |
| 3 | c | 1256 | GLU |
| 3 | c | 1460 | ALA |
| 3 | c | 1490 | LYS |
| 4 | d | 1017 | PRO |
| 4 | d | 1143 | SER |
| 4 | d | 1474 | GLU |
| 5 | e | 1036 | GLY |
| 5 | e | 1190 | SER |
| 6 | f | 1204 | PRO |
| 7 | g | 1063 | SER |
| 7 | g | 1250 | LEU |
| 7 | g | 1362 | TYR |
| 8 | h | 1013 | LEU |
| 8 | h | 1048 | PRO |
| 8 | h | 1146 | VAL |
| 8 | h | 1150 | ILE |
| 8 | h | 1178 | LEU |
| 8 | h | 1343 | ARG |
| 8 | h | 1378 | ILE |
| 8 | h | 1458 | VAL |
| 8 | h | 1460 | PRO |
| 8 | h | 1486 | GLU |
| 1 | i | 1335 | ALA |
| 1 | i | 1337 | LEU |
| 2 | j | 1015 | ALA |
| 2 | j | 1301 | LEU |
| 2 | j | 1467 | ILE |
| 2 | j | 1478 | THR |
| 3 | k | 1052 | MET |
| 3 | k | 1256 | GLU |
| 3 | k | 1460 | ALA |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | k | 1490 | LYS |
| 4 | l | 1017 | PRO |
| 4 | l | 1143 | SER |
| 4 | l | 1474 | GLU |
| 5 | m | 1036 | GLY |
| 5 | m | 1190 | SER |
| 6 | n | 1204 | PRO |
| 7 | o | 1063 | SER |
| 7 | o | 1250 | LEU |
| 7 | o | 1362 | TYR |
| 8 | p | 1006 | PRO |
| 8 | p | 1013 | LEU |
| 8 | p | 1048 | PRO |
| 8 | p | 1146 | VAL |
| 8 | p | 1150 | ILE |
| 8 | p | 1178 | LEU |
| 8 | p | 1343 | ARG |
| 8 | p | 1378 | ILE |
| 8 | p | 1458 | VAL |
| 8 | p | 1460 | PRO |
| 8 | p | 1486 | GLU |
| 1 | A | 74 | ASP |
| 1 | A | 121 | HIS |
| 1 | A | 267 | PRO |
| 1 | A | 518 | LEU |
| 2 | B | 16 | GLU |
| 2 | B | 202 | LYS |
| 2 | B | 246 | PHE |
| 2 | B | 327 | SER |
| 3 | C | 265 | LYS |
| 4 | D | 9 | ALA |
| 4 | D | 95 | SER |
| 4 | D | 382 | ALA |
| 5 | E | 274 | CYS |
| 5 | E | 462 | ARG |
| 6 | F | 167 | THR |
| 6 | F | 343 | LEU |
| 7 | G | 368 | CYS |
| 7 | G | 428 | SER |
| 8 | H | 122 | LEU |
| 8 | H | 233 | GLU |
| 8 | H | 356 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 8 | H | 373 | GLN |
| 1 | I | 74 | ASP |
| 1 | I | 121 | HIS |
| 1 | I | 267 | PRO |
| 1 | I | 518 | LEU |
| 2 | J | 16 | GLU |
| 2 | J | 202 | LYS |
| 2 | J | 246 | PHE |
| 2 | J | 327 | SER |
| 3 | K | 265 | LYS |
| 4 | L | 9 | ALA |
| 4 | L | 95 | SER |
| 4 | L | 382 | ALA |
| 5 | M | 274 | CYS |
| 5 | M | 462 | ARG |
| 6 | N | 167 | THR |
| 6 | N | 343 | LEU |
| 7 | O | 368 | CYS |
| 7 | O | 428 | SER |
| 8 | P | 122 | LEU |
| 8 | P | 233 | GLU |
| 8 | P | 356 | GLU |
| 8 | P | 373 | GLN |
| 1 | a | 1074 | ASP |
| 1 | a | 1121 | HIS |
| 1 | a | 1267 | PRO |
| 1 | a | 1518 | LEU |
| 2 | b | 1016 | GLU |
| 2 | b | 1202 | LYS |
| 2 | b | 1246 | PHE |
| 2 | b | 1327 | SER |
| 3 | c | 1265 | LYS |
| 4 | d | 1009 | ALA |
| 4 | d | 1095 | SER |
| 4 | d | 1382 | ALA |
| 5 | e | 1274 | CYS |
| 5 | e | 1462 | ARG |
| 6 | f | 1167 | THR |
| 6 | f | 1343 | LEU |
| 7 | g | 1368 | CYS |
| 7 | g | 1428 | SER |
| 8 | h | 1122 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 8 | h | 1233 | GLU |
| 8 | h | 1356 | GLU |
| 8 | h | 1373 | GLN |
| 1 | i | 1074 | ASP |
| 1 | i | 1121 | HIS |
| 1 | i | 1267 | PRO |
| 1 | i | 1518 | LEU |
| 2 | j | 1016 | GLU |
| 2 | j | 1202 | LYS |
| 2 | j | 1246 | PHE |
| 2 | j | 1327 | SER |
| 3 | k | 1265 | LYS |
| 4 | l | 1009 | ALA |
| 4 | l | 1095 | SER |
| 4 | l | 1382 | ALA |
| 5 | m | 1274 | CYS |
| 5 | m | 1462 | ARG |
| 6 | n | 1167 | THR |
| 6 | n | 1343 | LEU |
| 7 | o | 1368 | CYS |
| 7 | o | 1428 | SER |
| 8 | p | 1122 | LEU |
| 8 | p | 1233 | GLU |
| 8 | p | 1356 | GLU |
| 8 | p | 1373 | GLN |
| 1 | A | 199 | PRO |
| 1 | A | 367 | SER |
| 2 | B | 293 | TYR |
| 3 | C | 30 | ALA |
| 3 | C | 249 | PRO |
| 4 | D | 294 | ARG |
| 4 | D | 431 | SER |
| 5 | E | 147 | ALA |
| 5 | E | 279 | PRO |
| 5 | E | 376 | THR |
| 6 | F | 24 | THR |
| 6 | F | 188 | ASN |
| 7 | G | 337 | THR |
| 8 | H | 49 | CYS |
| 8 | H | 322 | LYS |
| 1 | I | 199 | PRO |
| 1 | I | 367 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | J | 293 | TYR |
| 3 | K | 30 | ALA |
| 3 | K | 249 | PRO |
| 4 | L | 294 | ARG |
| 4 | L | 431 | SER |
| 5 | M | 147 | ALA |
| 5 | M | 279 | PRO |
| 5 | M | 376 | THR |
| 6 | N | 24 | THR |
| 6 | N | 188 | ASN |
| 7 | O | 337 | THR |
| 8 | P | 49 | CYS |
| 8 | P | 322 | LYS |
| 1 | a | 1199 | PRO |
| 1 | a | 1367 | SER |
| 2 | b | 1293 | TYR |
| 3 | c | 1030 | ALA |
| 3 | c | 1249 | PRO |
| 4 | d | 1294 | ARG |
| 4 | d | 1431 | SER |
| 5 | e | 1147 | ALA |
| 5 | e | 1279 | PRO |
| 5 | e | 1376 | THR |
| 6 | f | 1024 | THR |
| 6 | f | 1188 | ASN |
| 7 | g | 1337 | THR |
| 8 | h | 1049 | CYS |
| 8 | h | 1322 | LYS |
| 1 | i | 1199 | PRO |
| 1 | i | 1367 | SER |
| 2 | j | 1293 | TYR |
| 3 | k | 1030 | ALA |
| 3 | k | 1249 | PRO |
| 4 | l | 1294 | ARG |
| 4 | l | 1431 | SER |
| 5 | m | 1147 | ALA |
| 5 | m | 1279 | PRO |
| 5 | m | 1376 | THR |
| 6 | n | 1024 | THR |
| 6 | n | 1188 | ASN |
| 7 | o | 1337 | THR |
| 8 | p | 1049 | CYS |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 8 | p | 1322 | LYS |
| 1 | A | 55 | ASP |
| 1 | A | 77 | HIS |
| 2 | B | 372 | ALA |
| 5 | E | 254 | MET |
| 6 | F | 183 | ASP |
| 7 | G | 67 | ALA |
| 7 | G | 479 | TYR |
| 8 | H | 187 | SER |
| 8 | H | 484 | VAL |
| 1 | I | 55 | ASP |
| 1 | I | 77 | HIS |
| 2 | J | 372 | ALA |
| 5 | M | 254 | MET |
| 6 | N | 183 | ASP |
| 7 | O | 67 | ALA |
| 7 | O | 479 | TYR |
| 8 | P | 187 | SER |
| 8 | P | 484 | VAL |
| 1 | a | 1055 | ASP |
| 1 | a | 1077 | HIS |
| 5 | e | 1254 | MET |
| 6 | f | 1183 | ASP |
| 7 | g | 1067 | ALA |
| 7 | g | 1479 | TYR |
| 8 | h | 1187 | SER |
| 8 | h | 1484 | VAL |
| 1 | i | 1055 | ASP |
| 1 | i | 1077 | HIS |
| 2 | j | 1372 | ALA |
| 5 | m | 1254 | MET |
| 6 | n | 1183 | ASP |
| 7 | o | 1067 | ALA |
| 7 | o | 1479 | TYR |
| 8 | p | 1187 | SER |
| 8 | p | 1484 | VAL |
| 1 | A | 22 | GLY |
| 1 | A | 376 | GLY |
| 1 | A | 549 | PRO |
| 2 | B | 117 | PRO |
| 3 | C | 410 | PRO |
| 5 | E | 493 | GLY |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 8 | H | 284 | ILE |
| 8 | H | 324 | PRO |
| 1 | I | 22 | GLY |
| 1 | I | 376 | GLY |
| 1 | I | 549 | PRO |
| 2 | J | 117 | PRO |
| 3 | K | 410 | PRO |
| 5 | M | 493 | GLY |
| 8 | P | 284 | ILE |
| 8 | P | 324 | PRO |
| 1 | a | 1022 | GLY |
| 1 | a | 1376 | GLY |
| 1 | a | 1549 | PRO |
| 2 | b | 1117 | PRO |
| 3 | c | 1410 | PRO |
| 5 | e | 1493 | GLY |
| 8 | h | 1284 | ILE |
| 8 | h | 1324 | PRO |
| 1 | i | 1022 | GLY |
| 1 | i | 1376 | GLY |
| 1 | i | 1549 | PRO |
| 2 | j | 1117 | PRO |
| 3 | k | 1410 | PRO |
| 5 | m | 1493 | GLY |
| 8 | p | 1284 | ILE |
| 8 | p | 1324 | PRO |
| 1 | A | 292 | GLY |
| 2 | B | 88 | VAL |
| 5 | E | 440 | VAL |
| 1 | I | 292 | GLY |
| 2 | J | 88 | VAL |
| 5 | M | 440 | VAL |
| 1 | a | 1292 | GLY |
| 2 | b | 1088 | VAL |
| 5 | e | 1440 | VAL |
| 1 | i | 1292 | GLY |
| 2 | j | 1088 | VAL |
| 5 | m | 1440 | VAL |
| 7 | G | 412 | GLY |
| 7 | G | 528 | GLY |
| 7 | O | 412 | GLY |
| 7 | O | 528 | GLY |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 7 | g | 1412 | GLY |
| 7 | g | 1528 | GLY |
| 7 | o | 1412 | GLY |
| 7 | o | 1528 | GLY |
| 3 | C | 142 | PRO |
| 5 | E | 386 | GLY |
| 6 | F | 412 | ILE |
| 7 | G | 62 | ILE |
| 3 | K | 142 | PRO |
| 5 | M | 386 | GLY |
| 6 | N | 412 | ILE |
| 6 | N | 512 | VAL |
| 7 | O | 62 | ILE |
| 3 | c | 1142 | PRO |
| 5 | e | 1386 | GLY |
| 6 | f | 1412 | ILE |
| 7 | g | 1062 | ILE |
| 3 | k | 1142 | PRO |
| 5 | m | 1386 | GLY |
| 6 | n | 1412 | ILE |
| 7 | o | 1062 | ILE |
| 3 | C | 50 | ASP |
| 5 | E | 507 | ILE |
| 6 | F | 512 | VAL |
| 3 | K | 50 | ASP |
| 5 | M | 507 | ILE |
| 5 | e | 1507 | ILE |
| 6 | f | 1512 | VAL |
| 3 | k | 1050 | ASP |
| 5 | m | 1507 | ILE |
| 6 | n | 1512 | VAL |

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1 | A | 301/471 (64%) | 274 (91%) | 27 (9%) | 9 | 37 |
| 1 | I | 301/471 (64%) | 274 (91%) | 27 (9%) | 9 | 37 |
| 1 | a | 301/471 (64%) | 274 (91%) | 27 (9%) | 9 | 37 |
| 1 | i | 301/471 (64%) | 274 (91%) | 27 (9%) | 9 | 37 |
| 2 | B | 320/441 (73%) | 263 (82%) | 57 (18%) | 2 | 12 |
| 2 | J | 320/441 (73%) | 263 (82%) | 57 (18%) | 2 | 12 |
| 2 | b | 320/441 (73%) | 262 (82%) | 58 (18%) | 1 | 12 |
| 2 | j | 319/441 (72%) | 262 (82%) | 57 (18%) | 2 | 12 |
| 3 | C | 295/497 (59%) | 268 (91%) | 27 (9%) | 9 | 35 |
| 3 | K | 296/497 (60%) | 269 (91%) | 27 (9%) | 9 | 36 |
| 3 | c | 297/497 (60%) | 270 (91%) | 27 (9%) | 9 | 36 |
| 3 | k | 297/497 (60%) | 270 (91%) | 27 (9%) | 9 | 36 |
| 4 | D | 290/454 (64%) | 261 (90%) | 29 (10%) | 7 | 32 |
| 4 | L | 290/454 (64%) | 261 (90%) | 29 (10%) | 7 | 32 |
| 4 | d | 290/454 (64%) | 261 (90%) | 29 (10%) | 7 | 32 |
| 4 | l | 290/454 (64%) | 261 (90%) | 29 (10%) | 7 | 32 |
| 5 | E | 293/483 (61%) | 257 (88%) | 36 (12%) | 4 | 24 |
| 5 | M | 293/483 (61%) | 257 (88%) | 36 (12%) | 4 | 24 |
| 5 | e | 293/483 (61%) | 257 (88%) | 36 (12%) | 4 | 24 |
| 5 | m | 293/483 (61%) | 257 (88%) | 36 (12%) | 4 | 24 |
| 6 | F | 334/463 (72%) | 273 (82%) | 61 (18%) | 1 | 11 |
| 6 | N | 333/463 (72%) | 273 (82%) | 60 (18%) | 1 | 12 |
| 6 | f | 334/463 (72%) | 272 (81%) | 62 (19%) | 1 | 11 |
| 6 | n | 333/463 (72%) | 272 (82%) | 61 (18%) | 1 | 11 |
| 7 | G | 275/454 (61%) | 241 (88%) | 34 (12%) | 4 | 24 |
| 7 | O | 274/454 (60%) | 240 (88%) | 34 (12%) | 4 | 24 |
| 7 | g | 274/454 (60%) | 240 (88%) | 34 (12%) | 4 | 24 |
| 7 | o | 274/454 (60%) | 240 (88%) | 34 (12%) | 4 | 24 |
| 8 | H | 307/473 (65%) | 276 (90%) | 31 (10%) | 7 | 32 |
| 8 | P | 307/473 (65%) | 276 (90%) | 31 (10%) | 7 | 32 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|------------|-------------|----|
| 8 | h | 306/473 (65%) | 275 (90%) | 31 (10%) | 7 | 32 |
| 8 | p | 307/473 (65%) | 276 (90%) | 31 (10%) | 7 | 32 |
| All | All | 9658/14944 (65%) | 8449 (88%) | 1209 (12%) | 4 | 24 |

All (1209) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 8 | SER |
| 1 | A | 13 | LEU |
| 1 | A | 44 | LEU |
| 1 | A | 50 | ASP |
| 1 | A | 74 | ASP |
| 1 | A | 76 | GLN |
| 1 | A | 90 | GLN |
| 1 | A | 91 | ASP |
| 1 | A | 119 | LYS |
| 1 | A | 120 | ILE |
| 1 | A | 187 | VAL |
| 1 | A | 204 | ASN |
| 1 | A | 225 | ASN |
| 1 | A | 226 | CYS |
| 1 | A | 228 | VAL |
| 1 | A | 248 | ASP |
| 1 | A | 255 | ARG |
| 1 | A | 344 | LEU |
| 1 | A | 350 | PHE |
| 1 | A | 402 | LEU |
| 1 | A | 404 | ASP |
| 1 | A | 419 | VAL |
| 1 | A | 446 | LEU |
| 1 | A | 484 | SER |
| 1 | A | 496 | SER |
| 1 | A | 532 | LEU |
| 1 | A | 548 | ASP |
| 2 | B | 4 | GLN |
| 2 | B | 5 | ILE |
| 2 | B | 8 | ASP |
| 2 | B | 19 | ARG |
| 2 | B | 27 | ILE |
| 2 | B | 31 | ASP |
| 2 | B | 32 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 33 | VAL |
| 2 | B | 43 | ASP |
| 2 | B | 57 | THR |
| 2 | B | 58 | ASN |
| 2 | B | 66 | SER |
| 2 | B | 80 | ILE |
| 2 | B | 92 | THR |
| 2 | B | 145 | ASP |
| 2 | B | 146 | LYS |
| 2 | B | 149 | PHE |
| 2 | B | 166 | LEU |
| 2 | B | 176 | LEU |
| 2 | B | 197 | LYS |
| 2 | B | 203 | LEU |
| 2 | B | 213 | ILE |
| 2 | B | 217 | LYS |
| 2 | B | 228 | ASN |
| 2 | B | 231 | ILE |
| 2 | B | 233 | ILE |
| 2 | B | 238 | LEU |
| 2 | B | 239 | ASP |
| 2 | B | 245 | ILE |
| 2 | B | 246 | PHE |
| 2 | B | 268 | LYS |
| 2 | B | 285 | ILE |
| 2 | B | 287 | ARG |
| 2 | B | 289 | LEU |
| 2 | B | 307 | GLU |
| 2 | B | 329 | PHE |
| 2 | B | 331 | GLU |
| 2 | B | 350 | GLU |
| 2 | B | 357 | SER |
| 2 | B | 375 | GLN |
| 2 | B | 379 | GLU |
| 2 | B | 382 | ARG |
| 2 | B | 399 | ARG |
| 2 | B | 406 | CYS |
| 2 | B | 409 | MET |
| 2 | B | 427 | SER |
| 2 | B | 444 | LEU |
| 2 | B | 462 | SER |
| 2 | B | 463 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 465 | ASN |
| 2 | B | 468 | SER |
| 2 | B | 474 | LEU |
| 2 | B | 475 | ASN |
| 2 | B | 490 | SER |
| 2 | B | 492 | LYS |
| 2 | B | 508 | LEU |
| 2 | B | 512 | ASP |
| 3 | C | 8 | MET |
| 3 | C | 25 | ILE |
| 3 | C | 26 | THR |
| 3 | C | 44 | MET |
| 3 | C | 48 | LEU |
| 3 | C | 57 | LEU |
| 3 | C | 64 | ILE |
| 3 | C | 143 | VAL |
| 3 | C | 165 | ILE |
| 3 | C | 170 | LYS |
| 3 | C | 182 | VAL |
| 3 | C | 184 | LYS |
| 3 | C | 209 | ILE |
| 3 | C | 225 | LEU |
| 3 | C | 226 | ASN |
| 3 | C | 239 | GLU |
| 3 | C | 248 | CYS |
| 3 | C | 250 | LEU |
| 3 | C | 259 | THR |
| 3 | C | 265 | LYS |
| 3 | C | 297 | THR |
| 3 | C | 302 | SER |
| 3 | C | 433 | GLN |
| 3 | C | 456 | LEU |
| 3 | C | 491 | ILE |
| 3 | C | 492 | VAL |
| 3 | C | 519 | LEU |
| 4 | D | 70 | ILE |
| 4 | D | 94 | THR |
| 4 | D | 98 | ILE |
| 4 | D | 100 | THR |
| 4 | D | 135 | LEU |
| 4 | D | 139 | CYS |
| 4 | D | 144 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | D | 146 | ASP |
| 4 | D | 147 | ARG |
| 4 | D | 161 | LYS |
| 4 | D | 175 | VAL |
| 4 | D | 187 | LYS |
| 4 | D | 193 | ASP |
| 4 | D | 194 | ILE |
| 4 | D | 198 | LYS |
| 4 | D | 209 | MET |
| 4 | D | 210 | ILE |
| 4 | D | 231 | LYS |
| 4 | D | 241 | ILE |
| 4 | D | 253 | ILE |
| 4 | D | 263 | ILE |
| 4 | D | 385 | MET |
| 4 | D | 392 | ARG |
| 4 | D | 410 | LEU |
| 4 | D | 424 | ARG |
| 4 | D | 461 | ASN |
| 4 | D | 482 | ILE |
| 4 | D | 502 | LEU |
| 4 | D | 528 | ARG |
| 5 | E | 61 | ILE |
| 5 | E | 82 | THR |
| 5 | E | 86 | ASP |
| 5 | E | 93 | GLN |
| 5 | E | 103 | LEU |
| 5 | E | 106 | GLN |
| 5 | E | 107 | LEU |
| 5 | E | 108 | SER |
| 5 | E | 109 | LYS |
| 5 | E | 148 | ASN |
| 5 | E | 150 | PHE |
| 5 | E | 165 | CYS |
| 5 | E | 169 | SER |
| 5 | E | 175 | LEU |
| 5 | E | 187 | SER |
| 5 | E | 210 | ASN |
| 5 | E | 222 | ASP |
| 5 | E | 236 | ASP |
| 5 | E | 241 | ASN |
| 5 | E | 245 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | E | 273 | THR |
| 5 | E | 296 | GLN |
| 5 | E | 324 | GLN |
| 5 | E | 325 | TRP |
| 5 | E | 351 | LEU |
| 5 | E | 352 | GLU |
| 5 | E | 368 | ASP |
| 5 | E | 382 | GLU |
| 5 | E | 396 | GLU |
| 5 | E | 431 | ARG |
| 5 | E | 440 | VAL |
| 5 | E | 469 | PHE |
| 5 | E | 492 | ILE |
| 5 | E | 507 | ILE |
| 5 | E | 535 | LYS |
| 5 | E | 547 | MET |
| 6 | F | 1 | MET |
| 6 | F | 3 | LEU |
| 6 | F | 4 | GLN |
| 6 | F | 5 | LEU |
| 6 | F | 6 | LEU |
| 6 | F | 16 | ASP |
| 6 | F | 27 | GLU |
| 6 | F | 37 | LEU |
| 6 | F | 43 | LEU |
| 6 | F | 53 | ILE |
| 6 | F | 68 | ILE |
| 6 | F | 93 | THR |
| 6 | F | 102 | LEU |
| 6 | F | 113 | VAL |
| 6 | F | 117 | ILE |
| 6 | F | 133 | LEU |
| 6 | F | 142 | ASN |
| 6 | F | 143 | LEU |
| 6 | F | 152 | GLN |
| 6 | F | 158 | LEU |
| 6 | F | 171 | THR |
| 6 | F | 183 | ASP |
| 6 | F | 196 | ILE |
| 6 | F | 197 | MET |
| 6 | F | 198 | GLN |
| 6 | F | 209 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | F | 213 | LEU |
| 6 | F | 243 | GLU |
| 6 | F | 294 | VAL |
| 6 | F | 295 | ILE |
| 6 | F | 321 | LYS |
| 6 | F | 323 | ARG |
| 6 | F | 328 | LEU |
| 6 | F | 330 | LEU |
| 6 | F | 370 | ASN |
| 6 | F | 376 | CYS |
| 6 | F | 378 | ILE |
| 6 | F | 390 | GLN |
| 6 | F | 407 | LYS |
| 6 | F | 409 | LYS |
| 6 | F | 424 | ARG |
| 6 | F | 433 | LYS |
| 6 | F | 434 | LEU |
| 6 | F | 437 | LYS |
| 6 | F | 440 | THR |
| 6 | F | 442 | THR |
| 6 | F | 454 | ILE |
| 6 | F | 457 | THR |
| 6 | F | 458 | LEU |
| 6 | F | 483 | SER |
| 6 | F | 484 | ASP |
| 6 | F | 486 | THR |
| 6 | F | 489 | VAL |
| 6 | F | 513 | LEU |
| 6 | F | 515 | ASN |
| 6 | F | 518 | THR |
| 6 | F | 538 | ARG |
| 6 | F | 540 | THR |
| 6 | F | 541 | LEU |
| 6 | F | 542 | LYS |
| 6 | F | 544 | THR |
| 7 | G | 36 | VAL |
| 7 | G | 37 | GLN |
| 7 | G | 43 | THR |
| 7 | G | 52 | LEU |
| 7 | G | 58 | GLN |
| 7 | G | 64 | ASN |
| 7 | G | 71 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | G | 82 | THR |
| 7 | G | 86 | ILE |
| 7 | G | 100 | SER |
| 7 | G | 120 | ILE |
| 7 | G | 123 | HIS |
| 7 | G | 156 | GLU |
| 7 | G | 157 | LEU |
| 7 | G | 174 | ASN |
| 7 | G | 191 | ARG |
| 7 | G | 232 | GLN |
| 7 | G | 234 | LYS |
| 7 | G | 282 | LEU |
| 7 | G | 285 | VAL |
| 7 | G | 305 | GLN |
| 7 | G | 312 | ILE |
| 7 | G | 346 | LEU |
| 7 | G | 376 | LEU |
| 7 | G | 377 | LEU |
| 7 | G | 393 | LEU |
| 7 | G | 399 | ILE |
| 7 | G | 408 | LEU |
| 7 | G | 410 | VAL |
| 7 | G | 418 | MET |
| 7 | G | 488 | ILE |
| 7 | G | 514 | THR |
| 7 | G | 516 | LEU |
| 7 | G | 527 | LYS |
| 8 | H | 15 | LYS |
| 8 | H | 27 | GLN |
| 8 | H | 28 | ILE |
| 8 | H | 29 | ILE |
| 8 | H | 32 | ILE |
| 8 | H | 62 | ILE |
| 8 | H | 66 | ASN |
| 8 | H | 74 | GLU |
| 8 | H | 76 | ASP |
| 8 | H | 77 | ILE |
| 8 | H | 92 | GLN |
| 8 | H | 153 | LYS |
| 8 | H | 175 | GLU |
| 8 | H | 209 | VAL |
| 8 | H | 237 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | H | 244 | LYS |
| 8 | H | 267 | LEU |
| 8 | H | 314 | ASN |
| 8 | H | 316 | TYR |
| 8 | H | 320 | VAL |
| 8 | H | 343 | ARG |
| 8 | H | 352 | LEU |
| 8 | H | 386 | LEU |
| 8 | H | 390 | THR |
| 8 | H | 408 | VAL |
| 8 | H | 430 | LEU |
| 8 | H | 451 | GLN |
| 8 | H | 466 | THR |
| 8 | H | 473 | GLU |
| 8 | H | 494 | HIS |
| 8 | H | 532 | THR |
| 1 | I | 8 | SER |
| 1 | I | 13 | LEU |
| 1 | I | 44 | LEU |
| 1 | I | 50 | ASP |
| 1 | I | 74 | ASP |
| 1 | I | 76 | GLN |
| 1 | I | 90 | GLN |
| 1 | I | 91 | ASP |
| 1 | I | 119 | LYS |
| 1 | I | 120 | ILE |
| 1 | I | 187 | VAL |
| 1 | I | 204 | ASN |
| 1 | I | 225 | ASN |
| 1 | I | 226 | CYS |
| 1 | I | 228 | VAL |
| 1 | I | 248 | ASP |
| 1 | I | 255 | ARG |
| 1 | I | 344 | LEU |
| 1 | I | 350 | PHE |
| 1 | I | 402 | LEU |
| 1 | I | 404 | ASP |
| 1 | I | 419 | VAL |
| 1 | I | 446 | LEU |
| 1 | I | 484 | SER |
| 1 | I | 496 | SER |
| 1 | I | 532 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | I | 548 | ASP |
| 2 | J | 4 | GLN |
| 2 | J | 5 | ILE |
| 2 | J | 8 | ASP |
| 2 | J | 19 | ARG |
| 2 | J | 27 | ILE |
| 2 | J | 31 | ASP |
| 2 | J | 32 | LEU |
| 2 | J | 33 | VAL |
| 2 | J | 43 | ASP |
| 2 | J | 57 | THR |
| 2 | J | 58 | ASN |
| 2 | J | 66 | SER |
| 2 | J | 80 | ILE |
| 2 | J | 92 | THR |
| 2 | J | 145 | ASP |
| 2 | J | 146 | LYS |
| 2 | J | 149 | PHE |
| 2 | J | 166 | LEU |
| 2 | J | 176 | LEU |
| 2 | J | 197 | LYS |
| 2 | J | 203 | LEU |
| 2 | J | 213 | ILE |
| 2 | J | 217 | LYS |
| 2 | J | 228 | ASN |
| 2 | J | 231 | ILE |
| 2 | J | 233 | ILE |
| 2 | J | 238 | LEU |
| 2 | J | 239 | ASP |
| 2 | J | 245 | ILE |
| 2 | J | 246 | PHE |
| 2 | J | 268 | LYS |
| 2 | J | 285 | ILE |
| 2 | J | 287 | ARG |
| 2 | J | 289 | LEU |
| 2 | J | 307 | GLU |
| 2 | J | 329 | PHE |
| 2 | J | 331 | GLU |
| 2 | J | 350 | GLU |
| 2 | J | 357 | SER |
| 2 | J | 375 | GLN |
| 2 | J | 379 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | J | 382 | ARG |
| 2 | J | 399 | ARG |
| 2 | J | 406 | CYS |
| 2 | J | 409 | MET |
| 2 | J | 427 | SER |
| 2 | J | 444 | LEU |
| 2 | J | 462 | SER |
| 2 | J | 463 | ILE |
| 2 | J | 465 | ASN |
| 2 | J | 468 | SER |
| 2 | J | 474 | LEU |
| 2 | J | 475 | ASN |
| 2 | J | 490 | SER |
| 2 | J | 492 | LYS |
| 2 | J | 508 | LEU |
| 2 | J | 512 | ASP |
| 3 | K | 8 | MET |
| 3 | K | 25 | ILE |
| 3 | K | 26 | THR |
| 3 | K | 44 | MET |
| 3 | K | 48 | LEU |
| 3 | K | 57 | LEU |
| 3 | K | 64 | ILE |
| 3 | K | 143 | VAL |
| 3 | K | 165 | ILE |
| 3 | K | 170 | LYS |
| 3 | K | 182 | VAL |
| 3 | K | 184 | LYS |
| 3 | K | 209 | ILE |
| 3 | K | 225 | LEU |
| 3 | K | 226 | ASN |
| 3 | K | 239 | GLU |
| 3 | K | 248 | CYS |
| 3 | K | 250 | LEU |
| 3 | K | 259 | THR |
| 3 | K | 265 | LYS |
| 3 | K | 297 | THR |
| 3 | K | 302 | SER |
| 3 | K | 433 | GLN |
| 3 | K | 456 | LEU |
| 3 | K | 491 | ILE |
| 3 | K | 492 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | K | 519 | LEU |
| 4 | L | 70 | ILE |
| 4 | L | 94 | THR |
| 4 | L | 98 | ILE |
| 4 | L | 100 | THR |
| 4 | L | 135 | LEU |
| 4 | L | 139 | CYS |
| 4 | L | 144 | LEU |
| 4 | L | 146 | ASP |
| 4 | L | 147 | ARG |
| 4 | L | 161 | LYS |
| 4 | L | 175 | VAL |
| 4 | L | 187 | LYS |
| 4 | L | 193 | ASP |
| 4 | L | 194 | ILE |
| 4 | L | 198 | LYS |
| 4 | L | 209 | MET |
| 4 | L | 210 | ILE |
| 4 | L | 231 | LYS |
| 4 | L | 241 | ILE |
| 4 | L | 253 | ILE |
| 4 | L | 263 | ILE |
| 4 | L | 385 | MET |
| 4 | L | 392 | ARG |
| 4 | L | 410 | LEU |
| 4 | L | 424 | ARG |
| 4 | L | 461 | ASN |
| 4 | L | 482 | ILE |
| 4 | L | 502 | LEU |
| 4 | L | 528 | ARG |
| 5 | M | 61 | ILE |
| 5 | M | 82 | THR |
| 5 | M | 86 | ASP |
| 5 | M | 93 | GLN |
| 5 | M | 103 | LEU |
| 5 | M | 106 | GLN |
| 5 | M | 107 | LEU |
| 5 | M | 108 | SER |
| 5 | M | 109 | LYS |
| 5 | M | 148 | ASN |
| 5 | M | 150 | PHE |
| 5 | M | 165 | CYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | M | 169 | SER |
| 5 | M | 175 | LEU |
| 5 | M | 187 | SER |
| 5 | M | 210 | ASN |
| 5 | M | 222 | ASP |
| 5 | M | 236 | ASP |
| 5 | M | 241 | ASN |
| 5 | M | 245 | LEU |
| 5 | M | 273 | THR |
| 5 | M | 296 | GLN |
| 5 | M | 324 | GLN |
| 5 | M | 325 | TRP |
| 5 | M | 351 | LEU |
| 5 | M | 352 | GLU |
| 5 | M | 368 | ASP |
| 5 | M | 382 | GLU |
| 5 | M | 396 | GLU |
| 5 | M | 431 | ARG |
| 5 | M | 440 | VAL |
| 5 | M | 469 | PHE |
| 5 | M | 492 | ILE |
| 5 | M | 507 | ILE |
| 5 | M | 535 | LYS |
| 5 | M | 547 | MET |
| 6 | N | 1 | MET |
| 6 | N | 3 | LEU |
| 6 | N | 4 | GLN |
| 6 | N | 5 | LEU |
| 6 | N | 6 | LEU |
| 6 | N | 16 | ASP |
| 6 | N | 27 | GLU |
| 6 | N | 37 | LEU |
| 6 | N | 53 | ILE |
| 6 | N | 68 | ILE |
| 6 | N | 93 | THR |
| 6 | N | 102 | LEU |
| 6 | N | 113 | VAL |
| 6 | N | 117 | ILE |
| 6 | N | 133 | LEU |
| 6 | N | 142 | ASN |
| 6 | N | 143 | LEU |
| 6 | N | 152 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | N | 158 | LEU |
| 6 | N | 171 | THR |
| 6 | N | 183 | ASP |
| 6 | N | 196 | ILE |
| 6 | N | 197 | MET |
| 6 | N | 198 | GLN |
| 6 | N | 209 | PHE |
| 6 | N | 213 | LEU |
| 6 | N | 243 | GLU |
| 6 | N | 294 | VAL |
| 6 | N | 295 | ILE |
| 6 | N | 321 | LYS |
| 6 | N | 323 | ARG |
| 6 | N | 328 | LEU |
| 6 | N | 330 | LEU |
| 6 | N | 370 | ASN |
| 6 | N | 376 | CYS |
| 6 | N | 378 | ILE |
| 6 | N | 390 | GLN |
| 6 | N | 407 | LYS |
| 6 | N | 409 | LYS |
| 6 | N | 424 | ARG |
| 6 | N | 433 | LYS |
| 6 | N | 434 | LEU |
| 6 | N | 437 | LYS |
| 6 | N | 440 | THR |
| 6 | N | 442 | THR |
| 6 | N | 454 | ILE |
| 6 | N | 457 | THR |
| 6 | N | 458 | LEU |
| 6 | N | 483 | SER |
| 6 | N | 484 | ASP |
| 6 | N | 486 | THR |
| 6 | N | 489 | VAL |
| 6 | N | 513 | LEU |
| 6 | N | 515 | ASN |
| 6 | N | 518 | THR |
| 6 | N | 538 | ARG |
| 6 | N | 540 | THR |
| 6 | N | 541 | LEU |
| 6 | N | 542 | LYS |
| 6 | N | 544 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | O | 36 | VAL |
| 7 | O | 37 | GLN |
| 7 | O | 43 | THR |
| 7 | O | 52 | LEU |
| 7 | O | 58 | GLN |
| 7 | O | 64 | ASN |
| 7 | O | 71 | LYS |
| 7 | O | 82 | THR |
| 7 | O | 86 | ILE |
| 7 | O | 100 | SER |
| 7 | O | 120 | ILE |
| 7 | O | 123 | HIS |
| 7 | O | 156 | GLU |
| 7 | O | 157 | LEU |
| 7 | O | 174 | ASN |
| 7 | O | 191 | ARG |
| 7 | O | 232 | GLN |
| 7 | O | 234 | LYS |
| 7 | O | 282 | LEU |
| 7 | O | 285 | VAL |
| 7 | O | 305 | GLN |
| 7 | O | 312 | ILE |
| 7 | O | 346 | LEU |
| 7 | O | 376 | LEU |
| 7 | O | 377 | LEU |
| 7 | O | 393 | LEU |
| 7 | O | 399 | ILE |
| 7 | O | 408 | LEU |
| 7 | O | 410 | VAL |
| 7 | O | 418 | MET |
| 7 | O | 488 | ILE |
| 7 | O | 514 | THR |
| 7 | O | 516 | LEU |
| 7 | O | 527 | LYS |
| 8 | P | 15 | LYS |
| 8 | P | 27 | GLN |
| 8 | P | 28 | ILE |
| 8 | P | 29 | ILE |
| 8 | P | 32 | ILE |
| 8 | P | 62 | ILE |
| 8 | P | 66 | ASN |
| 8 | P | 74 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 8 | P | 76 | ASP |
| 8 | P | 77 | ILE |
| 8 | P | 92 | GLN |
| 8 | P | 153 | LYS |
| 8 | P | 175 | GLU |
| 8 | P | 209 | VAL |
| 8 | P | 237 | LYS |
| 8 | P | 244 | LYS |
| 8 | P | 267 | LEU |
| 8 | P | 314 | ASN |
| 8 | P | 316 | TYR |
| 8 | P | 320 | VAL |
| 8 | P | 343 | ARG |
| 8 | P | 352 | LEU |
| 8 | P | 386 | LEU |
| 8 | P | 390 | THR |
| 8 | P | 408 | VAL |
| 8 | P | 430 | LEU |
| 8 | P | 451 | GLN |
| 8 | P | 466 | THR |
| 8 | P | 473 | GLU |
| 8 | P | 494 | HIS |
| 8 | P | 532 | THR |
| 1 | a | 1008 | SER |
| 1 | a | 1013 | LEU |
| 1 | a | 1044 | LEU |
| 1 | a | 1050 | ASP |
| 1 | a | 1074 | ASP |
| 1 | a | 1076 | GLN |
| 1 | a | 1090 | GLN |
| 1 | a | 1091 | ASP |
| 1 | a | 1119 | LYS |
| 1 | a | 1120 | ILE |
| 1 | a | 1187 | VAL |
| 1 | a | 1204 | ASN |
| 1 | a | 1225 | ASN |
| 1 | a | 1226 | CYS |
| 1 | a | 1228 | VAL |
| 1 | a | 1248 | ASP |
| 1 | a | 1255 | ARG |
| 1 | a | 1344 | LEU |
| 1 | a | 1350 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | a | 1402 | LEU |
| 1 | a | 1404 | ASP |
| 1 | a | 1419 | VAL |
| 1 | a | 1446 | LEU |
| 1 | a | 1484 | SER |
| 1 | a | 1496 | SER |
| 1 | a | 1532 | LEU |
| 1 | a | 1548 | ASP |
| 2 | b | 1004 | GLN |
| 2 | b | 1005 | ILE |
| 2 | b | 1008 | ASP |
| 2 | b | 1019 | ARG |
| 2 | b | 1027 | ILE |
| 2 | b | 1031 | ASP |
| 2 | b | 1032 | LEU |
| 2 | b | 1033 | VAL |
| 2 | b | 1043 | ASP |
| 2 | b | 1057 | THR |
| 2 | b | 1058 | ASN |
| 2 | b | 1066 | SER |
| 2 | b | 1080 | ILE |
| 2 | b | 1092 | THR |
| 2 | b | 1145 | ASP |
| 2 | b | 1146 | LYS |
| 2 | b | 1149 | PHE |
| 2 | b | 1166 | LEU |
| 2 | b | 1176 | LEU |
| 2 | b | 1197 | LYS |
| 2 | b | 1203 | LEU |
| 2 | b | 1213 | ILE |
| 2 | b | 1217 | LYS |
| 2 | b | 1228 | ASN |
| 2 | b | 1231 | ILE |
| 2 | b | 1233 | ILE |
| 2 | b | 1238 | LEU |
| 2 | b | 1239 | ASP |
| 2 | b | 1245 | ILE |
| 2 | b | 1246 | PHE |
| 2 | b | 1268 | LYS |
| 2 | b | 1285 | ILE |
| 2 | b | 1287 | ARG |
| 2 | b | 1289 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | b | 1307 | GLU |
| 2 | b | 1329 | PHE |
| 2 | b | 1331 | GLU |
| 2 | b | 1348 | LEU |
| 2 | b | 1350 | GLU |
| 2 | b | 1357 | SER |
| 2 | b | 1375 | GLN |
| 2 | b | 1379 | GLU |
| 2 | b | 1382 | ARG |
| 2 | b | 1399 | ARG |
| 2 | b | 1406 | CYS |
| 2 | b | 1409 | MET |
| 2 | b | 1427 | SER |
| 2 | b | 1444 | LEU |
| 2 | b | 1462 | SER |
| 2 | b | 1463 | ILE |
| 2 | b | 1465 | ASN |
| 2 | b | 1468 | SER |
| 2 | b | 1474 | LEU |
| 2 | b | 1475 | ASN |
| 2 | b | 1490 | SER |
| 2 | b | 1492 | LYS |
| 2 | b | 1508 | LEU |
| 2 | b | 1512 | ASP |
| 3 | c | 1008 | MET |
| 3 | c | 1025 | ILE |
| 3 | c | 1026 | THR |
| 3 | c | 1044 | MET |
| 3 | c | 1048 | LEU |
| 3 | c | 1057 | LEU |
| 3 | c | 1064 | ILE |
| 3 | c | 1143 | VAL |
| 3 | c | 1165 | ILE |
| 3 | c | 1170 | LYS |
| 3 | c | 1182 | VAL |
| 3 | c | 1184 | LYS |
| 3 | c | 1209 | ILE |
| 3 | c | 1225 | LEU |
| 3 | c | 1226 | ASN |
| 3 | c | 1239 | GLU |
| 3 | c | 1248 | CYS |
| 3 | c | 1250 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | c | 1259 | THR |
| 3 | c | 1265 | LYS |
| 3 | c | 1297 | THR |
| 3 | c | 1302 | SER |
| 3 | c | 1433 | GLN |
| 3 | c | 1456 | LEU |
| 3 | c | 1491 | ILE |
| 3 | c | 1492 | VAL |
| 3 | c | 1519 | LEU |
| 4 | d | 1070 | ILE |
| 4 | d | 1094 | THR |
| 4 | d | 1098 | ILE |
| 4 | d | 1100 | THR |
| 4 | d | 1135 | LEU |
| 4 | d | 1139 | CYS |
| 4 | d | 1144 | LEU |
| 4 | d | 1146 | ASP |
| 4 | d | 1147 | ARG |
| 4 | d | 1161 | LYS |
| 4 | d | 1175 | VAL |
| 4 | d | 1187 | LYS |
| 4 | d | 1193 | ASP |
| 4 | d | 1194 | ILE |
| 4 | d | 1198 | LYS |
| 4 | d | 1209 | MET |
| 4 | d | 1210 | ILE |
| 4 | d | 1231 | LYS |
| 4 | d | 1241 | ILE |
| 4 | d | 1253 | ILE |
| 4 | d | 1263 | ILE |
| 4 | d | 1385 | MET |
| 4 | d | 1392 | ARG |
| 4 | d | 1410 | LEU |
| 4 | d | 1424 | ARG |
| 4 | d | 1461 | ASN |
| 4 | d | 1482 | ILE |
| 4 | d | 1502 | LEU |
| 4 | d | 1528 | ARG |
| 5 | e | 1061 | ILE |
| 5 | e | 1082 | THR |
| 5 | e | 1086 | ASP |
| 5 | e | 1093 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 5 | e | 1103 | LEU |
| 5 | e | 1106 | GLN |
| 5 | e | 1107 | LEU |
| 5 | e | 1108 | SER |
| 5 | e | 1109 | LYS |
| 5 | e | 1148 | ASN |
| 5 | e | 1150 | PHE |
| 5 | e | 1165 | CYS |
| 5 | e | 1169 | SER |
| 5 | e | 1175 | LEU |
| 5 | e | 1187 | SER |
| 5 | e | 1210 | ASN |
| 5 | e | 1222 | ASP |
| 5 | e | 1236 | ASP |
| 5 | e | 1241 | ASN |
| 5 | e | 1245 | LEU |
| 5 | e | 1273 | THR |
| 5 | e | 1296 | GLN |
| 5 | e | 1324 | GLN |
| 5 | e | 1325 | TRP |
| 5 | e | 1351 | LEU |
| 5 | e | 1352 | GLU |
| 5 | e | 1368 | ASP |
| 5 | e | 1382 | GLU |
| 5 | e | 1396 | GLU |
| 5 | e | 1431 | ARG |
| 5 | e | 1440 | VAL |
| 5 | e | 1469 | PHE |
| 5 | e | 1492 | ILE |
| 5 | e | 1507 | ILE |
| 5 | e | 1535 | LYS |
| 5 | e | 1547 | MET |
| 6 | f | 1001 | MET |
| 6 | f | 1003 | LEU |
| 6 | f | 1004 | GLN |
| 6 | f | 1005 | LEU |
| 6 | f | 1006 | LEU |
| 6 | f | 1016 | ASP |
| 6 | f | 1027 | GLU |
| 6 | f | 1037 | LEU |
| 6 | f | 1043 | LEU |
| 6 | f | 1053 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 6 | f | 1068 | ILE |
| 6 | f | 1093 | THR |
| 6 | f | 1102 | LEU |
| 6 | f | 1113 | VAL |
| 6 | f | 1117 | ILE |
| 6 | f | 1133 | LEU |
| 6 | f | 1142 | ASN |
| 6 | f | 1143 | LEU |
| 6 | f | 1152 | GLN |
| 6 | f | 1158 | LEU |
| 6 | f | 1171 | THR |
| 6 | f | 1183 | ASP |
| 6 | f | 1196 | ILE |
| 6 | f | 1197 | MET |
| 6 | f | 1198 | GLN |
| 6 | f | 1209 | PHE |
| 6 | f | 1213 | LEU |
| 6 | f | 1243 | GLU |
| 6 | f | 1294 | VAL |
| 6 | f | 1295 | ILE |
| 6 | f | 1321 | LYS |
| 6 | f | 1323 | ARG |
| 6 | f | 1328 | LEU |
| 6 | f | 1330 | LEU |
| 6 | f | 1370 | ASN |
| 6 | f | 1376 | CYS |
| 6 | f | 1378 | ILE |
| 6 | f | 1390 | GLN |
| 6 | f | 1407 | LYS |
| 6 | f | 1409 | LYS |
| 6 | f | 1424 | ARG |
| 6 | f | 1433 | LYS |
| 6 | f | 1434 | LEU |
| 6 | f | 1437 | LYS |
| 6 | f | 1439 | LYS |
| 6 | f | 1440 | THR |
| 6 | f | 1442 | THR |
| 6 | f | 1454 | ILE |
| 6 | f | 1457 | THR |
| 6 | f | 1458 | LEU |
| 6 | f | 1483 | SER |
| 6 | f | 1484 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 6 | f | 1486 | THR |
| 6 | f | 1489 | VAL |
| 6 | f | 1513 | LEU |
| 6 | f | 1515 | ASN |
| 6 | f | 1518 | THR |
| 6 | f | 1538 | ARG |
| 6 | f | 1540 | THR |
| 6 | f | 1541 | LEU |
| 6 | f | 1542 | LYS |
| 6 | f | 1544 | THR |
| 7 | g | 1036 | VAL |
| 7 | g | 1037 | GLN |
| 7 | g | 1043 | THR |
| 7 | g | 1052 | LEU |
| 7 | g | 1058 | GLN |
| 7 | g | 1064 | ASN |
| 7 | g | 1071 | LYS |
| 7 | g | 1082 | THR |
| 7 | g | 1086 | ILE |
| 7 | g | 1100 | SER |
| 7 | g | 1120 | ILE |
| 7 | g | 1123 | HIS |
| 7 | g | 1156 | GLU |
| 7 | g | 1157 | LEU |
| 7 | g | 1174 | ASN |
| 7 | g | 1191 | ARG |
| 7 | g | 1232 | GLN |
| 7 | g | 1234 | LYS |
| 7 | g | 1282 | LEU |
| 7 | g | 1285 | VAL |
| 7 | g | 1305 | GLN |
| 7 | g | 1312 | ILE |
| 7 | g | 1346 | LEU |
| 7 | g | 1376 | LEU |
| 7 | g | 1377 | LEU |
| 7 | g | 1393 | LEU |
| 7 | g | 1399 | ILE |
| 7 | g | 1408 | LEU |
| 7 | g | 1410 | VAL |
| 7 | g | 1418 | MET |
| 7 | g | 1488 | ILE |
| 7 | g | 1514 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 7 | g | 1516 | LEU |
| 7 | g | 1527 | LYS |
| 8 | h | 1015 | LYS |
| 8 | h | 1027 | GLN |
| 8 | h | 1028 | ILE |
| 8 | h | 1029 | ILE |
| 8 | h | 1032 | ILE |
| 8 | h | 1062 | ILE |
| 8 | h | 1066 | ASN |
| 8 | h | 1074 | GLU |
| 8 | h | 1076 | ASP |
| 8 | h | 1077 | ILE |
| 8 | h | 1092 | GLN |
| 8 | h | 1153 | LYS |
| 8 | h | 1175 | GLU |
| 8 | h | 1209 | VAL |
| 8 | h | 1237 | LYS |
| 8 | h | 1244 | LYS |
| 8 | h | 1267 | LEU |
| 8 | h | 1314 | ASN |
| 8 | h | 1316 | TYR |
| 8 | h | 1320 | VAL |
| 8 | h | 1343 | ARG |
| 8 | h | 1352 | LEU |
| 8 | h | 1386 | LEU |
| 8 | h | 1390 | THR |
| 8 | h | 1408 | VAL |
| 8 | h | 1430 | LEU |
| 8 | h | 1451 | GLN |
| 8 | h | 1466 | THR |
| 8 | h | 1473 | GLU |
| 8 | h | 1494 | HIS |
| 8 | h | 1532 | THR |
| 1 | i | 1008 | SER |
| 1 | i | 1013 | LEU |
| 1 | i | 1044 | LEU |
| 1 | i | 1050 | ASP |
| 1 | i | 1074 | ASP |
| 1 | i | 1076 | GLN |
| 1 | i | 1090 | GLN |
| 1 | i | 1091 | ASP |
| 1 | i | 1119 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | i | 1120 | ILE |
| 1 | i | 1187 | VAL |
| 1 | i | 1204 | ASN |
| 1 | i | 1225 | ASN |
| 1 | i | 1226 | CYS |
| 1 | i | 1228 | VAL |
| 1 | i | 1248 | ASP |
| 1 | i | 1255 | ARG |
| 1 | i | 1344 | LEU |
| 1 | i | 1350 | PHE |
| 1 | i | 1402 | LEU |
| 1 | i | 1404 | ASP |
| 1 | i | 1419 | VAL |
| 1 | i | 1446 | LEU |
| 1 | i | 1484 | SER |
| 1 | i | 1496 | SER |
| 1 | i | 1532 | LEU |
| 1 | i | 1548 | ASP |
| 2 | j | 1004 | GLN |
| 2 | j | 1005 | ILE |
| 2 | j | 1008 | ASP |
| 2 | j | 1019 | ARG |
| 2 | j | 1027 | ILE |
| 2 | j | 1031 | ASP |
| 2 | j | 1032 | LEU |
| 2 | j | 1033 | VAL |
| 2 | j | 1043 | ASP |
| 2 | j | 1057 | THR |
| 2 | j | 1058 | ASN |
| 2 | j | 1066 | SER |
| 2 | j | 1080 | ILE |
| 2 | j | 1092 | THR |
| 2 | j | 1145 | ASP |
| 2 | j | 1146 | LYS |
| 2 | j | 1149 | PHE |
| 2 | j | 1166 | LEU |
| 2 | j | 1176 | LEU |
| 2 | j | 1197 | LYS |
| 2 | j | 1203 | LEU |
| 2 | j | 1213 | ILE |
| 2 | j | 1217 | LYS |
| 2 | j | 1228 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | j | 1231 | ILE |
| 2 | j | 1233 | ILE |
| 2 | j | 1238 | LEU |
| 2 | j | 1239 | ASP |
| 2 | j | 1245 | ILE |
| 2 | j | 1246 | PHE |
| 2 | j | 1268 | LYS |
| 2 | j | 1285 | ILE |
| 2 | j | 1287 | ARG |
| 2 | j | 1289 | LEU |
| 2 | j | 1307 | GLU |
| 2 | j | 1329 | PHE |
| 2 | j | 1331 | GLU |
| 2 | j | 1350 | GLU |
| 2 | j | 1357 | SER |
| 2 | j | 1375 | GLN |
| 2 | j | 1379 | GLU |
| 2 | j | 1382 | ARG |
| 2 | j | 1399 | ARG |
| 2 | j | 1406 | CYS |
| 2 | j | 1409 | MET |
| 2 | j | 1427 | SER |
| 2 | j | 1444 | LEU |
| 2 | j | 1462 | SER |
| 2 | j | 1463 | ILE |
| 2 | j | 1465 | ASN |
| 2 | j | 1468 | SER |
| 2 | j | 1474 | LEU |
| 2 | j | 1475 | ASN |
| 2 | j | 1490 | SER |
| 2 | j | 1492 | LYS |
| 2 | j | 1508 | LEU |
| 2 | j | 1512 | ASP |
| 3 | k | 1008 | MET |
| 3 | k | 1025 | ILE |
| 3 | k | 1026 | THR |
| 3 | k | 1044 | MET |
| 3 | k | 1048 | LEU |
| 3 | k | 1057 | LEU |
| 3 | k | 1064 | ILE |
| 3 | k | 1143 | VAL |
| 3 | k | 1165 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | k | 1170 | LYS |
| 3 | k | 1182 | VAL |
| 3 | k | 1184 | LYS |
| 3 | k | 1209 | ILE |
| 3 | k | 1225 | LEU |
| 3 | k | 1226 | ASN |
| 3 | k | 1239 | GLU |
| 3 | k | 1248 | CYS |
| 3 | k | 1250 | LEU |
| 3 | k | 1259 | THR |
| 3 | k | 1265 | LYS |
| 3 | k | 1297 | THR |
| 3 | k | 1302 | SER |
| 3 | k | 1433 | GLN |
| 3 | k | 1456 | LEU |
| 3 | k | 1491 | ILE |
| 3 | k | 1492 | VAL |
| 3 | k | 1519 | LEU |
| 4 | l | 1070 | ILE |
| 4 | l | 1094 | THR |
| 4 | l | 1098 | ILE |
| 4 | l | 1100 | THR |
| 4 | l | 1135 | LEU |
| 4 | l | 1139 | CYS |
| 4 | l | 1144 | LEU |
| 4 | l | 1146 | ASP |
| 4 | l | 1147 | ARG |
| 4 | l | 1161 | LYS |
| 4 | l | 1175 | VAL |
| 4 | l | 1187 | LYS |
| 4 | l | 1193 | ASP |
| 4 | l | 1194 | ILE |
| 4 | l | 1198 | LYS |
| 4 | l | 1209 | MET |
| 4 | l | 1210 | ILE |
| 4 | l | 1231 | LYS |
| 4 | l | 1241 | ILE |
| 4 | l | 1253 | ILE |
| 4 | l | 1263 | ILE |
| 4 | l | 1385 | MET |
| 4 | l | 1392 | ARG |
| 4 | l | 1410 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 4 | l | 1424 | ARG |
| 4 | l | 1461 | ASN |
| 4 | l | 1482 | ILE |
| 4 | l | 1502 | LEU |
| 4 | l | 1528 | ARG |
| 5 | m | 1061 | ILE |
| 5 | m | 1082 | THR |
| 5 | m | 1086 | ASP |
| 5 | m | 1093 | GLN |
| 5 | m | 1103 | LEU |
| 5 | m | 1106 | GLN |
| 5 | m | 1107 | LEU |
| 5 | m | 1108 | SER |
| 5 | m | 1109 | LYS |
| 5 | m | 1148 | ASN |
| 5 | m | 1150 | PHE |
| 5 | m | 1165 | CYS |
| 5 | m | 1169 | SER |
| 5 | m | 1175 | LEU |
| 5 | m | 1187 | SER |
| 5 | m | 1210 | ASN |
| 5 | m | 1222 | ASP |
| 5 | m | 1236 | ASP |
| 5 | m | 1241 | ASN |
| 5 | m | 1245 | LEU |
| 5 | m | 1273 | THR |
| 5 | m | 1296 | GLN |
| 5 | m | 1324 | GLN |
| 5 | m | 1325 | TRP |
| 5 | m | 1351 | LEU |
| 5 | m | 1352 | GLU |
| 5 | m | 1368 | ASP |
| 5 | m | 1382 | GLU |
| 5 | m | 1396 | GLU |
| 5 | m | 1431 | ARG |
| 5 | m | 1440 | VAL |
| 5 | m | 1469 | PHE |
| 5 | m | 1492 | ILE |
| 5 | m | 1507 | ILE |
| 5 | m | 1535 | LYS |
| 5 | m | 1547 | MET |
| 6 | n | 1001 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 6 | n | 1003 | LEU |
| 6 | n | 1004 | GLN |
| 6 | n | 1005 | LEU |
| 6 | n | 1006 | LEU |
| 6 | n | 1016 | ASP |
| 6 | n | 1027 | GLU |
| 6 | n | 1037 | LEU |
| 6 | n | 1043 | LEU |
| 6 | n | 1053 | ILE |
| 6 | n | 1068 | ILE |
| 6 | n | 1093 | THR |
| 6 | n | 1102 | LEU |
| 6 | n | 1113 | VAL |
| 6 | n | 1117 | ILE |
| 6 | n | 1133 | LEU |
| 6 | n | 1142 | ASN |
| 6 | n | 1143 | LEU |
| 6 | n | 1152 | GLN |
| 6 | n | 1158 | LEU |
| 6 | n | 1171 | THR |
| 6 | n | 1183 | ASP |
| 6 | n | 1196 | ILE |
| 6 | n | 1197 | MET |
| 6 | n | 1198 | GLN |
| 6 | n | 1209 | PHE |
| 6 | n | 1213 | LEU |
| 6 | n | 1243 | GLU |
| 6 | n | 1294 | VAL |
| 6 | n | 1295 | ILE |
| 6 | n | 1321 | LYS |
| 6 | n | 1323 | ARG |
| 6 | n | 1328 | LEU |
| 6 | n | 1330 | LEU |
| 6 | n | 1370 | ASN |
| 6 | n | 1376 | CYS |
| 6 | n | 1378 | ILE |
| 6 | n | 1390 | GLN |
| 6 | n | 1407 | LYS |
| 6 | n | 1409 | LYS |
| 6 | n | 1424 | ARG |
| 6 | n | 1433 | LYS |
| 6 | n | 1434 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 6 | n | 1437 | LYS |
| 6 | n | 1440 | THR |
| 6 | n | 1442 | THR |
| 6 | n | 1454 | ILE |
| 6 | n | 1457 | THR |
| 6 | n | 1458 | LEU |
| 6 | n | 1483 | SER |
| 6 | n | 1484 | ASP |
| 6 | n | 1486 | THR |
| 6 | n | 1489 | VAL |
| 6 | n | 1513 | LEU |
| 6 | n | 1515 | ASN |
| 6 | n | 1518 | THR |
| 6 | n | 1538 | ARG |
| 6 | n | 1540 | THR |
| 6 | n | 1541 | LEU |
| 6 | n | 1542 | LYS |
| 6 | n | 1544 | THR |
| 7 | o | 1036 | VAL |
| 7 | o | 1037 | GLN |
| 7 | o | 1043 | THR |
| 7 | o | 1052 | LEU |
| 7 | o | 1058 | GLN |
| 7 | o | 1064 | ASN |
| 7 | o | 1071 | LYS |
| 7 | o | 1082 | THR |
| 7 | o | 1086 | ILE |
| 7 | o | 1100 | SER |
| 7 | o | 1120 | ILE |
| 7 | o | 1123 | HIS |
| 7 | o | 1156 | GLU |
| 7 | o | 1157 | LEU |
| 7 | o | 1174 | ASN |
| 7 | o | 1191 | ARG |
| 7 | o | 1232 | GLN |
| 7 | o | 1234 | LYS |
| 7 | o | 1282 | LEU |
| 7 | o | 1285 | VAL |
| 7 | o | 1305 | GLN |
| 7 | o | 1312 | ILE |
| 7 | o | 1346 | LEU |
| 7 | o | 1376 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 7 | o | 1377 | LEU |
| 7 | o | 1393 | LEU |
| 7 | o | 1399 | ILE |
| 7 | o | 1408 | LEU |
| 7 | o | 1410 | VAL |
| 7 | o | 1418 | MET |
| 7 | o | 1488 | ILE |
| 7 | o | 1514 | THR |
| 7 | o | 1516 | LEU |
| 7 | o | 1527 | LYS |
| 8 | p | 1015 | LYS |
| 8 | p | 1027 | GLN |
| 8 | p | 1028 | ILE |
| 8 | p | 1029 | ILE |
| 8 | p | 1032 | ILE |
| 8 | p | 1062 | ILE |
| 8 | p | 1066 | ASN |
| 8 | p | 1074 | GLU |
| 8 | p | 1076 | ASP |
| 8 | p | 1077 | ILE |
| 8 | p | 1092 | GLN |
| 8 | p | 1153 | LYS |
| 8 | p | 1175 | GLU |
| 8 | p | 1209 | VAL |
| 8 | p | 1237 | LYS |
| 8 | p | 1244 | LYS |
| 8 | p | 1267 | LEU |
| 8 | p | 1314 | ASN |
| 8 | p | 1316 | TYR |
| 8 | p | 1320 | VAL |
| 8 | p | 1343 | ARG |
| 8 | p | 1352 | LEU |
| 8 | p | 1386 | LEU |
| 8 | p | 1390 | THR |
| 8 | p | 1408 | VAL |
| 8 | p | 1430 | LEU |
| 8 | p | 1451 | GLN |
| 8 | p | 1466 | THR |
| 8 | p | 1473 | GLU |
| 8 | p | 1494 | HIS |
| 8 | p | 1532 | THR |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (306) such

sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 64 | ASN |
| 1 | A | 90 | GLN |
| 1 | A | 121 | HIS |
| 1 | A | 178 | ASN |
| 1 | A | 204 | ASN |
| 1 | A | 209 | HIS |
| 1 | A | 250 | ASN |
| 1 | A | 252 | GLN |
| 1 | A | 363 | GLN |
| 1 | A | 391 | ASN |
| 1 | A | 435 | ASN |
| 2 | B | 4 | GLN |
| 2 | B | 9 | GLN |
| 2 | B | 58 | ASN |
| 2 | B | 116 | HIS |
| 2 | B | 228 | ASN |
| 2 | B | 260 | GLN |
| 2 | B | 271 | ASN |
| 2 | B | 286 | ASN |
| 2 | B | 375 | GLN |
| 2 | B | 385 | HIS |
| 2 | B | 393 | GLN |
| 2 | B | 439 | GLN |
| 2 | B | 475 | ASN |
| 3 | C | 9 | ASN |
| 3 | C | 59 | ASN |
| 3 | C | 85 | GLN |
| 3 | C | 166 | HIS |
| 3 | C | 281 | GLN |
| 3 | C | 325 | ASN |
| 3 | C | 433 | GLN |
| 3 | C | 439 | GLN |
| 3 | C | 508 | GLN |
| 4 | D | 59 | ASN |
| 4 | D | 72 | HIS |
| 4 | D | 217 | GLN |
| 4 | D | 238 | GLN |
| 4 | D | 259 | GLN |
| 4 | D | 384 | ASN |
| 4 | D | 461 | ASN |
| 4 | D | 499 | GLN |
| 5 | E | 37 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | E | 50 | HIS |
| 5 | E | 93 | GLN |
| 5 | E | 106 | GLN |
| 5 | E | 132 | GLN |
| 5 | E | 210 | ASN |
| 5 | E | 324 | GLN |
| 5 | E | 338 | ASN |
| 5 | E | 466 | GLN |
| 5 | E | 553 | ASN |
| 6 | F | 104 | GLN |
| 6 | F | 110 | GLN |
| 6 | F | 198 | GLN |
| 6 | F | 200 | GLN |
| 6 | F | 217 | HIS |
| 6 | F | 221 | HIS |
| 6 | F | 312 | HIS |
| 6 | F | 515 | ASN |
| 7 | G | 37 | GLN |
| 7 | G | 58 | GLN |
| 7 | G | 232 | GLN |
| 7 | G | 268 | GLN |
| 7 | G | 305 | GLN |
| 7 | G | 491 | ASN |
| 8 | H | 27 | GLN |
| 8 | H | 66 | ASN |
| 8 | H | 79 | HIS |
| 8 | H | 92 | GLN |
| 8 | H | 101 | ASN |
| 8 | H | 188 | HIS |
| 8 | H | 283 | GLN |
| 8 | H | 373 | GLN |
| 8 | H | 446 | GLN |
| 8 | H | 451 | GLN |
| 1 | I | 64 | ASN |
| 1 | I | 90 | GLN |
| 1 | I | 121 | HIS |
| 1 | I | 178 | ASN |
| 1 | I | 204 | ASN |
| 1 | I | 209 | HIS |
| 1 | I | 225 | ASN |
| 1 | I | 250 | ASN |
| 1 | I | 252 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | I | 363 | GLN |
| 1 | I | 391 | ASN |
| 1 | I | 435 | ASN |
| 2 | J | 4 | GLN |
| 2 | J | 9 | GLN |
| 2 | J | 58 | ASN |
| 2 | J | 116 | HIS |
| 2 | J | 228 | ASN |
| 2 | J | 235 | ASN |
| 2 | J | 260 | GLN |
| 2 | J | 271 | ASN |
| 2 | J | 286 | ASN |
| 2 | J | 375 | GLN |
| 2 | J | 393 | GLN |
| 2 | J | 439 | GLN |
| 2 | J | 475 | ASN |
| 3 | K | 9 | ASN |
| 3 | K | 12 | GLN |
| 3 | K | 59 | ASN |
| 3 | K | 85 | GLN |
| 3 | K | 117 | HIS |
| 3 | K | 166 | HIS |
| 3 | K | 270 | ASN |
| 3 | K | 281 | GLN |
| 3 | K | 325 | ASN |
| 3 | K | 433 | GLN |
| 3 | K | 439 | GLN |
| 3 | K | 508 | GLN |
| 4 | L | 59 | ASN |
| 4 | L | 72 | HIS |
| 4 | L | 217 | GLN |
| 4 | L | 238 | GLN |
| 4 | L | 259 | GLN |
| 4 | L | 384 | ASN |
| 4 | L | 461 | ASN |
| 4 | L | 499 | GLN |
| 5 | M | 37 | ASN |
| 5 | M | 50 | HIS |
| 5 | M | 93 | GLN |
| 5 | M | 132 | GLN |
| 5 | M | 142 | HIS |
| 5 | M | 210 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 5 | M | 324 | GLN |
| 5 | M | 338 | ASN |
| 5 | M | 466 | GLN |
| 6 | N | 104 | GLN |
| 6 | N | 110 | GLN |
| 6 | N | 198 | GLN |
| 6 | N | 200 | GLN |
| 6 | N | 217 | HIS |
| 6 | N | 221 | HIS |
| 6 | N | 312 | HIS |
| 6 | N | 515 | ASN |
| 7 | O | 37 | GLN |
| 7 | O | 58 | GLN |
| 7 | O | 231 | GLN |
| 7 | O | 232 | GLN |
| 7 | O | 305 | GLN |
| 7 | O | 491 | ASN |
| 8 | P | 27 | GLN |
| 8 | P | 66 | ASN |
| 8 | P | 79 | HIS |
| 8 | P | 92 | GLN |
| 8 | P | 101 | ASN |
| 8 | P | 188 | HIS |
| 8 | P | 283 | GLN |
| 8 | P | 373 | GLN |
| 8 | P | 446 | GLN |
| 8 | P | 451 | GLN |
| 1 | a | 1064 | ASN |
| 1 | a | 1090 | GLN |
| 1 | a | 1121 | HIS |
| 1 | a | 1178 | ASN |
| 1 | a | 1204 | ASN |
| 1 | a | 1209 | HIS |
| 1 | a | 1250 | ASN |
| 1 | a | 1252 | GLN |
| 1 | a | 1363 | GLN |
| 1 | a | 1391 | ASN |
| 1 | a | 1435 | ASN |
| 2 | b | 1004 | GLN |
| 2 | b | 1009 | GLN |
| 2 | b | 1058 | ASN |
| 2 | b | 1116 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | b | 1228 | ASN |
| 2 | b | 1235 | ASN |
| 2 | b | 1260 | GLN |
| 2 | b | 1271 | ASN |
| 2 | b | 1286 | ASN |
| 2 | b | 1375 | GLN |
| 2 | b | 1393 | GLN |
| 2 | b | 1439 | GLN |
| 2 | b | 1475 | ASN |
| 3 | c | 1009 | ASN |
| 3 | c | 1012 | GLN |
| 3 | c | 1059 | ASN |
| 3 | c | 1085 | GLN |
| 3 | c | 1117 | HIS |
| 3 | c | 1166 | HIS |
| 3 | c | 1270 | ASN |
| 3 | c | 1281 | GLN |
| 3 | c | 1325 | ASN |
| 3 | c | 1433 | GLN |
| 3 | c | 1439 | GLN |
| 3 | c | 1508 | GLN |
| 4 | d | 1059 | ASN |
| 4 | d | 1072 | HIS |
| 4 | d | 1217 | GLN |
| 4 | d | 1238 | GLN |
| 4 | d | 1259 | GLN |
| 4 | d | 1384 | ASN |
| 4 | d | 1461 | ASN |
| 4 | d | 1499 | GLN |
| 5 | e | 1037 | ASN |
| 5 | e | 1050 | HIS |
| 5 | e | 1093 | GLN |
| 5 | e | 1132 | GLN |
| 5 | e | 1142 | HIS |
| 5 | e | 1210 | ASN |
| 5 | e | 1324 | GLN |
| 5 | e | 1338 | ASN |
| 5 | e | 1466 | GLN |
| 6 | f | 1110 | GLN |
| 6 | f | 1198 | GLN |
| 6 | f | 1200 | GLN |
| 6 | f | 1217 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 6 | f | 1221 | HIS |
| 6 | f | 1312 | HIS |
| 6 | f | 1515 | ASN |
| 7 | g | 1037 | GLN |
| 7 | g | 1058 | GLN |
| 7 | g | 1232 | GLN |
| 7 | g | 1305 | GLN |
| 7 | g | 1356 | GLN |
| 7 | g | 1491 | ASN |
| 8 | h | 1027 | GLN |
| 8 | h | 1066 | ASN |
| 8 | h | 1079 | HIS |
| 8 | h | 1092 | GLN |
| 8 | h | 1101 | ASN |
| 8 | h | 1188 | HIS |
| 8 | h | 1373 | GLN |
| 8 | h | 1446 | GLN |
| 8 | h | 1451 | GLN |
| 8 | h | 1472 | ASN |
| 1 | i | 1064 | ASN |
| 1 | i | 1090 | GLN |
| 1 | i | 1121 | HIS |
| 1 | i | 1178 | ASN |
| 1 | i | 1204 | ASN |
| 1 | i | 1209 | HIS |
| 1 | i | 1250 | ASN |
| 1 | i | 1252 | GLN |
| 1 | i | 1363 | GLN |
| 1 | i | 1391 | ASN |
| 1 | i | 1435 | ASN |
| 2 | j | 1004 | GLN |
| 2 | j | 1009 | GLN |
| 2 | j | 1058 | ASN |
| 2 | j | 1116 | HIS |
| 2 | j | 1228 | ASN |
| 2 | j | 1235 | ASN |
| 2 | j | 1260 | GLN |
| 2 | j | 1271 | ASN |
| 2 | j | 1286 | ASN |
| 2 | j | 1375 | GLN |
| 2 | j | 1393 | GLN |
| 2 | j | 1439 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | j | 1475 | ASN |
| 3 | k | 1009 | ASN |
| 3 | k | 1012 | GLN |
| 3 | k | 1085 | GLN |
| 3 | k | 1117 | HIS |
| 3 | k | 1166 | HIS |
| 3 | k | 1270 | ASN |
| 3 | k | 1281 | GLN |
| 3 | k | 1325 | ASN |
| 3 | k | 1433 | GLN |
| 3 | k | 1439 | GLN |
| 3 | k | 1508 | GLN |
| 4 | l | 1059 | ASN |
| 4 | l | 1072 | HIS |
| 4 | l | 1217 | GLN |
| 4 | l | 1238 | GLN |
| 4 | l | 1259 | GLN |
| 4 | l | 1384 | ASN |
| 4 | l | 1461 | ASN |
| 4 | l | 1499 | GLN |
| 5 | m | 1037 | ASN |
| 5 | m | 1050 | HIS |
| 5 | m | 1093 | GLN |
| 5 | m | 1132 | GLN |
| 5 | m | 1210 | ASN |
| 5 | m | 1296 | GLN |
| 5 | m | 1324 | GLN |
| 5 | m | 1338 | ASN |
| 5 | m | 1466 | GLN |
| 5 | m | 1553 | ASN |
| 6 | n | 1104 | GLN |
| 6 | n | 1110 | GLN |
| 6 | n | 1198 | GLN |
| 6 | n | 1200 | GLN |
| 6 | n | 1217 | HIS |
| 6 | n | 1221 | HIS |
| 6 | n | 1312 | HIS |
| 6 | n | 1515 | ASN |
| 7 | o | 1037 | GLN |
| 7 | o | 1058 | GLN |
| 7 | o | 1231 | GLN |
| 7 | o | 1232 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 7 | o | 1305 | GLN |
| 7 | o | 1491 | ASN |
| 8 | p | 1027 | GLN |
| 8 | p | 1066 | ASN |
| 8 | p | 1079 | HIS |
| 8 | p | 1092 | GLN |
| 8 | p | 1101 | ASN |
| 8 | p | 1188 | HIS |
| 8 | p | 1283 | GLN |
| 8 | p | 1373 | GLN |
| 8 | p | 1446 | GLN |
| 8 | p | 1451 | GLN |

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

56 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 10 | BEF | f | 1602 | - | 0,3,3 | 0.00 | - | - | | |
| 11 | SO4 | K | 1101 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.21 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 11 | SO4 | O | 600 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.12 | 0 |
| 10 | BEF | P | 602 | - | 0,3,3 | 0.00 | - | - | | |
| 10 | BEF | l | 1602 | 9 | 0,3,3 | 0.00 | - | - | | |
| 10 | BEF | E | 602 | 9 | 0,3,3 | 0.00 | - | - | | |
| 9 | ADP | J | 601 | 10 | 24,29,29 | 2.06 | 9 (37%) | 29,45,45 | 2.13 | 10 (34%) |
| 10 | BEF | m | 1602 | - | 0,3,3 | 0.00 | - | - | | |
| 9 | ADP | a | 1601 | - | 24,29,29 | 2.06 | 9 (37%) | 29,45,45 | 2.09 | 8 (27%) |
| 9 | ADP | P | 601 | - | 24,29,29 | 2.03 | 9 (37%) | 29,45,45 | 1.92 | 9 (31%) |
| 9 | ADP | n | 1601 | - | 24,29,29 | 2.03 | 8 (33%) | 29,45,45 | 1.93 | 8 (27%) |
| 9 | ADP | m | 1601 | - | 24,29,29 | 2.08 | 9 (37%) | 29,45,45 | 2.01 | 6 (20%) |
| 11 | SO4 | o | 1600 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.10 | 0 |
| 11 | SO4 | j | 1600 | - | 4,4,4 | 0.10 | 0 | 6,6,6 | 0.20 | 0 |
| 10 | BEF | C | 1102 | - | 0,3,3 | 0.00 | - | - | | |
| 10 | BEF | H | 602 | - | 0,3,3 | 0.00 | - | - | | |
| 9 | ADP | p | 1601 | 10 | 24,29,29 | 2.09 | 9 (37%) | 29,45,45 | 1.92 | 8 (27%) |
| 10 | BEF | J | 602 | 9 | 0,3,3 | 0.00 | - | - | | |
| 9 | ADP | A | 601 | 10 | 24,29,29 | 2.07 | 9 (37%) | 29,45,45 | 2.09 | 9 (31%) |
| 11 | SO4 | I | 600 | - | 4,4,4 | 0.16 | 0 | 6,6,6 | 0.17 | 0 |
| 9 | ADP | e | 1601 | - | 24,29,29 | 2.05 | 9 (37%) | 29,45,45 | 2.02 | 8 (27%) |
| 9 | ADP | g | 1601 | - | 24,29,29 | 2.07 | 9 (37%) | 29,45,45 | 1.92 | 8 (27%) |
| 9 | ADP | b | 1601 | 10 | 24,29,29 | 2.08 | 9 (37%) | 29,45,45 | 2.07 | 8 (27%) |
| 10 | BEF | p | 1602 | 9 | 0,3,3 | 0.00 | - | - | | |
| 9 | ADP | B | 601 | 10 | 24,29,29 | 2.11 | 10 (41%) | 29,45,45 | 2.11 | 9 (31%) |
| 11 | SO4 | i | 1600 | - | 4,4,4 | 0.12 | 0 | 6,6,6 | 0.30 | 0 |
| 10 | BEF | g | 1602 | - | 0,3,3 | 0.00 | - | - | | |
| 10 | BEF | D | 602 | - | 0,3,3 | 0.00 | - | - | | |
| 9 | ADP | H | 601 | - | 24,29,29 | 2.05 | 9 (37%) | 29,45,45 | 1.95 | 8 (27%) |
| 10 | BEF | F | 602 | - | 0,3,3 | 0.00 | - | - | | |
| 10 | BEF | B | 602 | 9 | 0,3,3 | 0.00 | - | - | | |
| 9 | ADP | M | 601 | - | 24,29,29 | 2.03 | 10 (41%) | 29,45,45 | 1.98 | 6 (20%) |
| 10 | BEF | a | 1602 | - | 0,3,3 | 0.00 | - | - | | |
| 10 | BEF | b | 1602 | 9 | 0,3,3 | 0.00 | - | - | | |
| 10 | BEF | G | 602 | - | 0,3,3 | 0.00 | - | - | | |
| 11 | SO4 | c | 2101 | - | 4,4,4 | 0.18 | 0 | 6,6,6 | 0.18 | 0 |
| 9 | ADP | C | 1101 | - | 24,29,29 | 2.04 | 9 (37%) | 29,45,45 | 1.94 | 8 (27%) |
| 9 | ADP | N | 601 | 10 | 24,29,29 | 2.07 | 9 (37%) | 29,45,45 | 2.08 | 9 (31%) |
| 9 | ADP | D | 601 | - | 24,29,29 | 2.06 | 9 (37%) | 29,45,45 | 1.96 | 8 (27%) |
| 9 | ADP | F | 601 | - | 24,29,29 | 2.09 | 9 (37%) | 29,45,45 | 1.98 | 8 (27%) |
| 10 | BEF | h | 1602 | 9 | 0,3,3 | 0.00 | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 10 | BEF | k | 2102 | 9 | 0,3,3 | 0.00 | - | - | | |
| 10 | BEF | e | 1602 | - | 0,3,3 | 0.00 | - | - | | |
| 9 | ADP | l | 1601 | 10 | 24,29,29 | 2.10 | 9 (37%) | 29,45,45 | 2.15 | 9 (31%) |
| 10 | BEF | N | 602 | 9 | 0,3,3 | 0.00 | - | - | | |
| 10 | BEF | L | 602 | - | 0,3,3 | 0.00 | - | - | | |
| 10 | BEF | A | 602 | 9 | 0,3,3 | 0.00 | - | - | | |
| 9 | ADP | E | 601 | 10 | 24,29,29 | 2.09 | 9 (37%) | 29,45,45 | 2.15 | 9 (31%) |
| 9 | ADP | G | 601 | - | 24,29,29 | 2.11 | 9 (37%) | 29,45,45 | 2.13 | 9 (31%) |
| 9 | ADP | f | 1601 | - | 24,29,29 | 2.08 | 9 (37%) | 29,45,45 | 2.11 | 8 (27%) |
| 9 | ADP | L | 601 | - | 24,29,29 | 2.06 | 9 (37%) | 29,45,45 | 1.94 | 8 (27%) |
| 10 | BEF | M | 602 | - | 0,3,3 | 0.00 | - | - | | |
| 11 | SO4 | d | 1600 | - | 4,4,4 | 0.13 | 0 | 6,6,6 | 0.13 | 0 |
| 9 | ADP | h | 1601 | 10 | 24,29,29 | 2.06 | 9 (37%) | 29,45,45 | 1.82 | 8 (27%) |
| 10 | BEF | n | 1602 | - | 0,3,3 | 0.00 | - | - | | |
| 9 | ADP | k | 2101 | 10 | 24,29,29 | 2.04 | 9 (37%) | 29,45,45 | 1.97 | 9 (31%) |

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 |
|-----|------|-------|------|------|---------|------------|---------|
| 9 | ADP | J | 601 | 10 | 2/2/6/6 | 6/12/32/32 | 0/3/3/3 |
| 9 | ADP | a | 1601 | - | 2/2/6/6 | 7/12/32/32 | 0/3/3/3 |
| 9 | ADP | P | 601 | - | 1/1/6/6 | 1/12/32/32 | 0/3/3/3 |
| 9 | ADP | n | 1601 | - | 1/1/6/6 | 4/12/32/32 | 0/3/3/3 |
| 9 | ADP | m | 1601 | - | 2/2/6/6 | 5/12/32/32 | 0/3/3/3 |
| 9 | ADP | p | 1601 | 10 | 1/1/6/6 | 3/12/32/32 | 0/3/3/3 |
| 9 | ADP | A | 601 | 10 | 2/2/6/6 | 4/12/32/32 | 0/3/3/3 |
| 9 | ADP | e | 1601 | - | 2/2/6/6 | 5/12/32/32 | 0/3/3/3 |
| 9 | ADP | g | 1601 | - | 1/1/6/6 | 4/12/32/32 | 0/3/3/3 |
| 9 | ADP | b | 1601 | 10 | 2/2/6/6 | 8/12/32/32 | 0/3/3/3 |
| 9 | ADP | B | 601 | 10 | 2/2/6/6 | 3/12/32/32 | 0/3/3/3 |
| 9 | ADP | H | 601 | - | 1/1/6/6 | 4/12/32/32 | 0/3/3/3 |
| 9 | ADP | M | 601 | - | 2/2/6/6 | 7/12/32/32 | 0/3/3/3 |
| 9 | ADP | C | 1101 | - | 2/2/6/6 | 5/12/32/32 | 0/3/3/3 |
| 9 | ADP | N | 601 | 10 | 2/2/6/6 | 4/12/32/32 | 0/3/3/3 |
| 9 | ADP | D | 601 | - | 2/2/6/6 | 3/12/32/32 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|------------|---------|
| 9 | ADP | F | 601 | - | - | 8/12/32/32 | 0/3/3/3 |
| 9 | ADP | l | 1601 | 10 | - | 3/12/32/32 | 0/3/3/3 |
| 9 | ADP | E | 601 | 10 | 1/1/6/6 | 5/12/32/32 | 0/3/3/3 |
| 9 | ADP | G | 601 | - | 1/1/6/6 | 3/12/32/32 | 0/3/3/3 |
| 9 | ADP | f | 1601 | - | 2/2/6/6 | 4/12/32/32 | 0/3/3/3 |
| 9 | ADP | L | 601 | - | - | 4/12/32/32 | 0/3/3/3 |
| 9 | ADP | h | 1601 | 10 | 1/1/6/6 | 1/12/32/32 | 0/3/3/3 |
| 9 | ADP | k | 2101 | 10 | 2/2/6/6 | 4/12/32/32 | 0/3/3/3 |

All (217) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|------|-------------|----------|
| 9 | p | 1601 | ADP | PB-O1B | 4.77 | 1.65 | 1.50 |
| 9 | N | 601 | ADP | PB-O1B | 4.66 | 1.65 | 1.50 |
| 9 | l | 1601 | ADP | PB-O1B | 4.66 | 1.65 | 1.50 |
| 9 | E | 601 | ADP | PB-O1B | 4.66 | 1.65 | 1.50 |
| 9 | h | 1601 | ADP | PB-O1B | 4.65 | 1.65 | 1.50 |
| 9 | k | 2101 | ADP | PB-O1B | 4.65 | 1.65 | 1.50 |
| 9 | f | 1601 | ADP | PB-O1B | 4.63 | 1.65 | 1.50 |
| 9 | F | 601 | ADP | PB-O1B | 4.56 | 1.65 | 1.50 |
| 9 | B | 601 | ADP | PB-O1B | 4.55 | 1.65 | 1.50 |
| 9 | J | 601 | ADP | PB-O1B | 4.55 | 1.65 | 1.50 |
| 9 | g | 1601 | ADP | PB-O1B | 4.54 | 1.65 | 1.50 |
| 9 | A | 601 | ADP | PB-O1B | 4.53 | 1.65 | 1.50 |
| 9 | b | 1601 | ADP | PB-O1B | 4.47 | 1.65 | 1.50 |
| 9 | G | 601 | ADP | PB-O1B | 4.44 | 1.64 | 1.50 |
| 9 | M | 601 | ADP | PB-O1B | 4.43 | 1.64 | 1.50 |
| 9 | H | 601 | ADP | PB-O1B | 4.42 | 1.64 | 1.50 |
| 9 | L | 601 | ADP | PB-O1B | 4.41 | 1.64 | 1.50 |
| 9 | e | 1601 | ADP | PB-O1B | 4.39 | 1.64 | 1.50 |
| 9 | m | 1601 | ADP | PB-O1B | 4.39 | 1.64 | 1.50 |
| 9 | P | 601 | ADP | PB-O1B | 4.38 | 1.64 | 1.50 |
| 9 | G | 601 | ADP | PA-O1A | 4.37 | 1.66 | 1.50 |
| 9 | a | 1601 | ADP | PB-O1B | 4.37 | 1.64 | 1.50 |
| 9 | n | 1601 | ADP | PB-O1B | 4.32 | 1.64 | 1.50 |
| 9 | C | 1101 | ADP | PB-O1B | 4.29 | 1.64 | 1.50 |
| 9 | D | 601 | ADP | PB-O1B | 4.25 | 1.64 | 1.50 |
| 9 | A | 601 | ADP | PA-O1A | 4.21 | 1.65 | 1.50 |
| 9 | k | 2101 | ADP | PA-O1A | 4.11 | 1.65 | 1.50 |
| 9 | F | 601 | ADP | PA-O1A | 4.09 | 1.65 | 1.50 |
| 9 | P | 601 | ADP | PA-O1A | 4.07 | 1.65 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 9 | g | 1601 | ADP | PA-O1A | 4.07 | 1.65 | 1.50 |
| 9 | H | 601 | ADP | PA-O1A | 4.05 | 1.65 | 1.50 |
| 9 | a | 1601 | ADP | PA-O1A | 4.05 | 1.65 | 1.50 |
| 9 | C | 1101 | ADP | PA-O1A | 4.04 | 1.65 | 1.50 |
| 9 | N | 601 | ADP | PA-O1A | 4.04 | 1.65 | 1.50 |
| 9 | h | 1601 | ADP | PA-O1A | 4.04 | 1.65 | 1.50 |
| 9 | E | 601 | ADP | PA-O1A | 4.01 | 1.65 | 1.50 |
| 9 | f | 1601 | ADP | PA-O1A | 4.00 | 1.65 | 1.50 |
| 9 | n | 1601 | ADP | PA-O1A | 4.00 | 1.65 | 1.50 |
| 9 | b | 1601 | ADP | PA-O1A | 3.97 | 1.65 | 1.50 |
| 9 | m | 1601 | ADP | PA-O1A | 3.97 | 1.65 | 1.50 |
| 9 | e | 1601 | ADP | PA-O1A | 3.96 | 1.65 | 1.50 |
| 9 | l | 1601 | ADP | PA-O1A | 3.95 | 1.64 | 1.50 |
| 9 | B | 601 | ADP | PA-O1A | 3.95 | 1.64 | 1.50 |
| 9 | M | 601 | ADP | PA-O1A | 3.94 | 1.64 | 1.50 |
| 9 | L | 601 | ADP | PA-O1A | 3.93 | 1.64 | 1.50 |
| 9 | p | 1601 | ADP | PA-O1A | 3.91 | 1.64 | 1.50 |
| 9 | J | 601 | ADP | PA-O1A | 3.90 | 1.64 | 1.50 |
| 9 | D | 601 | ADP | PA-O1A | 3.88 | 1.64 | 1.50 |
| 9 | l | 1601 | ADP | C6-N6 | 3.27 | 1.46 | 1.34 |
| 9 | p | 1601 | ADP | C6-N6 | 3.26 | 1.45 | 1.34 |
| 9 | f | 1601 | ADP | C6-N6 | 3.25 | 1.45 | 1.34 |
| 9 | n | 1601 | ADP | C6-N6 | 3.23 | 1.45 | 1.34 |
| 9 | k | 2101 | ADP | C6-N6 | 3.22 | 1.45 | 1.34 |
| 9 | h | 1601 | ADP | C6-N6 | 3.21 | 1.45 | 1.34 |
| 9 | B | 601 | ADP | C6-N6 | 3.20 | 1.45 | 1.34 |
| 9 | M | 601 | ADP | C6-N6 | 3.19 | 1.45 | 1.34 |
| 9 | P | 601 | ADP | C6-N6 | 3.19 | 1.45 | 1.34 |
| 9 | b | 1601 | ADP | C6-N6 | 3.18 | 1.45 | 1.34 |
| 9 | m | 1601 | ADP | C6-N6 | 3.17 | 1.45 | 1.34 |
| 9 | e | 1601 | ADP | C6-N6 | 3.17 | 1.45 | 1.34 |
| 9 | C | 1101 | ADP | C6-N6 | 3.17 | 1.45 | 1.34 |
| 9 | J | 601 | ADP | C6-N6 | 3.16 | 1.45 | 1.34 |
| 9 | L | 601 | ADP | C6-N6 | 3.16 | 1.45 | 1.34 |
| 9 | N | 601 | ADP | C6-N6 | 3.16 | 1.45 | 1.34 |
| 9 | H | 601 | ADP | C6-N6 | 3.16 | 1.45 | 1.34 |
| 9 | D | 601 | ADP | C2'-C1' | -3.16 | 1.49 | 1.53 |
| 9 | a | 1601 | ADP | C6-N6 | 3.13 | 1.45 | 1.34 |
| 9 | F | 601 | ADP | C6-N6 | 3.13 | 1.45 | 1.34 |
| 9 | g | 1601 | ADP | C6-N6 | 3.12 | 1.45 | 1.34 |
| 9 | G | 601 | ADP | C6-N6 | 3.11 | 1.45 | 1.34 |
| 9 | A | 601 | ADP | C6-N6 | 3.11 | 1.45 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 9 | E | 601 | ADP | C6-N6 | 3.10 | 1.45 | 1.34 |
| 9 | l | 1601 | ADP | C2'-C1' | -3.08 | 1.49 | 1.53 |
| 9 | D | 601 | ADP | C6-N6 | 3.05 | 1.45 | 1.34 |
| 9 | G | 601 | ADP | PB-O2B | 2.94 | 1.66 | 1.54 |
| 9 | g | 1601 | ADP | PB-O2B | 2.92 | 1.66 | 1.54 |
| 9 | B | 601 | ADP | PB-O2B | 2.91 | 1.66 | 1.54 |
| 9 | L | 601 | ADP | C2'-C1' | -2.84 | 1.49 | 1.53 |
| 9 | b | 1601 | ADP | C2'-C1' | -2.82 | 1.49 | 1.53 |
| 9 | a | 1601 | ADP | PB-O2B | 2.81 | 1.65 | 1.54 |
| 9 | m | 1601 | ADP | PB-O2B | 2.80 | 1.65 | 1.54 |
| 9 | L | 601 | ADP | PB-O2B | 2.78 | 1.65 | 1.54 |
| 9 | e | 1601 | ADP | PB-O2B | 2.77 | 1.65 | 1.54 |
| 9 | f | 1601 | ADP | C2-N3 | 2.77 | 1.36 | 1.32 |
| 9 | B | 601 | ADP | C2'-C1' | -2.77 | 1.49 | 1.53 |
| 9 | k | 2101 | ADP | PB-O2B | 2.77 | 1.65 | 1.54 |
| 9 | l | 1601 | ADP | PB-O2B | 2.76 | 1.65 | 1.54 |
| 9 | F | 601 | ADP | PB-O2B | 2.73 | 1.65 | 1.54 |
| 9 | E | 601 | ADP | PB-O2B | 2.70 | 1.65 | 1.54 |
| 9 | C | 1101 | ADP | C2'-C1' | -2.70 | 1.49 | 1.53 |
| 9 | m | 1601 | ADP | C2'-C1' | -2.70 | 1.49 | 1.53 |
| 9 | M | 601 | ADP | PB-O2B | 2.69 | 1.65 | 1.54 |
| 9 | H | 601 | ADP | PB-O2B | 2.69 | 1.65 | 1.54 |
| 9 | G | 601 | ADP | C2-N3 | 2.69 | 1.36 | 1.32 |
| 9 | p | 1601 | ADP | PB-O2B | 2.69 | 1.65 | 1.54 |
| 9 | N | 601 | ADP | PB-O2B | 2.67 | 1.65 | 1.54 |
| 9 | n | 1601 | ADP | PB-O2B | 2.67 | 1.65 | 1.54 |
| 9 | P | 601 | ADP | PB-O2B | 2.67 | 1.65 | 1.54 |
| 9 | m | 1601 | ADP | C2-N3 | 2.66 | 1.36 | 1.32 |
| 9 | f | 1601 | ADP | PB-O2B | 2.65 | 1.65 | 1.54 |
| 9 | p | 1601 | ADP | C2'-C1' | -2.65 | 1.49 | 1.53 |
| 9 | J | 601 | ADP | PB-O2B | 2.64 | 1.65 | 1.54 |
| 9 | D | 601 | ADP | PB-O2B | 2.62 | 1.64 | 1.54 |
| 9 | M | 601 | ADP | C2'-C1' | -2.60 | 1.49 | 1.53 |
| 9 | b | 1601 | ADP | PB-O2B | 2.59 | 1.64 | 1.54 |
| 9 | a | 1601 | ADP | C2'-C1' | -2.59 | 1.49 | 1.53 |
| 9 | N | 601 | ADP | C2-N3 | 2.59 | 1.36 | 1.32 |
| 9 | H | 601 | ADP | C2'-C1' | -2.59 | 1.49 | 1.53 |
| 9 | h | 1601 | ADP | PB-O2B | 2.58 | 1.64 | 1.54 |
| 9 | A | 601 | ADP | C2-N3 | 2.58 | 1.36 | 1.32 |
| 9 | f | 1601 | ADP | C2'-C1' | -2.58 | 1.49 | 1.53 |
| 9 | n | 1601 | ADP | C2-N3 | 2.57 | 1.36 | 1.32 |
| 9 | A | 601 | ADP | PB-O2B | 2.57 | 1.64 | 1.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 9 | p | 1601 | ADP | C2-N3 | 2.56 | 1.36 | 1.32 |
| 9 | D | 601 | ADP | C2-N3 | 2.55 | 1.36 | 1.32 |
| 9 | n | 1601 | ADP | C2'-C1' | -2.54 | 1.49 | 1.53 |
| 9 | F | 601 | ADP | C2'-C1' | -2.54 | 1.49 | 1.53 |
| 9 | N | 601 | ADP | C2'-C1' | -2.54 | 1.49 | 1.53 |
| 9 | f | 1601 | ADP | C8-N7 | 2.53 | 1.39 | 1.34 |
| 9 | E | 601 | ADP | C2'-C1' | -2.53 | 1.49 | 1.53 |
| 9 | C | 1101 | ADP | PB-O2B | 2.51 | 1.64 | 1.54 |
| 9 | g | 1601 | ADP | C2-N3 | 2.51 | 1.36 | 1.32 |
| 9 | J | 601 | ADP | C2'-C1' | -2.50 | 1.50 | 1.53 |
| 9 | E | 601 | ADP | C8-N7 | 2.49 | 1.39 | 1.34 |
| 9 | M | 601 | ADP | C2-N3 | 2.48 | 1.36 | 1.32 |
| 9 | A | 601 | ADP | C8-N7 | 2.48 | 1.39 | 1.34 |
| 9 | e | 1601 | ADP | C2'-C1' | -2.47 | 1.50 | 1.53 |
| 9 | C | 1101 | ADP | C2-N3 | 2.45 | 1.36 | 1.32 |
| 9 | a | 1601 | ADP | C2-N3 | 2.45 | 1.36 | 1.32 |
| 9 | H | 601 | ADP | C5-C4 | -2.45 | 1.34 | 1.40 |
| 9 | B | 601 | ADP | C2-N3 | 2.44 | 1.36 | 1.32 |
| 9 | L | 601 | ADP | C2-N3 | 2.44 | 1.36 | 1.32 |
| 9 | F | 601 | ADP | C5-C4 | -2.43 | 1.34 | 1.40 |
| 9 | m | 1601 | ADP | C8-N7 | 2.43 | 1.39 | 1.34 |
| 9 | F | 601 | ADP | C2-N3 | 2.43 | 1.36 | 1.32 |
| 9 | J | 601 | ADP | C8-N7 | 2.42 | 1.39 | 1.34 |
| 9 | b | 1601 | ADP | C2-N3 | 2.41 | 1.36 | 1.32 |
| 9 | l | 1601 | ADP | C2-N3 | 2.41 | 1.36 | 1.32 |
| 9 | n | 1601 | ADP | C8-N7 | 2.40 | 1.39 | 1.34 |
| 9 | B | 601 | ADP | C8-N7 | 2.40 | 1.39 | 1.34 |
| 9 | C | 1101 | ADP | C8-N7 | 2.40 | 1.39 | 1.34 |
| 9 | h | 1601 | ADP | C2'-C1' | -2.40 | 1.50 | 1.53 |
| 9 | F | 601 | ADP | C8-N7 | 2.39 | 1.39 | 1.34 |
| 9 | l | 1601 | ADP | C8-N7 | 2.39 | 1.39 | 1.34 |
| 9 | e | 1601 | ADP | C5-C4 | -2.38 | 1.34 | 1.40 |
| 9 | k | 2101 | ADP | C2-N3 | 2.38 | 1.35 | 1.32 |
| 9 | g | 1601 | ADP | C5-C4 | -2.38 | 1.34 | 1.40 |
| 9 | e | 1601 | ADP | C8-N7 | 2.37 | 1.38 | 1.34 |
| 9 | N | 601 | ADP | C8-N7 | 2.37 | 1.38 | 1.34 |
| 9 | M | 601 | ADP | C8-N7 | 2.37 | 1.38 | 1.34 |
| 9 | H | 601 | ADP | C2-N3 | 2.35 | 1.35 | 1.32 |
| 9 | G | 601 | ADP | C2'-C1' | -2.35 | 1.50 | 1.53 |
| 9 | P | 601 | ADP | C2-N3 | 2.35 | 1.35 | 1.32 |
| 9 | b | 1601 | ADP | C8-N7 | 2.35 | 1.38 | 1.34 |
| 9 | a | 1601 | ADP | C5-C4 | -2.35 | 1.34 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 9 | C | 1101 | ADP | C5-C4 | -2.33 | 1.34 | 1.40 |
| 9 | h | 1601 | ADP | C2-N3 | 2.33 | 1.35 | 1.32 |
| 9 | p | 1601 | ADP | C8-N7 | 2.33 | 1.38 | 1.34 |
| 9 | E | 601 | ADP | C5-C4 | -2.33 | 1.34 | 1.40 |
| 9 | J | 601 | ADP | C5-C4 | -2.32 | 1.34 | 1.40 |
| 9 | D | 601 | ADP | C8-N7 | 2.32 | 1.38 | 1.34 |
| 9 | H | 601 | ADP | C8-N7 | 2.32 | 1.38 | 1.34 |
| 9 | h | 1601 | ADP | C8-N7 | 2.32 | 1.38 | 1.34 |
| 9 | P | 601 | ADP | C8-N7 | 2.31 | 1.38 | 1.34 |
| 9 | g | 1601 | ADP | C2'-C1' | -2.31 | 1.50 | 1.53 |
| 9 | p | 1601 | ADP | PB-O3B | -2.31 | 1.46 | 1.54 |
| 9 | P | 601 | ADP | C5-C4 | -2.31 | 1.34 | 1.40 |
| 9 | E | 601 | ADP | C2-N3 | 2.30 | 1.35 | 1.32 |
| 9 | E | 601 | ADP | PB-O3B | -2.30 | 1.46 | 1.54 |
| 9 | h | 1601 | ADP | C5-C4 | -2.30 | 1.34 | 1.40 |
| 9 | J | 601 | ADP | C2-N3 | 2.29 | 1.35 | 1.32 |
| 9 | D | 601 | ADP | C5-C4 | -2.29 | 1.34 | 1.40 |
| 9 | k | 2101 | ADP | C8-N7 | 2.28 | 1.38 | 1.34 |
| 9 | p | 1601 | ADP | C5-C4 | -2.28 | 1.34 | 1.40 |
| 9 | e | 1601 | ADP | C2-N3 | 2.28 | 1.35 | 1.32 |
| 9 | B | 601 | ADP | C5-C4 | -2.28 | 1.34 | 1.40 |
| 9 | L | 601 | ADP | C8-N7 | 2.27 | 1.38 | 1.34 |
| 9 | l | 1601 | ADP | C5-C4 | -2.26 | 1.34 | 1.40 |
| 9 | m | 1601 | ADP | C5-C4 | -2.26 | 1.34 | 1.40 |
| 9 | M | 601 | ADP | C5-C4 | -2.25 | 1.35 | 1.40 |
| 9 | A | 601 | ADP | PB-O3B | -2.25 | 1.46 | 1.54 |
| 9 | l | 1601 | ADP | PB-O3B | -2.25 | 1.46 | 1.54 |
| 9 | b | 1601 | ADP | C5-C4 | -2.24 | 1.35 | 1.40 |
| 9 | k | 2101 | ADP | C5-C4 | -2.24 | 1.35 | 1.40 |
| 9 | n | 1601 | ADP | C5-C4 | -2.24 | 1.35 | 1.40 |
| 9 | G | 601 | ADP | C5-C4 | -2.24 | 1.35 | 1.40 |
| 9 | N | 601 | ADP | C5-C4 | -2.23 | 1.35 | 1.40 |
| 9 | G | 601 | ADP | C8-N7 | 2.23 | 1.38 | 1.34 |
| 9 | k | 2101 | ADP | PB-O3B | -2.22 | 1.46 | 1.54 |
| 9 | a | 1601 | ADP | C8-N7 | 2.22 | 1.38 | 1.34 |
| 9 | P | 601 | ADP | C2'-C1' | -2.21 | 1.50 | 1.53 |
| 9 | L | 601 | ADP | PB-O3B | -2.21 | 1.46 | 1.54 |
| 9 | k | 2101 | ADP | C2'-C1' | -2.21 | 1.50 | 1.53 |
| 9 | A | 601 | ADP | C2'-C1' | -2.21 | 1.50 | 1.53 |
| 9 | B | 601 | ADP | PB-O3B | -2.20 | 1.46 | 1.54 |
| 9 | G | 601 | ADP | PB-O3B | -2.20 | 1.46 | 1.54 |
| 9 | m | 1601 | ADP | PB-O3B | -2.19 | 1.46 | 1.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 9 | J | 601 | ADP | PB-O3B | -2.19 | 1.46 | 1.54 |
| 9 | H | 601 | ADP | PB-O3B | -2.18 | 1.46 | 1.54 |
| 9 | F | 601 | ADP | PB-O3B | -2.18 | 1.46 | 1.54 |
| 9 | L | 601 | ADP | C5-C4 | -2.17 | 1.35 | 1.40 |
| 9 | C | 1101 | ADP | PB-O3B | -2.16 | 1.46 | 1.54 |
| 9 | e | 1601 | ADP | PB-O3B | -2.15 | 1.46 | 1.54 |
| 9 | g | 1601 | ADP | PB-O3B | -2.14 | 1.46 | 1.54 |
| 9 | P | 601 | ADP | PB-O3B | -2.14 | 1.46 | 1.54 |
| 9 | A | 601 | ADP | C5-C4 | -2.13 | 1.35 | 1.40 |
| 9 | h | 1601 | ADP | PB-O3B | -2.13 | 1.46 | 1.54 |
| 9 | g | 1601 | ADP | C8-N7 | 2.13 | 1.38 | 1.34 |
| 9 | M | 601 | ADP | PB-O3B | -2.13 | 1.46 | 1.54 |
| 9 | a | 1601 | ADP | PB-O3B | -2.12 | 1.46 | 1.54 |
| 9 | b | 1601 | ADP | PB-O3B | -2.10 | 1.46 | 1.54 |
| 9 | D | 601 | ADP | PB-O3B | -2.09 | 1.46 | 1.54 |
| 9 | B | 601 | ADP | PA-O2A | -2.05 | 1.45 | 1.55 |
| 9 | f | 1601 | ADP | PB-O3B | -2.04 | 1.47 | 1.54 |
| 9 | N | 601 | ADP | PB-O3B | -2.03 | 1.47 | 1.54 |
| 9 | f | 1601 | ADP | C5-C4 | -2.02 | 1.35 | 1.40 |
| 9 | M | 601 | ADP | PA-O2A | -2.01 | 1.45 | 1.55 |

All (198) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 9 | G | 601 | ADP | PA-O3A-PB | -6.32 | 111.12 | 132.83 |
| 9 | J | 601 | ADP | N3-C2-N1 | -5.96 | 119.36 | 128.68 |
| 9 | H | 601 | ADP | N3-C2-N1 | -5.82 | 119.58 | 128.68 |
| 9 | l | 1601 | ADP | N3-C2-N1 | -5.71 | 119.76 | 128.68 |
| 9 | a | 1601 | ADP | N3-C2-N1 | -5.65 | 119.86 | 128.68 |
| 9 | P | 601 | ADP | N3-C2-N1 | -5.58 | 119.96 | 128.68 |
| 9 | E | 601 | ADP | N3-C2-N1 | -5.57 | 119.97 | 128.68 |
| 9 | M | 601 | ADP | N3-C2-N1 | -5.56 | 119.99 | 128.68 |
| 9 | C | 1101 | ADP | N3-C2-N1 | -5.56 | 119.99 | 128.68 |
| 9 | k | 2101 | ADP | N3-C2-N1 | -5.53 | 120.03 | 128.68 |
| 9 | L | 601 | ADP | N3-C2-N1 | -5.53 | 120.04 | 128.68 |
| 9 | p | 1601 | ADP | N3-C2-N1 | -5.52 | 120.06 | 128.68 |
| 9 | F | 601 | ADP | N3-C2-N1 | -5.51 | 120.06 | 128.68 |
| 9 | D | 601 | ADP | N3-C2-N1 | -5.51 | 120.07 | 128.68 |
| 9 | h | 1601 | ADP | N3-C2-N1 | -5.49 | 120.10 | 128.68 |
| 9 | e | 1601 | ADP | PA-O3A-PB | -5.48 | 114.03 | 132.83 |
| 9 | B | 601 | ADP | N3-C2-N1 | -5.46 | 120.14 | 128.68 |
| 9 | m | 1601 | ADP | N3-C2-N1 | -5.46 | 120.14 | 128.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 9 | E | 601 | ADP | PA-O3A-PB | -5.46 | 114.09 | 132.83 |
| 9 | a | 1601 | ADP | PA-O3A-PB | -5.44 | 114.15 | 132.83 |
| 9 | e | 1601 | ADP | N3-C2-N1 | -5.44 | 120.17 | 128.68 |
| 9 | A | 601 | ADP | N3-C2-N1 | -5.40 | 120.23 | 128.68 |
| 9 | N | 601 | ADP | PA-O3A-PB | -5.38 | 114.36 | 132.83 |
| 9 | N | 601 | ADP | N3-C2-N1 | -5.37 | 120.28 | 128.68 |
| 9 | f | 1601 | ADP | N3-C2-N1 | -5.32 | 120.36 | 128.68 |
| 9 | n | 1601 | ADP | N3-C2-N1 | -5.30 | 120.39 | 128.68 |
| 9 | G | 601 | ADP | N3-C2-N1 | -5.24 | 120.49 | 128.68 |
| 9 | g | 1601 | ADP | N3-C2-N1 | -5.22 | 120.52 | 128.68 |
| 9 | b | 1601 | ADP | N3-C2-N1 | -5.21 | 120.54 | 128.68 |
| 9 | m | 1601 | ADP | PA-O3A-PB | -5.08 | 115.39 | 132.83 |
| 9 | C | 1101 | ADP | PA-O3A-PB | -4.99 | 115.70 | 132.83 |
| 9 | f | 1601 | ADP | PA-O3A-PB | -4.90 | 116.02 | 132.83 |
| 9 | b | 1601 | ADP | PA-O3A-PB | -4.74 | 116.55 | 132.83 |
| 9 | A | 601 | ADP | PA-O3A-PB | -4.73 | 116.60 | 132.83 |
| 9 | B | 601 | ADP | PA-O3A-PB | -4.72 | 116.62 | 132.83 |
| 9 | n | 1601 | ADP | PA-O3A-PB | -4.59 | 117.06 | 132.83 |
| 9 | H | 601 | ADP | PA-O3A-PB | -4.51 | 117.35 | 132.83 |
| 9 | g | 1601 | ADP | PA-O3A-PB | -4.49 | 117.40 | 132.83 |
| 9 | l | 1601 | ADP | PA-O3A-PB | -4.43 | 117.64 | 132.83 |
| 9 | J | 601 | ADP | PA-O3A-PB | -4.26 | 118.20 | 132.83 |
| 9 | P | 601 | ADP | PA-O3A-PB | -4.22 | 118.35 | 132.83 |
| 9 | F | 601 | ADP | PA-O3A-PB | -4.17 | 118.52 | 132.83 |
| 9 | E | 601 | ADP | O3'-C3'-C4' | 4.14 | 123.03 | 111.05 |
| 9 | D | 601 | ADP | O4'-C4'-C5' | 4.11 | 122.90 | 109.37 |
| 9 | L | 601 | ADP | PA-O3A-PB | -4.11 | 118.72 | 132.83 |
| 9 | D | 601 | ADP | O5'-C5'-C4' | 4.04 | 122.90 | 108.99 |
| 9 | k | 2101 | ADP | PA-O3A-PB | -4.00 | 119.11 | 132.83 |
| 9 | a | 1601 | ADP | O4'-C4'-C5' | 3.92 | 122.28 | 109.37 |
| 9 | k | 2101 | ADP | O4'-C4'-C5' | 3.91 | 122.25 | 109.37 |
| 9 | f | 1601 | ADP | O4'-C4'-C5' | 3.82 | 121.95 | 109.37 |
| 9 | f | 1601 | ADP | O5'-C5'-C4' | 3.79 | 122.05 | 108.99 |
| 9 | M | 601 | ADP | O4'-C4'-C5' | 3.67 | 121.45 | 109.37 |
| 9 | p | 1601 | ADP | PA-O3A-PB | -3.66 | 120.26 | 132.83 |
| 9 | A | 601 | ADP | O3'-C3'-C4' | 3.66 | 121.62 | 111.05 |
| 9 | f | 1601 | ADP | O3'-C3'-C4' | 3.65 | 121.60 | 111.05 |
| 9 | B | 601 | ADP | O3'-C3'-C4' | 3.65 | 121.59 | 111.05 |
| 9 | N | 601 | ADP | O3'-C3'-C4' | 3.58 | 121.39 | 111.05 |
| 9 | g | 1601 | ADP | O4'-C4'-C5' | 3.57 | 121.12 | 109.37 |
| 9 | G | 601 | ADP | O4'-C4'-C5' | 3.57 | 121.10 | 109.37 |
| 9 | J | 601 | ADP | O4'-C4'-C5' | 3.56 | 121.07 | 109.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 9 | m | 1601 | ADP | O3'-C3'-C4' | 3.52 | 121.22 | 111.05 |
| 9 | n | 1601 | ADP | O4'-C4'-C5' | 3.50 | 120.89 | 109.37 |
| 9 | J | 601 | ADP | O5'-C5'-C4' | 3.49 | 121.01 | 108.99 |
| 9 | h | 1601 | ADP | PA-O3A-PB | -3.47 | 120.93 | 132.83 |
| 9 | B | 601 | ADP | O5'-C5'-C4' | 3.46 | 120.90 | 108.99 |
| 9 | F | 601 | ADP | O5'-C5'-C4' | 3.44 | 120.85 | 108.99 |
| 9 | b | 1601 | ADP | O5'-C5'-C4' | 3.43 | 120.78 | 108.99 |
| 9 | M | 601 | ADP | PA-O3A-PB | -3.41 | 121.12 | 132.83 |
| 9 | H | 601 | ADP | O3'-C3'-C4' | 3.40 | 120.88 | 111.05 |
| 9 | D | 601 | ADP | PA-O3A-PB | -3.40 | 121.17 | 132.83 |
| 9 | p | 1601 | ADP | O3'-C3'-C4' | 3.40 | 120.87 | 111.05 |
| 9 | M | 601 | ADP | O3'-C3'-C4' | 3.36 | 120.77 | 111.05 |
| 9 | l | 1601 | ADP | O4'-C4'-C5' | 3.34 | 120.37 | 109.37 |
| 9 | A | 601 | ADP | O4'-C4'-C5' | 3.34 | 120.37 | 109.37 |
| 9 | B | 601 | ADP | O4'-C4'-C5' | 3.31 | 120.27 | 109.37 |
| 9 | b | 1601 | ADP | O4'-C4'-C5' | 3.28 | 120.16 | 109.37 |
| 9 | m | 1601 | ADP | O4'-C4'-C5' | 3.20 | 119.92 | 109.37 |
| 9 | p | 1601 | ADP | O3'-C3'-C2' | 3.19 | 122.13 | 111.82 |
| 9 | k | 2101 | ADP | O3'-C3'-C4' | 3.18 | 120.26 | 111.05 |
| 9 | l | 1601 | ADP | O3'-C3'-C4' | 3.18 | 120.25 | 111.05 |
| 9 | N | 601 | ADP | O4'-C4'-C5' | 3.15 | 119.74 | 109.37 |
| 9 | A | 601 | ADP | O5'-C5'-C4' | 3.14 | 119.81 | 108.99 |
| 9 | E | 601 | ADP | O4'-C4'-C5' | 3.13 | 119.67 | 109.37 |
| 9 | J | 601 | ADP | O3'-C3'-C4' | 3.12 | 120.08 | 111.05 |
| 9 | N | 601 | ADP | O5'-C5'-C4' | 3.12 | 119.73 | 108.99 |
| 9 | l | 1601 | ADP | C3'-C2'-C1' | 3.12 | 105.67 | 100.98 |
| 9 | P | 601 | ADP | O3'-C3'-C4' | 3.11 | 120.05 | 111.05 |
| 9 | e | 1601 | ADP | O3'-C3'-C4' | 3.11 | 120.03 | 111.05 |
| 9 | e | 1601 | ADP | O4'-C4'-C5' | 3.10 | 119.56 | 109.37 |
| 9 | b | 1601 | ADP | O3'-C3'-C4' | 3.08 | 119.95 | 111.05 |
| 9 | M | 601 | ADP | O5'-C5'-C4' | 3.05 | 119.50 | 108.99 |
| 9 | L | 601 | ADP | O4'-C4'-C5' | 3.04 | 119.38 | 109.37 |
| 9 | F | 601 | ADP | O4'-C4'-C5' | 3.03 | 119.35 | 109.37 |
| 9 | n | 1601 | ADP | O3'-C3'-C2' | 3.02 | 121.59 | 111.82 |
| 9 | l | 1601 | ADP | O5'-C5'-C4' | 3.02 | 119.37 | 108.99 |
| 9 | n | 1601 | ADP | O3'-C3'-C4' | 3.01 | 119.77 | 111.05 |
| 9 | C | 1101 | ADP | O4'-C4'-C5' | 3.01 | 119.28 | 109.37 |
| 9 | h | 1601 | ADP | O3'-C3'-C4' | 3.01 | 119.75 | 111.05 |
| 9 | p | 1601 | ADP | O4'-C4'-C3' | -2.99 | 99.20 | 105.11 |
| 9 | E | 601 | ADP | O3'-C3'-C2' | 2.97 | 121.43 | 111.82 |
| 9 | P | 601 | ADP | O4'-C4'-C3' | -2.89 | 99.40 | 105.11 |
| 9 | l | 1601 | ADP | O2'-C2'-C3' | 2.87 | 121.11 | 111.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 9 | a | 1601 | ADP | O5'-C5'-C4' | 2.85 | 118.80 | 108.99 |
| 9 | m | 1601 | ADP | O3'-C3'-C2' | 2.83 | 120.97 | 111.82 |
| 9 | D | 601 | ADP | O3'-C3'-C4' | 2.83 | 119.22 | 111.05 |
| 9 | E | 601 | ADP | O2'-C2'-C3' | 2.79 | 120.85 | 111.82 |
| 9 | A | 601 | ADP | O2'-C2'-C1' | 2.79 | 121.15 | 110.85 |
| 9 | F | 601 | ADP | O2'-C2'-C1' | 2.78 | 121.12 | 110.85 |
| 9 | L | 601 | ADP | O5'-C5'-C4' | 2.78 | 118.55 | 108.99 |
| 9 | a | 1601 | ADP | O3'-C3'-C4' | 2.75 | 118.99 | 111.05 |
| 9 | h | 1601 | ADP | O4'-C4'-C5' | 2.74 | 118.40 | 109.37 |
| 9 | l | 1601 | ADP | O3'-C3'-C2' | 2.73 | 120.64 | 111.82 |
| 9 | L | 601 | ADP | O3'-C3'-C4' | 2.71 | 118.89 | 111.05 |
| 9 | L | 601 | ADP | O2'-C2'-C3' | 2.69 | 120.52 | 111.82 |
| 9 | G | 601 | ADP | O3'-C3'-C4' | 2.69 | 118.82 | 111.05 |
| 9 | M | 601 | ADP | O3'-C3'-C2' | 2.67 | 120.47 | 111.82 |
| 9 | h | 1601 | ADP | O3'-C3'-C2' | 2.67 | 120.47 | 111.82 |
| 9 | b | 1601 | ADP | O4'-C4'-C3' | -2.66 | 99.84 | 105.11 |
| 9 | F | 601 | ADP | O2'-C2'-C3' | 2.66 | 120.44 | 111.82 |
| 9 | f | 1601 | ADP | O3'-C3'-C2' | 2.66 | 120.42 | 111.82 |
| 9 | J | 601 | ADP | O2'-C2'-C3' | 2.66 | 120.41 | 111.82 |
| 9 | h | 1601 | ADP | O4'-C4'-C3' | -2.65 | 99.87 | 105.11 |
| 9 | N | 601 | ADP | O3'-C3'-C2' | 2.65 | 120.38 | 111.82 |
| 9 | e | 1601 | ADP | O3'-C3'-C2' | 2.63 | 120.33 | 111.82 |
| 9 | p | 1601 | ADP | O4'-C4'-C5' | 2.62 | 117.98 | 109.37 |
| 9 | e | 1601 | ADP | O2'-C2'-C1' | 2.61 | 120.49 | 110.85 |
| 9 | G | 601 | ADP | O4'-C4'-C3' | -2.61 | 99.96 | 105.11 |
| 9 | g | 1601 | ADP | O3'-C3'-C4' | 2.59 | 118.55 | 111.05 |
| 9 | m | 1601 | ADP | O5'-C5'-C4' | 2.58 | 117.88 | 108.99 |
| 9 | B | 601 | ADP | O2'-C2'-C1' | 2.57 | 120.36 | 110.85 |
| 9 | k | 2101 | ADP | O2'-C2'-C1' | 2.57 | 120.33 | 110.85 |
| 9 | C | 1101 | ADP | O3'-C3'-C4' | 2.57 | 118.47 | 111.05 |
| 9 | G | 601 | ADP | O2'-C2'-C1' | 2.56 | 120.31 | 110.85 |
| 9 | b | 1601 | ADP | O3'-C3'-C2' | 2.54 | 120.03 | 111.82 |
| 9 | k | 2101 | ADP | C3'-C2'-C1' | 2.53 | 104.79 | 100.98 |
| 9 | A | 601 | ADP | O2'-C2'-C3' | 2.53 | 120.00 | 111.82 |
| 9 | P | 601 | ADP | O3'-C3'-C2' | 2.50 | 119.92 | 111.82 |
| 9 | B | 601 | ADP | C3'-C2'-C1' | 2.50 | 104.75 | 100.98 |
| 9 | b | 1601 | ADP | O2'-C2'-C3' | 2.49 | 119.89 | 111.82 |
| 9 | g | 1601 | ADP | O2'-C2'-C1' | 2.48 | 120.01 | 110.85 |
| 9 | P | 601 | ADP | O4'-C4'-C5' | 2.48 | 117.53 | 109.37 |
| 9 | P | 601 | ADP | O5'-C5'-C4' | 2.48 | 117.52 | 108.99 |
| 9 | H | 601 | ADP | O3'-C3'-C2' | 2.47 | 119.82 | 111.82 |
| 9 | N | 601 | ADP | O2'-C2'-C1' | 2.47 | 119.99 | 110.85 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 9 | C | 1101 | ADP | O3'-C3'-C2' | 2.45 | 119.76 | 111.82 |
| 9 | L | 601 | ADP | O2'-C2'-C1' | 2.45 | 119.91 | 110.85 |
| 9 | E | 601 | ADP | O2'-C2'-C1' | 2.44 | 119.88 | 110.85 |
| 9 | k | 2101 | ADP | O3'-C3'-C2' | 2.43 | 119.68 | 111.82 |
| 9 | e | 1601 | ADP | O2'-C2'-C3' | 2.40 | 119.60 | 111.82 |
| 9 | g | 1601 | ADP | O3'-C3'-C2' | 2.40 | 119.59 | 111.82 |
| 9 | J | 601 | ADP | O3'-C3'-C2' | 2.39 | 119.57 | 111.82 |
| 9 | J | 601 | ADP | O2'-C2'-C1' | 2.38 | 119.65 | 110.85 |
| 9 | l | 1601 | ADP | O2'-C2'-C1' | 2.37 | 119.62 | 110.85 |
| 9 | p | 1601 | ADP | O5'-C5'-C4' | 2.36 | 117.13 | 108.99 |
| 9 | a | 1601 | ADP | O2'-C2'-C3' | 2.35 | 119.42 | 111.82 |
| 9 | G | 601 | ADP | O5'-C5'-C4' | 2.35 | 117.07 | 108.99 |
| 9 | a | 1601 | ADP | O3'-C3'-C2' | 2.34 | 119.41 | 111.82 |
| 9 | J | 601 | ADP | O4'-C4'-C3' | -2.34 | 100.47 | 105.11 |
| 9 | J | 601 | ADP | C3'-C2'-C1' | 2.34 | 104.50 | 100.98 |
| 9 | n | 1601 | ADP | O5'-C5'-C4' | 2.32 | 116.98 | 108.99 |
| 9 | e | 1601 | ADP | O5'-C5'-C4' | 2.31 | 116.94 | 108.99 |
| 9 | H | 601 | ADP | O4'-C4'-C3' | -2.29 | 100.58 | 105.11 |
| 9 | A | 601 | ADP | C3'-C2'-C1' | 2.29 | 104.42 | 100.98 |
| 9 | D | 601 | ADP | O2'-C2'-C3' | 2.29 | 119.23 | 111.82 |
| 9 | n | 1601 | ADP | O3B-PB-O3A | 2.28 | 112.29 | 104.64 |
| 9 | g | 1601 | ADP | O4'-C4'-C3' | -2.27 | 100.61 | 105.11 |
| 9 | L | 601 | ADP | O3'-C3'-C2' | 2.27 | 119.15 | 111.82 |
| 9 | g | 1601 | ADP | O5'-C5'-C4' | 2.25 | 116.73 | 108.99 |
| 9 | A | 601 | ADP | O3'-C3'-C2' | 2.25 | 119.09 | 111.82 |
| 9 | E | 601 | ADP | O5'-C5'-C4' | 2.23 | 116.67 | 108.99 |
| 9 | H | 601 | ADP | O2'-C2'-C1' | 2.23 | 119.09 | 110.85 |
| 9 | h | 1601 | ADP | O5'-C5'-C4' | 2.23 | 116.66 | 108.99 |
| 9 | D | 601 | ADP | O3'-C3'-C2' | 2.22 | 119.02 | 111.82 |
| 9 | C | 1101 | ADP | O2B-PB-O3A | 2.22 | 112.08 | 104.64 |
| 9 | H | 601 | ADP | O2'-C2'-C3' | 2.22 | 119.00 | 111.82 |
| 9 | P | 601 | ADP | O2'-C2'-C1' | 2.22 | 119.04 | 110.85 |
| 9 | F | 601 | ADP | O3'-C3'-C4' | 2.21 | 117.44 | 111.05 |
| 9 | P | 601 | ADP | O2'-C2'-C3' | 2.19 | 118.92 | 111.82 |
| 9 | f | 1601 | ADP | O2'-C2'-C1' | 2.19 | 118.94 | 110.85 |
| 9 | p | 1601 | ADP | O2'-C2'-C3' | 2.19 | 118.90 | 111.82 |
| 9 | n | 1601 | ADP | O2'-C2'-C1' | 2.17 | 118.88 | 110.85 |
| 9 | N | 601 | ADP | O2'-C2'-C3' | 2.17 | 118.84 | 111.82 |
| 9 | a | 1601 | ADP | O2'-C2'-C1' | 2.16 | 118.83 | 110.85 |
| 9 | H | 601 | ADP | O4'-C4'-C5' | 2.16 | 116.47 | 109.37 |
| 9 | G | 601 | ADP | O3'-C3'-C2' | 2.14 | 118.75 | 111.82 |
| 9 | F | 601 | ADP | C2'-C3'-C4' | -2.12 | 98.52 | 102.64 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 9 | B | 601 | ADP | O2'-C2'-C3' | 2.11 | 118.65 | 111.82 |
| 9 | C | 1101 | ADP | O5'-C5'-C4' | 2.11 | 116.24 | 108.99 |
| 9 | G | 601 | ADP | O2'-C2'-C3' | 2.08 | 118.55 | 111.82 |
| 9 | k | 2101 | ADP | O2'-C2'-C3' | 2.08 | 118.55 | 111.82 |
| 9 | E | 601 | ADP | O2B-PB-O3A | 2.07 | 111.58 | 104.64 |
| 9 | N | 601 | ADP | O3B-PB-O3A | 2.07 | 111.57 | 104.64 |
| 9 | B | 601 | ADP | C5'-C4'-C3' | 2.03 | 122.79 | 115.18 |
| 9 | D | 601 | ADP | O2'-C2'-C1' | 2.03 | 118.33 | 110.85 |
| 9 | h | 1601 | ADP | O2'-C2'-C3' | 2.02 | 118.37 | 111.82 |
| 9 | f | 1601 | ADP | C5'-C4'-C3' | 2.01 | 122.71 | 115.18 |
| 9 | k | 2101 | ADP | C5'-C4'-C3' | 2.00 | 122.68 | 115.18 |
| 9 | C | 1101 | ADP | O2'-C2'-C3' | 2.00 | 118.29 | 111.82 |

All (34) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|------|------|------|
| 9 | J | 601 | ADP | C4' |
| 9 | J | 601 | ADP | C3' |
| 9 | a | 1601 | ADP | C4' |
| 9 | a | 1601 | ADP | C3' |
| 9 | P | 601 | ADP | C4' |
| 9 | n | 1601 | ADP | C2' |
| 9 | m | 1601 | ADP | C4' |
| 9 | m | 1601 | ADP | C3' |
| 9 | p | 1601 | ADP | C4' |
| 9 | A | 601 | ADP | C4' |
| 9 | A | 601 | ADP | C3' |
| 9 | e | 1601 | ADP | C4' |
| 9 | e | 1601 | ADP | C3' |
| 9 | g | 1601 | ADP | C3' |
| 9 | b | 1601 | ADP | C4' |
| 9 | b | 1601 | ADP | C3' |
| 9 | B | 601 | ADP | C4' |
| 9 | B | 601 | ADP | C3' |
| 9 | H | 601 | ADP | C4' |
| 9 | M | 601 | ADP | C4' |
| 9 | M | 601 | ADP | C3' |
| 9 | C | 1101 | ADP | C4' |
| 9 | C | 1101 | ADP | C3' |
| 9 | N | 601 | ADP | C2' |
| 9 | N | 601 | ADP | C3' |
| 9 | D | 601 | ADP | C4' |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|------|------|------|
| 9 | D | 601 | ADP | C3' |
| 9 | E | 601 | ADP | C4' |
| 9 | G | 601 | ADP | C3' |
| 9 | f | 1601 | ADP | C2' |
| 9 | f | 1601 | ADP | C3' |
| 9 | h | 1601 | ADP | C4' |
| 9 | k | 2101 | ADP | C4' |
| 9 | k | 2101 | ADP | C3' |

All (105) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 9 | J | 601 | ADP | C5'-O5'-PA-O2A |
| 9 | a | 1601 | ADP | PA-O3A-PB-O2B |
| 9 | a | 1601 | ADP | PB-O3A-PA-O5' |
| 9 | a | 1601 | ADP | C5'-O5'-PA-O3A |
| 9 | n | 1601 | ADP | PA-O3A-PB-O3B |
| 9 | n | 1601 | ADP | C5'-O5'-PA-O3A |
| 9 | m | 1601 | ADP | PB-O3A-PA-O5' |
| 9 | m | 1601 | ADP | C5'-O5'-PA-O1A |
| 9 | m | 1601 | ADP | C3'-C4'-C5'-O5' |
| 9 | p | 1601 | ADP | O4'-C4'-C5'-O5' |
| 9 | p | 1601 | ADP | C3'-C4'-C5'-O5' |
| 9 | A | 601 | ADP | C5'-O5'-PA-O3A |
| 9 | e | 1601 | ADP | PA-O3A-PB-O2B |
| 9 | e | 1601 | ADP | C3'-C4'-C5'-O5' |
| 9 | b | 1601 | ADP | PA-O3A-PB-O2B |
| 9 | b | 1601 | ADP | C5'-O5'-PA-O1A |
| 9 | b | 1601 | ADP | C5'-O5'-PA-O3A |
| 9 | b | 1601 | ADP | O4'-C4'-C5'-O5' |
| 9 | B | 601 | ADP | PB-O3A-PA-O5' |
| 9 | M | 601 | ADP | PA-O3A-PB-O2B |
| 9 | M | 601 | ADP | PA-O3A-PB-O3B |
| 9 | M | 601 | ADP | C5'-O5'-PA-O3A |
| 9 | C | 1101 | ADP | C5'-O5'-PA-O1A |
| 9 | C | 1101 | ADP | C5'-O5'-PA-O3A |
| 9 | N | 601 | ADP | C5'-O5'-PA-O1A |
| 9 | D | 601 | ADP | C4'-C5'-O5'-PA |
| 9 | F | 601 | ADP | PA-O3A-PB-O3B |
| 9 | F | 601 | ADP | C5'-O5'-PA-O1A |
| 9 | F | 601 | ADP | C5'-O5'-PA-O2A |
| 9 | l | 1601 | ADP | C5'-O5'-PA-O1A |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 9 | l | 1601 | ADP | C5'-O5'-PA-O2A |
| 9 | l | 1601 | ADP | C5'-O5'-PA-O3A |
| 9 | E | 601 | ADP | C5'-O5'-PA-O1A |
| 9 | E | 601 | ADP | C5'-O5'-PA-O2A |
| 9 | G | 601 | ADP | C5'-O5'-PA-O1A |
| 9 | f | 1601 | ADP | PA-O3A-PB-O3B |
| 9 | f | 1601 | ADP | C5'-O5'-PA-O1A |
| 9 | L | 601 | ADP | PA-O3A-PB-O2B |
| 9 | L | 601 | ADP | PA-O3A-PB-O3B |
| 9 | k | 2101 | ADP | C3'-C4'-C5'-O5' |
| 9 | J | 601 | ADP | O4'-C4'-C5'-O5' |
| 9 | a | 1601 | ADP | O4'-C4'-C5'-O5' |
| 9 | B | 601 | ADP | O4'-C4'-C5'-O5' |
| 9 | C | 1101 | ADP | C3'-C4'-C5'-O5' |
| 9 | A | 601 | ADP | O4'-C4'-C5'-O5' |
| 9 | e | 1601 | ADP | O4'-C4'-C5'-O5' |
| 9 | g | 1601 | ADP | O4'-C4'-C5'-O5' |
| 9 | g | 1601 | ADP | C3'-C4'-C5'-O5' |
| 9 | E | 601 | ADP | C3'-C4'-C5'-O5' |
| 9 | G | 601 | ADP | O4'-C4'-C5'-O5' |
| 9 | L | 601 | ADP | O4'-C4'-C5'-O5' |
| 9 | k | 2101 | ADP | O4'-C4'-C5'-O5' |
| 9 | H | 601 | ADP | O4'-C4'-C5'-O5' |
| 9 | k | 2101 | ADP | C4'-C5'-O5'-PA |
| 9 | m | 1601 | ADP | C4'-C5'-O5'-PA |
| 9 | g | 1601 | ADP | C4'-C5'-O5'-PA |
| 9 | b | 1601 | ADP | C4'-C5'-O5'-PA |
| 9 | B | 601 | ADP | C4'-C5'-O5'-PA |
| 9 | F | 601 | ADP | C4'-C5'-O5'-PA |
| 9 | G | 601 | ADP | C4'-C5'-O5'-PA |
| 9 | J | 601 | ADP | PB-O3A-PA-O5' |
| 9 | g | 1601 | ADP | PB-O3A-PA-O5' |
| 9 | b | 1601 | ADP | PB-O3A-PA-O5' |
| 9 | M | 601 | ADP | PB-O3A-PA-O5' |
| 9 | C | 1101 | ADP | PB-O3A-PA-O5' |
| 9 | D | 601 | ADP | PB-O3A-PA-O5' |
| 9 | E | 601 | ADP | PB-O3A-PA-O5' |
| 9 | J | 601 | ADP | C4'-C5'-O5'-PA |
| 9 | a | 1601 | ADP | C4'-C5'-O5'-PA |
| 9 | A | 601 | ADP | C4'-C5'-O5'-PA |
| 9 | e | 1601 | ADP | PA-O3A-PB-O3B |
| 9 | H | 601 | ADP | PA-O3A-PB-O2B |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 9 | D | 601 | ADP | PA-O3A-PB-O2B |
| 9 | k | 2101 | ADP | PA-O3A-PB-O3B |
| 9 | J | 601 | ADP | C5'-O5'-PA-O3A |
| 9 | m | 1601 | ADP | C5'-O5'-PA-O3A |
| 9 | N | 601 | ADP | C5'-O5'-PA-O3A |
| 9 | F | 601 | ADP | C5'-O5'-PA-O3A |
| 9 | f | 1601 | ADP | C5'-O5'-PA-O3A |
| 9 | h | 1601 | ADP | PB-O3A-PA-O2A |
| 9 | J | 601 | ADP | C5'-O5'-PA-O1A |
| 9 | a | 1601 | ADP | C5'-O5'-PA-O1A |
| 9 | n | 1601 | ADP | C5'-O5'-PA-O1A |
| 9 | A | 601 | ADP | C5'-O5'-PA-O1A |
| 9 | M | 601 | ADP | C5'-O5'-PA-O1A |
| 9 | H | 601 | ADP | C3'-C4'-C5'-O5' |
| 9 | N | 601 | ADP | O4'-C4'-C5'-O5' |
| 9 | f | 1601 | ADP | PA-O3A-PB-O1B |
| 9 | F | 601 | ADP | PB-O3A-PA-O2A |
| 9 | F | 601 | ADP | PA-O3A-PB-O1B |
| 9 | b | 1601 | ADP | C3'-C4'-C5'-O5' |
| 9 | P | 601 | ADP | PB-O3A-PA-O2A |
| 9 | p | 1601 | ADP | PB-O3A-PA-O2A |
| 9 | H | 601 | ADP | PB-O3A-PA-O2A |
| 9 | n | 1601 | ADP | PA-O3A-PB-O1B |
| 9 | e | 1601 | ADP | PA-O3A-PB-O1B |
| 9 | b | 1601 | ADP | PA-O3A-PB-O1B |
| 9 | C | 1101 | ADP | O4'-C4'-C5'-O5' |
| 9 | a | 1601 | ADP | PA-O3A-PB-O3B |
| 9 | E | 601 | ADP | C5'-O5'-PA-O3A |
| 9 | M | 601 | ADP | O4'-C4'-C5'-O5' |
| 9 | F | 601 | ADP | PB-O3A-PA-O1A |
| 9 | N | 601 | ADP | C4'-C5'-O5'-PA |
| 9 | L | 601 | ADP | C5'-O5'-PA-O2A |
| 9 | M | 601 | ADP | PA-O3A-PB-O1B |

There are no ring outliers.

17 monomers are involved in 79 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 9 | J | 601 | ADP | 5 | 0 |
| 9 | P | 601 | ADP | 5 | 0 |
| 10 | C | 1102 | BEF | 3 | 0 |
| 9 | A | 601 | ADP | 3 | 0 |

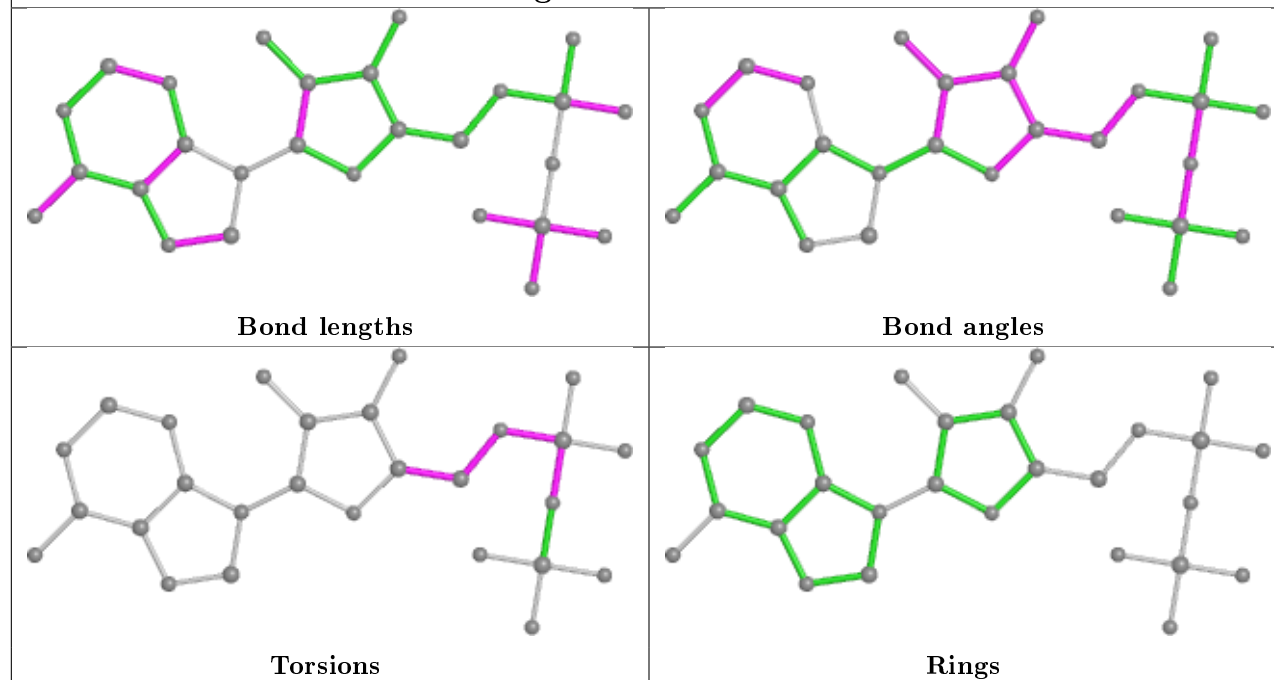
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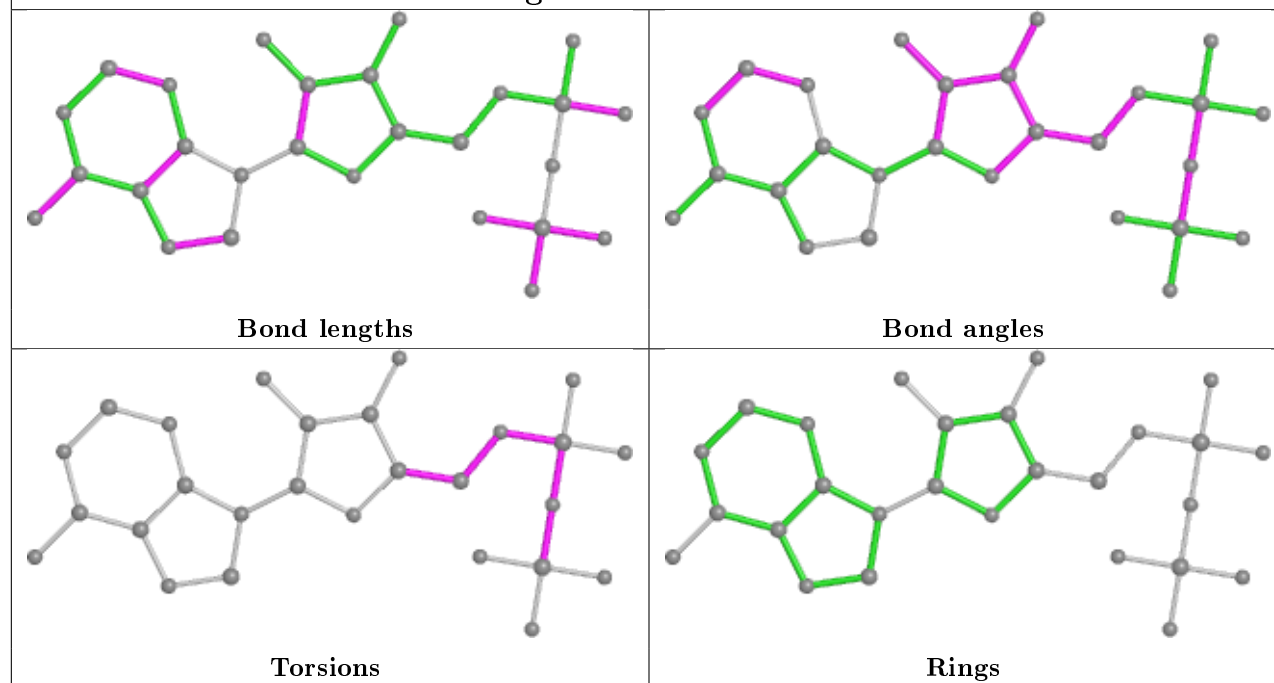
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 9 | B | 601 | ADP | 8 | 0 |
| 9 | H | 601 | ADP | 3 | 0 |
| 10 | F | 602 | BEF | 2 | 0 |
| 9 | M | 601 | ADP | 6 | 0 |
| 9 | C | 1101 | ADP | 7 | 0 |
| 9 | N | 601 | ADP | 6 | 0 |
| 9 | D | 601 | ADP | 8 | 0 |
| 9 | F | 601 | ADP | 6 | 0 |
| 10 | N | 602 | BEF | 3 | 0 |
| 10 | L | 602 | BEF | 1 | 0 |
| 9 | E | 601 | ADP | 2 | 0 |
| 9 | G | 601 | ADP | 5 | 0 |
| 9 | L | 601 | ADP | 7 | 0 |

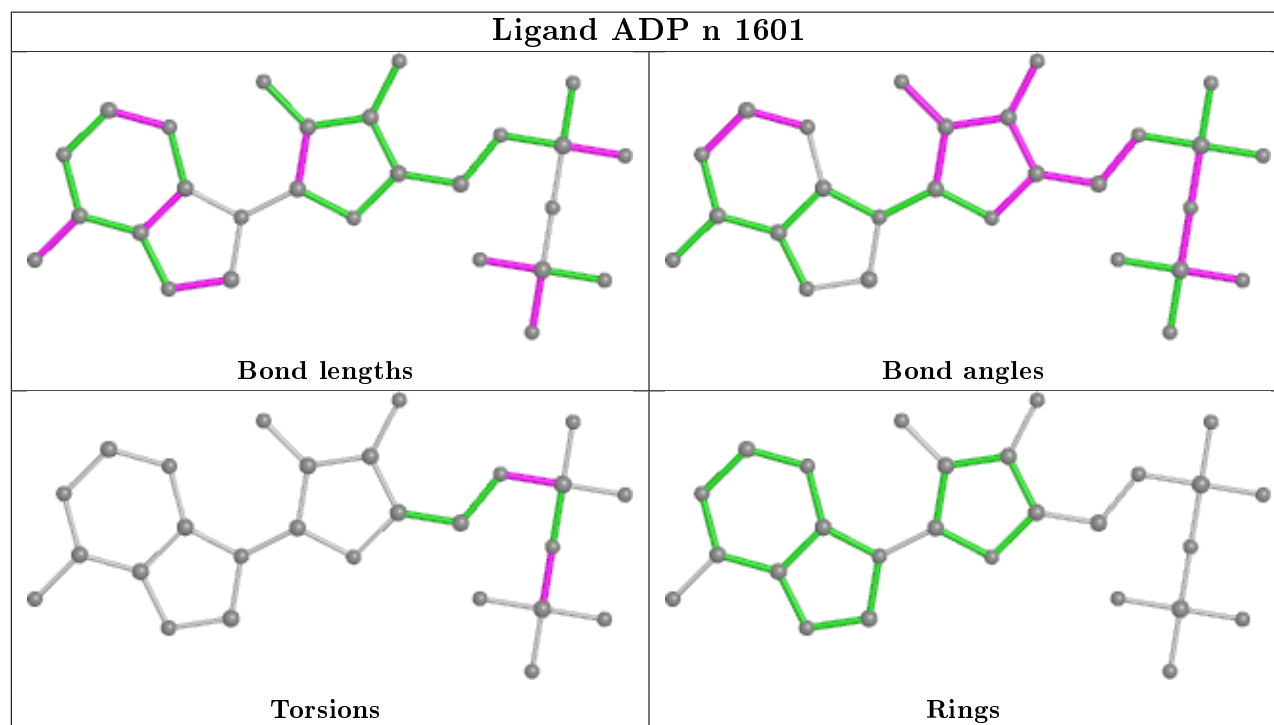
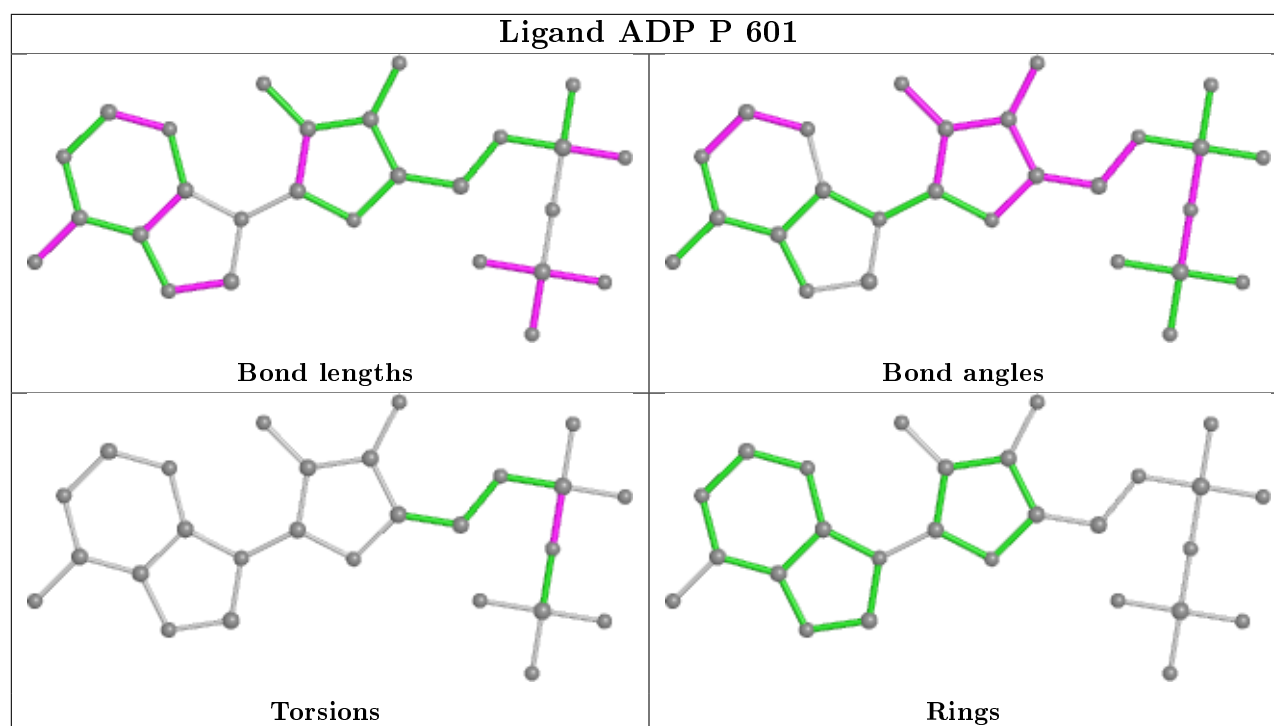
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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 ADP J 601

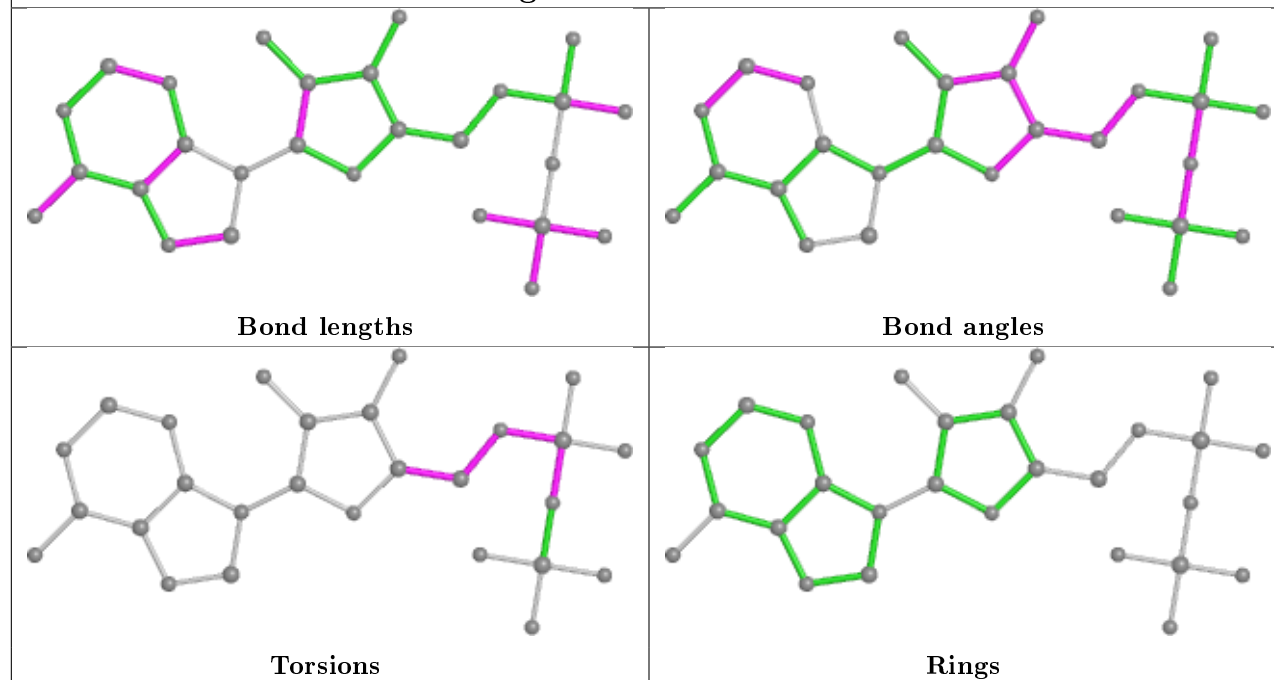


Ligand ADP a 1601

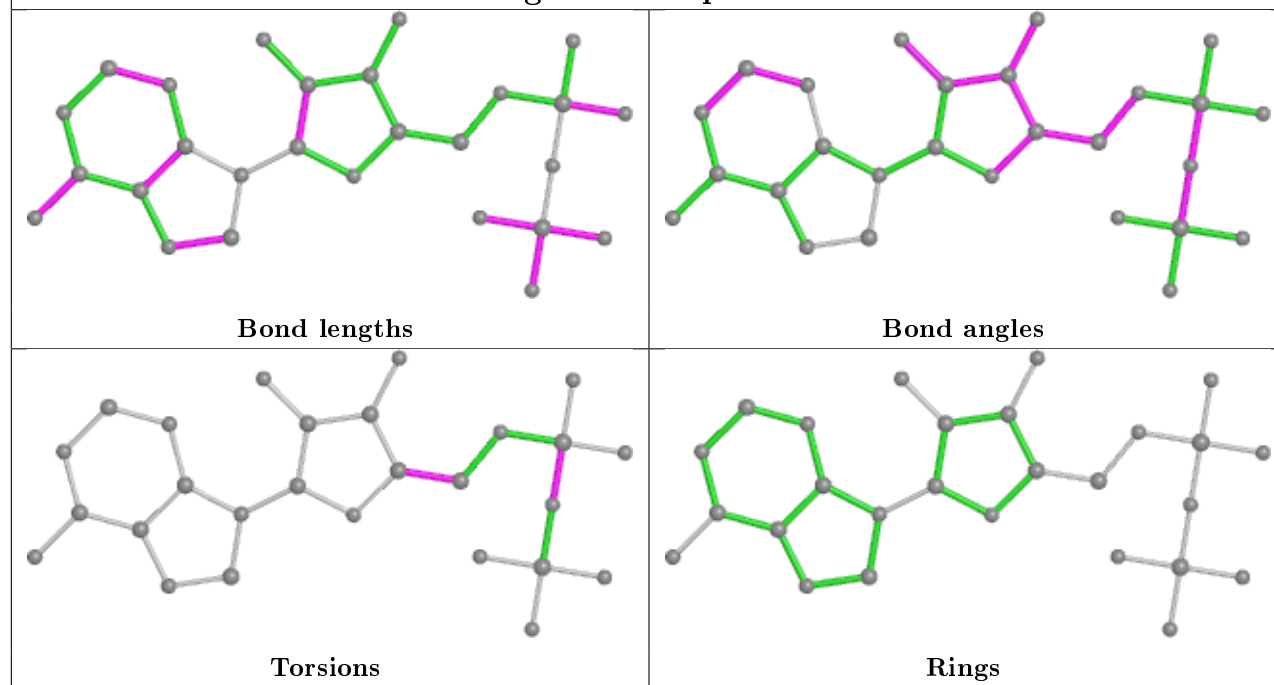


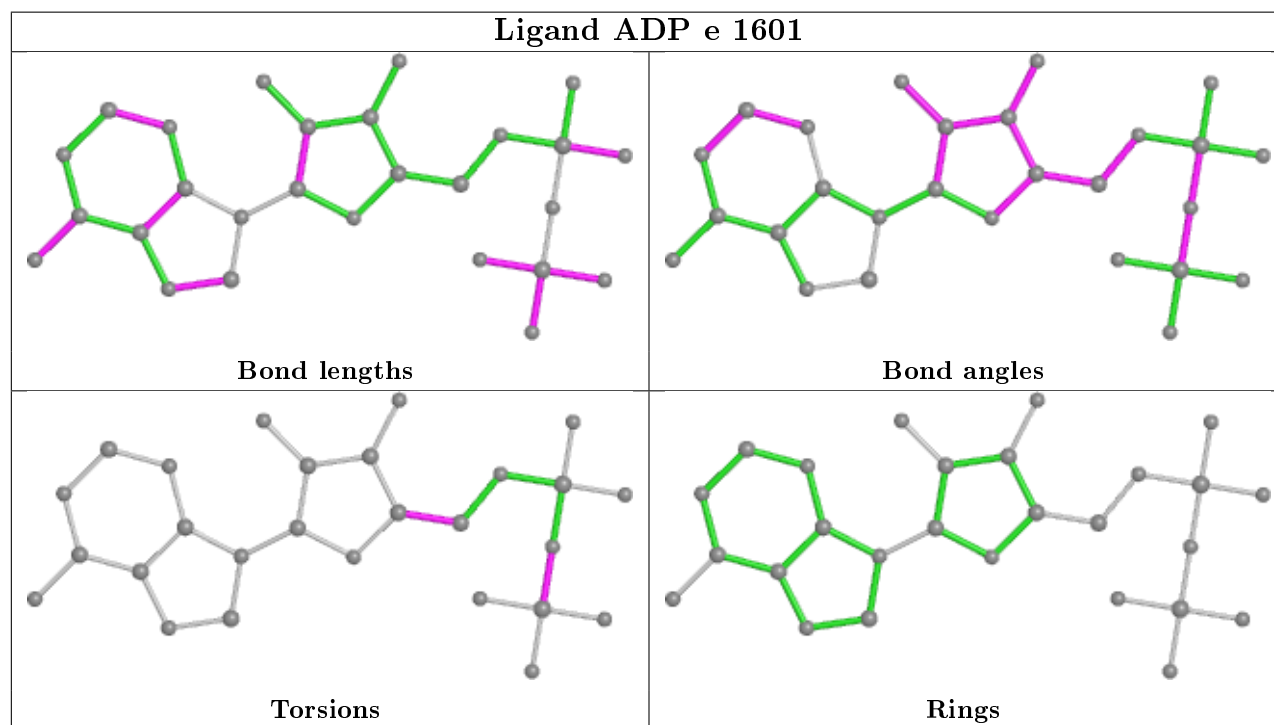
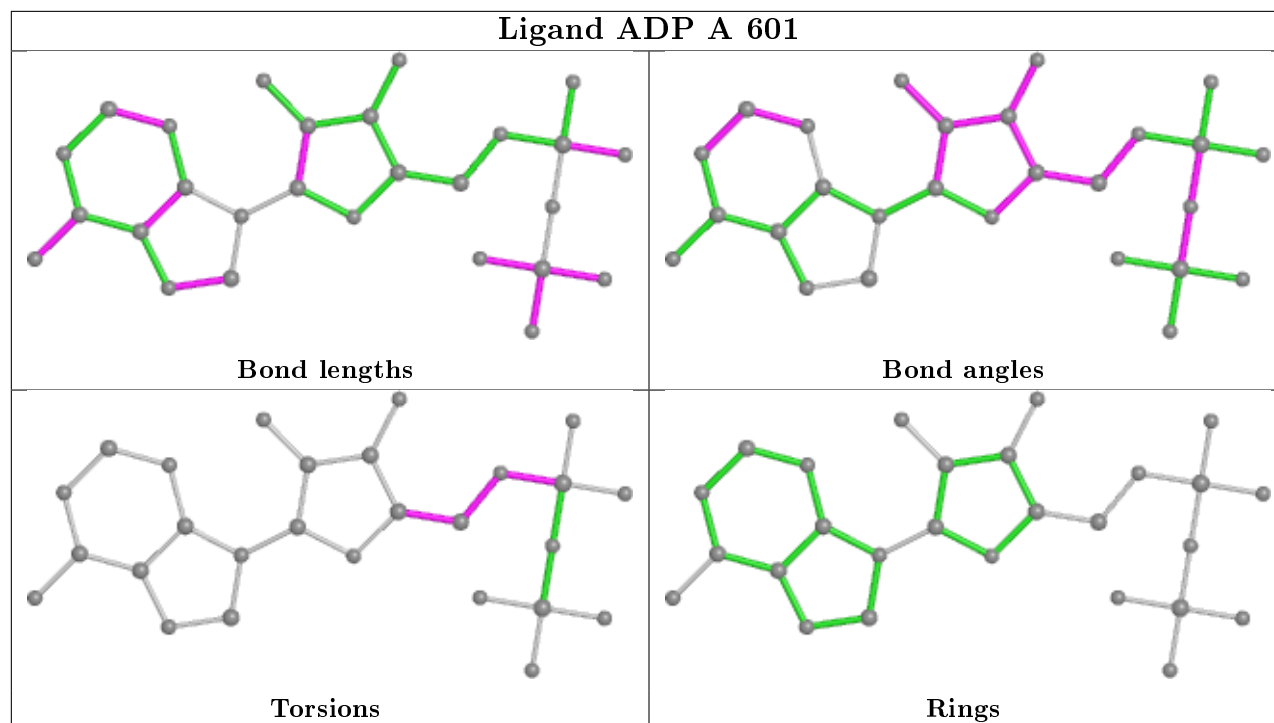


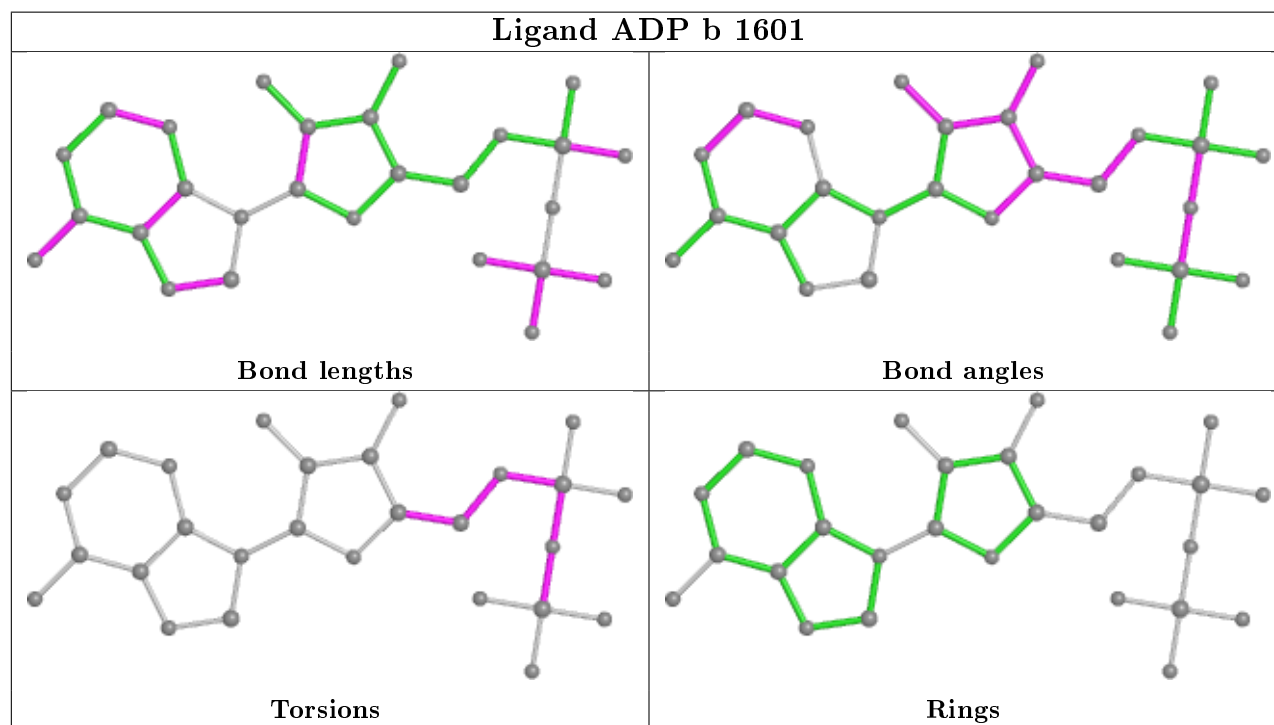
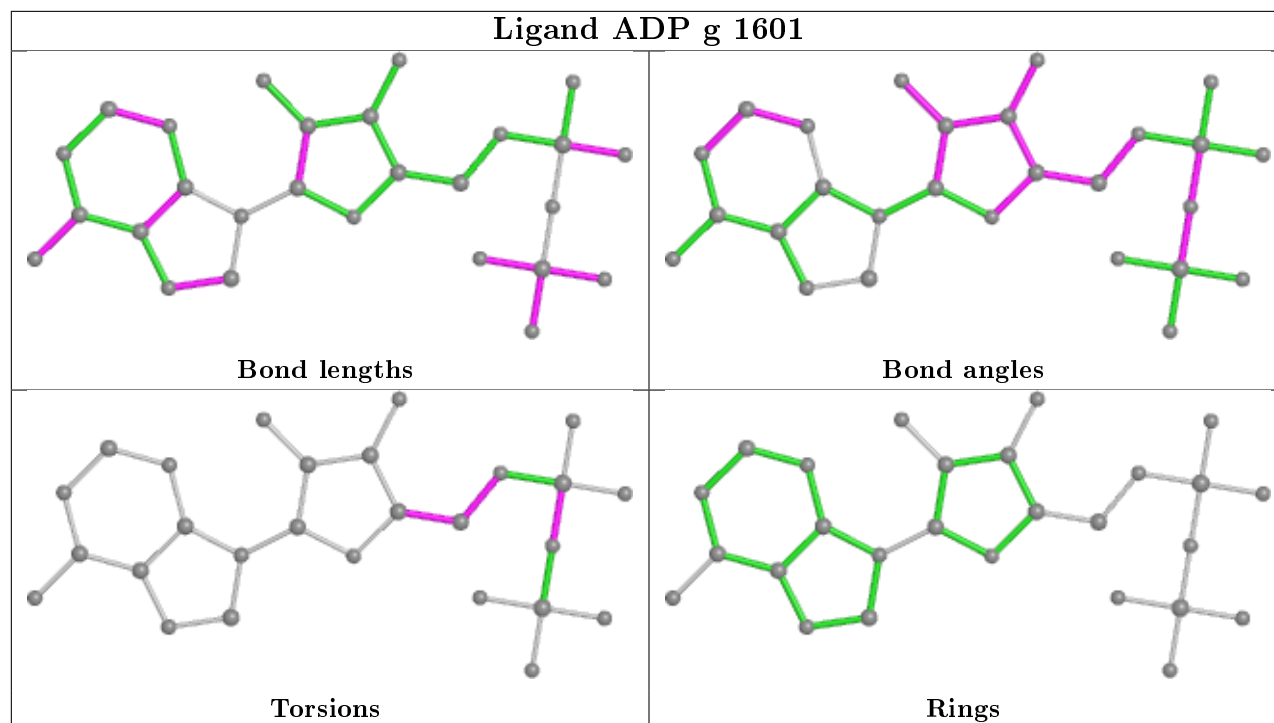
Ligand ADP m 1601

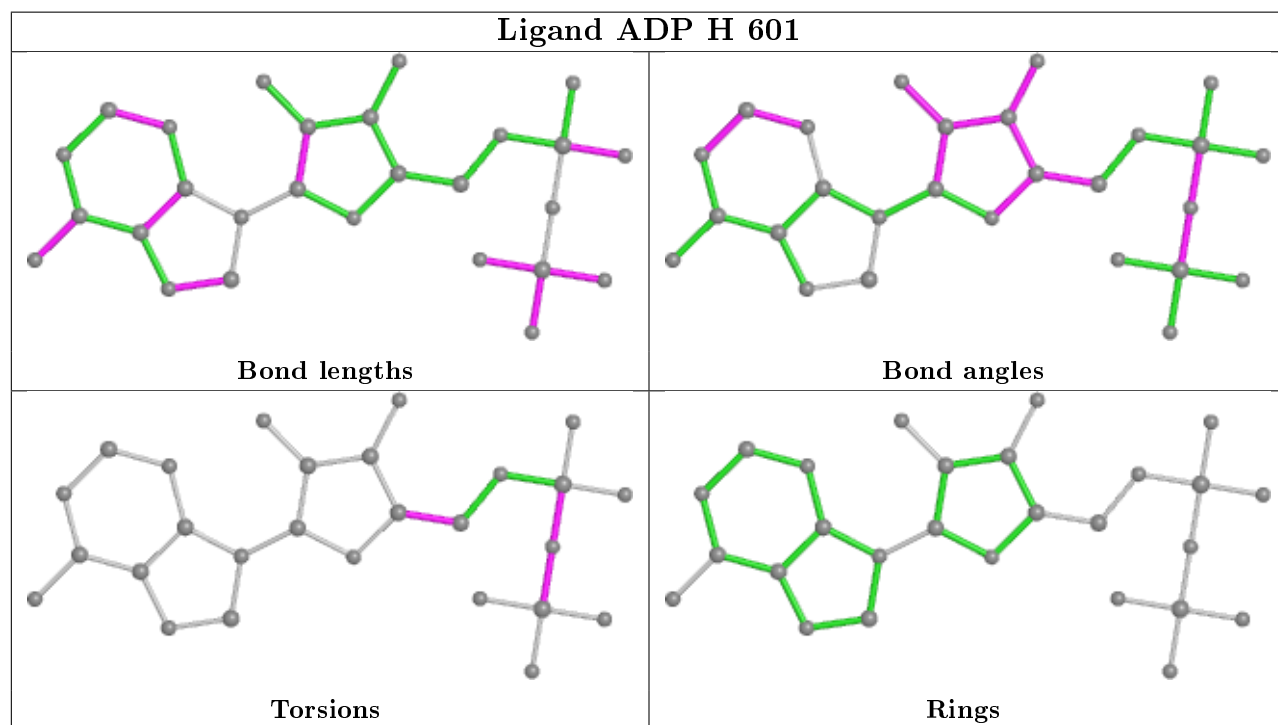
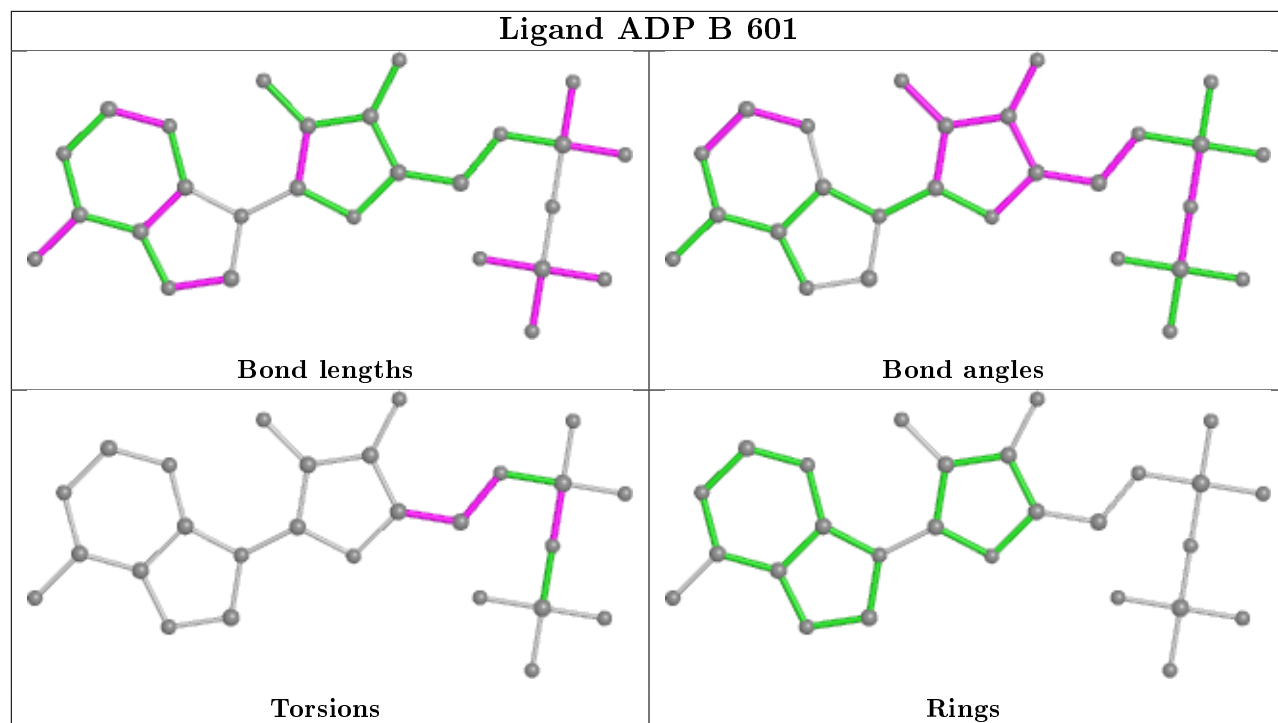


Ligand ADP p 1601

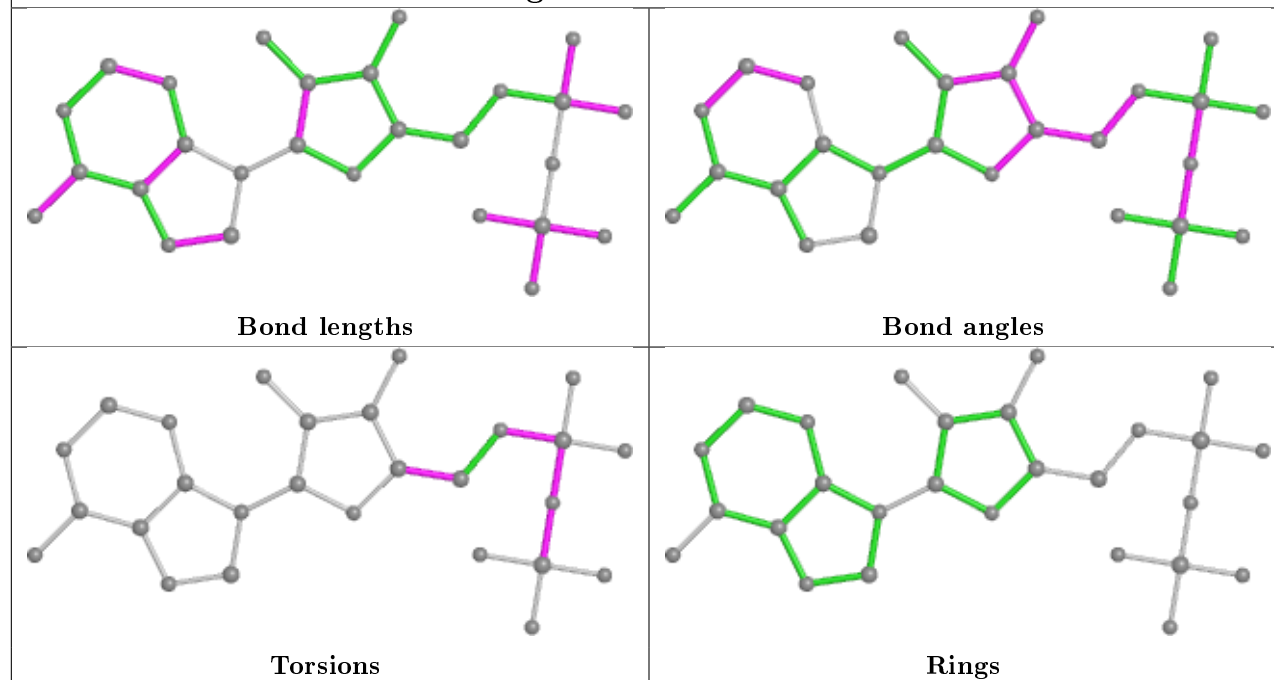




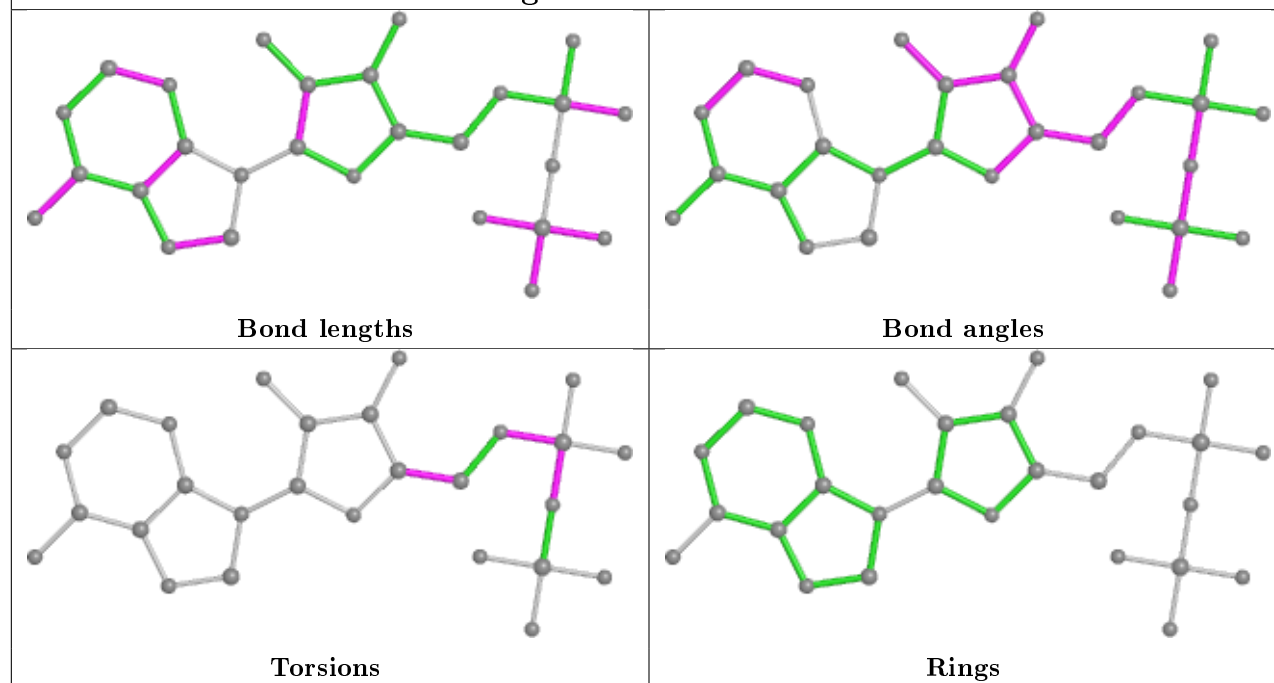


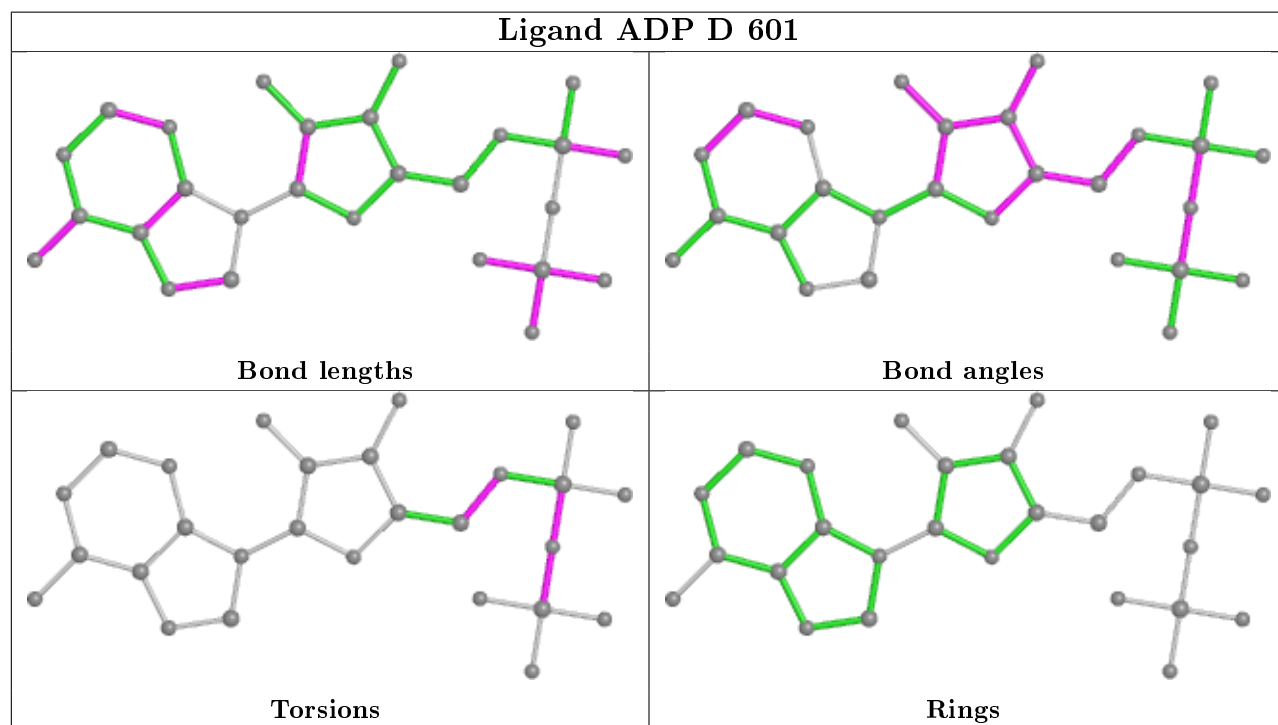
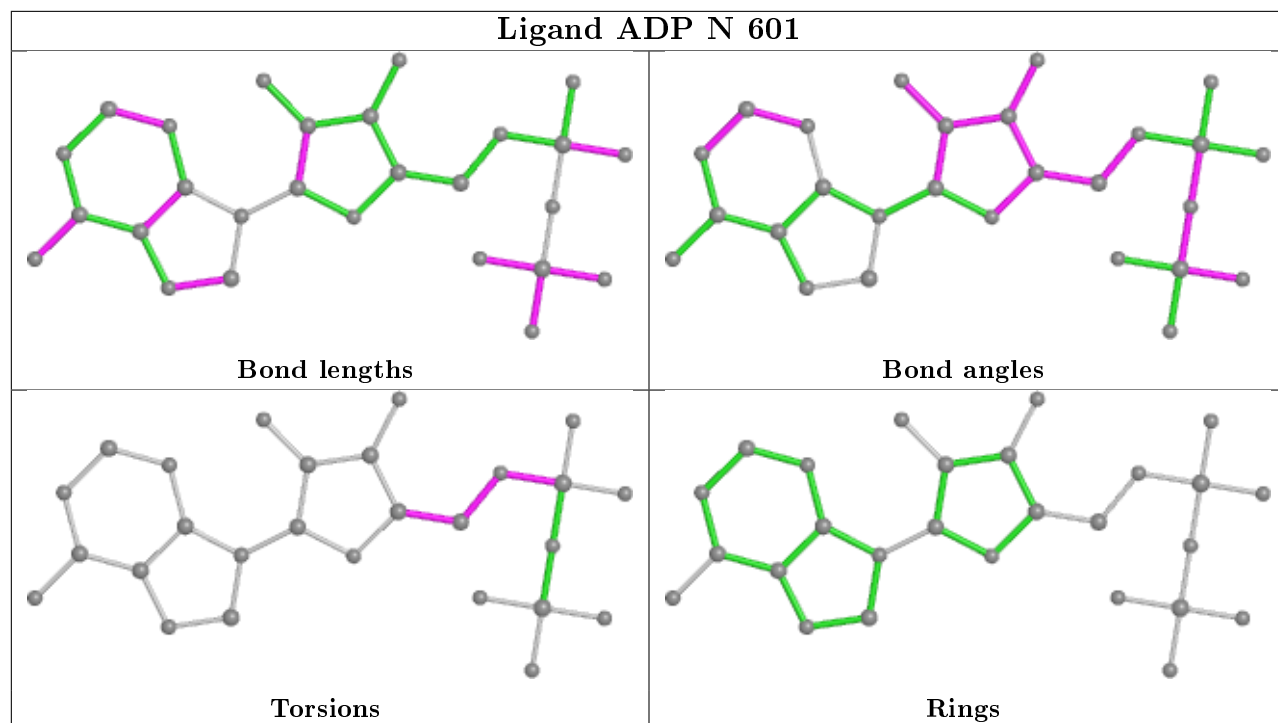


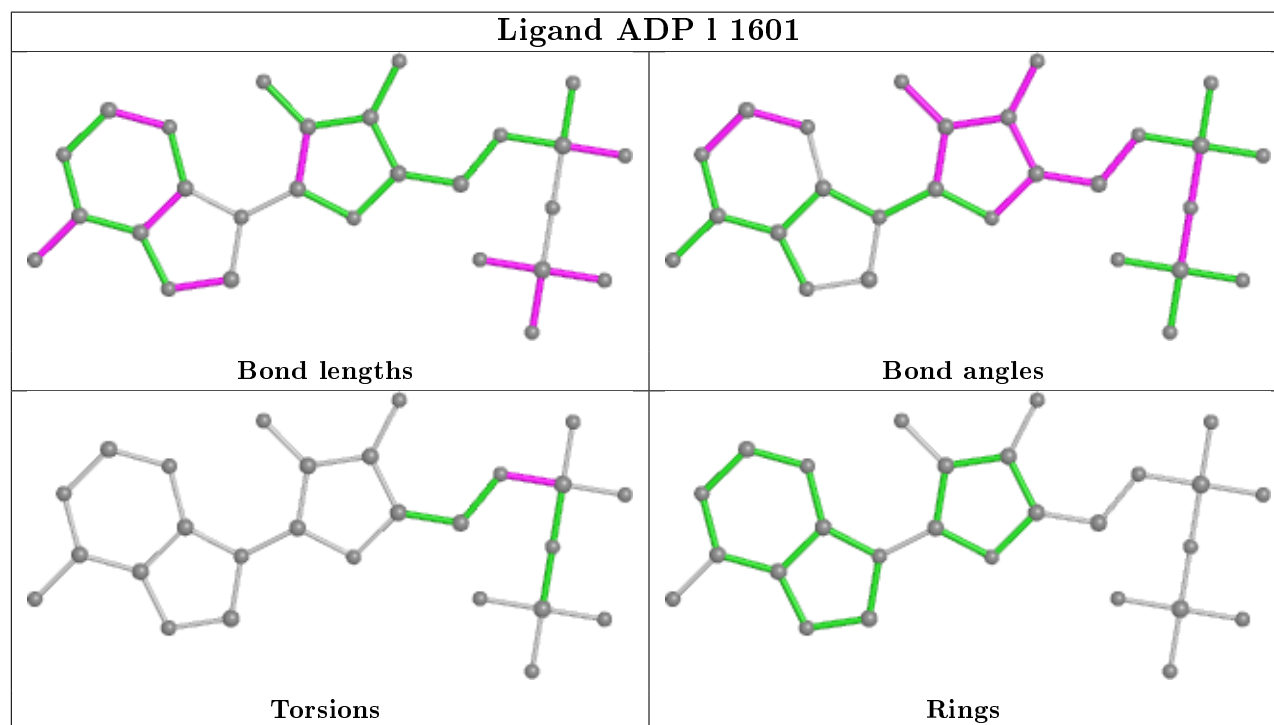
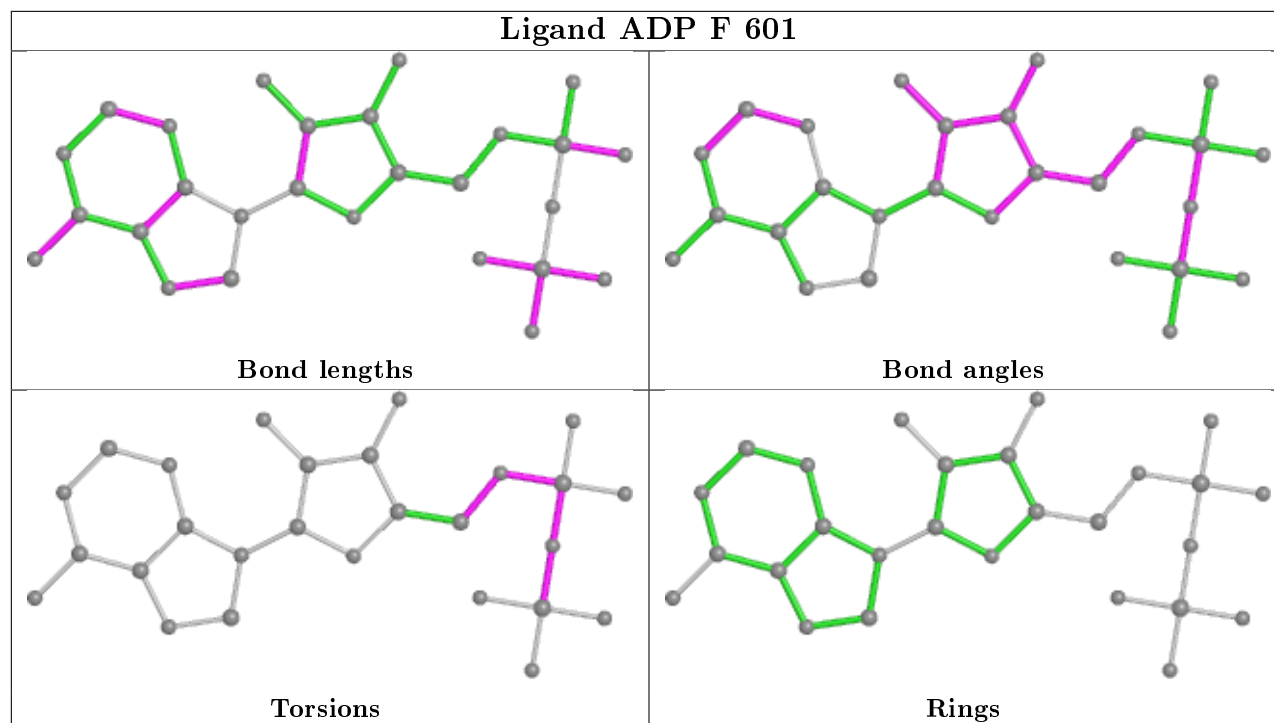
Ligand ADP M 601

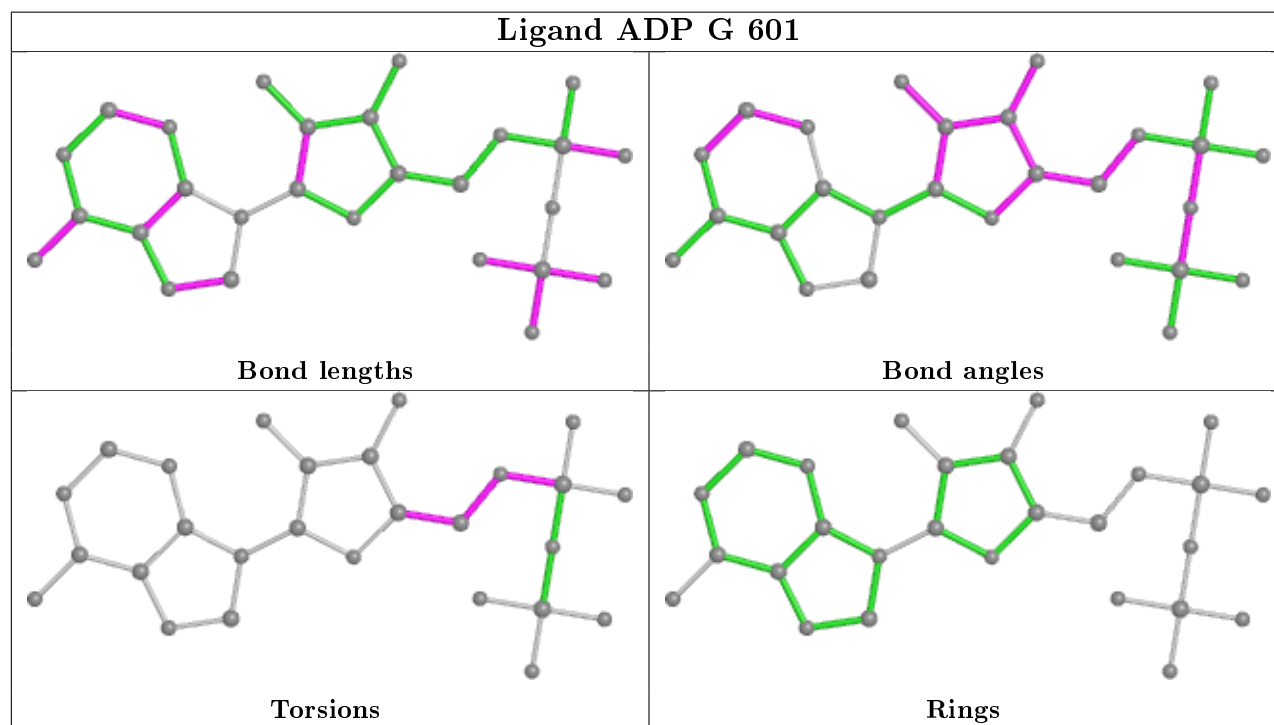
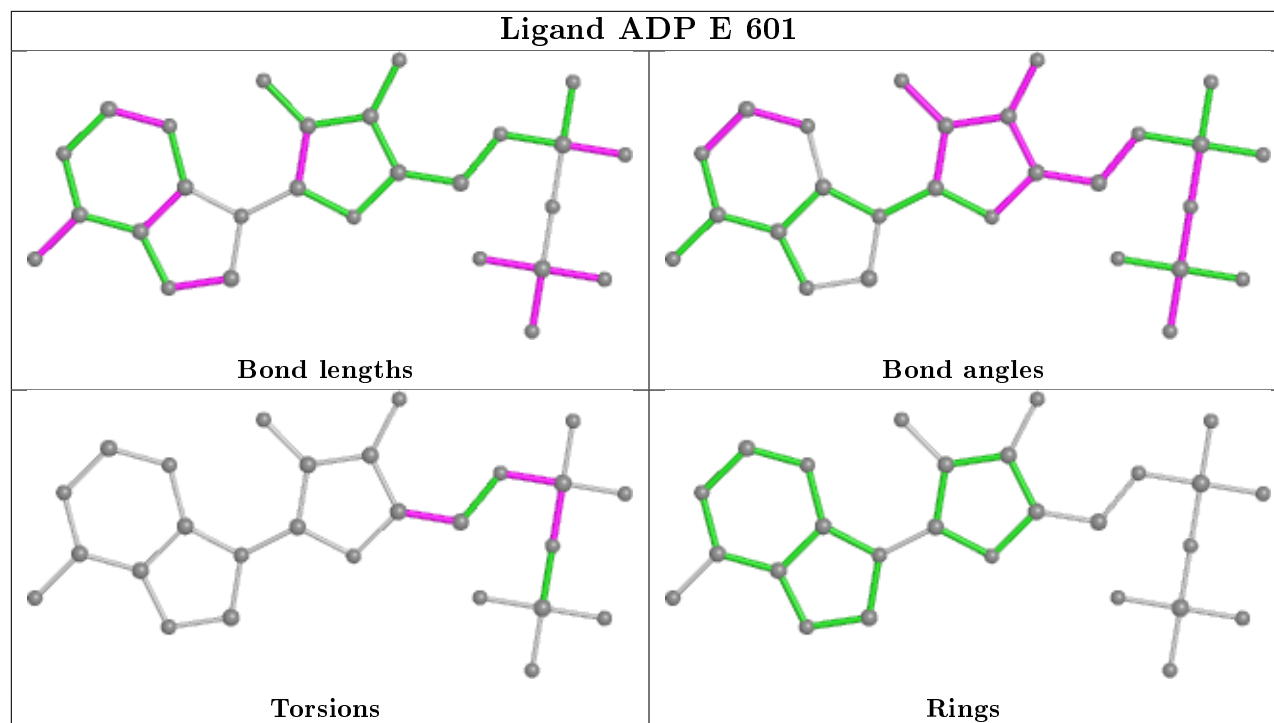


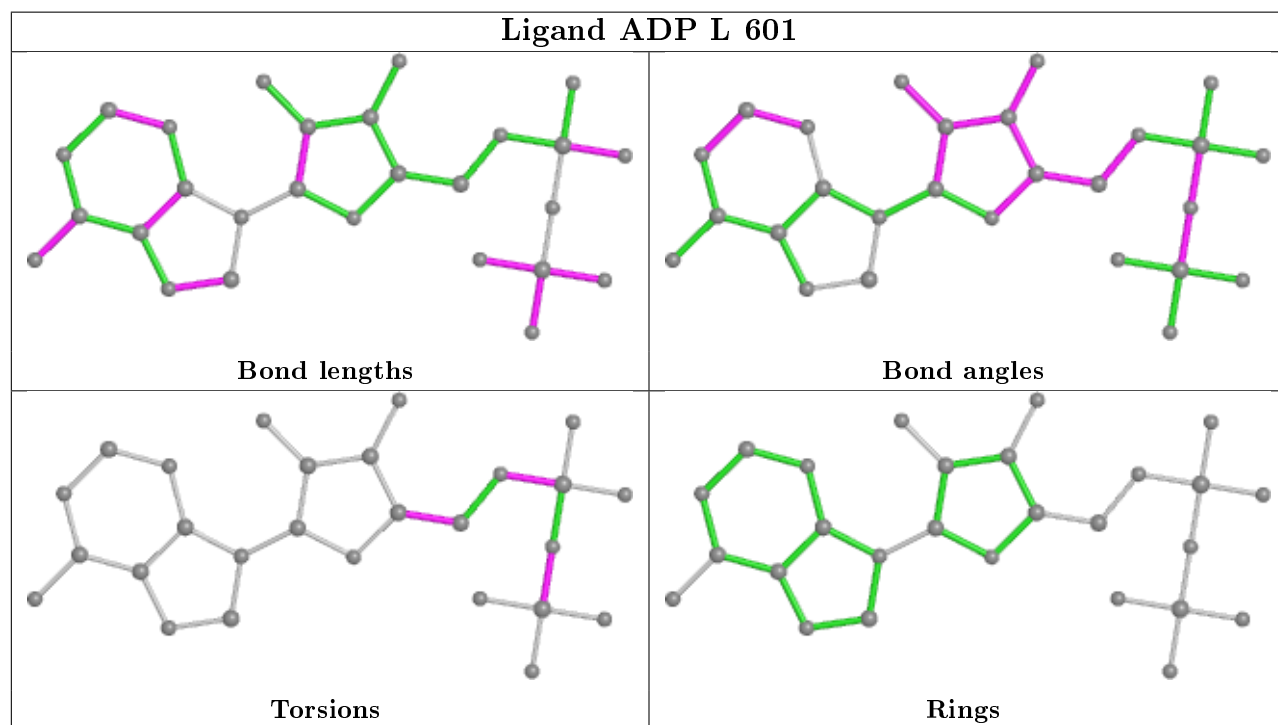
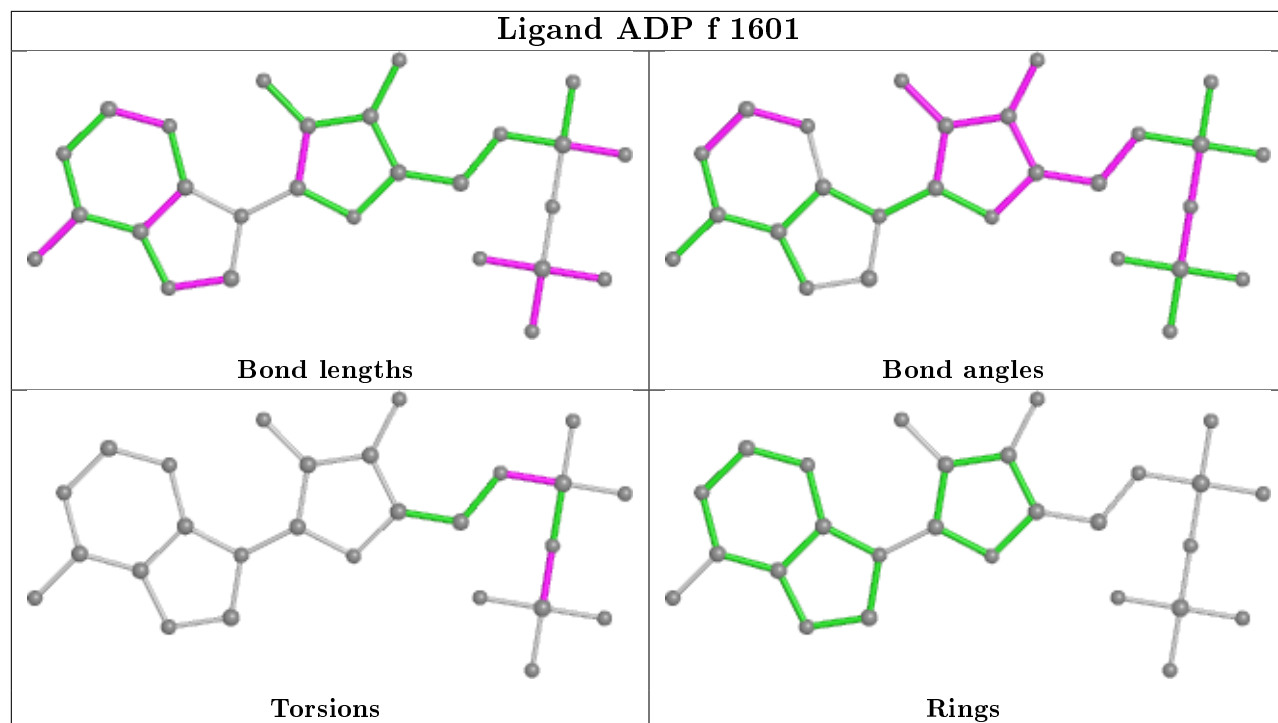
Ligand ADP C 1101

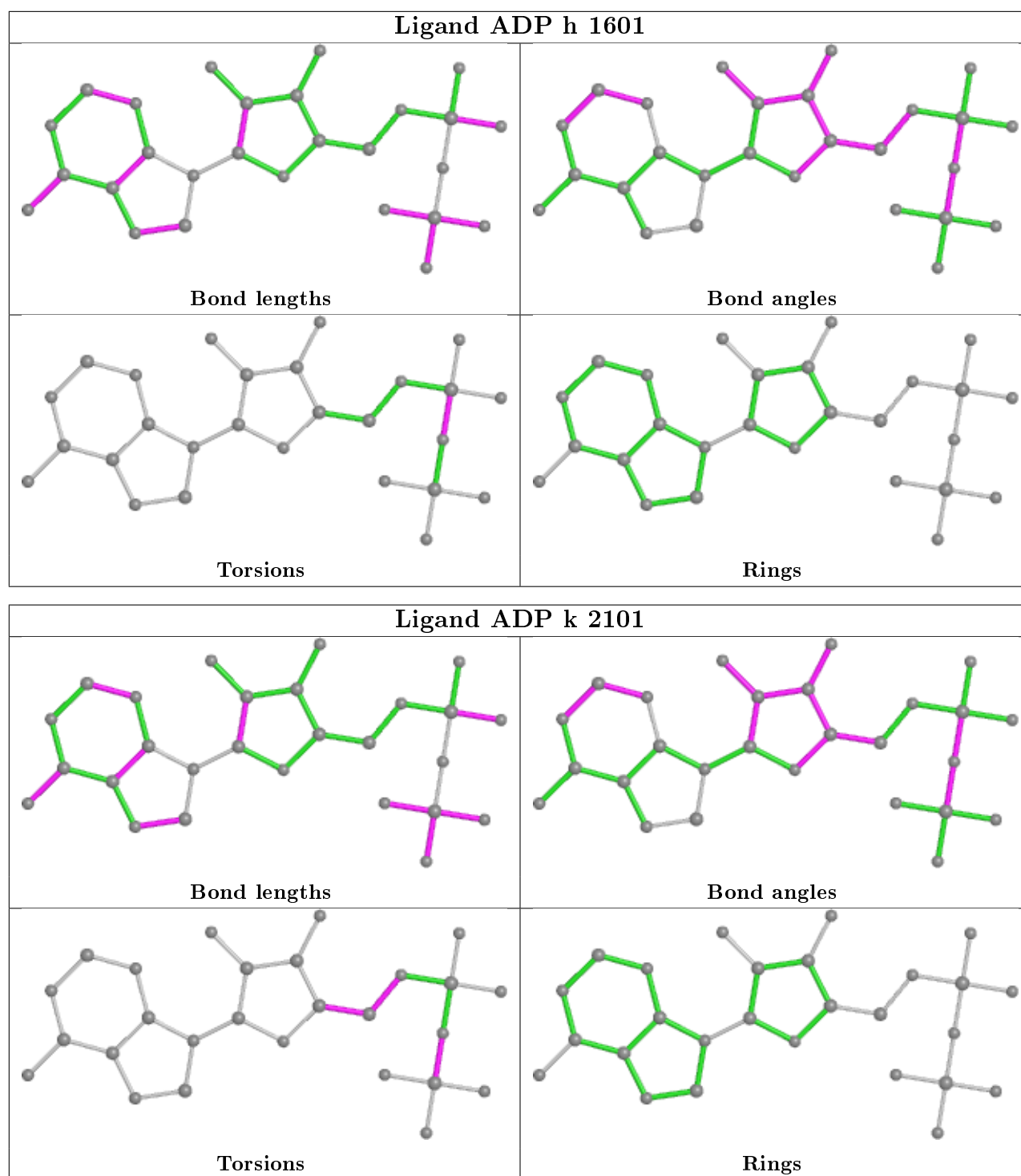












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | | | OWAB(Å ²) | Q<0.9 |
|-----|-------|---------------|--------|---------|----|----|-----------------------|-------|
| 1 | A | 544/559 (97%) | -0.00 | 13 (2%) | 59 | 50 | 72, 134, 206, 254 | 0 |
| 1 | I | 544/559 (97%) | 0.02 | 27 (4%) | 28 | 25 | 72, 134, 206, 254 | 0 |
| 1 | a | 544/559 (97%) | -0.09 | 15 (2%) | 53 | 43 | 72, 134, 206, 254 | 0 |
| 1 | i | 544/559 (97%) | -0.06 | 14 (2%) | 56 | 47 | 72, 134, 206, 254 | 0 |
| 2 | B | 513/527 (97%) | -0.11 | 5 (0%) | 82 | 76 | 47, 120, 192, 236 | 0 |
| 2 | J | 513/527 (97%) | 0.05 | 18 (3%) | 44 | 36 | 47, 120, 192, 236 | 0 |
| 2 | b | 513/527 (97%) | -0.10 | 8 (1%) | 72 | 64 | 47, 120, 192, 236 | 0 |
| 2 | j | 513/527 (97%) | -0.09 | 7 (1%) | 75 | 68 | 47, 120, 192, 236 | 0 |
| 3 | C | 514/590 (87%) | 0.06 | 10 (1%) | 66 | 59 | 73, 141, 205, 295 | 0 |
| 3 | K | 514/590 (87%) | 0.01 | 18 (3%) | 44 | 36 | 73, 141, 205, 295 | 0 |
| 3 | c | 514/590 (87%) | 0.03 | 18 (3%) | 44 | 36 | 73, 141, 205, 295 | 0 |
| 3 | k | 514/590 (87%) | -0.08 | 10 (1%) | 66 | 59 | 73, 141, 205, 295 | 0 |
| 4 | D | 522/528 (98%) | 0.00 | 15 (2%) | 51 | 42 | 70, 149, 232, 297 | 0 |
| 4 | L | 522/528 (98%) | 0.07 | 26 (4%) | 28 | 25 | 70, 149, 232, 297 | 0 |
| 4 | d | 522/528 (98%) | 0.01 | 15 (2%) | 51 | 42 | 70, 149, 232, 297 | 0 |
| 4 | l | 522/528 (98%) | 0.09 | 21 (4%) | 38 | 32 | 70, 149, 232, 297 | 0 |
| 5 | E | 525/562 (93%) | 0.05 | 16 (3%) | 50 | 40 | 56, 138, 238, 297 | 0 |
| 5 | M | 525/562 (93%) | 0.22 | 31 (5%) | 22 | 18 | 56, 138, 238, 297 | 0 |
| 5 | e | 525/562 (93%) | 0.02 | 20 (3%) | 40 | 33 | 56, 138, 238, 297 | 0 |
| 5 | m | 525/562 (93%) | -0.06 | 15 (2%) | 51 | 42 | 56, 138, 238, 297 | 0 |
| 6 | F | 533/546 (97%) | 0.11 | 27 (5%) | 28 | 24 | 42, 116, 214, 301 | 0 |
| 6 | N | 533/546 (97%) | 0.05 | 18 (3%) | 45 | 37 | 42, 116, 214, 301 | 0 |
| 6 | f | 533/546 (97%) | 0.07 | 20 (3%) | 40 | 33 | 42, 116, 214, 301 | 0 |
| 6 | n | 533/546 (97%) | 0.05 | 19 (3%) | 42 | 35 | 42, 116, 214, 301 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | | | OWAB(Å ²) | Q<0.9 |
|-----|-------|-------------------|--------|----------|----|----|-----------------------|-------|
| 7 | G | 509/550 (92%) | 0.03 | 13 (2%) | 56 | 47 | 65, 136, 207, 264 | 0 |
| 7 | O | 509/550 (92%) | 0.13 | 23 (4%) | 33 | 28 | 65, 136, 207, 264 | 0 |
| 7 | g | 509/550 (92%) | -0.05 | 15 (2%) | 51 | 42 | 65, 136, 207, 264 | 0 |
| 7 | o | 509/550 (92%) | 0.09 | 23 (4%) | 33 | 28 | 65, 136, 207, 264 | 0 |
| 8 | H | 525/568 (92%) | 0.01 | 11 (2%) | 63 | 55 | 70, 148, 236, 294 | 0 |
| 8 | P | 525/568 (92%) | 0.26 | 37 (7%) | 16 | 12 | 70, 148, 236, 294 | 0 |
| 8 | h | 525/568 (92%) | 0.16 | 27 (5%) | 28 | 24 | 70, 148, 236, 294 | 0 |
| 8 | p | 525/568 (92%) | 0.11 | 26 (4%) | 28 | 25 | 70, 148, 236, 294 | 0 |
| All | All | 16740/17720 (94%) | 0.03 | 581 (3%) | 44 | 36 | 42, 136, 217, 301 | 0 |

All (581) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 5 | e | 1387 | THR | 13.7 |
| 5 | M | 387 | THR | 12.0 |
| 7 | o | 1228 | GLY | 11.4 |
| 5 | m | 1387 | THR | 9.9 |
| 1 | a | 1552 | PRO | 8.9 |
| 6 | n | 1539 | SER | 8.5 |
| 5 | e | 1388 | THR | 7.9 |
| 6 | F | 223 | ASP | 7.9 |
| 5 | m | 1398 | SER | 7.7 |
| 4 | D | 283 | CYS | 7.2 |
| 6 | n | 1001 | MET | 7.1 |
| 6 | F | 539 | SER | 6.8 |
| 7 | O | 530 | GLU | 6.5 |
| 6 | N | 223 | ASP | 6.2 |
| 6 | n | 1466 | PRO | 6.0 |
| 5 | M | 388 | THR | 5.9 |
| 1 | I | 556 | PRO | 5.9 |
| 4 | L | 251 | ASN | 5.7 |
| 7 | o | 1207 | GLY | 5.7 |
| 7 | G | 228 | GLY | 5.6 |
| 6 | F | 187 | ASP | 5.6 |
| 5 | m | 1358 | THR | 5.6 |
| 4 | L | 292 | ILE | 5.6 |
| 7 | o | 1227 | ALA | 5.5 |
| 6 | f | 1487 | ARG | 5.5 |
| 5 | M | 249 | PHE | 5.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 6 | N | 487 | ARG | 5.4 |
| 4 | L | 252 | ILE | 5.4 |
| 6 | n | 1002 | SER | 5.4 |
| 6 | n | 1467 | LEU | 5.4 |
| 3 | K | 258 | GLN | 5.2 |
| 7 | O | 373 | THR | 5.2 |
| 4 | l | 1284 | ASN | 5.2 |
| 1 | a | 1342 | SER | 5.2 |
| 1 | I | 14 | PHE | 5.2 |
| 1 | a | 1341 | MET | 5.1 |
| 6 | f | 1465 | ASP | 5.1 |
| 1 | i | 1146 | THR | 5.1 |
| 7 | O | 371 | ALA | 5.1 |
| 6 | F | 368 | THR | 5.0 |
| 4 | l | 1374 | THR | 5.0 |
| 7 | g | 1371 | ALA | 4.9 |
| 8 | P | 235 | HIS | 4.9 |
| 3 | K | 257 | SER | 4.9 |
| 7 | O | 372 | LYS | 4.8 |
| 6 | f | 1466 | PRO | 4.8 |
| 5 | M | 169 | SER | 4.8 |
| 1 | I | 186 | ALA | 4.8 |
| 1 | A | 15 | LEU | 4.7 |
| 4 | D | 364 | THR | 4.7 |
| 4 | L | 298 | ASN | 4.7 |
| 7 | O | 529 | SER | 4.7 |
| 4 | D | 374 | THR | 4.7 |
| 6 | n | 1372 | ASP | 4.7 |
| 3 | C | 484 | ILE | 4.6 |
| 8 | p | 1379 | SER | 4.6 |
| 7 | g | 1370 | GLN | 4.5 |
| 5 | e | 1509 | ASN | 4.5 |
| 7 | G | 369 | PRO | 4.5 |
| 5 | e | 1166 | ASP | 4.5 |
| 7 | O | 228 | GLY | 4.5 |
| 4 | d | 1298 | ASN | 4.5 |
| 8 | P | 138 | THR | 4.4 |
| 6 | N | 544 | THR | 4.4 |
| 5 | M | 164 | THR | 4.4 |
| 6 | F | 540 | THR | 4.4 |
| 3 | C | 483 | GLY | 4.3 |
| 2 | j | 1294 | PRO | 4.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | i | 1149 | ASP | 4.3 |
| 1 | a | 1553 | LYS | 4.3 |
| 6 | N | 252 | PHE | 4.3 |
| 3 | c | 1351 | ASN | 4.3 |
| 6 | F | 487 | ARG | 4.2 |
| 4 | L | 364 | THR | 4.2 |
| 6 | n | 1544 | THR | 4.2 |
| 3 | C | 500 | TRP | 4.2 |
| 8 | P | 355 | VAL | 4.2 |
| 8 | p | 1006 | PRO | 4.2 |
| 1 | I | 555 | ASP | 4.2 |
| 5 | E | 381 | TYR | 4.2 |
| 6 | F | 467 | LEU | 4.1 |
| 6 | F | 468 | ASP | 4.1 |
| 5 | M | 398 | SER | 4.1 |
| 5 | m | 1388 | THR | 4.1 |
| 7 | O | 370 | GLN | 4.1 |
| 8 | P | 321 | LEU | 4.1 |
| 8 | h | 1370 | VAL | 4.1 |
| 5 | M | 410 | GLY | 4.0 |
| 4 | l | 1283 | CYS | 4.0 |
| 4 | D | 291 | SER | 4.0 |
| 7 | G | 227 | ALA | 4.0 |
| 8 | P | 300 | VAL | 4.0 |
| 1 | I | 380 | HIS | 4.0 |
| 5 | e | 1290 | SER | 4.0 |
| 8 | P | 336 | CYS | 3.9 |
| 8 | P | 248 | ALA | 3.9 |
| 1 | I | 270 | LEU | 3.9 |
| 1 | I | 557 | HIS | 3.9 |
| 4 | l | 1257 | TYR | 3.9 |
| 6 | F | 466 | PRO | 3.9 |
| 5 | m | 1217 | LYS | 3.9 |
| 8 | P | 268 | HIS | 3.9 |
| 3 | K | 362 | ASP | 3.9 |
| 5 | e | 1291 | SER | 3.8 |
| 4 | L | 283 | CYS | 3.8 |
| 4 | L | 373 | PRO | 3.8 |
| 4 | L | 253 | ILE | 3.8 |
| 4 | L | 291 | SER | 3.8 |
| 5 | e | 1289 | ILE | 3.8 |
| 8 | H | 370 | VAL | 3.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 2 | J | 249 | LYS | 3.8 |
| 8 | P | 257 | ALA | 3.7 |
| 4 | l | 1298 | ASN | 3.7 |
| 6 | F | 225 | PRO | 3.7 |
| 6 | n | 1223 | ASP | 3.7 |
| 4 | L | 219 | ALA | 3.7 |
| 2 | J | 282 | ASN | 3.7 |
| 6 | N | 1 | MET | 3.7 |
| 4 | L | 297 | VAL | 3.7 |
| 3 | C | 485 | ASP | 3.7 |
| 4 | d | 1480 | ASP | 3.7 |
| 4 | L | 284 | ASN | 3.7 |
| 6 | N | 368 | THR | 3.7 |
| 5 | M | 386 | GLY | 3.6 |
| 3 | c | 1336 | ILE | 3.6 |
| 7 | o | 1165 | ALA | 3.6 |
| 1 | a | 1554 | GLU | 3.5 |
| 5 | M | 514 | CYS | 3.5 |
| 5 | m | 1168 | ILE | 3.5 |
| 8 | h | 1249 | VAL | 3.5 |
| 3 | c | 1146 | GLU | 3.5 |
| 6 | N | 539 | SER | 3.5 |
| 8 | P | 267 | LEU | 3.5 |
| 7 | o | 1530 | GLU | 3.5 |
| 3 | c | 1365 | PHE | 3.5 |
| 3 | c | 1370 | ASN | 3.5 |
| 5 | M | 349 | GLN | 3.5 |
| 4 | D | 163 | VAL | 3.5 |
| 1 | I | 264 | ILE | 3.5 |
| 6 | f | 1186 | ALA | 3.5 |
| 7 | O | 263 | HIS | 3.5 |
| 6 | N | 468 | ASP | 3.4 |
| 6 | F | 188 | ASN | 3.4 |
| 4 | L | 293 | LEU | 3.4 |
| 8 | H | 149 | GLU | 3.4 |
| 4 | l | 1162 | ILE | 3.4 |
| 4 | l | 1163 | VAL | 3.4 |
| 4 | L | 363 | VAL | 3.4 |
| 2 | J | 490 | SER | 3.4 |
| 2 | J | 250 | PHE | 3.4 |
| 4 | L | 528 | ARG | 3.4 |
| 4 | l | 1297 | VAL | 3.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 8 | p | 1322 | LYS | 3.4 |
| 3 | K | 359 | MET | 3.4 |
| 1 | I | 16 | GLY | 3.3 |
| 3 | k | 1500 | TRP | 3.3 |
| 8 | h | 1329 | LEU | 3.3 |
| 8 | p | 1455 | ALA | 3.3 |
| 8 | P | 234 | GLY | 3.3 |
| 8 | P | 483 | ASN | 3.3 |
| 8 | p | 1372 | LYS | 3.3 |
| 6 | f | 1222 | PRO | 3.3 |
| 7 | o | 1223 | THR | 3.3 |
| 8 | h | 1258 | ASN | 3.3 |
| 1 | I | 146 | THR | 3.3 |
| 6 | n | 1142 | ASN | 3.3 |
| 4 | D | 222 | SER | 3.3 |
| 6 | N | 365 | THR | 3.3 |
| 5 | e | 1231 | GLY | 3.3 |
| 5 | e | 1386 | GLY | 3.3 |
| 2 | J | 478 | THR | 3.3 |
| 8 | p | 1249 | VAL | 3.3 |
| 5 | m | 1359 | ASN | 3.3 |
| 5 | M | 451 | SER | 3.3 |
| 7 | g | 1016 | GLY | 3.3 |
| 5 | M | 358 | THR | 3.2 |
| 5 | m | 1167 | ASP | 3.2 |
| 4 | L | 312 | VAL | 3.2 |
| 6 | f | 1254 | SER | 3.2 |
| 6 | n | 1187 | ASP | 3.2 |
| 7 | G | 368 | CYS | 3.2 |
| 4 | d | 1188 | ASN | 3.2 |
| 6 | f | 1248 | ASN | 3.2 |
| 7 | O | 227 | ALA | 3.2 |
| 1 | I | 552 | PRO | 3.2 |
| 3 | c | 1260 | ASN | 3.2 |
| 6 | F | 372 | ASP | 3.2 |
| 6 | f | 1223 | ASP | 3.2 |
| 8 | p | 1321 | LEU | 3.2 |
| 1 | I | 338 | VAL | 3.2 |
| 1 | I | 554 | GLU | 3.2 |
| 3 | C | 186 | LEU | 3.2 |
| 3 | c | 1264 | GLU | 3.2 |
| 1 | a | 1557 | HIS | 3.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 8 | p | 1336 | CYS | 3.2 |
| 1 | I | 266 | ASP | 3.2 |
| 1 | I | 15 | LEU | 3.2 |
| 8 | p | 1378 | ILE | 3.2 |
| 7 | g | 1167 | SER | 3.1 |
| 2 | b | 1282 | ASN | 3.1 |
| 2 | j | 1419 | ALA | 3.1 |
| 7 | o | 1166 | MET | 3.1 |
| 4 | D | 298 | ASN | 3.1 |
| 3 | k | 1012 | GLN | 3.1 |
| 1 | a | 1263 | ASN | 3.1 |
| 3 | c | 1269 | TRP | 3.1 |
| 3 | K | 218 | ARG | 3.1 |
| 3 | c | 1369 | ASP | 3.1 |
| 8 | h | 1155 | ASP | 3.1 |
| 8 | h | 1330 | ARG | 3.1 |
| 2 | J | 303 | ILE | 3.1 |
| 1 | I | 553 | LYS | 3.1 |
| 2 | b | 1283 | THR | 3.1 |
| 5 | M | 166 | ASP | 3.0 |
| 8 | p | 1300 | VAL | 3.0 |
| 3 | c | 1265 | LYS | 3.0 |
| 4 | L | 311 | MET | 3.0 |
| 2 | J | 252 | VAL | 3.0 |
| 4 | l | 1219 | ALA | 3.0 |
| 7 | O | 264 | VAL | 3.0 |
| 6 | N | 355 | TYR | 3.0 |
| 6 | F | 227 | ARG | 3.0 |
| 3 | C | 145 | VAL | 3.0 |
| 3 | K | 331 | VAL | 3.0 |
| 4 | l | 1296 | ALA | 3.0 |
| 5 | E | 218 | ASP | 3.0 |
| 1 | I | 185 | LEU | 3.0 |
| 7 | g | 1166 | MET | 3.0 |
| 8 | h | 1372 | LYS | 3.0 |
| 6 | f | 1187 | ASP | 3.0 |
| 7 | o | 1017 | THR | 3.0 |
| 8 | h | 1227 | VAL | 3.0 |
| 8 | H | 450 | LYS | 3.0 |
| 4 | l | 1007 | SER | 3.0 |
| 6 | f | 1461 | ASN | 3.0 |
| 8 | P | 275 | ASP | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 7 | g | 1252 | ALA | 2.9 |
| 5 | E | 362 | ILE | 2.9 |
| 1 | a | 1226 | CYS | 2.9 |
| 3 | K | 223 | VAL | 2.9 |
| 4 | d | 1255 | ASN | 2.9 |
| 8 | P | 269 | ASN | 2.9 |
| 3 | k | 1384 | GLY | 2.9 |
| 1 | A | 146 | THR | 2.9 |
| 3 | k | 1184 | LYS | 2.9 |
| 6 | n | 1465 | ASP | 2.9 |
| 7 | o | 1220 | PHE | 2.9 |
| 8 | p | 1236 | VAL | 2.9 |
| 7 | g | 1223 | THR | 2.9 |
| 8 | P | 330 | ARG | 2.9 |
| 8 | h | 1150 | ILE | 2.9 |
| 6 | f | 1372 | ASP | 2.9 |
| 3 | C | 41 | PRO | 2.8 |
| 8 | h | 1490 | VAL | 2.8 |
| 5 | E | 357 | SER | 2.8 |
| 5 | M | 512 | VAL | 2.8 |
| 8 | H | 235 | HIS | 2.8 |
| 1 | i | 1317 | GLY | 2.8 |
| 6 | F | 346 | GLN | 2.8 |
| 6 | F | 541 | LEU | 2.8 |
| 5 | E | 295 | TYR | 2.8 |
| 7 | G | 337 | THR | 2.8 |
| 6 | F | 226 | THR | 2.8 |
| 4 | L | 348 | ASP | 2.8 |
| 5 | e | 1288 | ASP | 2.8 |
| 2 | J | 398 | THR | 2.8 |
| 3 | k | 1243 | VAL | 2.8 |
| 1 | I | 340 | SER | 2.8 |
| 7 | o | 1480 | GLY | 2.8 |
| 2 | J | 400 | THR | 2.8 |
| 5 | m | 1215 | ASP | 2.8 |
| 6 | f | 1001 | MET | 2.8 |
| 2 | b | 1232 | LEU | 2.8 |
| 4 | L | 296 | ALA | 2.8 |
| 5 | m | 1386 | GLY | 2.8 |
| 7 | g | 1165 | ALA | 2.8 |
| 1 | i | 1552 | PRO | 2.8 |
| 1 | i | 1186 | ALA | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 4 | D | 330 | CYS | 2.8 |
| 6 | F | 324 | ASN | 2.8 |
| 8 | h | 1151 | THR | 2.8 |
| 1 | A | 380 | HIS | 2.7 |
| 1 | I | 262 | ILE | 2.7 |
| 7 | O | 306 | PHE | 2.7 |
| 6 | F | 375 | SER | 2.7 |
| 1 | I | 293 | ALA | 2.7 |
| 3 | K | 256 | GLU | 2.7 |
| 8 | H | 298 | CYS | 2.7 |
| 7 | g | 1241 | ILE | 2.7 |
| 4 | D | 284 | ASN | 2.7 |
| 7 | O | 259 | VAL | 2.7 |
| 1 | a | 1555 | ASP | 2.7 |
| 7 | G | 294 | LEU | 2.7 |
| 4 | l | 1291 | SER | 2.7 |
| 6 | F | 544 | THR | 2.7 |
| 1 | A | 14 | PHE | 2.7 |
| 5 | m | 1031 | ILE | 2.7 |
| 8 | h | 1489 | ALA | 2.7 |
| 1 | a | 1551 | PRO | 2.7 |
| 7 | O | 461 | ALA | 2.7 |
| 2 | B | 218 | PHE | 2.7 |
| 2 | B | 51 | SER | 2.7 |
| 6 | n | 1461 | ASN | 2.7 |
| 2 | B | 192 | HIS | 2.7 |
| 8 | P | 296 | VAL | 2.7 |
| 7 | g | 1355 | MET | 2.6 |
| 1 | I | 371 | CYS | 2.6 |
| 5 | M | 520 | ASN | 2.6 |
| 3 | k | 1185 | ASP | 2.6 |
| 4 | l | 1367 | ARG | 2.6 |
| 4 | l | 1437 | ALA | 2.6 |
| 8 | p | 1368 | VAL | 2.6 |
| 3 | K | 159 | ILE | 2.6 |
| 8 | h | 1373 | GLN | 2.6 |
| 5 | e | 1230 | VAL | 2.6 |
| 5 | m | 1323 | CYS | 2.6 |
| 3 | K | 16 | THR | 2.6 |
| 4 | l | 1251 | ASN | 2.6 |
| 3 | k | 1144 | ASP | 2.6 |
| 5 | e | 1264 | SER | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 5 | e | 1398 | SER | 2.6 |
| 6 | n | 1324 | ASN | 2.6 |
| 4 | d | 1481 | GLY | 2.6 |
| 6 | N | 383 | SER | 2.6 |
| 5 | M | 67 | PRO | 2.6 |
| 8 | P | 320 | VAL | 2.6 |
| 8 | p | 1428 | ILE | 2.6 |
| 5 | M | 403 | THR | 2.6 |
| 3 | K | 25 | ILE | 2.6 |
| 5 | M | 170 | ALA | 2.6 |
| 6 | f | 1249 | SER | 2.6 |
| 8 | p | 1369 | THR | 2.6 |
| 8 | P | 427 | GLU | 2.6 |
| 8 | h | 1389 | ALA | 2.6 |
| 1 | i | 1342 | SER | 2.6 |
| 6 | f | 1431 | MET | 2.5 |
| 5 | e | 1232 | GLY | 2.5 |
| 4 | l | 1370 | ASN | 2.5 |
| 6 | n | 1346 | GLN | 2.5 |
| 8 | h | 1226 | MET | 2.5 |
| 8 | P | 369 | THR | 2.5 |
| 1 | a | 1346 | GLY | 2.5 |
| 4 | D | 370 | ASN | 2.5 |
| 5 | M | 559 | LYS | 2.5 |
| 6 | n | 1295 | ILE | 2.5 |
| 3 | K | 363 | GLU | 2.5 |
| 3 | c | 1331 | VAL | 2.5 |
| 8 | p | 1373 | GLN | 2.5 |
| 6 | F | 465 | ASP | 2.5 |
| 3 | c | 1350 | THR | 2.5 |
| 7 | o | 1380 | GLY | 2.5 |
| 3 | C | 144 | ASP | 2.5 |
| 8 | p | 1250 | PHE | 2.5 |
| 2 | J | 251 | LYS | 2.5 |
| 6 | N | 467 | LEU | 2.5 |
| 3 | K | 207 | GLU | 2.5 |
| 1 | A | 304 | ASP | 2.5 |
| 2 | j | 1190 | LEU | 2.5 |
| 3 | K | 380 | MET | 2.5 |
| 8 | H | 267 | LEU | 2.5 |
| 6 | F | 347 | ILE | 2.5 |
| 1 | a | 1556 | PRO | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 8 | h | 1379 | SER | 2.5 |
| 1 | A | 208 | ALA | 2.5 |
| 7 | G | 432 | ALA | 2.5 |
| 8 | P | 265 | VAL | 2.5 |
| 5 | E | 387 | THR | 2.5 |
| 6 | f | 1540 | THR | 2.5 |
| 8 | P | 382 | SER | 2.5 |
| 8 | H | 215 | GLY | 2.5 |
| 5 | M | 497 | THR | 2.5 |
| 4 | L | 295 | ASP | 2.4 |
| 1 | a | 1261 | GLN | 2.4 |
| 7 | G | 111 | GLU | 2.4 |
| 1 | i | 1239 | GLY | 2.4 |
| 6 | N | 317 | LEU | 2.4 |
| 3 | k | 1483 | GLY | 2.4 |
| 8 | h | 1380 | ARG | 2.4 |
| 8 | p | 1248 | ALA | 2.4 |
| 1 | A | 186 | ALA | 2.4 |
| 8 | P | 25 | ASP | 2.4 |
| 7 | O | 336 | SER | 2.4 |
| 6 | F | 355 | TYR | 2.4 |
| 4 | D | 162 | ILE | 2.4 |
| 6 | N | 465 | ASP | 2.4 |
| 4 | D | 363 | VAL | 2.4 |
| 6 | f | 1227 | ARG | 2.4 |
| 8 | P | 489 | ALA | 2.4 |
| 7 | O | 234 | LYS | 2.4 |
| 1 | i | 1244 | ILE | 2.4 |
| 4 | L | 527 | SER | 2.4 |
| 2 | J | 190 | LEU | 2.4 |
| 7 | o | 1242 | LEU | 2.4 |
| 8 | P | 354 | LEU | 2.4 |
| 1 | a | 1264 | ILE | 2.4 |
| 7 | o | 1325 | ARG | 2.4 |
| 7 | O | 342 | LYS | 2.4 |
| 1 | i | 1369 | ASP | 2.4 |
| 4 | d | 1312 | VAL | 2.4 |
| 5 | E | 173 | ASP | 2.4 |
| 8 | P | 298 | CYS | 2.4 |
| 3 | c | 1263 | ILE | 2.4 |
| 5 | M | 476 | LEU | 2.4 |
| 7 | o | 1481 | VAL | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 6 | F | 486 | THR | 2.4 |
| 1 | A | 187 | VAL | 2.3 |
| 5 | e | 1175 | LEU | 2.3 |
| 1 | I | 265 | ASP | 2.3 |
| 3 | C | 159 | ILE | 2.3 |
| 4 | L | 220 | ILE | 2.3 |
| 7 | O | 241 | ILE | 2.3 |
| 7 | O | 341 | ILE | 2.3 |
| 1 | A | 488 | LYS | 2.3 |
| 5 | E | 217 | LYS | 2.3 |
| 4 | L | 255 | ASN | 2.3 |
| 2 | b | 1198 | ILE | 2.3 |
| 7 | O | 262 | GLU | 2.3 |
| 8 | h | 1149 | GLU | 2.3 |
| 3 | c | 1186 | LEU | 2.3 |
| 4 | d | 1189 | VAL | 2.3 |
| 4 | d | 1253 | ILE | 2.3 |
| 5 | e | 1115 | ILE | 2.3 |
| 8 | P | 301 | ALA | 2.3 |
| 2 | J | 189 | ASN | 2.3 |
| 3 | c | 1248 | CYS | 2.3 |
| 3 | C | 295 | VAL | 2.3 |
| 6 | N | 228 | VAL | 2.3 |
| 8 | h | 1215 | GLY | 2.3 |
| 2 | j | 1371 | GLY | 2.3 |
| 8 | h | 1299 | ILE | 2.3 |
| 2 | J | 325 | VAL | 2.3 |
| 7 | o | 1016 | GLY | 2.3 |
| 8 | H | 389 | ALA | 2.3 |
| 5 | m | 1030 | ILE | 2.3 |
| 1 | A | 381 | SER | 2.3 |
| 3 | k | 1229 | VAL | 2.3 |
| 5 | M | 114 | GLU | 2.3 |
| 5 | M | 513 | ASP | 2.3 |
| 5 | e | 1249 | PHE | 2.3 |
| 6 | F | 221 | HIS | 2.3 |
| 7 | o | 1178 | PHE | 2.3 |
| 1 | a | 1293 | ALA | 2.3 |
| 7 | G | 349 | CYS | 2.3 |
| 6 | F | 366 | TYR | 2.3 |
| 6 | f | 1002 | SER | 2.3 |
| 1 | A | 259 | GLY | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 4 | L | 140 | HIS | 2.3 |
| 4 | d | 1198 | LYS | 2.3 |
| 4 | l | 1213 | VAL | 2.3 |
| 5 | M | 255 | PRO | 2.3 |
| 5 | E | 166 | ASP | 2.3 |
| 8 | h | 1264 | THR | 2.3 |
| 5 | E | 509 | ASN | 2.3 |
| 6 | N | 303 | PRO | 2.3 |
| 7 | o | 1311 | ASN | 2.3 |
| 1 | I | 316 | MET | 2.2 |
| 2 | J | 281 | ILE | 2.2 |
| 6 | n | 1226 | THR | 2.2 |
| 5 | M | 264 | SER | 2.2 |
| 6 | n | 1225 | PRO | 2.2 |
| 8 | H | 249 | VAL | 2.2 |
| 8 | p | 1370 | VAL | 2.2 |
| 2 | J | 248 | THR | 2.2 |
| 7 | o | 1370 | GLN | 2.2 |
| 3 | K | 158 | SER | 2.2 |
| 5 | e | 1214 | LYS | 2.2 |
| 7 | g | 1230 | GLU | 2.2 |
| 8 | P | 319 | LEU | 2.2 |
| 2 | b | 1248 | THR | 2.2 |
| 6 | n | 1213 | LEU | 2.2 |
| 7 | O | 335 | GLN | 2.2 |
| 4 | D | 373 | PRO | 2.2 |
| 2 | J | 280 | GLY | 2.2 |
| 1 | i | 1557 | HIS | 2.2 |
| 4 | L | 443 | PHE | 2.2 |
| 2 | J | 277 | SER | 2.2 |
| 4 | d | 1162 | ILE | 2.2 |
| 1 | I | 90 | GLN | 2.2 |
| 5 | E | 379 | ARG | 2.2 |
| 7 | G | 526 | ASN | 2.2 |
| 5 | M | 353 | HIS | 2.2 |
| 8 | h | 1280 | GLU | 2.2 |
| 8 | h | 1382 | SER | 2.2 |
| 6 | f | 1296 | ILE | 2.2 |
| 1 | I | 93 | GLU | 2.2 |
| 3 | K | 328 | ILE | 2.2 |
| 2 | B | 209 | ASP | 2.2 |
| 2 | B | 469 | THR | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 2 | b | 1478 | THR | 2.2 |
| 2 | b | 1249 | LYS | 2.2 |
| 4 | l | 1392 | ARG | 2.2 |
| 5 | E | 167 | ASP | 2.2 |
| 5 | M | 261 | LYS | 2.2 |
| 6 | F | 383 | SER | 2.2 |
| 5 | m | 1164 | THR | 2.2 |
| 7 | O | 346 | LEU | 2.2 |
| 4 | l | 1431 | SER | 2.2 |
| 4 | l | 1373 | PRO | 2.2 |
| 8 | p | 1483 | ASN | 2.2 |
| 3 | K | 12 | GLN | 2.2 |
| 5 | E | 252 | PRO | 2.1 |
| 2 | j | 1254 | SER | 2.1 |
| 5 | e | 1220 | ASP | 2.1 |
| 7 | O | 243 | SER | 2.1 |
| 7 | g | 1262 | GLU | 2.1 |
| 7 | o | 1241 | ILE | 2.1 |
| 3 | K | 436 | GLY | 2.1 |
| 6 | f | 1142 | ASN | 2.1 |
| 7 | G | 216 | ASN | 2.1 |
| 7 | O | 178 | PHE | 2.1 |
| 5 | E | 410 | GLY | 2.1 |
| 7 | g | 1097 | GLY | 2.1 |
| 6 | f | 1225 | PRO | 2.1 |
| 8 | p | 1005 | LEU | 2.1 |
| 8 | p | 1230 | ARG | 2.1 |
| 5 | M | 250 | SER | 2.1 |
| 7 | G | 370 | GLN | 2.1 |
| 1 | i | 1185 | LEU | 2.1 |
| 4 | d | 1377 | VAL | 2.1 |
| 8 | P | 247 | VAL | 2.1 |
| 3 | c | 1500 | TRP | 2.1 |
| 8 | p | 1380 | ARG | 2.1 |
| 8 | h | 1475 | LEU | 2.1 |
| 2 | b | 1276 | ILE | 2.1 |
| 2 | j | 1121 | ILE | 2.1 |
| 6 | N | 187 | ASP | 2.1 |
| 8 | p | 1299 | ILE | 2.1 |
| 8 | h | 1341 | LEU | 2.1 |
| 8 | p | 1367 | ARG | 2.1 |
| 8 | H | 240 | SER | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 4 | D | 265 | LYS | 2.1 |
| 8 | P | 233 | GLU | 2.1 |
| 8 | P | 504 | GLU | 2.1 |
| 8 | h | 1321 | LEU | 2.1 |
| 8 | P | 226 | MET | 2.1 |
| 3 | c | 1261 | ILE | 2.1 |
| 4 | d | 1115 | ILE | 2.1 |
| 8 | H | 247 | VAL | 2.1 |
| 8 | P | 113 | VAL | 2.1 |
| 4 | l | 1223 | ALA | 2.1 |
| 4 | d | 1482 | ILE | 2.1 |
| 5 | E | 168 | ILE | 2.1 |
| 6 | N | 295 | ILE | 2.1 |
| 8 | P | 299 | ILE | 2.1 |
| 4 | L | 519 | LEU | 2.1 |
| 4 | d | 1409 | GLY | 2.1 |
| 8 | P | 169 | SER | 2.1 |
| 1 | i | 1147 | SER | 2.1 |
| 7 | o | 1167 | SER | 2.1 |
| 5 | m | 1514 | CYS | 2.1 |
| 8 | P | 242 | ASP | 2.1 |
| 2 | j | 1288 | GLN | 2.1 |
| 1 | i | 1093 | GLU | 2.1 |
| 7 | o | 1461 | ALA | 2.0 |
| 5 | M | 167 | ASP | 2.0 |
| 3 | c | 1244 | VAL | 2.0 |
| 3 | k | 1186 | LEU | 2.0 |
| 7 | o | 1520 | VAL | 2.0 |
| 8 | p | 1302 | GLY | 2.0 |
| 8 | P | 256 | ILE | 2.0 |
| 7 | G | 129 | TYR | 2.0 |
| 8 | h | 1474 | VAL | 2.0 |
| 2 | J | 142 | ASN | 2.0 |
| 4 | D | 168 | SER | 2.0 |
| 1 | A | 518 | LEU | 2.0 |
| 7 | g | 1193 | ASP | 2.0 |
| 8 | P | 372 | LYS | 2.0 |
| 5 | M | 324 | GLN | 2.0 |
| 6 | n | 1375 | SER | 2.0 |
| 5 | M | 352 | GLU | 2.0 |
| 7 | o | 1018 | ASP | 2.0 |
| 1 | I | 169 | ILE | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | A | 185 | LEU | 2.0 |
| 1 | i | 1150 | THR | 2.0 |
| 7 | g | 1381 | GLY | 2.0 |
| 8 | p | 1427 | GLU | 2.0 |
| 5 | e | 1380 | ILE | 2.0 |
| 5 | E | 114 | GLU | 2.0 |
| 1 | I | 226 | CYS | 2.0 |
| 4 | d | 1254 | VAL | 2.0 |
| 6 | F | 345 | PRO | 2.0 |

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 10 | BEF | M | 602 | 4/4 | 0.78 | 0.23 | 152,158,161,170 | 0 |
| 10 | BEF | J | 602 | 4/4 | 0.80 | 0.29 | 235,236,240,246 | 0 |
| 10 | BEF | a | 1602 | 4/4 | 0.85 | 0.24 | 235,239,240,241 | 0 |
| 10 | BEF | E | 602 | 4/4 | 0.87 | 0.44 | 240,241,242,244 | 0 |
| 9 | ADP | l | 1601 | 27/27 | 0.87 | 0.29 | 62,105,189,226 | 0 |
| 9 | ADP | M | 601 | 27/27 | 0.87 | 0.26 | 43,113,256,333 | 0 |
| 10 | BEF | B | 602 | 4/4 | 0.89 | 0.33 | 210,215,215,215 | 0 |
| 10 | BEF | G | 602 | 4/4 | 0.89 | 0.42 | 236,237,238,239 | 0 |
| 9 | ADP | B | 601 | 27/27 | 0.90 | 0.27 | 62,105,202,218 | 0 |
| 9 | ADP | m | 1601 | 27/27 | 0.90 | 0.24 | 13,87,195,273 | 0 |
| 10 | BEF | A | 602 | 4/4 | 0.90 | 0.36 | 246,247,249,251 | 0 |
| 9 | ADP | f | 1601 | 27/27 | 0.90 | 0.28 | 13,50,316,499 | 0 |
| 9 | ADP | L | 601 | 27/27 | 0.90 | 0.24 | 102,157,212,241 | 0 |
| 9 | ADP | A | 601 | 27/27 | 0.90 | 0.35 | 46,110,243,330 | 0 |

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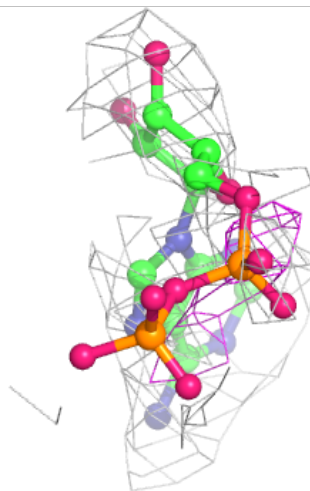
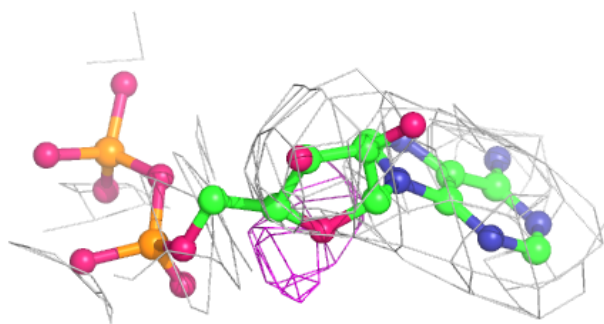
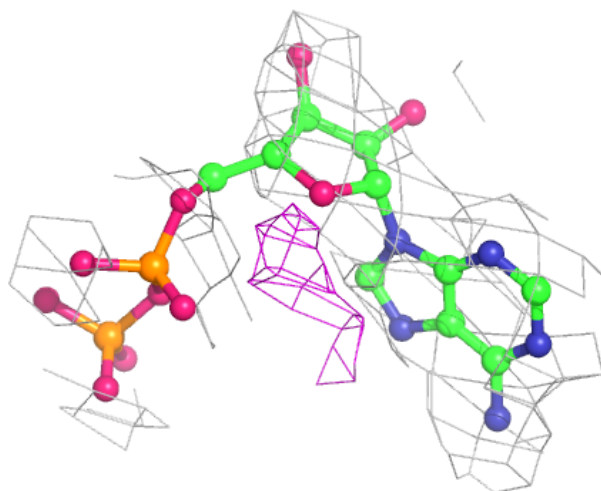
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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 10 | BEF | b | 1602 | 4/4 | 0.91 | 0.19 | 154,158,161,163 | 0 |
| 10 | BEF | C | 1102 | 4/4 | 0.91 | 0.21 | 104,105,105,120 | 0 |
| 9 | ADP | E | 601 | 27/27 | 0.91 | 0.32 | 11,102,242,288 | 0 |
| 9 | ADP | G | 601 | 27/27 | 0.92 | 0.21 | 12,133,240,248 | 0 |
| 9 | ADP | a | 1601 | 27/27 | 0.92 | 0.23 | 50,112,239,328 | 0 |
| 11 | SO4 | j | 1600 | 5/5 | 0.92 | 0.29 | 79,96,98,100 | 0 |
| 9 | ADP | C | 1101 | 27/27 | 0.92 | 0.28 | 38,135,163,237 | 0 |
| 9 | ADP | J | 601 | 27/27 | 0.93 | 0.24 | 74,85,241,279 | 0 |
| 10 | BEF | L | 602 | 4/4 | 0.93 | 0.17 | 172,177,177,180 | 0 |
| 9 | ADP | n | 1601 | 27/27 | 0.93 | 0.26 | 27,94,337,491 | 0 |
| 9 | ADP | e | 1601 | 27/27 | 0.93 | 0.20 | 30,116,232,274 | 0 |
| 9 | ADP | h | 1601 | 27/27 | 0.93 | 0.33 | 40,139,153,188 | 0 |
| 9 | ADP | g | 1601 | 27/27 | 0.94 | 0.19 | 26,159,211,215 | 0 |
| 9 | ADP | p | 1601 | 27/27 | 0.94 | 0.21 | 11,114,136,239 | 0 |
| 9 | ADP | H | 601 | 27/27 | 0.94 | 0.24 | 11,112,145,153 | 0 |
| 9 | ADP | D | 601 | 27/27 | 0.94 | 0.20 | 41,92,238,264 | 0 |
| 10 | BEF | k | 2102 | 4/4 | 0.94 | 0.09 | 68,69,80,82 | 0 |
| 11 | SO4 | I | 600 | 5/5 | 0.94 | 0.28 | 98,103,110,113 | 0 |
| 9 | ADP | P | 601 | 27/27 | 0.94 | 0.24 | 73,153,161,164 | 0 |
| 10 | BEF | N | 602 | 4/4 | 0.95 | 0.31 | 112,120,121,122 | 0 |
| 10 | BEF | f | 1602 | 4/4 | 0.95 | 0.23 | 167,170,171,173 | 0 |
| 11 | SO4 | c | 2101 | 5/5 | 0.95 | 0.28 | 82,98,107,111 | 0 |
| 11 | SO4 | O | 600 | 5/5 | 0.95 | 0.27 | 78,79,92,100 | 0 |
| 9 | ADP | N | 601 | 27/27 | 0.95 | 0.24 | 11,88,232,484 | 0 |
| 10 | BEF | m | 1602 | 4/4 | 0.95 | 0.26 | 185,193,195,196 | 0 |
| 9 | ADP | F | 601 | 27/27 | 0.95 | 0.30 | 11,105,323,481 | 0 |
| 11 | SO4 | o | 1600 | 5/5 | 0.95 | 0.23 | 107,107,115,117 | 0 |
| 11 | SO4 | d | 1600 | 5/5 | 0.95 | 0.28 | 106,109,115,118 | 0 |
| 9 | ADP | b | 1601 | 27/27 | 0.95 | 0.20 | 44,69,220,243 | 0 |
| 9 | ADP | k | 2101 | 27/27 | 0.95 | 0.28 | 80,131,164,321 | 0 |
| 11 | SO4 | i | 1600 | 5/5 | 0.96 | 0.28 | 91,94,103,116 | 0 |
| 10 | BEF | l | 1602 | 4/4 | 0.96 | 0.13 | 28,61,73,75 | 0 |
| 11 | SO4 | K | 1101 | 5/5 | 0.96 | 0.35 | 84,89,97,102 | 0 |
| 10 | BEF | e | 1602 | 4/4 | 0.96 | 0.21 | 201,205,207,207 | 0 |
| 10 | BEF | F | 602 | 4/4 | 0.97 | 0.26 | 157,163,163,171 | 0 |
| 10 | BEF | g | 1602 | 4/4 | 0.97 | 0.18 | 162,165,165,166 | 0 |
| 10 | BEF | D | 602 | 4/4 | 0.97 | 0.11 | 81,84,91,92 | 0 |
| 10 | BEF | n | 1602 | 4/4 | 0.97 | 0.23 | 163,167,167,173 | 0 |
| 10 | BEF | p | 1602 | 4/4 | 0.97 | 0.13 | 84,99,102,108 | 0 |
| 10 | BEF | h | 1602 | 4/4 | 0.98 | 0.15 | 85,93,93,106 | 0 |
| 10 | BEF | P | 602 | 4/4 | 0.99 | 0.12 | 158,158,158,162 | 0 |
| 10 | BEF | H | 602 | 4/4 | 0.99 | 0.12 | 101,103,104,110 | 0 |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

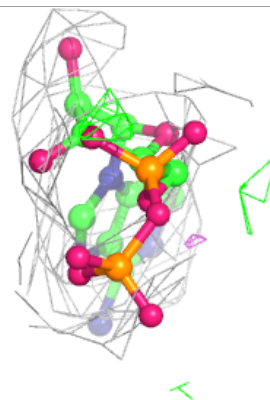
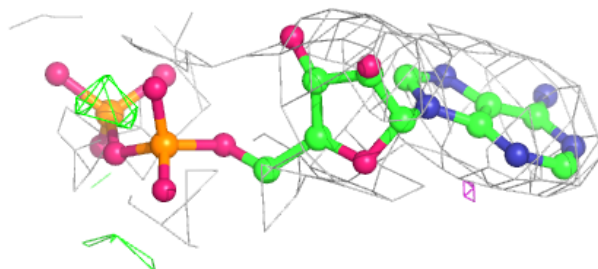
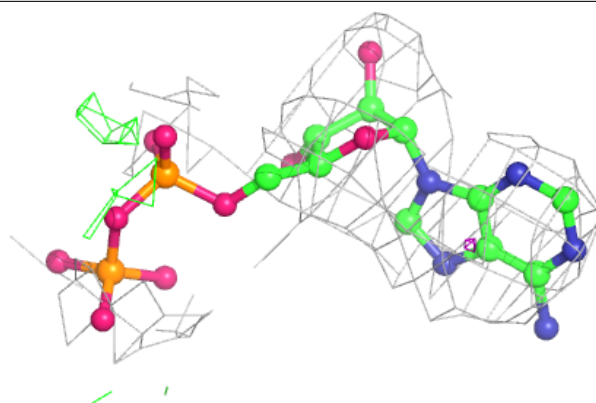
Electron density around ADP 1 1601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

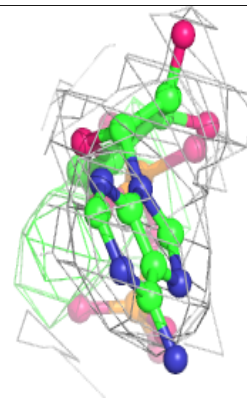
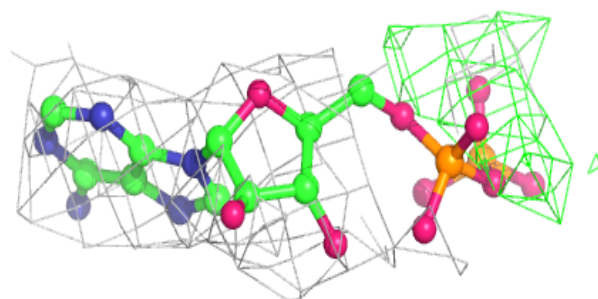
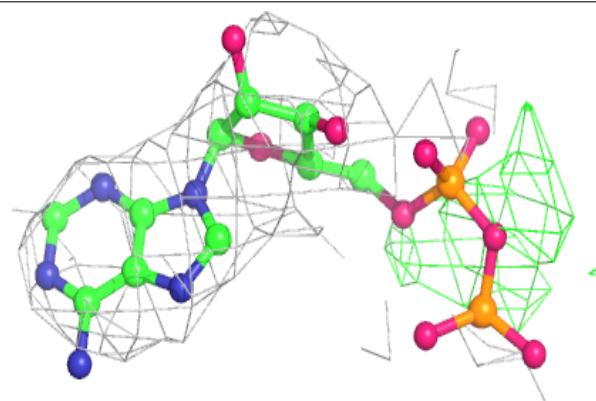


Electron density around ADP M 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

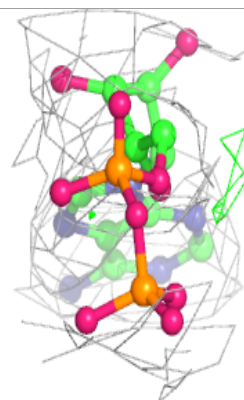
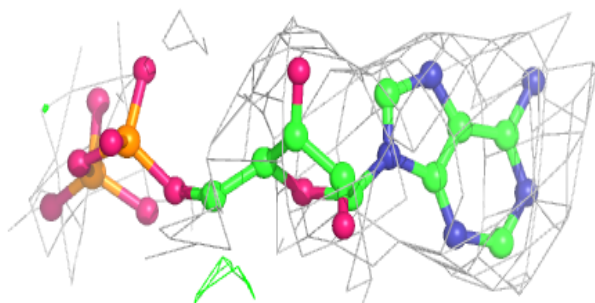
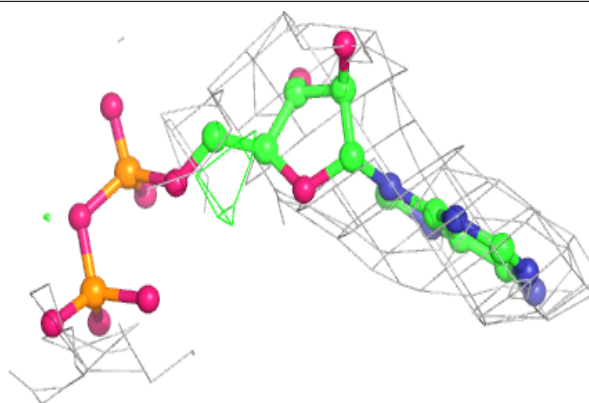
**Electron density around ADP B 601:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

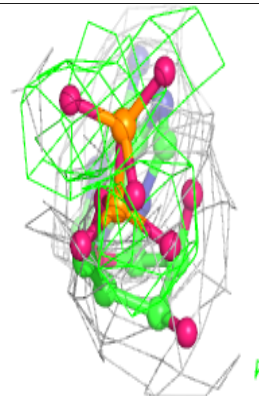
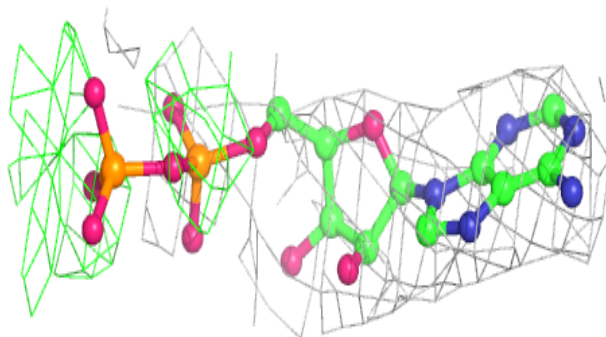
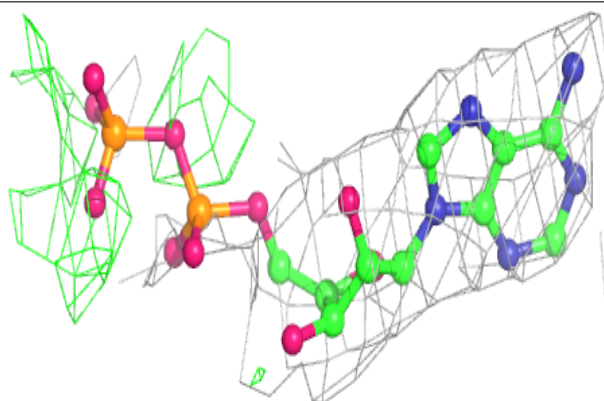


Electron density around ADP m 1601:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

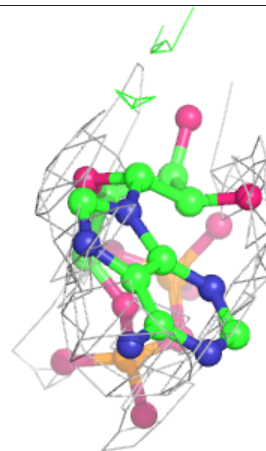
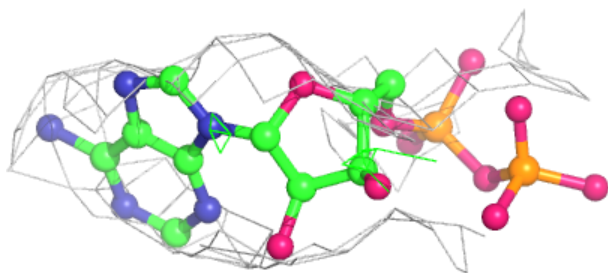
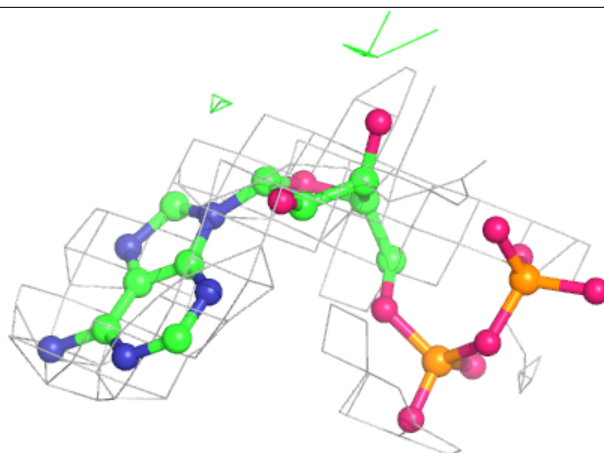
**Electron density around ADP f 1601:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

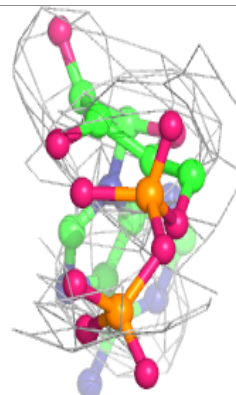
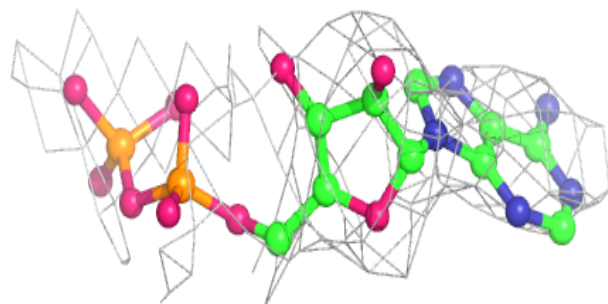
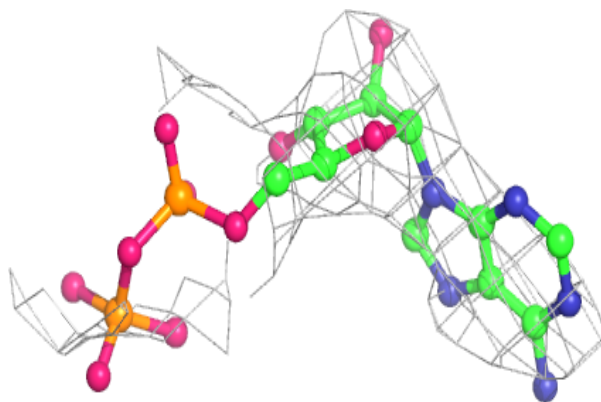


Electron density around ADP L 601:

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and green (positive)

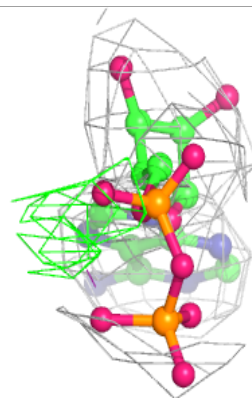
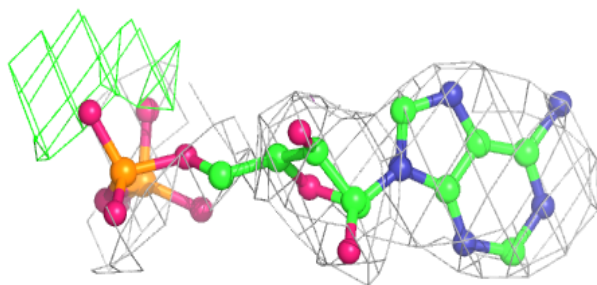
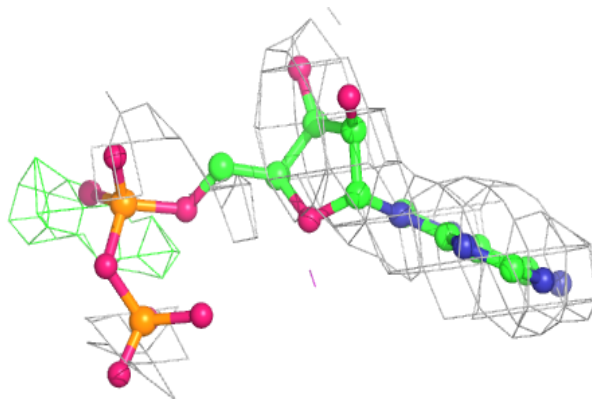
**Electron density around ADP A 601:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

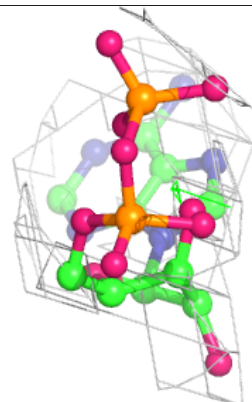
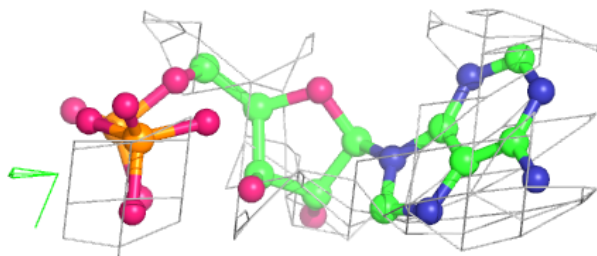
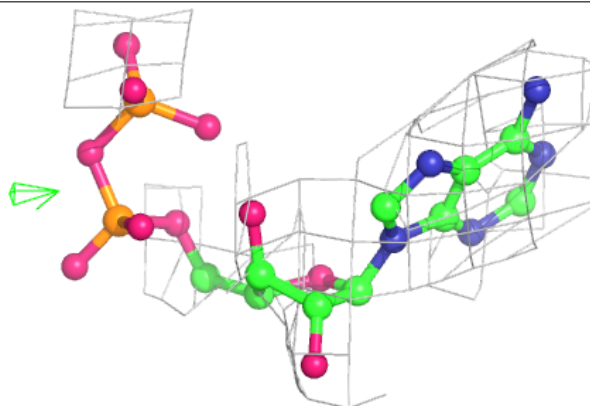


Electron density around ADP E 601:

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and green (positive)

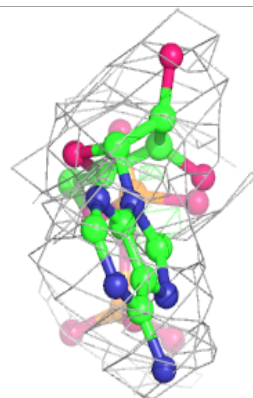
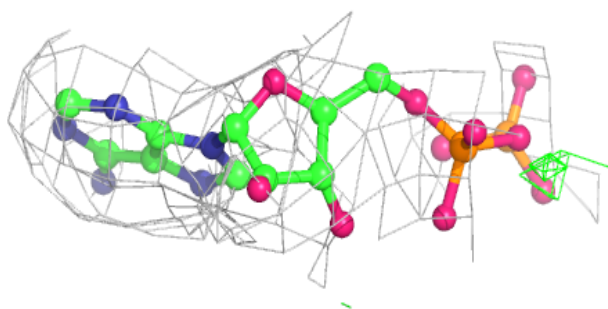
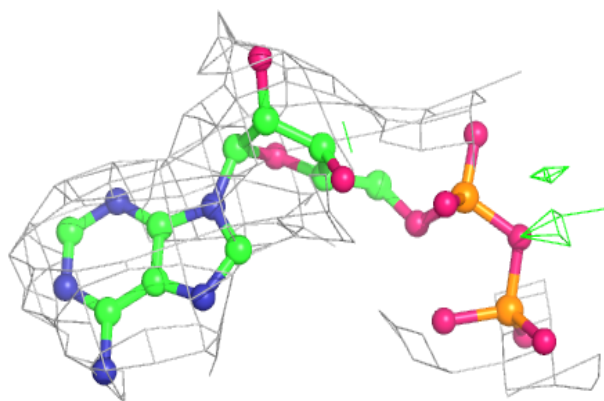
**Electron density around ADP G 601:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

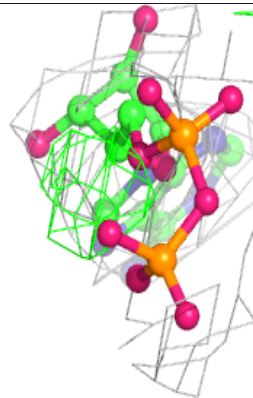
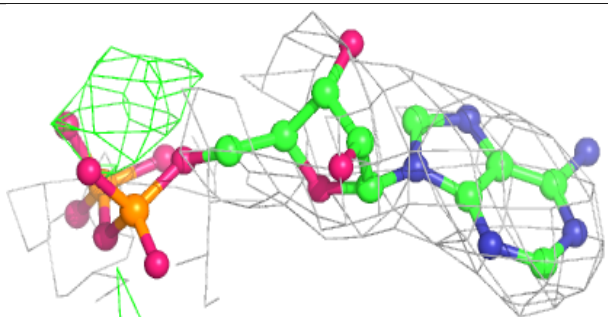
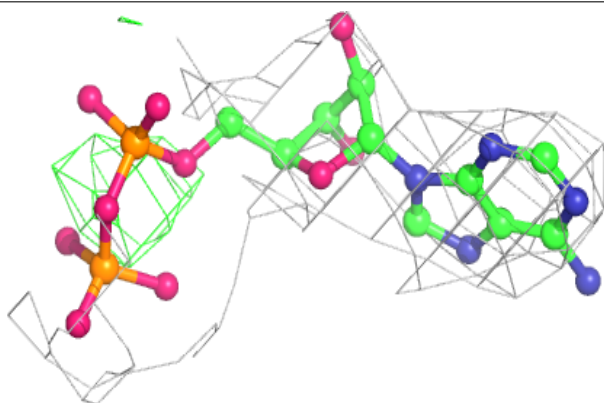


Electron density around ADP a 1601:

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and green (positive)

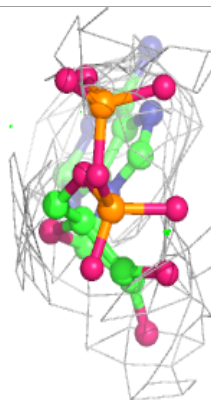
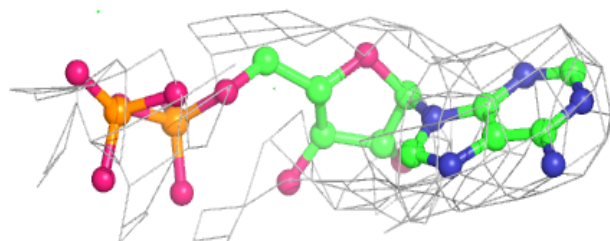
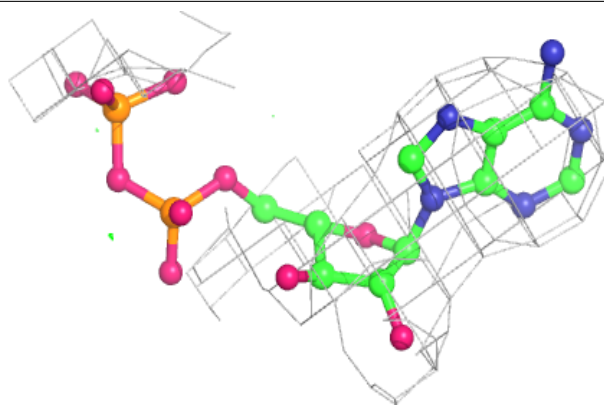
**Electron density around ADP C 1101:**

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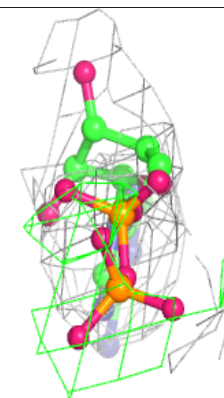
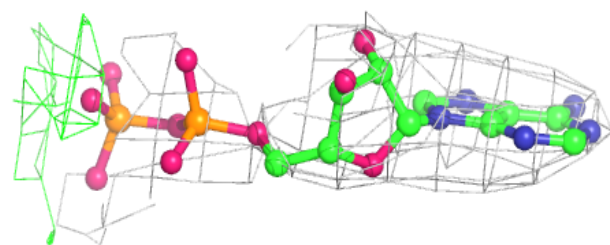
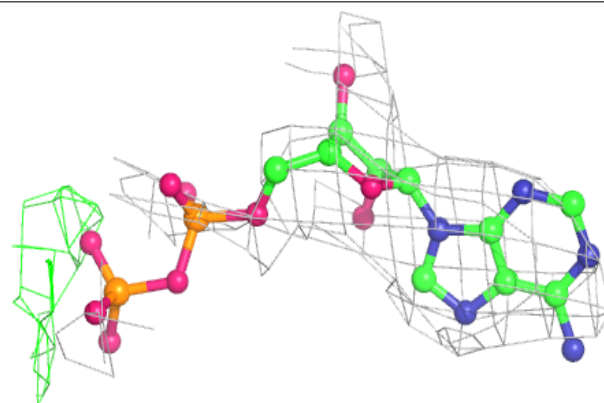


Electron density around ADP J 601:

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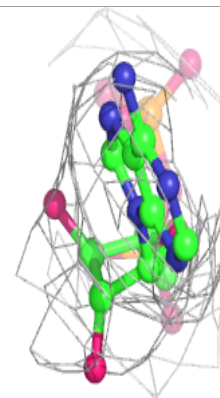
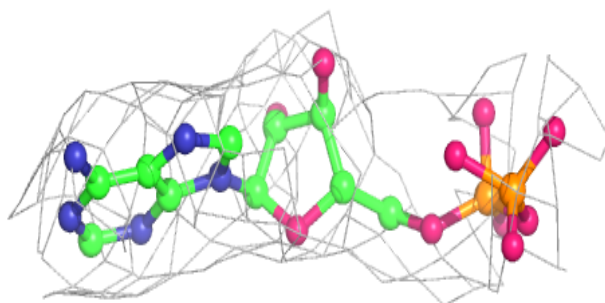
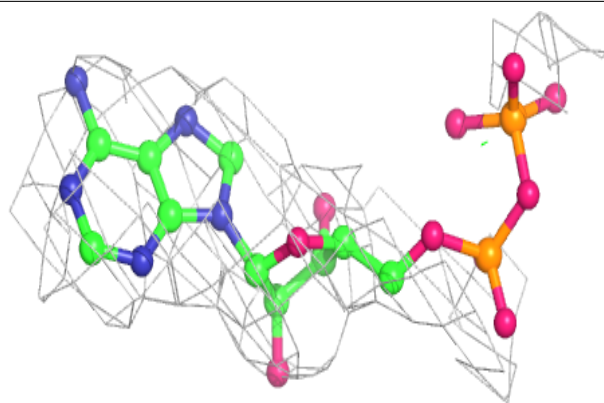
**Electron density around ADP n 1601:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

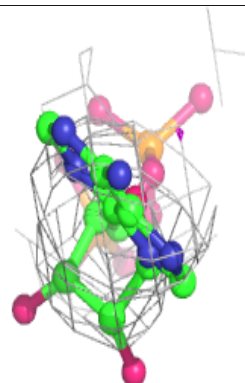
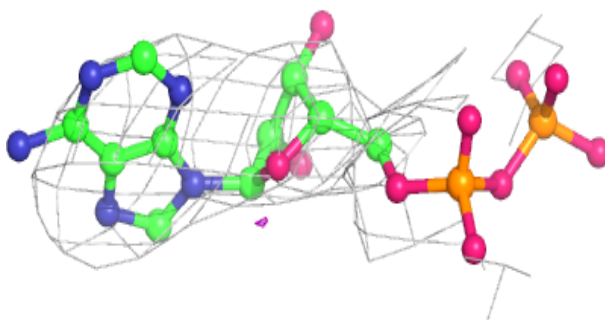
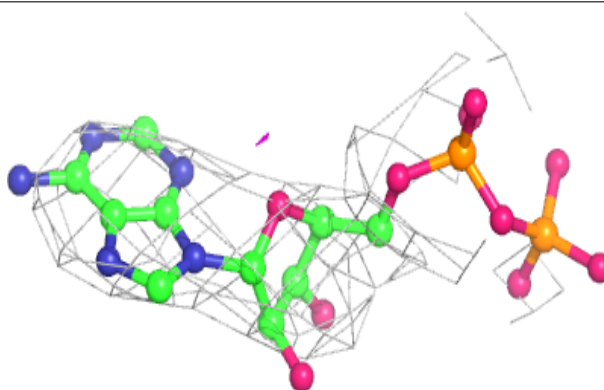


Electron density around ADP e 1601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

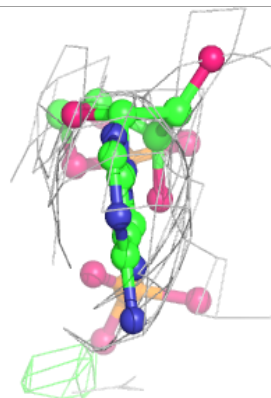
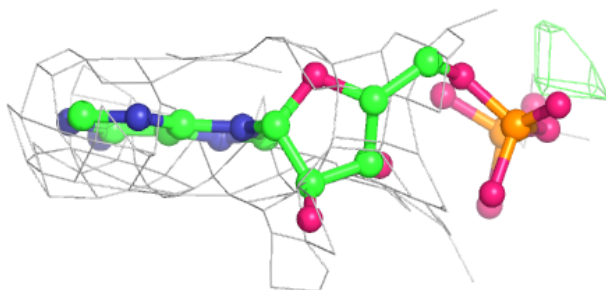
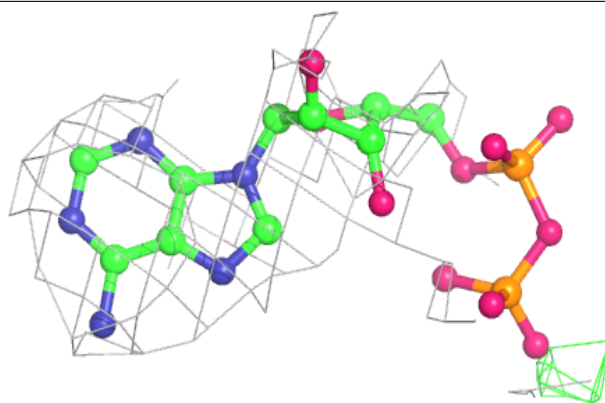
**Electron density around ADP h 1601:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

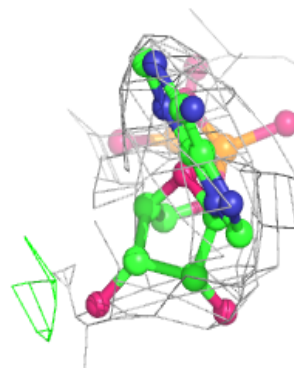
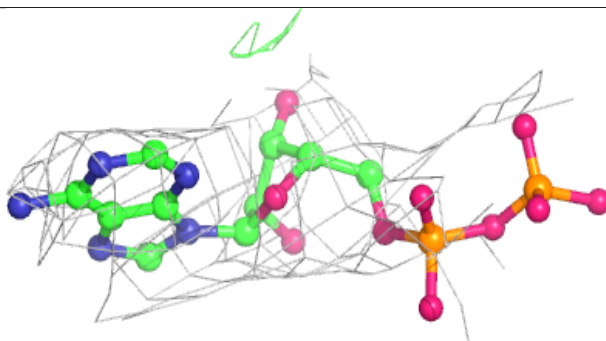
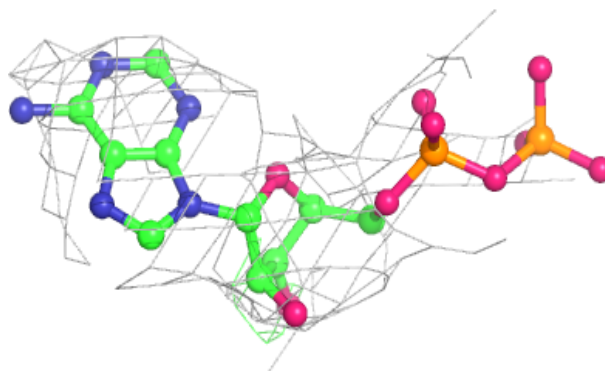


Electron density around ADP g 1601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

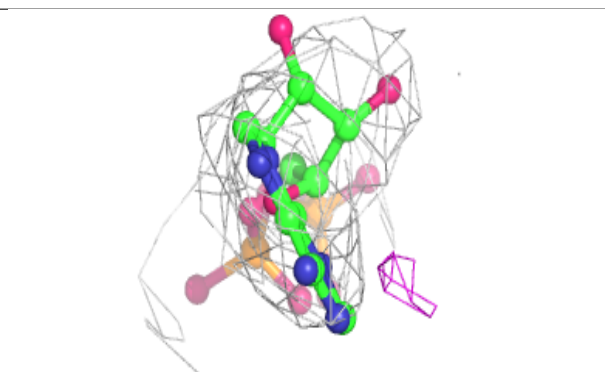
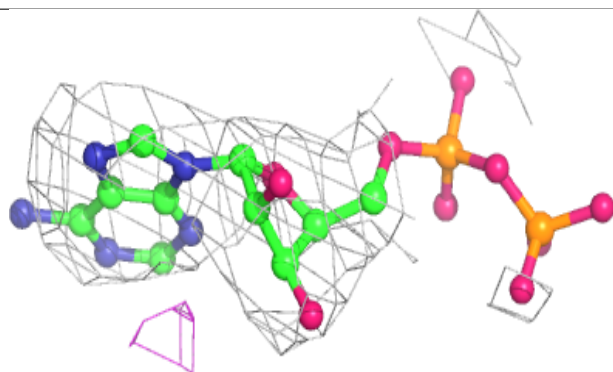
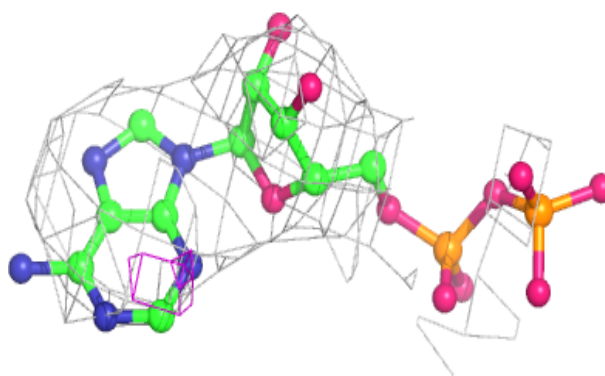
**Electron density around ADP p 1601:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

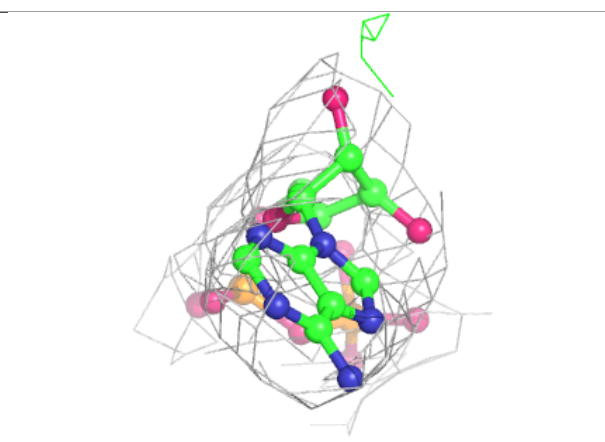
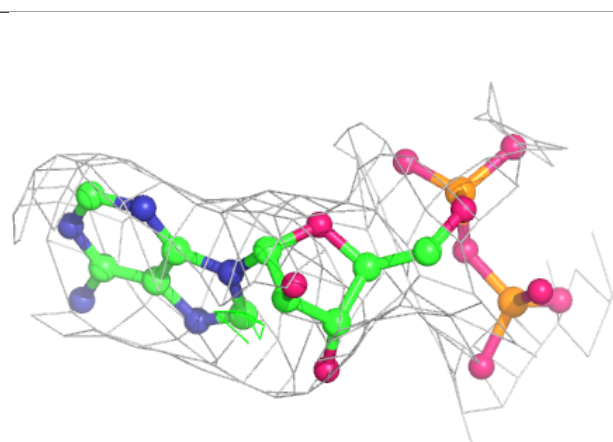
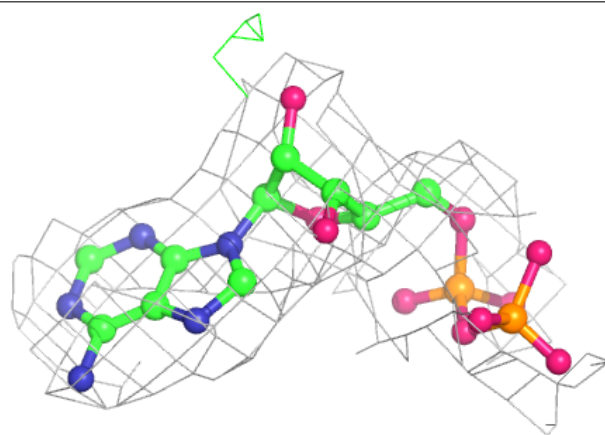


Electron density around ADP H 601:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

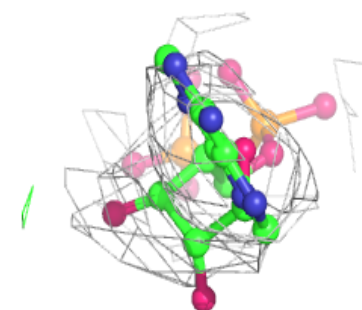
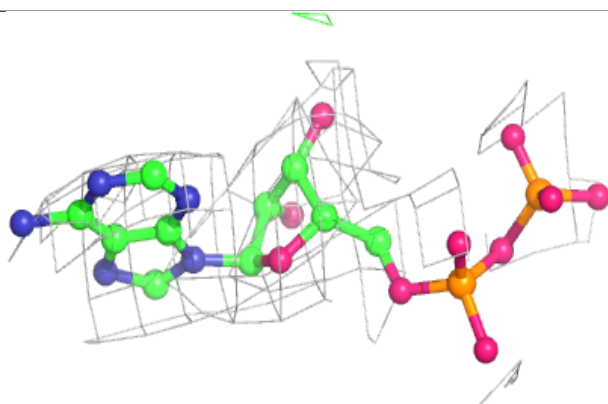
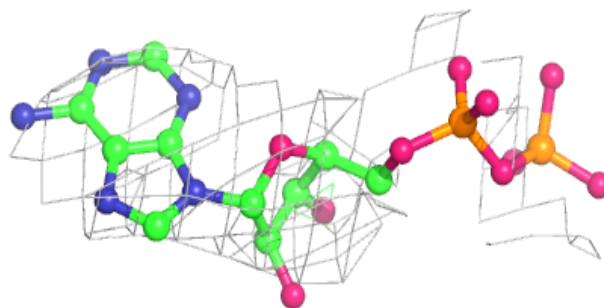
**Electron density around ADP D 601:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

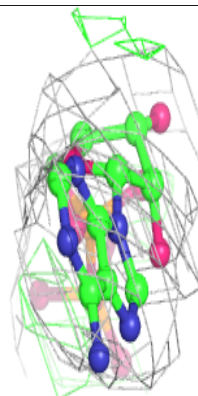
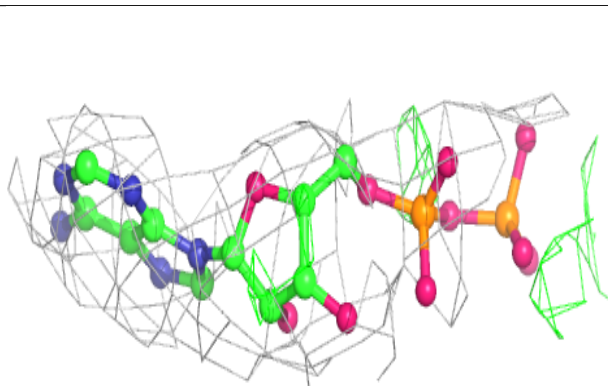
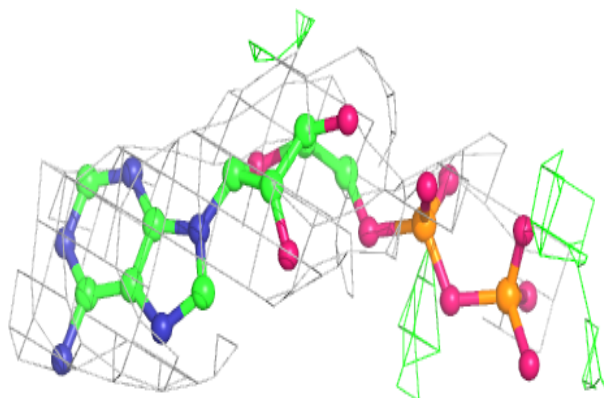


Electron density around ADP P 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

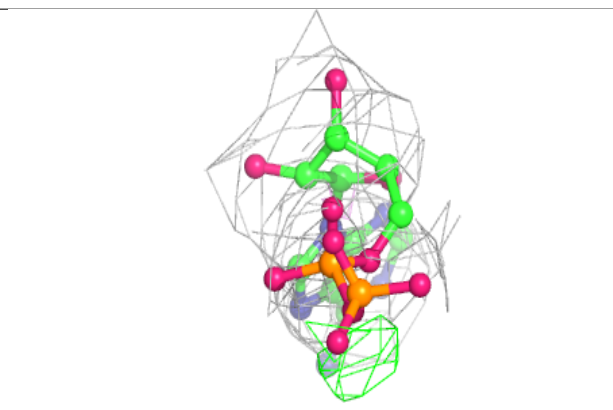
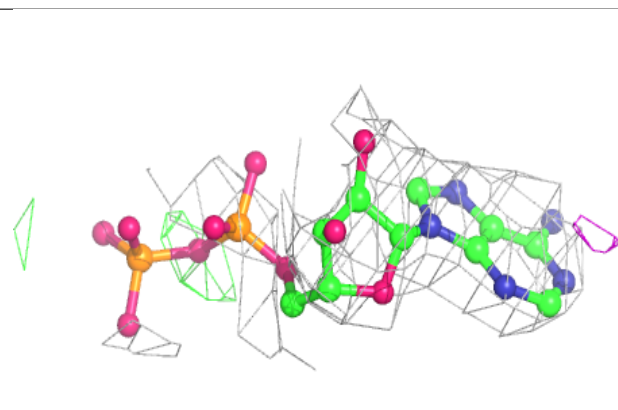
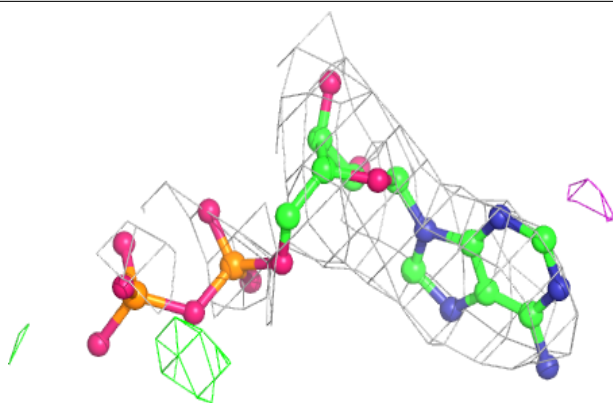
**Electron density around ADP N 601:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

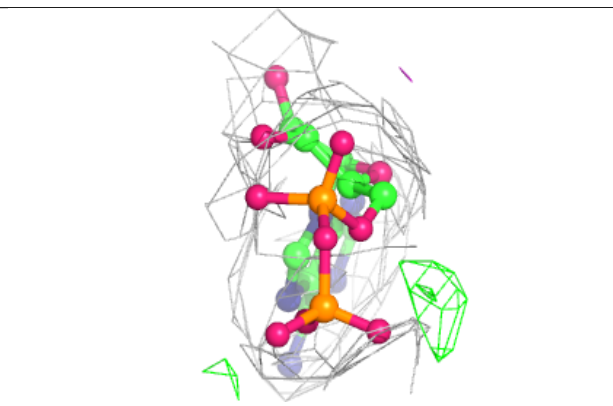
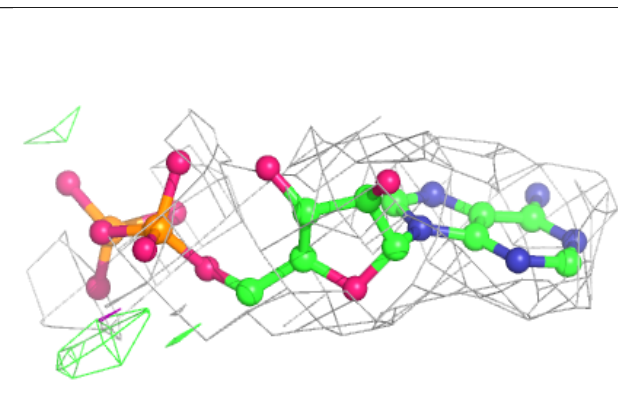
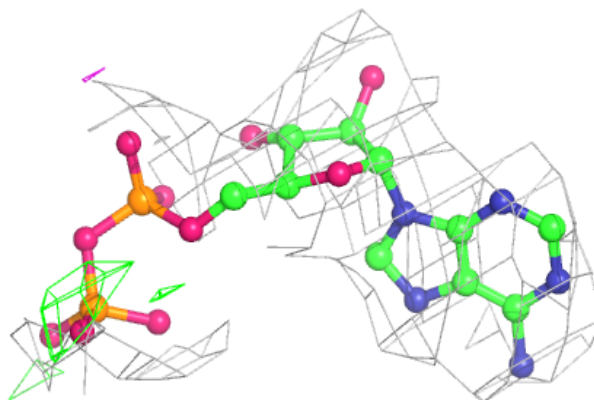


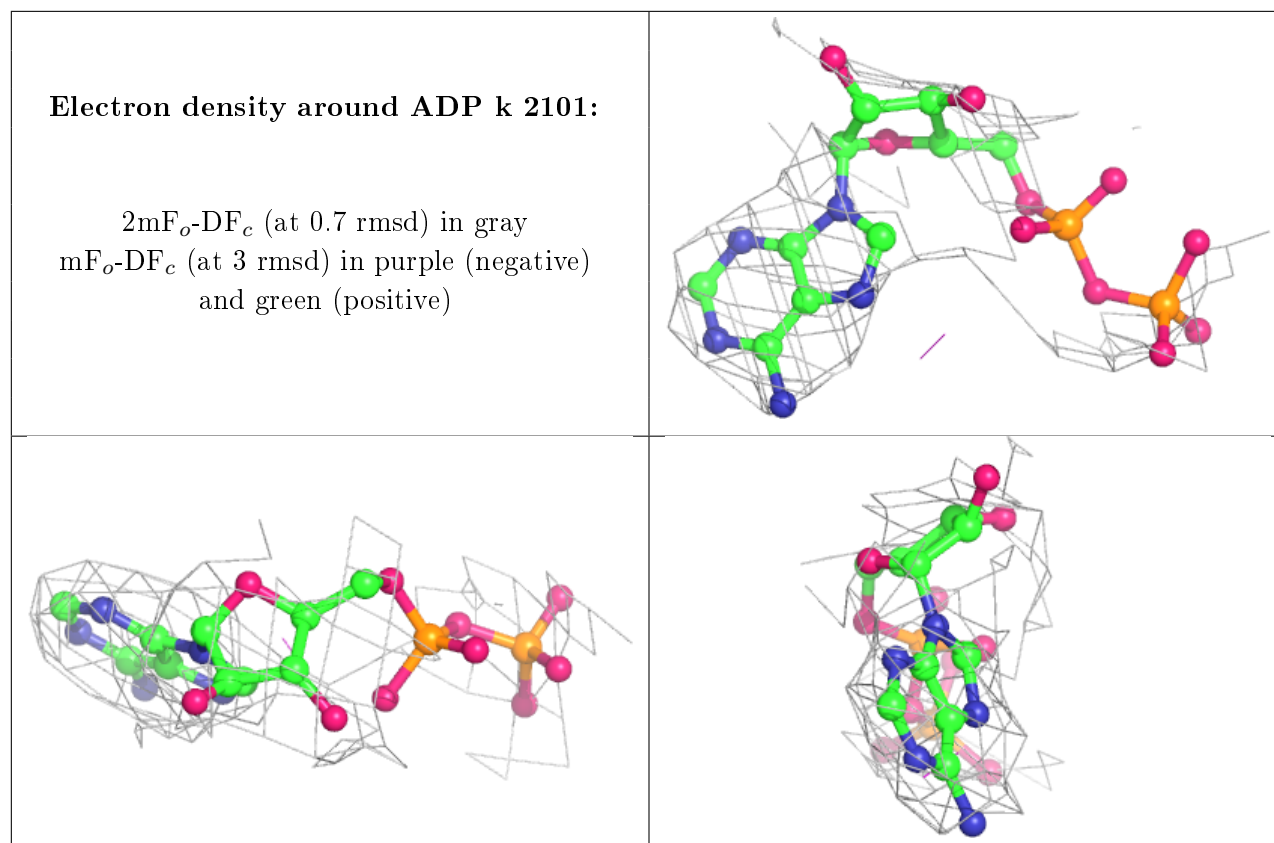
Electron density around ADP F 601:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around ADP b 1601:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.