



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Feb 20, 2018 – 05:58 am GMT

PDB ID : 5G04
EMDB ID: : EMD-3385
Title : Structure of the human APC-Cdc20-Hsl1 complex
Authors : Zhang, S.; Chang, L.; Alfieri, C.; Zhang, Z.; Yang, J.; Maslen, S.; Skehel, M.;
Barford, D.
Deposited on : 2016-03-16
Resolution : 4.00 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

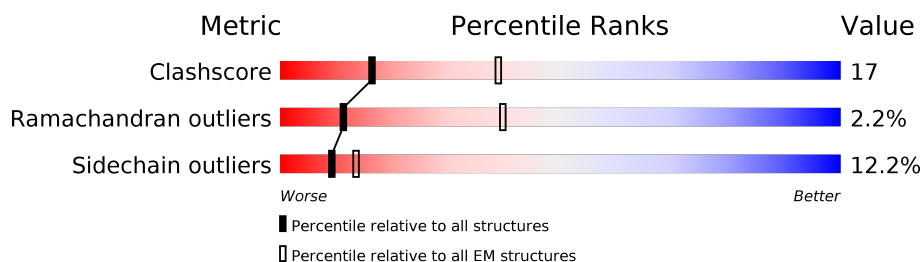
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 Å.

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






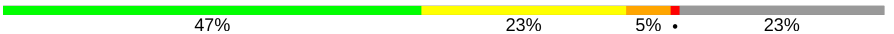


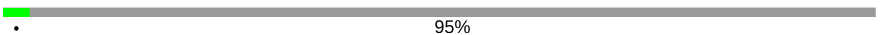


| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore | 136279 | 1886 |
| Ramachandran outliers | 132675 | 1663 |
| Sidechain outliers | 132484 | 1531 |

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|-------------------|
| 1 | A | 1944 | 41% 26% 6% • 26% |
| 2 | B | 84 | 69% 23% 6% • |
| 3 | C | 597 | 44% 34% 10% • 12% |
| 3 | P | 597 | 53% 24% 5% 18% |
| 4 | D | 121 | 26% 17% • 55% |
| 5 | E | 110 | 35% 15% • 49% |
| 6 | F | 824 | 41% 17% • 40% |
| 6 | H | 824 | 41% 16% • 41% |
| 7 | G | 85 | 19% 11% 71% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 7 | W | 85 |  |
| 8 | I | 808 |  |
| 9 | J | 620 |  |
| 9 | K | 620 |  |
| 10 | L | 184 |  |
| 11 | M | 74 |  |
| 12 | N | 822 |  |
| 13 | O | 755 |  |
| 14 | R | 499 |  |
| 15 | S | 206 |  |
| 16 | X | 599 |  |
| 16 | Y | 599 |  |

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 65481 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 1 | A | 1437 | Total | C | N | O | S | 0 | 0 |
| | | | 10925 | 7025 | 1849 | 1977 | 74 | | |

- Molecule 2 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---------|-------|
| 2 | B | 84 | Total | C | N | O | S | 1 | 0 |
| | | | 649 | 416 | 117 | 99 | 17 | | |

- Molecule 3 is a protein called CELL DIVISION CYCLE PROTEIN 23 HOMOLOG.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3 | C | 524 | Total | C | N | O | S | 0 | 0 |
| | | | 4306 | 2774 | 727 | 781 | 24 | | |
| 3 | P | 491 | Total | C | N | O | S | 0 | 0 |
| | | | 4039 | 2608 | 678 | 729 | 24 | | |

- Molecule 4 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 15.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 4 | D | 55 | Total | C | N | O | 0 | 0 |
| | | | 436 | 277 | 73 | 86 | | |

- Molecule 5 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 5 | E | 56 | Total | C | N | O | S | 0 | 0 |
| | | | 450 | 290 | 74 | 85 | 1 | | |

- Molecule 6 is a protein called CELL DIVISION CYCLE PROTEIN 27 HOMOLOG.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 6 | F | 498 | Total | C | N | O | S | 0 | 0 |
| | | | 3923 | 2514 | 664 | 719 | 26 | | |
| 6 | H | 483 | Total | C | N | O | S | 0 | 0 |
| | | | 3853 | 2473 | 650 | 704 | 26 | | |

- Molecule 7 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT CDC26.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 7 | G | 25 | Total | C | N | O | S | 0 | 0 |
| | | | 213 | 133 | 40 | 39 | 1 | | |
| 7 | W | 25 | Total | C | N | O | S | 0 | 0 |
| | | | 213 | 133 | 40 | 39 | 1 | | |

- Molecule 8 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| 8 | I | 730 | Total | C | N | O | S | 0 | 0 |
| | | | 5709 | 3660 | 950 | 1066 | 33 | | |

- Molecule 9 is a protein called CELL DIVISION CYCLE PROTEIN 16 HOMOLOG.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 9 | J | 504 | Total | C | N | O | S | 0 | 0 |
| | | | 4047 | 2601 | 684 | 737 | 25 | | |
| 9 | K | 493 | Total | C | N | O | S | 0 | 0 |
| | | | 3988 | 2563 | 672 | 729 | 24 | | |

- Molecule 10 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10 | L | 182 | Total | C | N | O | S | 0 | 0 |
| | | | 1435 | 898 | 263 | 268 | 6 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| L | ? | - | ARG | deletion | UNP Q9UM13 |

- Molecule 11 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|-------|
| 11 | M | 59 | Total | C | N | O | S | 0 | 0 |
| | | | 493 | 310 | 79 | 102 | 2 | | |

- Molecule 12 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 12 | N | 631 | Total | C | N | O | S | 0 | 0 |
| | | | 4837 | 3067 | 880 | 868 | 22 | | |

- Molecule 13 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 13 | O | 685 | Total | C | N | O | S | 0 | 0 |
| | | | 5395 | 3440 | 940 | 987 | 28 | | |

- Molecule 14 is a protein called CELL DIVISION CYCLE PROTEIN 20 HOMOLOG.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 14 | R | 370 | Total | C | N | O | S | 2 | 0 |
| | | | 2869 | 1801 | 524 | 532 | 12 | | |

- Molecule 15 is a protein called PROBABLE SERINE/THREONINE-PROTEIN KINASE HSL1.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 15 | S | 10 | Total | C | N | O | 0 | 0 |
| | | | 72 | 42 | 14 | 16 | | |

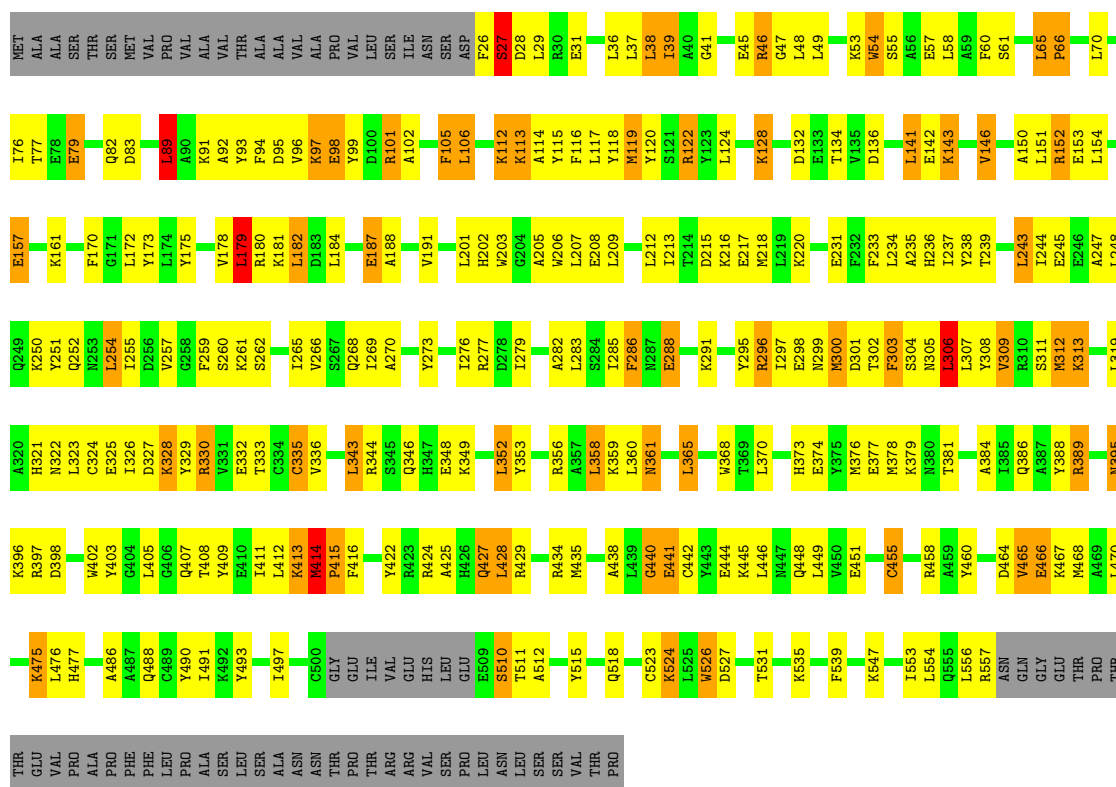
- Molecule 16 is a protein called ANAPHASE-PROMOTING COMPLEX SUBUNIT 7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 16 | X | 484 | Total | C | N | O | S | 0 | 0 |
| | | | 3767 | 2390 | 649 | 704 | 24 | | |
| 16 | Y | 496 | Total | C | N | O | S | 0 | 0 |
| | | | 3859 | 2444 | 666 | 724 | 25 | | |

- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

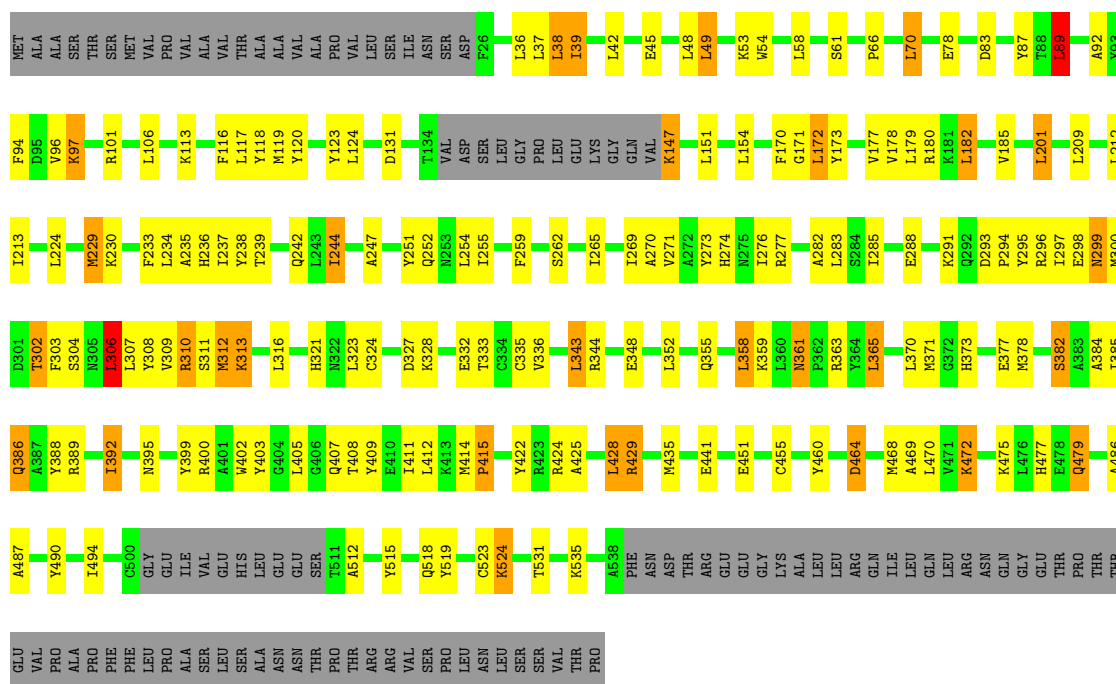
| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 17 | B | 3 | Total | Zn | 0 |
| | | | 3 | 3 | |



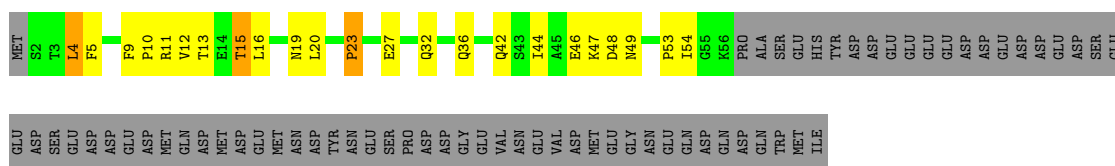
• Molecule 3: CELL DIVISION CYCLE PROTEIN 23 HOMOLOG

Chain P:

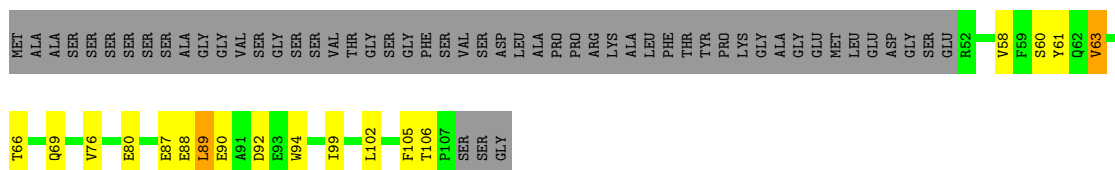
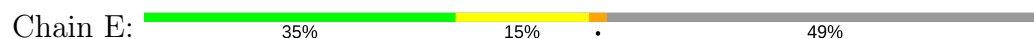


• Molecule 4: ANAPHASE-PROMOTING COMPLEX SUBUNIT 15

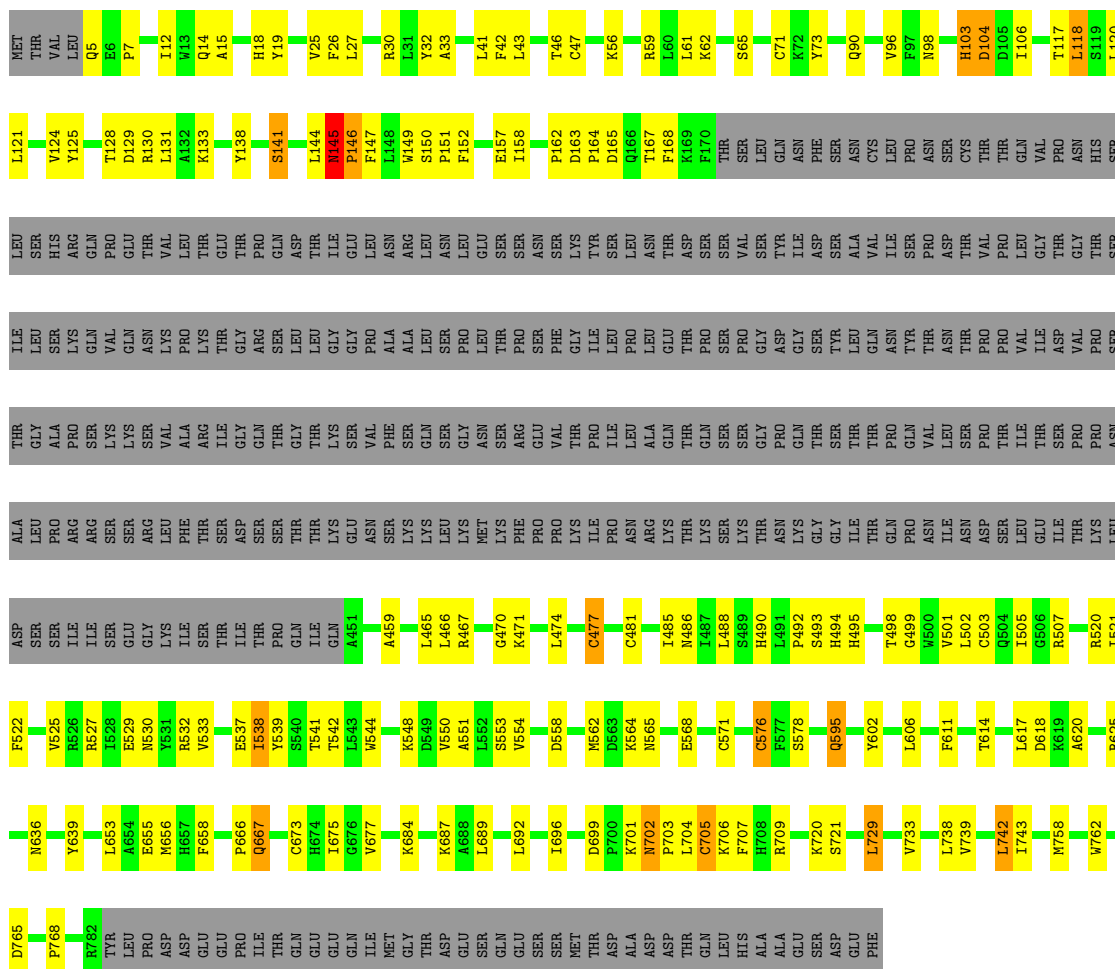
Chain D:



• Molecule 5: ANAPHASE-PROMOTING COMPLEX SUBUNIT 16

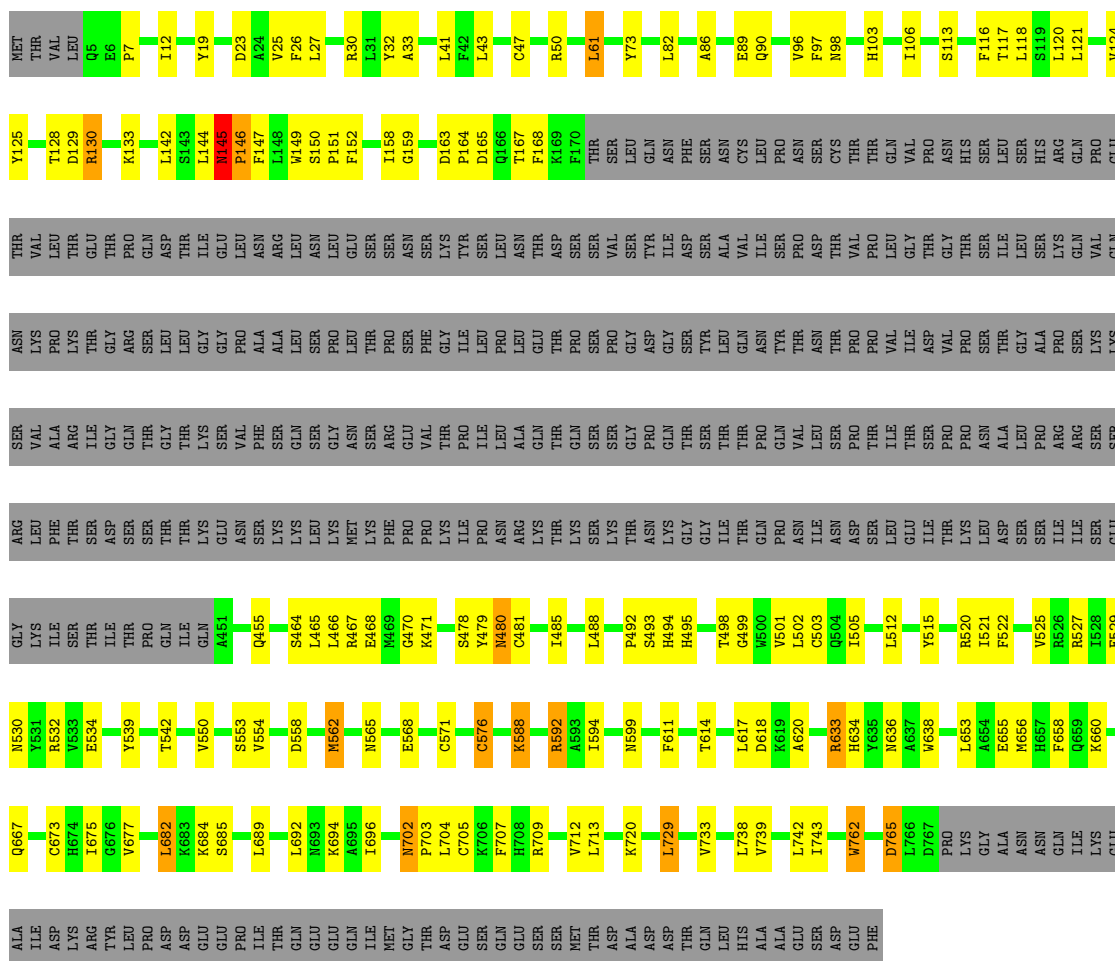


• Molecule 6: CELL DIVISION CYCLE PROTEIN 27 HOMOLOG



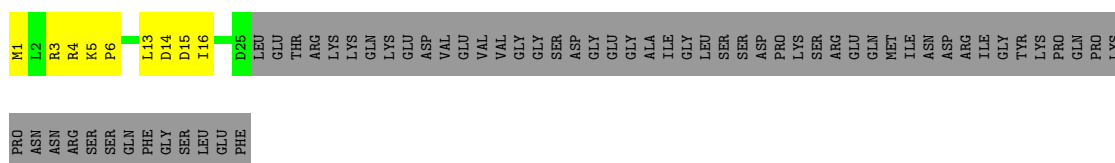
• Molecule 6: CELL DIVISION CYCLE PROTEIN 27 HOMOLOG





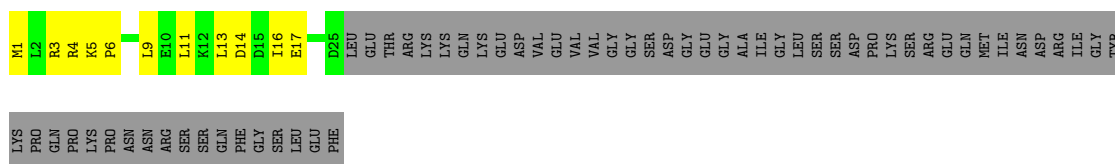
- Molecule 7: ANAPHASE-PROMOTING COMPLEX SUBUNIT CDC26

Chain G: 19% 11% 71%



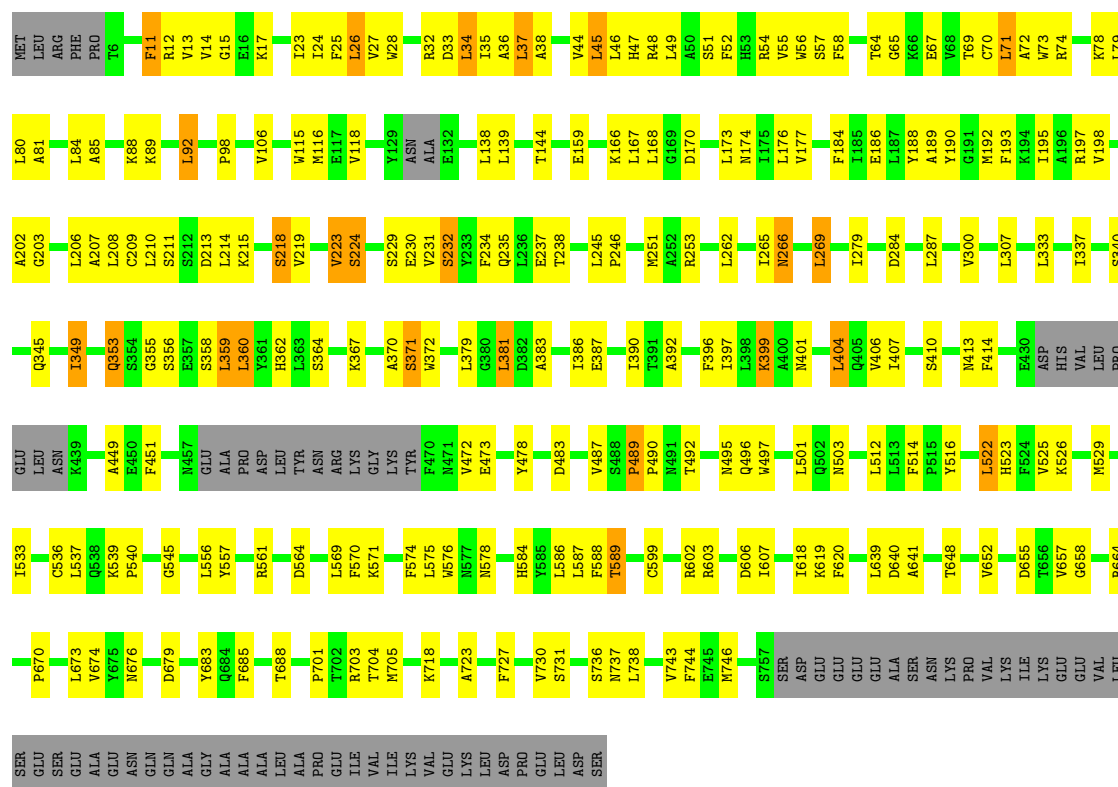
● Molecule 7: ANAPHASE-PROMOTING COMPLEX SUBUNIT CDC26

Chain W:  16% 13% 71%



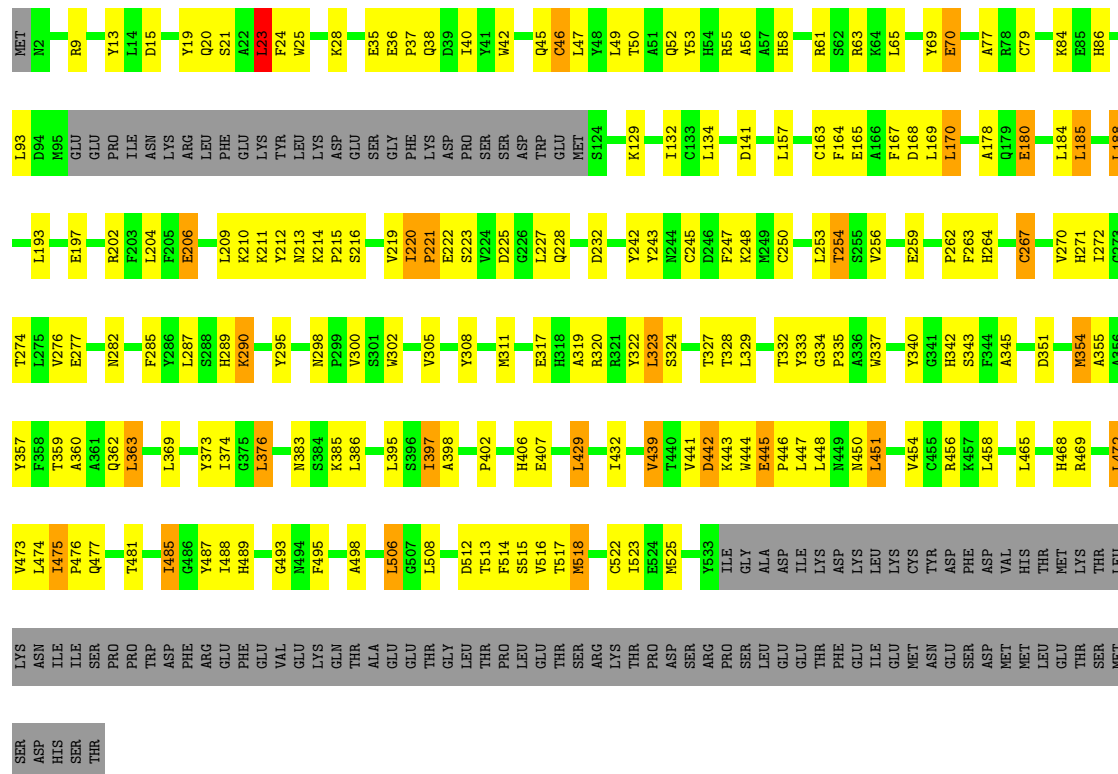
- Molecule 8: ANAPHASE-PROMOTING COMPLEX SUBUNIT 4

Chain I:  62% 26% 10%



• Molecule 9: CELL DIVISION CYCLE PROTEIN 16 HOMOLOG

Chain J: 50% 26% 19%



• Molecule 9: CELL DIVISION CYCLE PROTEIN 16 HOMOLOG

| Frequency | Percentage |
|-----------|------------|
| Daily | 51% |
| Weekly | 24% |
| Monthly | 2% |
| Never | 20% |



| Response | Percentage |
|--|------------|
| U.S. should take action to protect the environment | 59% |
| U.S. should not take action to protect the environment | 36% |
| Don't know | 5% |

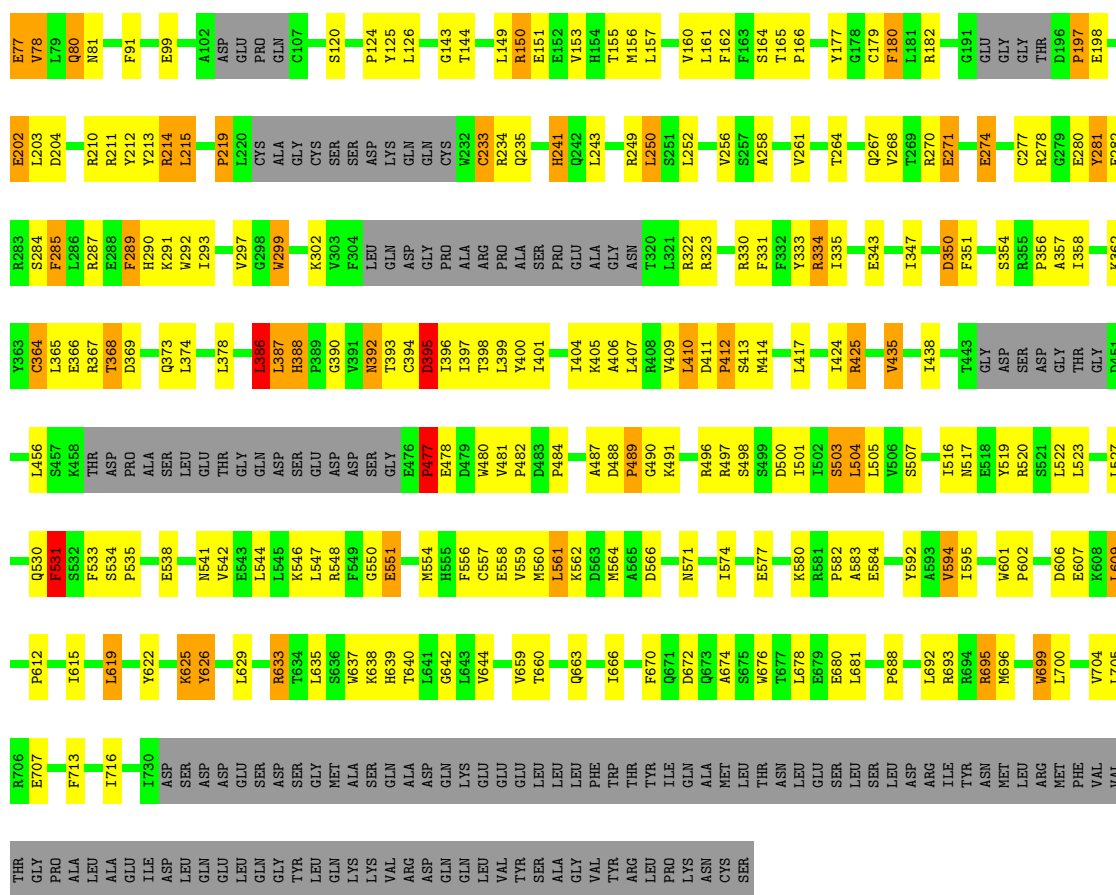


| Frequency | Percentage |
|-----------|------------|
| Daily | 49% |
| Often | 20% |
| Sometimes | 9% |
| Rarely | 20% |
| Never | 2% |



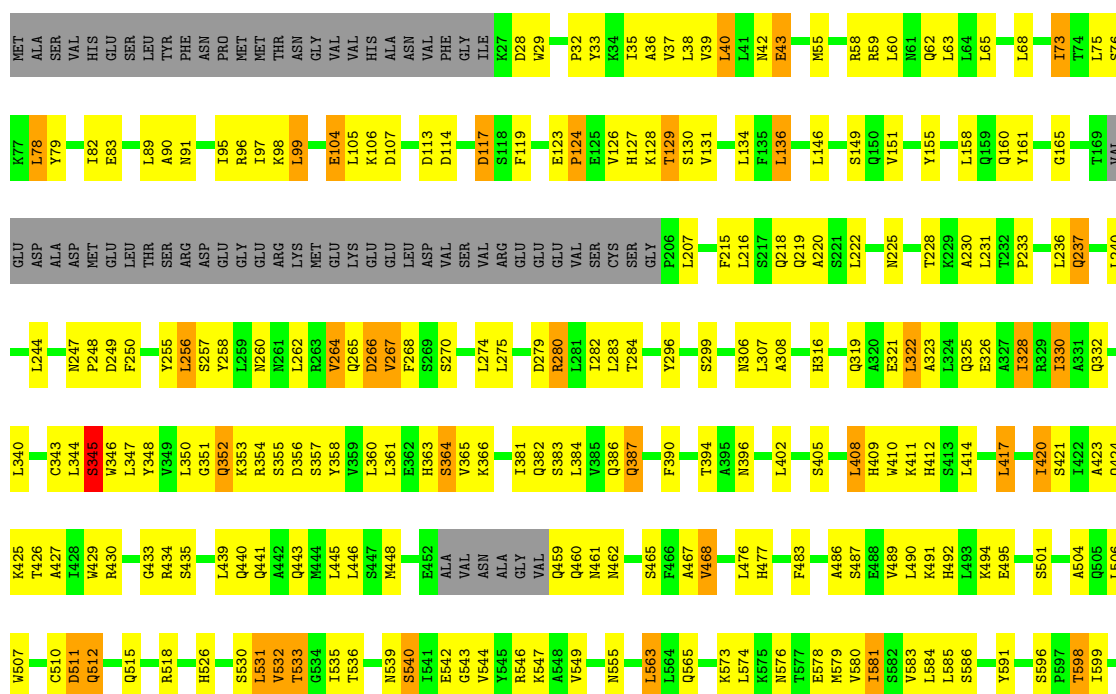
| Frequency | Percentage |
|-----------|------------|
| Daily | 47% |
| Often | 23% |
| Sometimes | 5% |
| Never | 23% |



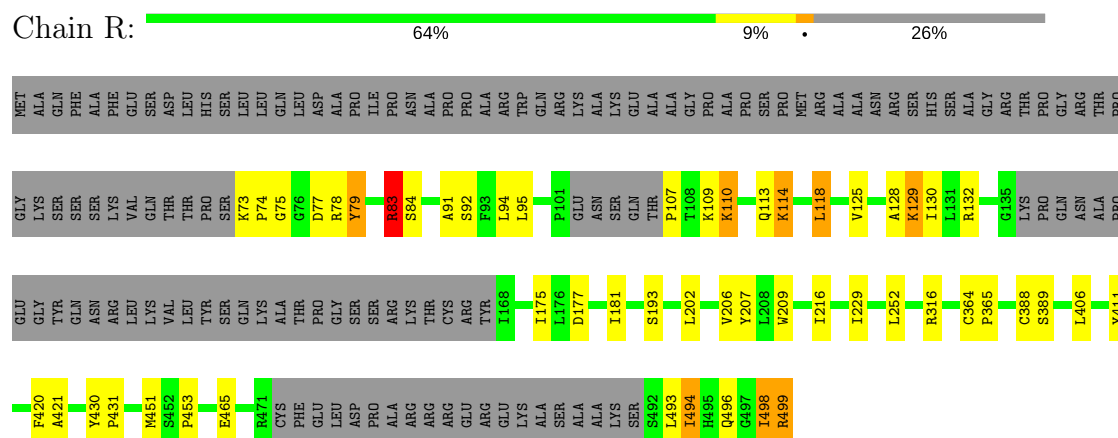


• Molecule 13: ANAPHASE-PROMOTING COMPLEX SUBUNIT 5

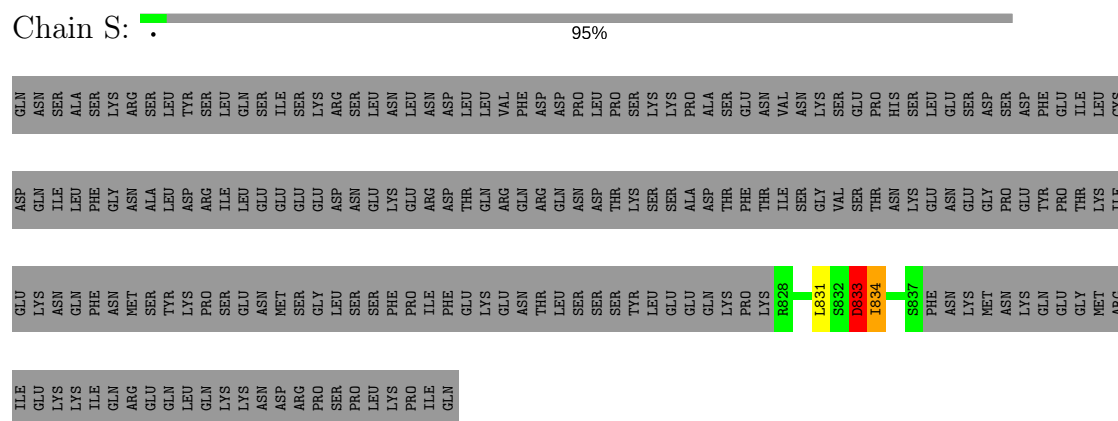
Chain O: 50% 33% 6% 9%



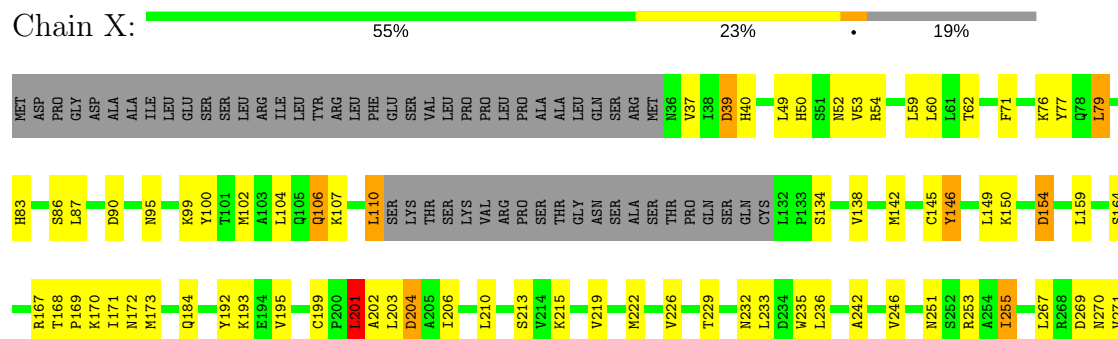
- Molecule 14: CELL DIVISION CYCLE PROTEIN 20 HOMOLOG

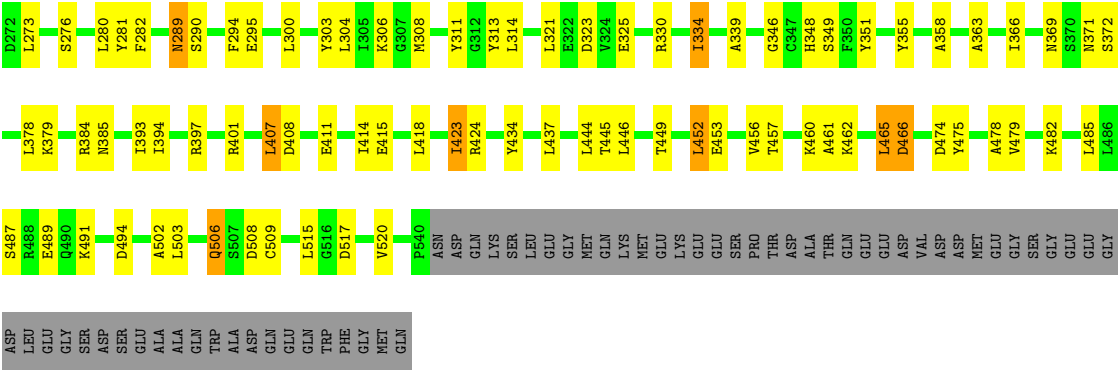


- Molecule 15: PROBABLE SERINE/THREONINE-PROTEIN KINASE HSL1



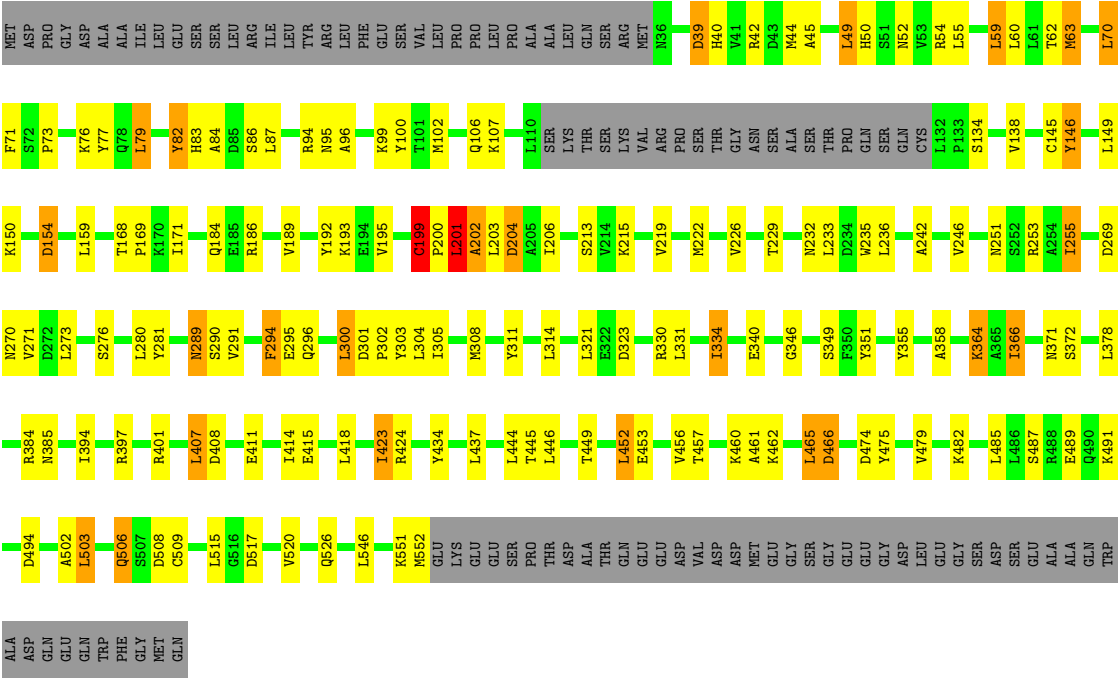
- Molecule 16: ANAPHASE-PROMOTING COMPLEX SUBUNIT 7





• Molecule 16: ANAPHASE-PROMOTING COMPLEX SUBUNIT 7

Chain Y: 56% 22% 17%



4 Experimental information

| Property | Value | Source |
|--------------------------------------|-------------------------|-----------|
| Reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 179660 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | Not provided | Depositor |
| Microscope | FEI POLARA 300 | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 27 | Depositor |
| Minimum defocus (nm) | 2000 | Depositor |
| Maximum defocus (nm) | 4000 | Depositor |
| Magnification | 78000 | Depositor |
| Image detector | FEI FALCON II (4k x 4k) | Depositor |

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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 | $\# Z > 2$ | RMSZ | $\# Z > 2$ |
| 1 | A | 0.58 | 0/11165 | 0.89 | 29/15204 (0.2%) |
| 10 | L | 0.67 | 0/1468 | 0.88 | 1/1993 (0.1%) |
| 11 | M | 0.63 | 1/502 (0.2%) | 0.95 | 0/680 |
| 12 | N | 0.54 | 0/4915 | 0.88 | 15/6645 (0.2%) |
| 13 | O | 0.61 | 1/5493 (0.0%) | 0.92 | 14/7421 (0.2%) |
| 14 | R | 0.54 | 2/2940 (0.1%) | 0.72 | 1/3996 (0.0%) |
| 15 | S | 0.50 | 0/71 | 1.09 | 1/95 (1.1%) |
| 16 | X | 0.55 | 0/3826 | 0.80 | 6/5177 (0.1%) |
| 16 | Y | 0.55 | 0/3919 | 0.82 | 10/5301 (0.2%) |
| 2 | B | 0.67 | 0/674 | 0.91 | 0/913 |
| 3 | C | 0.65 | 0/4404 | 0.94 | 8/5945 (0.1%) |
| 3 | P | 0.63 | 0/4134 | 0.91 | 7/5583 (0.1%) |
| 4 | D | 0.58 | 0/446 | 0.85 | 1/610 (0.2%) |
| 5 | E | 0.57 | 0/459 | 0.78 | 0/619 |
| 6 | F | 0.58 | 0/4013 | 0.83 | 4/5428 (0.1%) |
| 6 | H | 0.59 | 0/3942 | 0.82 | 3/5326 (0.1%) |
| 7 | G | 0.59 | 0/214 | 0.92 | 1/284 (0.4%) |
| 7 | W | 0.64 | 0/214 | 0.86 | 0/284 |
| 8 | I | 0.65 | 0/5827 | 0.93 | 12/7899 (0.2%) |
| 9 | J | 0.69 | 1/4146 (0.0%) | 0.94 | 6/5616 (0.1%) |
| 9 | K | 0.70 | 1/4086 (0.0%) | 0.93 | 5/5534 (0.1%) |
| All | All | 0.61 | 6/66858 (0.0%) | 0.88 | 124/90553 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | A | 0 | 1 |
| 10 | L | 0 | 1 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 11 | M | 0 | 1 |
| 12 | N | 0 | 4 |
| 16 | Y | 0 | 1 |
| 3 | P | 0 | 1 |
| 6 | F | 0 | 1 |
| 6 | H | 0 | 1 |
| 8 | I | 0 | 3 |
| 9 | J | 0 | 1 |
| All | All | 0 | 15 |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 13 | O | 268 | PHE | CG-CD2 | 7.98 | 1.50 | 1.38 |
| 9 | J | 302 | TRP | CB-CG | -6.32 | 1.38 | 1.50 |
| 14 | R | 79 | TYR | CB-CG | 5.73 | 1.60 | 1.51 |
| 11 | M | 19 | TRP | CB-CG | 5.53 | 1.60 | 1.50 |
| 14 | R | 79 | TYR | CE1-CZ | 5.37 | 1.45 | 1.38 |
| 9 | K | 302 | TRP | CB-CG | -5.22 | 1.40 | 1.50 |

All (124) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 3 | P | 358 | LEU | CA-CB-CG | 9.86 | 137.98 | 115.30 |
| 13 | O | 730 | ARG | NE-CZ-NH1 | 9.15 | 124.88 | 120.30 |
| 3 | C | 440 | GLY | N-CA-C | -8.87 | 90.94 | 113.10 |
| 9 | K | 351 | ASP | CB-CG-OD1 | 8.76 | 126.19 | 118.30 |
| 1 | A | 1235 | LEU | CA-CB-CG | 8.41 | 134.65 | 115.30 |
| 16 | Y | 70 | LEU | CB-CG-CD1 | 7.62 | 123.96 | 111.00 |
| 3 | P | 89 | LEU | CB-CG-CD2 | 7.55 | 123.84 | 111.00 |
| 3 | C | 179 | LEU | CA-CB-CG | 7.42 | 132.38 | 115.30 |
| 13 | O | 751 | LEU | CA-CB-CG | 7.31 | 132.12 | 115.30 |
| 13 | O | 117 | ASP | CB-CG-OD1 | -7.30 | 111.73 | 118.30 |
| 13 | O | 616 | LEU | CA-CB-CG | 7.10 | 131.62 | 115.30 |
| 12 | N | 477 | PRO | N-CA-CB | 7.05 | 111.76 | 103.30 |
| 4 | D | 23 | PRO | N-CA-CB | 7.03 | 111.74 | 103.30 |
| 12 | N | 63 | ARG | C-N-CA | 7.02 | 137.05 | 122.30 |
| 1 | A | 1415 | LEU | CA-CB-CG | 6.96 | 131.31 | 115.30 |
| 13 | O | 117 | ASP | CB-CG-OD2 | 6.81 | 124.43 | 118.30 |
| 8 | I | 223 | VAL | CB-CA-C | -6.78 | 98.51 | 111.40 |
| 12 | N | 219 | PRO | N-CA-CB | 6.74 | 111.39 | 103.30 |
| 13 | O | 632 | LEU | CA-CB-CG | 6.65 | 130.59 | 115.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 8 | I | 620 | PHE | CG-CD1-CE1 | 6.53 | 127.98 | 120.80 |
| 9 | J | 188 | LEU | CA-CB-CG | 6.47 | 130.18 | 115.30 |
| 1 | A | 1168 | LEU | CA-CB-CG | 6.38 | 129.97 | 115.30 |
| 13 | O | 730 | ARG | NE-CZ-NH2 | -6.31 | 117.14 | 120.30 |
| 1 | A | 1748 | LEU | CA-CB-CG | 6.26 | 129.70 | 115.30 |
| 1 | A | 1409 | LEU | CB-CG-CD2 | 6.26 | 121.64 | 111.00 |
| 12 | N | 215 | LEU | CA-CB-CG | 6.20 | 129.56 | 115.30 |
| 9 | K | 451 | LEU | CB-CG-CD2 | -6.19 | 100.48 | 111.00 |
| 10 | L | 171 | PRO | N-CA-CB | 6.17 | 110.70 | 103.30 |
| 13 | O | 625 | LEU | CA-CB-CG | 6.14 | 129.42 | 115.30 |
| 1 | A | 1556 | LEU | CA-CB-CG | 6.11 | 129.36 | 115.30 |
| 3 | C | 89 | LEU | CA-CB-CG | 6.11 | 129.35 | 115.30 |
| 16 | Y | 59 | LEU | CA-CB-CG | 6.11 | 129.34 | 115.30 |
| 16 | X | 110 | LEU | CA-CB-CG | 6.05 | 129.22 | 115.30 |
| 1 | A | 1409 | LEU | CA-CB-CG | 5.99 | 129.08 | 115.30 |
| 12 | N | 16 | PRO | N-CA-CB | 5.98 | 110.48 | 103.30 |
| 12 | N | 386 | LEU | CA-CB-CG | 5.95 | 128.99 | 115.30 |
| 8 | I | 11 | PHE | CB-CG-CD1 | -5.95 | 116.64 | 120.80 |
| 1 | A | 1934 | PRO | N-CA-CB | 5.95 | 110.43 | 103.30 |
| 1 | A | 1925 | PRO | N-CA-CB | 5.94 | 110.43 | 103.30 |
| 12 | N | 489 | PRO | N-CA-CB | 5.93 | 110.41 | 103.30 |
| 1 | A | 1603 | LEU | CA-CB-CG | 5.90 | 128.86 | 115.30 |
| 16 | Y | 146 | TYR | CB-CG-CD1 | -5.89 | 117.46 | 121.00 |
| 6 | F | 689 | LEU | CA-CB-CG | 5.89 | 128.85 | 115.30 |
| 12 | N | 197 | PRO | N-CA-CB | 5.88 | 110.36 | 103.30 |
| 8 | I | 602 | ARG | NE-CZ-NH1 | 5.86 | 123.23 | 120.30 |
| 1 | A | 442 | LEU | CA-CB-CG | 5.84 | 128.73 | 115.30 |
| 13 | O | 608 | LEU | CA-CB-CG | 5.83 | 128.71 | 115.30 |
| 3 | C | 556 | LEU | CA-CB-CG | 5.83 | 128.70 | 115.30 |
| 6 | H | 682 | LEU | CA-CB-CG | 5.82 | 128.68 | 115.30 |
| 14 | R | 83 | ARG | NE-CZ-NH1 | 5.81 | 123.20 | 120.30 |
| 1 | A | 214 | LEU | CA-CB-CG | 5.79 | 128.61 | 115.30 |
| 9 | J | 23 | LEU | CA-CB-CG | 5.78 | 128.58 | 115.30 |
| 1 | A | 1770 | LEU | CA-CB-CG | 5.76 | 128.56 | 115.30 |
| 1 | A | 1670 | GLY | C-N-CD | -5.76 | 107.92 | 120.60 |
| 6 | F | 768 | PRO | N-CA-CB | 5.76 | 110.21 | 103.30 |
| 8 | I | 589 | THR | CA-CB-CG2 | -5.76 | 104.34 | 112.40 |
| 16 | X | 446 | LEU | CA-CB-CG | 5.74 | 128.51 | 115.30 |
| 12 | N | 395 | ASP | N-CA-C | 5.72 | 126.44 | 111.00 |
| 1 | A | 412 | LEU | CA-CB-CG | 5.70 | 128.40 | 115.30 |
| 13 | O | 408 | LEU | CA-CB-CG | 5.69 | 128.38 | 115.30 |
| 13 | O | 574 | LEU | CA-CB-CG | 5.64 | 128.27 | 115.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 12 | N | 125 | TYR | C-N-CA | 5.59 | 135.68 | 121.70 |
| 1 | A | 271 | LEU | CA-CB-CG | 5.59 | 128.16 | 115.30 |
| 1 | A | 651 | PRO | N-CA-CB | 5.58 | 110.00 | 103.30 |
| 16 | Y | 146 | TYR | CB-CG-CD2 | 5.57 | 124.34 | 121.00 |
| 12 | N | 63 | ARG | N-CA-C | 5.57 | 126.03 | 111.00 |
| 16 | X | 418 | LEU | CA-CB-CG | 5.55 | 128.06 | 115.30 |
| 12 | N | 482 | PRO | N-CA-CB | 5.54 | 109.94 | 103.30 |
| 1 | A | 1313 | LEU | CA-CB-CG | 5.53 | 128.03 | 115.30 |
| 6 | F | 118 | LEU | CA-CB-CG | 5.53 | 128.02 | 115.30 |
| 16 | X | 201 | LEU | CA-CB-CG | 5.52 | 127.99 | 115.30 |
| 8 | I | 11 | PHE | CB-CG-CD2 | 5.50 | 124.65 | 120.80 |
| 16 | Y | 199 | CYS | N-CA-C | 5.49 | 125.82 | 111.00 |
| 16 | Y | 446 | LEU | CA-CB-CG | 5.48 | 127.91 | 115.30 |
| 3 | C | 38 | LEU | CA-CB-CG | 5.45 | 127.83 | 115.30 |
| 8 | I | 307 | LEU | CA-CB-CG | 5.45 | 127.83 | 115.30 |
| 3 | P | 38 | LEU | CA-CB-CG | 5.44 | 127.81 | 115.30 |
| 1 | A | 793 | LEU | CA-CB-CG | 5.43 | 127.79 | 115.30 |
| 13 | O | 563 | LEU | CA-CB-CG | 5.41 | 127.75 | 115.30 |
| 1 | A | 1405 | LEU | CA-CB-CG | 5.40 | 127.72 | 115.30 |
| 1 | A | 1609 | LEU | CA-CB-CG | -5.39 | 102.91 | 115.30 |
| 3 | P | 358 | LEU | CB-CA-C | 5.37 | 120.39 | 110.20 |
| 16 | Y | 82 | TYR | CB-CG-CD1 | 5.37 | 124.22 | 121.00 |
| 8 | I | 603 | ARG | NE-CZ-NH1 | 5.35 | 122.97 | 120.30 |
| 3 | C | 54 | TRP | CB-CA-C | -5.33 | 99.75 | 110.40 |
| 8 | I | 45 | LEU | CB-CG-CD2 | 5.33 | 120.06 | 111.00 |
| 6 | H | 617 | LEU | CA-CB-CG | 5.30 | 127.50 | 115.30 |
| 8 | I | 606 | ASP | CB-CG-OD1 | 5.29 | 123.06 | 118.30 |
| 1 | A | 773 | LEU | CA-CB-CG | 5.29 | 127.46 | 115.30 |
| 3 | C | 306 | LEU | CA-CB-CG | 5.28 | 127.43 | 115.30 |
| 1 | A | 1227 | LEU | CA-CB-CG | 5.27 | 127.42 | 115.30 |
| 12 | N | 484 | PRO | N-CA-CB | 5.27 | 109.62 | 103.30 |
| 3 | P | 172 | LEU | CA-CB-CG | 5.23 | 127.34 | 115.30 |
| 7 | G | 14 | ASP | CB-CG-OD2 | 5.23 | 123.00 | 118.30 |
| 1 | A | 1882 | LEU | CA-CB-CG | 5.21 | 127.29 | 115.30 |
| 9 | J | 225 | ASP | CB-CG-OD2 | 5.21 | 122.98 | 118.30 |
| 1 | A | 1059 | ASP | CB-CG-OD2 | 5.20 | 122.98 | 118.30 |
| 16 | Y | 418 | LEU | CA-CB-CG | 5.20 | 127.25 | 115.30 |
| 15 | S | 833 | ASP | CB-CG-OD2 | 5.19 | 122.97 | 118.30 |
| 16 | Y | 466 | ASP | CB-CG-OD2 | 5.18 | 122.97 | 118.30 |
| 8 | I | 664 | ARG | NE-CZ-NH1 | 5.18 | 122.89 | 120.30 |
| 12 | N | 522 | LEU | CA-CB-CG | 5.18 | 127.21 | 115.30 |
| 9 | J | 376 | LEU | CA-CB-CG | 5.17 | 127.18 | 115.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 16 | X | 466 | ASP | CB-CG-OD2 | 5.16 | 122.94 | 118.30 |
| 16 | X | 146 | TYR | CB-CG-CD1 | -5.15 | 117.91 | 121.00 |
| 12 | N | 63 | ARG | CA-C-N | 5.14 | 126.49 | 116.20 |
| 3 | P | 229 | MET | CG-SD-CE | 5.14 | 108.42 | 100.20 |
| 1 | A | 797 | LEU | CA-CB-CG | 5.12 | 127.08 | 115.30 |
| 1 | A | 1188 | LEU | CA-CB-CG | 5.12 | 127.07 | 115.30 |
| 9 | K | 188 | LEU | CA-CB-CG | 5.11 | 127.06 | 115.30 |
| 6 | F | 118 | LEU | CB-CG-CD1 | 5.11 | 119.69 | 111.00 |
| 9 | J | 134 | LEU | CA-CB-CG | 5.10 | 127.04 | 115.30 |
| 1 | A | 1538 | LEU | CA-CB-CG | 5.10 | 127.03 | 115.30 |
| 16 | Y | 546 | LEU | CA-CB-CG | 5.10 | 127.03 | 115.30 |
| 9 | K | 451 | LEU | CA-CB-CG | 5.10 | 127.02 | 115.30 |
| 6 | H | 82 | LEU | CA-CB-CG | 5.06 | 126.94 | 115.30 |
| 13 | O | 322 | LEU | CA-CB-CG | 5.06 | 126.94 | 115.30 |
| 3 | C | 89 | LEU | CB-CG-CD2 | 5.06 | 119.60 | 111.00 |
| 3 | P | 306 | LEU | CA-CB-CG | 5.05 | 126.92 | 115.30 |
| 13 | O | 268 | PHE | CB-CG-CD2 | 5.03 | 124.32 | 120.80 |
| 1 | A | 1533 | LEU | CA-CB-CG | 5.03 | 126.87 | 115.30 |
| 8 | I | 683 | TYR | CB-CG-CD2 | 5.03 | 124.02 | 121.00 |
| 9 | J | 232 | ASP | CB-CG-OD1 | 5.03 | 122.82 | 118.30 |
| 9 | K | 7 | ARG | NE-CZ-NH2 | -5.01 | 117.79 | 120.30 |

There are no chirality outliers.

All (15) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 1 | A | 124 | GLN | Peptide |
| 6 | F | 565 | ASN | Peptide |
| 6 | H | 565 | ASN | Peptide |
| 8 | I | 489 | PRO | Peptide |
| 8 | I | 658 | GLY | Peptide |
| 8 | I | 727 | PHE | Peptide |
| 9 | J | 220 | ILE | Peptide |
| 10 | L | 36 | CYS | Peptide |
| 11 | M | 62 | LEU | Peptide |
| 12 | N | 143 | GLY | Peptide |
| 12 | N | 367 | ARG | Peptide |
| 12 | N | 387 | LEU | Peptide |
| 12 | N | 394 | CYS | Peptide |
| 3 | P | 147 | LYS | Peptide |
| 16 | Y | 199 | CYS | Peptide |

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 | 10925 | 0 | 10669 | 471 | 0 |
| 2 | B | 649 | 0 | 595 | 26 | 0 |
| 3 | C | 4306 | 0 | 4273 | 274 | 0 |
| 3 | P | 4039 | 0 | 3989 | 120 | 0 |
| 4 | D | 436 | 0 | 396 | 27 | 0 |
| 5 | E | 450 | 0 | 435 | 12 | 0 |
| 6 | F | 3923 | 0 | 3819 | 115 | 0 |
| 6 | H | 3853 | 0 | 3793 | 110 | 0 |
| 7 | G | 213 | 0 | 220 | 16 | 0 |
| 7 | W | 213 | 0 | 220 | 9 | 0 |
| 8 | I | 5709 | 0 | 5597 | 188 | 0 |
| 9 | J | 4047 | 0 | 3949 | 185 | 0 |
| 9 | K | 3988 | 0 | 3908 | 148 | 0 |
| 10 | L | 1435 | 0 | 1382 | 43 | 0 |
| 11 | M | 493 | 0 | 469 | 17 | 0 |
| 12 | N | 4837 | 0 | 4534 | 155 | 0 |
| 13 | O | 5395 | 0 | 5429 | 231 | 0 |
| 14 | R | 2869 | 0 | 2772 | 59 | 0 |
| 15 | S | 72 | 0 | 71 | 10 | 0 |
| 16 | X | 3767 | 0 | 3819 | 136 | 0 |
| 16 | Y | 3859 | 0 | 3908 | 150 | 0 |
| 17 | B | 3 | 0 | 0 | 0 | 0 |
| All | All | 65481 | 0 | 64247 | 2216 | 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 17.

All (2216) 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) |
|------------------|-------------------|--------------------------|-------------------|
| 12:N:362:LYS:HG3 | 12:N:410:LEU:CD2 | 1.38 | 1.52 |
| 9:J:223:SER:CB | 9:J:228:GLN:HE21 | 1.29 | 1.44 |
| 12:N:362:LYS:CG | 12:N:410:LEU:HD23 | 1.60 | 1.31 |
| 12:N:362:LYS:CB | 12:N:410:LEU:HD21 | 1.67 | 1.24 |
| 14:R:177:ASP:OD2 | 15:S:834:ILE:HD11 | 1.30 | 1.23 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1332:GLY:O | 1:A:1358:ILE:HD12 | 1.34 | 1.23 |
| 12:N:362:LYS:CG | 12:N:410:LEU:CD2 | 2.15 | 1.23 |
| 3:C:98:GLU:OE1 | 3:C:101:ARG:HB3 | 1.39 | 1.21 |
| 13:O:42:ASN:ND2 | 13:O:43:GLU:OE1 | 1.72 | 1.21 |
| 16:Y:42:ARG:HA | 16:Y:82:TYR:CE2 | 1.75 | 1.20 |
| 14:R:177:ASP:CG | 15:S:834:ILE:HD11 | 1.64 | 1.17 |
| 9:J:223:SER:CB | 9:J:228:GLN:NE2 | 2.07 | 1.17 |
| 1:A:1229:SER:HA | 1:A:1235:LEU:HG | 1.17 | 1.16 |
| 9:J:383:ASN:HB3 | 9:J:386:LEU:HD13 | 1.24 | 1.16 |
| 9:K:250:CYS:SG | 9:K:274:THR:HG21 | 1.85 | 1.14 |
| 9:J:223:SER:HB2 | 9:J:228:GLN:NE2 | 1.60 | 1.11 |
| 1:A:39:LEU:HD13 | 13:O:248:PRO:HB3 | 1.30 | 1.11 |
| 1:A:23:PHE:HB2 | 1:A:111:LEU:HD22 | 1.33 | 1.11 |
| 16:X:37:VAL:CG2 | 16:Y:232:ASN:HB2 | 1.81 | 1.09 |
| 3:C:101:ARG:HH11 | 3:C:101:ARG:HG2 | 1.02 | 1.08 |
| 1:A:1332:GLY:O | 1:A:1358:ILE:CD1 | 2.01 | 1.07 |
| 9:K:129:LYS:O | 9:K:133:CYS:SG | 2.13 | 1.06 |
| 14:R:128:ALA:HB1 | 14:R:129:LYS:HA | 1.37 | 1.06 |
| 6:H:479:TYR:C | 6:H:480:ASN:N | 2.09 | 1.05 |
| 8:I:56:TRP:CE3 | 8:I:98:PRO:HB3 | 1.92 | 1.04 |
| 14:R:177:ASP:OD2 | 15:S:834:ILE:CD1 | 2.06 | 1.03 |
| 16:X:37:VAL:HG21 | 16:Y:232:ASN:CB | 1.89 | 1.03 |
| 12:N:362:LYS:HB2 | 12:N:410:LEU:HD21 | 1.39 | 1.02 |
| 3:C:251:TYR:HA | 3:C:254:LEU:HD12 | 1.38 | 1.02 |
| 16:X:235:TRP:NE1 | 16:Y:63:MET:HE1 | 1.75 | 1.02 |
| 16:X:235:TRP:HE1 | 16:Y:63:MET:HE1 | 1.22 | 1.01 |
| 9:J:454:VAL:O | 9:J:458:LEU:HD12 | 1.59 | 1.01 |
| 16:X:37:VAL:HG21 | 16:Y:232:ASN:HB2 | 1.05 | 1.01 |
| 1:A:1237:PRO:HB2 | 1:A:1238:PRO:HD3 | 1.40 | 1.01 |
| 12:N:414:MET:SD | 12:N:498:SER:HA | 2.02 | 0.99 |
| 1:A:1225:THR:O | 1:A:1229:SER:N | 1.96 | 0.99 |
| 12:N:425:ARG:HH11 | 12:N:425:ARG:HG2 | 1.26 | 0.98 |
| 8:I:209:CYS:SG | 8:I:584:HIS:CE1 | 2.56 | 0.98 |
| 9:J:254:THR:HG23 | 9:J:271:HIS:HD2 | 1.27 | 0.97 |
| 14:R:177:ASP:CG | 15:S:834:ILE:CD1 | 2.33 | 0.97 |
| 1:A:48:LEU:HD22 | 1:A:49:TRP:N | 1.80 | 0.97 |
| 8:I:279:ILE:HD11 | 8:I:337:ILE:HA | 1.44 | 0.96 |
| 9:K:263:PHE:HZ | 9:K:290:LYS:HG2 | 1.30 | 0.96 |
| 12:N:538:GLU:HG2 | 12:N:561:LEU:HG | 1.44 | 0.96 |
| 12:N:211:ARG:O | 12:N:215:LEU:HG | 1.66 | 0.96 |
| 3:C:98:GLU:OE2 | 3:C:101:ARG:HD3 | 1.66 | 0.96 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:P:233:PHE:CE2 | 3:P:237:ILE:HD11 | 1.99 | 0.96 |
| 9:J:223:SER:HB2 | 9:J:228:GLN:HE21 | 0.80 | 0.96 |
| 1:A:1433:ILE:HD13 | 1:A:1433:ILE:H | 1.26 | 0.95 |
| 3:P:487:ALA:HB1 | 3:P:519:TYR:CD1 | 2.02 | 0.95 |
| 9:J:332:THR:HA | 9:J:363:LEU:HD21 | 1.46 | 0.95 |
| 16:X:235:TRP:CD1 | 16:Y:63:MET:CE | 2.50 | 0.94 |
| 6:F:130:ARG:HG3 | 16:Y:506:GLN:HB2 | 1.48 | 0.94 |
| 1:A:248:PHE:HB2 | 1:A:430:VAL:CG2 | 1.97 | 0.94 |
| 16:X:355:TYR:CZ | 16:X:385:ASN:HB3 | 2.02 | 0.94 |
| 8:I:144:THR:HG21 | 8:I:159:GLU:HA | 1.50 | 0.93 |
| 8:I:34:LEU:HD12 | 8:I:46:LEU:HD21 | 1.51 | 0.93 |
| 13:O:435:SER:HB3 | 13:O:654:ASP:HB2 | 1.50 | 0.93 |
| 3:C:283:LEU:HD13 | 3:C:306:LEU:CD1 | 1.97 | 0.93 |
| 16:Y:42:ARG:HG3 | 16:Y:82:TYR:OH | 1.67 | 0.92 |
| 12:N:362:LYS:CB | 12:N:410:LEU:CD2 | 2.44 | 0.92 |
| 3:C:296:ARG:HH11 | 3:C:296:ARG:CG | 1.82 | 0.92 |
| 16:X:201:LEU:HD11 | 16:Y:40:HIS:HB3 | 1.52 | 0.92 |
| 3:C:441:GLU:HA | 3:C:444:GLU:HB3 | 1.52 | 0.92 |
| 8:I:209:CYS:SG | 8:I:584:HIS:ND1 | 2.43 | 0.92 |
| 3:C:54:TRP:HZ3 | 3:C:207:LEU:HD22 | 1.32 | 0.91 |
| 8:I:26:LEU:HB3 | 8:I:37:LEU:HB3 | 1.52 | 0.91 |
| 8:I:266:ASN:HA | 8:I:526:LYS:HZ3 | 1.36 | 0.91 |
| 3:C:296:ARG:HH12 | 3:C:299:ASN:H | 1.17 | 0.91 |
| 9:K:214:LYS:O | 9:K:216:SER:N | 2.04 | 0.91 |
| 3:C:296:ARG:HH11 | 3:C:296:ARG:HG3 | 1.34 | 0.91 |
| 3:C:414:MET:HG2 | 13:O:330:ILE:HG12 | 1.54 | 0.90 |
| 16:X:267:LEU:HD11 | 16:Y:59:LEU:HD11 | 1.49 | 0.90 |
| 1:A:1636:VAL:HB | 1:A:1663:LEU:HD11 | 1.51 | 0.90 |
| 9:J:476:PRO:HG2 | 3:P:182:LEU:HG | 1.54 | 0.90 |
| 9:K:174:HIS:CE1 | 9:K:211:LYS:HD3 | 2.06 | 0.90 |
| 13:O:55:MET:SD | 13:O:58:ARG:CZ | 2.60 | 0.90 |
| 1:A:1739:SER:HA | 1:A:1740:ALA:HB3 | 1.54 | 0.90 |
| 9:K:472:LEU:HG | 9:K:481:THR:HG21 | 1.52 | 0.90 |
| 16:X:235:TRP:NE1 | 16:Y:63:MET:CE | 2.36 | 0.89 |
| 1:A:1145:LEU:HD22 | 1:A:1611:VAL:HG21 | 1.54 | 0.89 |
| 9:J:263:PHE:HZ | 9:J:290:LYS:HG2 | 1.37 | 0.89 |
| 13:O:55:MET:SD | 13:O:58:ARG:NH1 | 2.46 | 0.89 |
| 3:P:233:PHE:CZ | 3:P:237:ILE:HD11 | 2.07 | 0.89 |
| 3:C:113:LYS:HE2 | 3:C:113:LYS:H | 1.38 | 0.89 |
| 1:A:1255:VAL:HG11 | 1:A:1606:LEU:HD21 | 1.55 | 0.88 |
| 9:J:185:LEU:HD12 | 9:J:209:LEU:HD21 | 1.55 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:248:PHE:HB3 | 1:A:257:MET:CB | 2.03 | 0.88 |
| 8:I:514:PHE:HE2 | 13:O:440:GLN:HA | 1.36 | 0.88 |
| 3:C:101:ARG:HG2 | 3:C:101:ARG:NH1 | 1.80 | 0.88 |
| 9:J:354:MET:HE1 | 9:J:374:ILE:HA | 1.55 | 0.87 |
| 12:N:289:PHE:HA | 12:N:292:TRP:HB3 | 1.56 | 0.87 |
| 3:C:46:ARG:HH21 | 3:C:48:LEU:HD11 | 1.39 | 0.87 |
| 3:C:234:LEU:HD23 | 3:C:250:LYS:HE3 | 1.56 | 0.87 |
| 4:D:9:PHE:HD2 | 13:O:346:TRP:CZ3 | 1.91 | 0.87 |
| 1:A:433:THR:HG22 | 1:A:481:PRO:HB3 | 1.55 | 0.87 |
| 9:J:295:TYR:OH | 9:K:54:HIS:HB2 | 1.74 | 0.86 |
| 16:Y:42:ARG:HA | 16:Y:82:TYR:HE2 | 1.34 | 0.86 |
| 1:A:1492:ALA:O | 1:A:1496:MET:HG3 | 1.75 | 0.86 |
| 8:I:209:CYS:HG | 8:I:584:HIS:CE1 | 1.92 | 0.86 |
| 3:C:308:TYR:CD2 | 14:R:78:ARG:HD2 | 2.11 | 0.86 |
| 1:A:1567:LEU:HD22 | 1:A:1574:LEU:HD23 | 1.58 | 0.86 |
| 1:A:1239:THR:HB | 1:A:1240:SER:HA | 1.56 | 0.86 |
| 1:A:1877:LEU:HD22 | 1:A:1881:GLN:HE22 | 1.39 | 0.86 |
| 1:A:1086:MET:SD | 1:A:1564:LEU:HD13 | 2.16 | 0.86 |
| 1:A:1089:LEU:HD11 | 1:A:1611:VAL:HG23 | 1.57 | 0.85 |
| 1:A:252:ASP:HB3 | 1:A:253:PRO:HD3 | 1.57 | 0.85 |
| 8:I:186:GLU:OE2 | 8:I:197:ARG:NH1 | 2.10 | 0.85 |
| 9:J:254:THR:HG23 | 9:J:271:HIS:CD2 | 2.10 | 0.85 |
| 3:C:46:ARG:HH22 | 3:C:170:PHE:HB3 | 1.42 | 0.84 |
| 9:K:292:VAL:HG21 | 11:M:57:TRP:HB3 | 1.60 | 0.84 |
| 16:X:267:LEU:HD11 | 16:Y:59:LEU:CD1 | 2.08 | 0.84 |
| 16:X:235:TRP:HE1 | 16:Y:63:MET:CE | 1.89 | 0.84 |
| 1:A:433:THR:CG2 | 1:A:481:PRO:HB3 | 2.09 | 0.83 |
| 3:C:449:LEU:HD22 | 3:C:476:LEU:CD2 | 2.09 | 0.83 |
| 16:Y:42:ARG:HA | 16:Y:82:TYR:CZ | 2.13 | 0.83 |
| 8:I:56:TRP:HZ3 | 8:I:58:PHE:HB2 | 1.42 | 0.83 |
| 1:A:1573:SER:OG | 1:A:1656:LEU:HD22 | 1.77 | 0.83 |
| 1:A:1229:SER:CA | 1:A:1235:LEU:HG | 2.05 | 0.83 |
| 8:I:209:CYS:HG | 8:I:584:HIS:HD1 | 1.27 | 0.82 |
| 9:J:441:VAL:HG21 | 9:J:444:TRP:HD1 | 1.42 | 0.82 |
| 9:K:383:ASN:HB3 | 9:K:386:LEU:HD13 | 1.60 | 0.82 |
| 12:N:531:PHE:O | 12:N:533:PHE:HA | 1.80 | 0.82 |
| 1:A:44:PRO:HA | 1:A:45:ALA:HB2 | 1.62 | 0.82 |
| 13:O:231:LEU:HD23 | 13:O:236:LEU:HA | 1.62 | 0.82 |
| 1:A:210:MET:HB3 | 1:A:223:LEU:HB2 | 1.63 | 0.81 |
| 3:C:61:SER:HB2 | 3:C:262:SER:HB2 | 1.62 | 0.81 |
| 3:C:283:LEU:HD13 | 3:C:306:LEU:HD11 | 1.61 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:J:406:HIS:CE1 | 9:J:450:ASN:HD22 | 1.98 | 0.81 |
| 13:O:578:GLU:HA | 13:O:616:LEU:HD11 | 1.60 | 0.81 |
| 16:X:235:TRP:CD1 | 16:Y:63:MET:HE1 | 2.15 | 0.81 |
| 1:A:248:PHE:HB2 | 1:A:430:VAL:HG23 | 1.61 | 0.81 |
| 3:C:95:ASP:O | 3:C:97:LYS:HG2 | 1.79 | 0.81 |
| 13:O:539:ASN:HD22 | 13:O:542:GLU:CB | 1.93 | 0.81 |
| 1:A:185:TYR:HE1 | 1:A:273:ARG:HH11 | 1.28 | 0.80 |
| 9:J:167:PHE:O | 9:J:170:LEU:HD23 | 1.80 | 0.80 |
| 8:I:356:SER:HB3 | 8:I:397:ILE:HG12 | 1.63 | 0.80 |
| 3:C:175:TYR:O | 3:C:179:LEU:HD23 | 1.81 | 0.80 |
| 1:A:1373:MET:HA | 1:A:1376:LEU:HD12 | 1.63 | 0.80 |
| 3:C:285:ILE:O | 3:C:288:GLU:OE1 | 2.00 | 0.80 |
| 6:F:707:PHE:HB2 | 6:F:729:LEU:HD11 | 1.63 | 0.80 |
| 12:N:368:THR:OG1 | 12:N:369:ASP:HA | 1.81 | 0.80 |
| 12:N:362:LYS:CA | 12:N:410:LEU:HD21 | 2.11 | 0.79 |
| 1:A:1177:MET:HB2 | 1:A:1207:GLY:HA2 | 1.64 | 0.79 |
| 16:Y:84:ALA:HB1 | 16:Y:100:TYR:CE2 | 2.17 | 0.79 |
| 9:J:397:ILE:HG22 | 9:J:398:ALA:H | 1.48 | 0.79 |
| 13:O:32:PRO:O | 13:O:35:ILE:HG22 | 1.82 | 0.79 |
| 1:A:248:PHE:HB2 | 1:A:430:VAL:HG21 | 1.65 | 0.78 |
| 8:I:266:ASN:HA | 8:I:526:LYS:NZ | 1.97 | 0.78 |
| 13:O:539:ASN:HD22 | 13:O:542:GLU:HB3 | 1.45 | 0.78 |
| 8:I:73:TRP:CZ2 | 8:I:80:LEU:HD22 | 2.17 | 0.78 |
| 9:J:37:PRO:HB3 | 9:J:69:TYR:CE2 | 2.19 | 0.78 |
| 10:L:50:LEU:O | 10:L:154:ARG:HD3 | 1.84 | 0.78 |
| 12:N:165:THR:H | 12:N:166:PRO:HA | 1.46 | 0.78 |
| 8:I:177:VAL:HG12 | 8:I:208:LEU:HD13 | 1.64 | 0.78 |
| 12:N:519:TYR:OH | 12:N:541:ASN:HB3 | 1.83 | 0.78 |
| 1:A:1320:ASN:HB3 | 1:A:1323:GLU:HG2 | 1.65 | 0.78 |
| 1:A:1360:VAL:HB | 1:A:1364:CYS:HB2 | 1.66 | 0.78 |
| 2:B:39:VAL:CB | 2:B:43:ASP:HB2 | 2.14 | 0.78 |
| 11:M:2:ASP:HB2 | 3:P:123:TYR:CE2 | 2.18 | 0.78 |
| 11:M:2:ASP:HB2 | 3:P:123:TYR:HE2 | 1.49 | 0.78 |
| 13:O:581:ILE:HD11 | 13:O:619:LEU:HB3 | 1.66 | 0.78 |
| 1:A:1093:HIS:ND1 | 1:A:1151:SER:HB3 | 1.99 | 0.78 |
| 6:F:7:PRO:HG3 | 6:H:455:GLN:HG2 | 1.66 | 0.78 |
| 6:F:537:GLU:OE1 | 6:F:602:TYR:HB3 | 1.84 | 0.78 |
| 3:P:61:SER:HB2 | 3:P:262:SER:HB2 | 1.66 | 0.77 |
| 16:Y:45:ALA:HB3 | 16:Y:82:TYR:CE2 | 2.19 | 0.77 |
| 12:N:165:THR:N | 12:N:166:PRO:HA | 2.00 | 0.77 |
| 3:P:373:HIS:O | 3:P:377:GLU:HG2 | 1.84 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:438:ALA:HA | 14:R:83:ARG:HH11 | 1.48 | 0.77 |
| 3:C:449:LEU:HD22 | 3:C:476:LEU:HD21 | 1.64 | 0.77 |
| 3:C:403:TYR:HD2 | 3:C:435:MET:SD | 2.08 | 0.77 |
| 3:C:309:VAL:HG23 | 14:R:78:ARG:HG3 | 1.67 | 0.77 |
| 16:X:199:CYS:SG | 16:Y:44:MET:HG2 | 2.25 | 0.77 |
| 3:C:206:TRP:HZ3 | 3:C:233:PHE:CD2 | 2.02 | 0.77 |
| 16:X:235:TRP:CD1 | 16:Y:63:MET:HE3 | 2.19 | 0.77 |
| 8:I:679:ASP:OD1 | 8:I:703:ARG:NH2 | 2.18 | 0.77 |
| 3:C:440:GLY:O | 3:C:442:CYS:N | 2.17 | 0.77 |
| 1:A:1332:GLY:O | 1:A:1358:ILE:CG1 | 2.32 | 0.77 |
| 8:I:514:PHE:CE2 | 13:O:440:GLN:HA | 2.20 | 0.77 |
| 3:C:54:TRP:HH2 | 3:C:207:LEU:HD13 | 1.50 | 0.76 |
| 3:C:370:LEU:HG | 14:R:79:TYR:HE1 | 1.49 | 0.76 |
| 3:C:373:HIS:O | 3:C:377:GLU:HG2 | 1.85 | 0.76 |
| 8:I:224:SER:CB | 8:I:229:SER:HA | 2.14 | 0.76 |
| 1:A:248:PHE:HB3 | 1:A:257:MET:HB2 | 1.65 | 0.76 |
| 3:C:54:TRP:CH2 | 3:C:207:LEU:HD13 | 2.21 | 0.76 |
| 9:J:55:ARG:HH11 | 9:K:264:HIS:HA | 1.50 | 0.76 |
| 3:P:313:LYS:HE3 | 3:P:344:ARG:HD2 | 1.66 | 0.76 |
| 3:C:413:LYS:O | 3:C:415:PRO:HD2 | 1.86 | 0.76 |
| 1:A:1791:ILE:HB | 13:O:598:THR:HG21 | 1.67 | 0.76 |
| 9:J:441:VAL:HG21 | 9:J:444:TRP:CD1 | 2.19 | 0.76 |
| 3:C:46:ARG:NH2 | 3:C:170:PHE:HB3 | 2.01 | 0.75 |
| 12:N:213:TYR:N | 12:N:215:LEU:H | 1.82 | 0.75 |
| 6:H:653:LEU:HD22 | 9:K:523:ILE:HG21 | 1.66 | 0.75 |
| 3:P:487:ALA:HB1 | 3:P:519:TYR:HD1 | 1.50 | 0.75 |
| 1:A:1573:SER:HB2 | 1:A:1617:ARG:HH21 | 1.50 | 0.75 |
| 6:H:707:PHE:HB2 | 6:H:729:LEU:HD11 | 1.67 | 0.75 |
| 3:P:494:ILE:HG12 | 3:P:512:ALA:HB1 | 1.69 | 0.75 |
| 1:A:1409:LEU:HG | 1:A:1470:LEU:HD23 | 1.69 | 0.75 |
| 9:K:177:THR:HG22 | 9:K:365:LYS:HB3 | 1.69 | 0.75 |
| 8:I:88:LYS:O | 8:I:106:VAL:HG22 | 1.87 | 0.74 |
| 13:O:35:ILE:HG21 | 13:O:158:LEU:HD13 | 1.68 | 0.74 |
| 16:Y:271:VAL:HG12 | 16:Y:304:LEU:HD21 | 1.68 | 0.74 |
| 8:I:65:GLY:H | 8:I:84:LEU:HG | 1.51 | 0.74 |
| 16:X:452:LEU:HB3 | 16:X:461:ALA:HB2 | 1.70 | 0.74 |
| 1:A:1433:ILE:N | 1:A:1433:ILE:HD13 | 2.02 | 0.74 |
| 1:A:39:LEU:HD13 | 13:O:248:PRO:CB | 2.15 | 0.74 |
| 3:C:296:ARG:HH12 | 3:C:299:ASN:N | 1.85 | 0.74 |
| 3:C:94:PHE:O | 3:C:97:LYS:HB3 | 1.86 | 0.74 |
| 1:A:1877:LEU:HD22 | 1:A:1881:GLN:NE2 | 2.03 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:119:MET:O | 3:C:122:ARG:HG2 | 1.88 | 0.74 |
| 3:C:114:ALA:O | 3:C:116:PHE:N | 2.20 | 0.74 |
| 9:K:45:GLN:HE21 | 9:K:45:GLN:HA | 1.51 | 0.74 |
| 1:A:175:PHE:CD1 | 1:A:191:ARG:HG3 | 2.23 | 0.73 |
| 3:P:382:SER:HA | 3:P:385:ILE:HD12 | 1.69 | 0.73 |
| 1:A:1293:SER:HB3 | 1:A:1600:ARG:O | 1.88 | 0.73 |
| 3:C:115:TYR:OH | 3:C:161:LYS:CD | 2.36 | 0.73 |
| 10:L:126:ASP:HB2 | 10:L:132:THR:HG23 | 1.70 | 0.73 |
| 1:A:1229:SER:HA | 1:A:1235:LEU:CG | 2.09 | 0.73 |
| 3:C:99:TYR:HE2 | 3:C:128:LYS:HG3 | 1.52 | 0.73 |
| 8:I:26:LEU:CB | 8:I:37:LEU:HB3 | 2.18 | 0.73 |
| 12:N:531:PHE:HB3 | 12:N:534:SER:HB2 | 1.71 | 0.73 |
| 16:X:62:THR:HG21 | 16:Y:270:ASN:HA | 1.69 | 0.73 |
| 16:X:407:LEU:HD22 | 16:X:437:LEU:HD21 | 1.71 | 0.73 |
| 3:C:77:THR:OG1 | 3:C:79:GLU:OE1 | 2.06 | 0.73 |
| 9:J:354:MET:CE | 9:J:354:MET:HA | 2.19 | 0.73 |
| 1:A:431:PHE:O | 1:A:431:PHE:CD1 | 2.42 | 0.73 |
| 16:Y:466:ASP:OD1 | 16:Y:482:LYS:HE3 | 1.88 | 0.73 |
| 4:D:9:PHE:HD2 | 13:O:346:TRP:HZ3 | 1.34 | 0.73 |
| 1:A:1470:LEU:HA | 1:A:1522:SER:OG | 1.89 | 0.73 |
| 16:Y:452:LEU:HB3 | 16:Y:461:ALA:HB2 | 1.70 | 0.73 |
| 6:F:502:LEU:HB3 | 6:F:525:VAL:HG22 | 1.69 | 0.72 |
| 8:I:48:ARG:HG3 | 8:I:55:VAL:HG22 | 1.71 | 0.72 |
| 14:R:177:ASP:OD1 | 15:S:834:ILE:HD11 | 1.88 | 0.72 |
| 13:O:652:LEU:HD23 | 13:O:660:LYS:HG3 | 1.70 | 0.72 |
| 1:A:793:LEU:HD22 | 1:A:794:ALA:HA | 1.71 | 0.72 |
| 3:C:173:TYR:CD1 | 3:C:202:HIS:HE1 | 2.07 | 0.72 |
| 10:L:86:ASP:HB3 | 10:L:89:TYR:HB2 | 1.71 | 0.72 |
| 5:E:63:VAL:HG21 | 16:Y:364:LYS:HD2 | 1.70 | 0.72 |
| 8:I:674:VAL:O | 8:I:703:ARG:NH1 | 2.22 | 0.72 |
| 9:J:465:LEU:HA | 9:J:488:ILE:HD12 | 1.71 | 0.72 |
| 3:C:96:VAL:HG21 | 3:P:53:LYS:HD3 | 1.72 | 0.72 |
| 1:A:1848:VAL:O | 1:A:1852:ILE:HG12 | 1.90 | 0.72 |
| 1:A:248:PHE:HB3 | 1:A:257:MET:HB3 | 1.70 | 0.72 |
| 6:H:502:LEU:HB3 | 6:H:525:VAL:HG22 | 1.72 | 0.72 |
| 8:I:46:LEU:HD22 | 8:I:56:TRP:HE1 | 1.55 | 0.72 |
| 3:P:271:VAL:HG22 | 3:P:302:THR:HG21 | 1.72 | 0.71 |
| 6:H:703:PRO:HB3 | 6:H:733:VAL:HG21 | 1.71 | 0.71 |
| 6:H:765:ASP:OD1 | 16:X:397:ARG:HG2 | 1.90 | 0.71 |
| 9:K:63:ARG:HB2 | 9:K:65:LEU:CD1 | 2.21 | 0.71 |
| 1:A:1791:ILE:HB | 13:O:598:THR:CG2 | 2.21 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:I:231:VAL:HG21 | 8:I:557:TYR:CZ | 2.25 | 0.71 |
| 1:A:87:VAL:HG12 | 1:A:88:ASP:N | 2.05 | 0.71 |
| 3:C:296:ARG:NH1 | 3:C:296:ARG:HG3 | 2.06 | 0.71 |
| 3:C:407:GLN:O | 3:C:411:ILE:HG12 | 1.91 | 0.71 |
| 9:J:254:THR:CG2 | 9:J:271:HIS:CD2 | 2.74 | 0.71 |
| 13:O:672:VAL:HG11 | 13:O:720:LEU:HD11 | 1.71 | 0.71 |
| 16:X:466:ASP:OD1 | 16:X:482:LYS:HE3 | 1.91 | 0.71 |
| 9:K:263:PHE:CZ | 9:K:290:LYS:HG2 | 2.20 | 0.71 |
| 9:J:223:SER:OG | 9:J:228:GLN:NE2 | 2.24 | 0.71 |
| 9:J:485:ILE:O | 9:J:488:ILE:HG12 | 1.90 | 0.71 |
| 12:N:120:SER:O | 12:N:124:PRO:HD3 | 1.91 | 0.71 |
| 3:P:276:ILE:HG22 | 3:P:277:ARG:N | 2.06 | 0.71 |
| 6:F:130:ARG:HG3 | 16:Y:506:GLN:HE21 | 1.56 | 0.70 |
| 12:N:350:ASP:CB | 12:N:351:PHE:HA | 2.21 | 0.70 |
| 16:Y:77:TYR:HB2 | 16:Y:106:GLN:HG3 | 1.73 | 0.70 |
| 1:A:1405:LEU:HD13 | 1:A:1467:GLY:HA2 | 1.73 | 0.70 |
| 13:O:544:VAL:HA | 13:O:547:LYS:HB3 | 1.73 | 0.70 |
| 14:R:114:LYS:HE2 | 14:R:118:LEU:HD12 | 1.73 | 0.70 |
| 6:F:738:LEU:HD12 | 14:R:494:ILE:HG12 | 1.72 | 0.70 |
| 6:H:685:SER:O | 6:H:689:LEU:HD12 | 1.92 | 0.70 |
| 3:P:407:GLN:O | 3:P:411:ILE:HG12 | 1.91 | 0.70 |
| 6:H:130:ARG:HH12 | 9:K:473:VAL:HG22 | 1.55 | 0.70 |
| 3:C:231:GLU:O | 3:C:250:LYS:NZ | 2.25 | 0.70 |
| 3:C:283:LEU:CD1 | 3:C:306:LEU:HD11 | 2.20 | 0.70 |
| 8:I:48:ARG:HG3 | 8:I:55:VAL:CG2 | 2.21 | 0.70 |
| 9:J:254:THR:CG2 | 9:J:271:HIS:HD2 | 2.01 | 0.70 |
| 6:H:689:LEU:HD11 | 6:H:712:VAL:HG12 | 1.72 | 0.70 |
| 3:C:53:LYS:HD3 | 3:P:96:VAL:HG21 | 1.73 | 0.70 |
| 1:A:1777:GLU:HA | 1:A:1780:THR:HG22 | 1.74 | 0.70 |
| 9:J:305:VAL:HG11 | 11:M:31:ILE:HD11 | 1.74 | 0.70 |
| 1:A:1239:THR:CB | 1:A:1240:SER:HA | 2.22 | 0.70 |
| 1:A:641:TRP:HD1 | 1:A:663:CYS:HB2 | 1.56 | 0.70 |
| 3:C:259:PHE:HB3 | 3:C:265:ILE:HD12 | 1.74 | 0.70 |
| 3:C:99:TYR:CE2 | 3:C:128:LYS:HG3 | 2.27 | 0.70 |
| 8:I:56:TRP:CE3 | 8:I:98:PRO:CB | 2.74 | 0.70 |
| 1:A:1177:MET:HB2 | 1:A:1207:GLY:CA | 2.22 | 0.69 |
| 8:I:214:LEU:O | 8:I:238:THR:OG1 | 2.10 | 0.69 |
| 8:I:269:LEU:HB2 | 8:I:526:LYS:HZ2 | 1.56 | 0.69 |
| 3:P:180:ARG:HG3 | 3:P:212:LEU:HD21 | 1.74 | 0.69 |
| 16:X:170:LYS:HA | 16:Y:49:LEU:HD21 | 1.74 | 0.69 |
| 1:A:1196:TYR:HB2 | 1:A:1208:LEU:HD11 | 1.74 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:594:ARG:HB3 | 1:A:606:ARG:HE | 1.57 | 0.69 |
| 3:C:54:TRP:CZ3 | 3:C:207:LEU:HD22 | 2.22 | 0.69 |
| 12:N:663:GLN:HE21 | 12:N:695:ARG:HG3 | 1.57 | 0.69 |
| 16:X:170:LYS:HA | 16:Y:49:LEU:CD2 | 2.22 | 0.69 |
| 1:A:272:ARG:O | 1:A:407:LEU:HA | 1.92 | 0.69 |
| 3:C:477:HIS:HB3 | 3:C:486:ALA:HB2 | 1.74 | 0.69 |
| 4:D:44:ILE:HA | 4:D:47:LYS:HG2 | 1.74 | 0.69 |
| 8:I:116:MET:SD | 8:I:210:LEU:HG | 2.33 | 0.69 |
| 3:C:234:LEU:HB3 | 3:C:250:LYS:NZ | 2.06 | 0.69 |
| 4:D:5:PHE:CE1 | 13:O:390:PHE:HZ | 2.11 | 0.69 |
| 6:F:554:VAL:HG22 | 9:K:285:PHE:CD2 | 2.28 | 0.69 |
| 6:H:696:ILE:HG13 | 6:H:705:CYS:SG | 2.33 | 0.69 |
| 1:A:1209:LEU:HD22 | 1:A:1228:LEU:HD23 | 1.75 | 0.69 |
| 7:G:6:PRO:HB3 | 9:J:406:HIS:CD2 | 2.27 | 0.69 |
| 3:C:234:LEU:HB3 | 3:C:250:LYS:HZ1 | 1.57 | 0.69 |
| 1:A:125:GLN:HE21 | 1:A:179:ASN:HA | 1.58 | 0.69 |
| 8:I:24:ILE:O | 8:I:569:LEU:HD22 | 1.92 | 0.69 |
| 16:X:201:LEU:HD11 | 16:Y:40:HIS:CB | 2.22 | 0.69 |
| 8:I:353:GLN:HE21 | 8:I:353:GLN:HA | 1.56 | 0.69 |
| 12:N:76:VAL:O | 12:N:80:GLN:HB3 | 1.93 | 0.69 |
| 16:Y:503:LEU:O | 16:Y:506:GLN:NE2 | 2.26 | 0.69 |
| 1:A:1237:PRO:HB2 | 1:A:1238:PRO:CD | 2.20 | 0.68 |
| 1:A:1606:LEU:HD23 | 1:A:1609:LEU:HD13 | 1.75 | 0.68 |
| 8:I:279:ILE:CD1 | 8:I:337:ILE:HA | 2.21 | 0.68 |
| 13:O:114:ASP:HA | 13:O:117:ASP:OD1 | 1.94 | 0.68 |
| 13:O:426:THR:O | 13:O:430:ARG:HB2 | 1.94 | 0.68 |
| 13:O:512:GLN:HA | 13:O:512:GLN:OE1 | 1.93 | 0.68 |
| 9:K:184:LEU:O | 9:K:188:LEU:HD23 | 1.93 | 0.68 |
| 1:A:629:LEU:HB2 | 1:A:630:PRO:HD2 | 1.76 | 0.68 |
| 8:I:251:MET:HE2 | 8:I:379:LEU:HD13 | 1.74 | 0.68 |
| 9:J:332:THR:CA | 9:J:363:LEU:HD21 | 2.22 | 0.68 |
| 16:X:52:ASN:HD22 | 16:Y:202:ALA:HB1 | 1.57 | 0.68 |
| 1:A:185:TYR:O | 1:A:214:LEU:HD23 | 1.94 | 0.68 |
| 3:C:46:ARG:NH2 | 3:C:170:PHE:CG | 2.62 | 0.68 |
| 13:O:114:ASP:O | 13:O:117:ASP:OD1 | 2.12 | 0.68 |
| 3:P:477:HIS:HB3 | 3:P:486:ALA:HB2 | 1.76 | 0.68 |
| 16:X:503:LEU:O | 16:X:506:GLN:NE2 | 2.27 | 0.68 |
| 1:A:1145:LEU:CD2 | 1:A:1611:VAL:HG21 | 2.23 | 0.68 |
| 6:F:703:PRO:HB3 | 6:F:733:VAL:HG21 | 1.74 | 0.68 |
| 3:P:487:ALA:CB | 3:P:519:TYR:HD1 | 2.07 | 0.68 |
| 9:K:372:LEU:HD22 | 9:K:404:VAL:HG22 | 1.76 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:I:81:ALA:HB2 | 8:I:92:LEU:HB3 | 1.76 | 0.67 |
| 12:N:407:LEU:HB2 | 12:N:417:LEU:HD12 | 1.75 | 0.67 |
| 3:P:409:TYR:HA | 3:P:412:LEU:HD12 | 1.75 | 0.67 |
| 1:A:1877:LEU:HD13 | 1:A:1885:LEU:CD1 | 2.25 | 0.67 |
| 1:A:24:GLY:O | 1:A:28:CYS:N | 2.24 | 0.67 |
| 16:X:235:TRP:HD1 | 16:Y:63:MET:HE3 | 1.57 | 0.67 |
| 1:A:1141:VAL:HA | 1:A:1178:ALA:HB2 | 1.77 | 0.67 |
| 3:C:46:ARG:NH2 | 3:C:170:PHE:CB | 2.57 | 0.67 |
| 6:F:502:LEU:CB | 6:F:525:VAL:HG22 | 2.24 | 0.67 |
| 6:F:533:VAL:HG13 | 6:F:568:GLU:OE1 | 1.94 | 0.67 |
| 3:P:244:ILE:HG12 | 3:P:276:ILE:HG13 | 1.76 | 0.67 |
| 3:C:259:PHE:HB3 | 3:C:265:ILE:CD1 | 2.25 | 0.67 |
| 3:P:385:ILE:HD11 | 3:P:412:LEU:HD11 | 1.76 | 0.67 |
| 16:X:355:TYR:CE1 | 16:X:385:ASN:HB3 | 2.29 | 0.67 |
| 6:H:502:LEU:CB | 6:H:525:VAL:HG22 | 2.25 | 0.67 |
| 9:J:263:PHE:HZ | 9:J:290:LYS:CG | 2.06 | 0.67 |
| 9:J:495:PHE:HD2 | 9:J:522:CYS:HG | 1.41 | 0.67 |
| 9:K:210:LYS:O | 9:K:212:TYR:N | 2.23 | 0.67 |
| 13:O:648:ILE:HA | 13:O:651:ILE:HD12 | 1.77 | 0.67 |
| 3:C:119:MET:HA | 3:C:122:ARG:HD2 | 1.76 | 0.67 |
| 3:C:273:TYR:HB3 | 3:C:282:ALA:HB2 | 1.77 | 0.67 |
| 3:C:370:LEU:HG | 14:R:79:TYR:CE1 | 2.29 | 0.67 |
| 4:D:9:PHE:CD2 | 13:O:346:TRP:HZ3 | 2.11 | 0.67 |
| 9:J:477:GLN:O | 9:J:508:LEU:HD13 | 1.95 | 0.67 |
| 1:A:1239:THR:HB | 1:A:1240:SER:CA | 2.25 | 0.67 |
| 1:A:1181:LEU:HB3 | 1:A:1611:VAL:HG11 | 1.76 | 0.67 |
| 3:C:279:ILE:HD12 | 3:C:279:ILE:H | 1.60 | 0.67 |
| 13:O:146:LEU:HB2 | 13:O:151:VAL:HG23 | 1.77 | 0.67 |
| 16:X:271:VAL:HG12 | 16:X:304:LEU:HD21 | 1.75 | 0.67 |
| 8:I:73:TRP:CG | 8:I:80:LEU:HD13 | 2.30 | 0.67 |
| 9:J:19:TYR:CD1 | 9:J:49:LEU:HD13 | 2.29 | 0.67 |
| 11:M:2:ASP:OD2 | 3:P:177:VAL:HG13 | 1.95 | 0.67 |
| 6:H:656:MET:O | 6:H:660:LYS:HG3 | 1.94 | 0.66 |
| 8:I:574:PHE:CE1 | 8:I:576:TRP:HB2 | 2.30 | 0.66 |
| 8:I:574:PHE:HE1 | 8:I:576:TRP:HB2 | 1.60 | 0.66 |
| 1:A:44:PRO:HA | 1:A:45:ALA:CB | 2.25 | 0.66 |
| 7:G:3:ARG:HA | 9:J:373:TYR:OH | 1.95 | 0.66 |
| 1:A:1229:SER:HB3 | 1:A:1236:LEU:HA | 1.78 | 0.66 |
| 1:A:210:MET:HB3 | 1:A:223:LEU:CB | 2.24 | 0.66 |
| 12:N:333:TYR:HD1 | 12:N:364:CYS:HG | 1.43 | 0.66 |
| 3:C:413:LYS:C | 3:C:415:PRO:HD2 | 2.16 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:I:26:LEU:HB3 | 8:I:37:LEU:CB | 2.24 | 0.66 |
| 7:G:3:ARG:NH1 | 9:J:243:TYR:HD1 | 1.93 | 0.66 |
| 3:P:283:LEU:HD13 | 3:P:306:LEU:HD11 | 1.76 | 0.66 |
| 9:K:285:PHE:HB2 | 9:K:308:TYR:CE1 | 2.29 | 0.66 |
| 13:O:490:LEU:HD13 | 13:O:511:ASP:HB2 | 1.77 | 0.66 |
| 16:Y:304:LEU:O | 16:Y:308:MET:HG2 | 1.95 | 0.66 |
| 8:I:13:VAL:HG22 | 8:I:744:PHE:CE2 | 2.30 | 0.66 |
| 3:P:242:GLN:HE22 | 3:P:429:ARG:HG3 | 1.60 | 0.66 |
| 3:C:416:PHE:HB3 | 13:O:326:GLU:HG2 | 1.77 | 0.66 |
| 12:N:362:LYS:HG3 | 12:N:410:LEU:HD23 | 0.68 | 0.66 |
| 13:O:328:ILE:O | 13:O:332:GLN:HG3 | 1.96 | 0.66 |
| 13:O:609:ALA:HA | 13:O:612:LYS:HE3 | 1.76 | 0.66 |
| 3:C:308:TYR:HD2 | 14:R:78:ARG:HD2 | 1.57 | 0.66 |
| 1:A:1674:TRP:CD1 | 1:A:1674:TRP:N | 2.64 | 0.66 |
| 3:C:236:HIS:O | 3:C:239:THR:HG22 | 1.95 | 0.66 |
| 3:C:386:GLN:HE22 | 13:O:282:ILE:HG12 | 1.60 | 0.66 |
| 13:O:477:HIS:HB3 | 13:O:486:ALA:HB2 | 1.77 | 0.66 |
| 13:O:641:LEU:HG | 13:O:670:CYS:HB3 | 1.77 | 0.65 |
| 1:A:1610:TYR:C | 1:A:1610:TYR:CD1 | 2.69 | 0.65 |
| 9:J:285:PHE:HB2 | 9:J:308:TYR:CE1 | 2.31 | 0.65 |
| 9:K:254:THR:HG23 | 9:K:271:HIS:CD2 | 2.32 | 0.65 |
| 12:N:538:GLU:CG | 12:N:561:LEU:HG | 2.25 | 0.65 |
| 12:N:666:ILE:HG12 | 12:N:681:LEU:HD21 | 1.77 | 0.65 |
| 3:P:236:HIS:O | 3:P:239:THR:HG22 | 1.96 | 0.65 |
| 1:A:1209:LEU:HD13 | 1:A:1253:ALA:HB2 | 1.76 | 0.65 |
| 1:A:668:MET:HG2 | 1:A:759:ILE:HG12 | 1.79 | 0.65 |
| 3:C:208:GLU:HA | 3:C:208:GLU:OE1 | 1.97 | 0.65 |
| 13:O:343:CYS:O | 13:O:347:LEU:HB2 | 1.97 | 0.65 |
| 3:C:438:ALA:HA | 14:R:83:ARG:NH1 | 2.11 | 0.65 |
| 8:I:269:LEU:HB2 | 8:I:526:LYS:NZ | 2.11 | 0.65 |
| 9:J:386:LEU:HD12 | 9:J:386:LEU:H | 1.59 | 0.65 |
| 9:J:55:ARG:NH1 | 9:K:264:HIS:HA | 2.11 | 0.65 |
| 1:A:1255:VAL:HG21 | 1:A:1606:LEU:HD11 | 1.79 | 0.65 |
| 16:X:445:THR:O | 16:X:449:THR:HG23 | 1.97 | 0.65 |
| 1:A:1193:ILE:HG23 | 1:A:1208:LEU:HD22 | 1.79 | 0.65 |
| 3:C:101:ARG:HH11 | 3:C:101:ARG:CG | 1.92 | 0.65 |
| 16:Y:445:THR:O | 16:Y:449:THR:HG23 | 1.96 | 0.65 |
| 1:A:799:LEU:O | 1:A:801:PRO:HD2 | 1.97 | 0.65 |
| 8:I:73:TRP:CD1 | 8:I:80:LEU:HD13 | 2.31 | 0.65 |
| 9:J:263:PHE:CZ | 9:J:290:LYS:HG2 | 2.27 | 0.65 |
| 1:A:1307:LEU:HD21 | 1:A:1579:SER:HA | 1.79 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:L:141:VAL:HG11 | 10:L:151:THR:HG21 | 1.78 | 0.64 |
| 14:R:209:TRP:HB2 | 15:S:831:LEU:HD13 | 1.77 | 0.64 |
| 1:A:1405:LEU:HD13 | 1:A:1467:GLY:CA | 2.27 | 0.64 |
| 12:N:362:LYS:HA | 12:N:410:LEU:HD21 | 1.79 | 0.64 |
| 1:A:185:TYR:CE1 | 1:A:273:ARG:HD3 | 2.33 | 0.64 |
| 16:Y:45:ALA:CB | 16:Y:82:TYR:CE2 | 2.80 | 0.64 |
| 1:A:773:LEU:HD22 | 1:A:779:MET:HG3 | 1.79 | 0.64 |
| 6:F:550:VAL:HG21 | 9:K:289:HIS:CG | 2.33 | 0.64 |
| 9:K:185:LEU:HA | 9:K:188:LEU:HD21 | 1.79 | 0.64 |
| 13:O:420:ILE:O | 13:O:424:GLN:N | 2.26 | 0.64 |
| 6:H:89:GLU:HB2 | 6:H:124:VAL:HG11 | 1.80 | 0.64 |
| 6:H:478:SER:HA | 6:H:633:ARG:HH22 | 1.61 | 0.64 |
| 8:I:15:GLY:O | 8:I:743:VAL:N | 2.27 | 0.64 |
| 8:I:206:LEU:HD22 | 8:I:570:PHE:CG | 2.32 | 0.64 |
| 3:C:46:ARG:HH22 | 3:C:170:PHE:CB | 2.11 | 0.64 |
| 3:C:475:LYS:HD2 | 3:C:490:TYR:OH | 1.96 | 0.64 |
| 16:Y:349:SER:HB2 | 16:Y:358:ALA:HB2 | 1.80 | 0.64 |
| 8:I:72:ALA:O | 8:I:80:LEU:HD12 | 1.97 | 0.64 |
| 9:K:300:VAL:HG12 | 9:K:333:TYR:OH | 1.98 | 0.64 |
| 9:K:19:TYR:CD1 | 9:K:49:LEU:HD13 | 2.33 | 0.64 |
| 13:O:354:ARG:HD3 | 13:O:573:LYS:O | 1.98 | 0.64 |
| 3:C:89:LEU:HD21 | 3:C:101:ARG:HH22 | 1.62 | 0.64 |
| 9:K:386:LEU:HD12 | 9:K:386:LEU:H | 1.62 | 0.64 |
| 3:P:327:ASP:O | 3:P:333:THR:HG21 | 1.98 | 0.64 |
| 3:C:93:TYR:CE2 | 3:C:101:ARG:NH2 | 2.65 | 0.64 |
| 3:C:389:ARG:HG2 | 13:O:279:ASP:HB3 | 1.80 | 0.64 |
| 3:P:273:TYR:HB3 | 3:P:282:ALA:HB2 | 1.80 | 0.64 |
| 2:B:14:TRP:HA | 2:B:15:LEU:HG | 1.80 | 0.63 |
| 8:I:67:GLU:O | 8:I:85:ALA:N | 2.25 | 0.63 |
| 13:O:220:ALA:HB2 | 13:O:256:LEU:HD21 | 1.80 | 0.63 |
| 1:A:1413:LEU:HD22 | 1:A:1416:TRP:HZ3 | 1.63 | 0.63 |
| 1:A:15:ARG:HE | 13:O:526:HIS:HB2 | 1.63 | 0.63 |
| 3:C:115:TYR:OH | 3:C:161:LYS:HD2 | 1.97 | 0.63 |
| 3:C:277:ARG:O | 3:C:279:ILE:HD12 | 1.99 | 0.63 |
| 4:D:5:PHE:CZ | 13:O:390:PHE:CZ | 2.86 | 0.63 |
| 9:J:24:PHE:CE1 | 9:J:28:LYS:HE3 | 2.33 | 0.63 |
| 9:J:77:ALA:HB1 | 9:J:93:LEU:HD11 | 1.79 | 0.63 |
| 6:F:554:VAL:HG22 | 9:K:285:PHE:CE2 | 2.33 | 0.63 |
| 4:D:10:PRO:HD2 | 13:O:346:TRP:CE3 | 2.34 | 0.63 |
| 6:H:481:CYS:HB3 | 6:H:512:LEU:HD13 | 1.79 | 0.63 |
| 16:X:304:LEU:O | 16:X:308:MET:HG2 | 1.97 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:Y:462:LYS:HG2 | 16:Y:485:LEU:HD13 | 1.80 | 0.63 |
| 1:A:78:LYS:HD3 | 1:A:592:HIS:HB2 | 1.80 | 0.63 |
| 3:C:409:TYR:HA | 3:C:412:LEU:HD12 | 1.80 | 0.63 |
| 12:N:425:ARG:HG2 | 12:N:425:ARG:NH1 | 2.04 | 0.63 |
| 1:A:1638:TYR:N | 1:A:1638:TYR:CD1 | 2.66 | 0.63 |
| 1:A:185:TYR:HE1 | 1:A:273:ARG:NH1 | 1.95 | 0.63 |
| 1:A:641:TRP:CD1 | 1:A:663:CYS:HB2 | 2.33 | 0.63 |
| 9:K:174:HIS:HA | 9:K:211:LYS:HZ3 | 1.63 | 0.63 |
| 3:P:276:ILE:HG22 | 3:P:277:ARG:H | 1.64 | 0.63 |
| 3:C:235:ALA:N | 3:C:250:LYS:HZ2 | 1.97 | 0.63 |
| 9:J:429:LEU:HA | 9:J:432:ILE:HG22 | 1.79 | 0.63 |
| 2:B:8:TRP:CD1 | 12:N:644:VAL:HG12 | 2.34 | 0.63 |
| 1:A:776:ASN:HD22 | 1:A:779:MET:HG2 | 1.64 | 0.63 |
| 1:A:1170:ASN:O | 1:A:1173:ALA:HB3 | 1.99 | 0.63 |
| 1:A:1409:LEU:HD23 | 1:A:1471:SER:HA | 1.81 | 0.63 |
| 9:J:219:VAL:HG12 | 9:J:221:PRO:HD3 | 1.80 | 0.62 |
| 16:X:462:LYS:HG2 | 16:X:485:LEU:HD13 | 1.81 | 0.62 |
| 1:A:585:HIS:HB3 | 1:A:598:GLU:O | 1.99 | 0.62 |
| 3:C:327:ASP:O | 3:C:333:THR:HG21 | 1.99 | 0.62 |
| 1:A:1218:GLY:N | 1:A:1259:LEU:O | 2.32 | 0.62 |
| 1:A:1595:HIS:NE2 | 1:A:1598:ASP:HB2 | 2.13 | 0.62 |
| 3:C:115:TYR:OH | 3:C:161:LYS:HD3 | 1.98 | 0.62 |
| 7:G:4:ARG:HH21 | 9:J:345:ALA:HB1 | 1.63 | 0.62 |
| 13:O:275:LEU:HD11 | 13:O:307:LEU:HD13 | 1.82 | 0.62 |
| 8:I:231:VAL:HG21 | 8:I:557:TYR:CE1 | 2.34 | 0.62 |
| 16:X:104:LEU:HD11 | 16:X:142:MET:SD | 2.39 | 0.62 |
| 1:A:950:GLY:H | 1:A:1813:GLN:HG2 | 1.65 | 0.62 |
| 6:H:142:LEU:HD21 | 6:H:152:PHE:HB2 | 1.80 | 0.62 |
| 6:H:729:LEU:HD13 | 6:H:739:VAL:HG22 | 1.82 | 0.62 |
| 16:X:355:TYR:CE1 | 16:X:385:ASN:CB | 2.82 | 0.62 |
| 16:Y:407:LEU:HD22 | 16:Y:437:LEU:HD21 | 1.81 | 0.62 |
| 2:B:14:TRP:HA | 2:B:15:LEU:CG | 2.30 | 0.62 |
| 3:C:265:ILE:O | 3:C:269:ILE:HG12 | 1.99 | 0.62 |
| 9:J:167:PHE:HA | 9:J:170:LEU:CD2 | 2.30 | 0.62 |
| 13:O:222:LEU:HB3 | 13:O:230:ALA:HB2 | 1.81 | 0.62 |
| 1:A:1536:LEU:HD23 | 1:A:1562:LEU:HD23 | 1.82 | 0.62 |
| 1:A:1877:LEU:HD13 | 1:A:1885:LEU:HD13 | 1.82 | 0.62 |
| 6:F:502:LEU:HA | 6:F:505:ILE:HD12 | 1.82 | 0.62 |
| 9:K:250:CYS:SG | 9:K:274:THR:CG2 | 2.76 | 0.62 |
| 1:A:1201:HIS:CE1 | 1:A:1203:MET:HB2 | 2.35 | 0.62 |
| 1:A:1323:GLU:HG3 | 1:A:1324:GLN:N | 2.15 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1739:SER:HA | 1:A:1740:ALA:CB | 2.27 | 0.62 |
| 6:H:502:LEU:HA | 6:H:505:ILE:HD12 | 1.82 | 0.62 |
| 8:I:607:ILE:HD12 | 8:I:607:ILE:H | 1.65 | 0.62 |
| 12:N:404:ILE:HA | 12:N:417:LEU:HD11 | 1.82 | 0.62 |
| 13:O:467:ALA:HB1 | 13:O:506:LEU:HD11 | 1.82 | 0.62 |
| 16:X:235:TRP:NE1 | 16:Y:63:MET:SD | 2.73 | 0.62 |
| 3:C:58:LEU:HB3 | 3:C:259:PHE:HE2 | 1.65 | 0.61 |
| 6:H:673:CYS:O | 6:H:677:VAL:HG23 | 2.00 | 0.61 |
| 8:I:28:TRP:NE1 | 8:I:723:ALA:O | 2.30 | 0.61 |
| 9:K:472:LEU:HG | 9:K:481:THR:CG2 | 2.27 | 0.61 |
| 12:N:258:ALA:HA | 12:N:261:VAL:HG22 | 1.82 | 0.61 |
| 1:A:115:LYS:HD3 | 13:O:267:VAL:HG21 | 1.82 | 0.61 |
| 1:A:1871:TYR:HB2 | 1:A:1877:LEU:HD21 | 1.81 | 0.61 |
| 1:A:222:PRO:HD2 | 1:A:405:PRO:HA | 1.82 | 0.61 |
| 9:K:174:HIS:HA | 9:K:211:LYS:NZ | 2.14 | 0.61 |
| 9:K:77:ALA:HB1 | 9:K:93:LEU:HD11 | 1.81 | 0.61 |
| 3:P:39:ILE:HD13 | 3:P:201:LEU:HB2 | 1.81 | 0.61 |
| 3:P:304:SER:HB2 | 3:P:336:VAL:HG22 | 1.82 | 0.61 |
| 6:F:541:THR:HG23 | 14:R:499:ARG:HG2 | 1.81 | 0.61 |
| 16:X:222:MET:O | 16:X:226:VAL:HG23 | 2.00 | 0.61 |
| 9:K:280:LYS:HB3 | 9:K:283:GLU:HG2 | 1.82 | 0.61 |
| 9:K:372:LEU:HD11 | 9:K:407:GLU:HG3 | 1.80 | 0.61 |
| 13:O:657:ILE:HA | 13:O:660:LYS:HB2 | 1.81 | 0.61 |
| 1:A:1238:PRO:HA | 1:A:1239:THR:C | 2.21 | 0.61 |
| 1:A:1519:VAL:HG13 | 1:A:1520:LEU:N | 2.15 | 0.61 |
| 1:A:72:GLU:HG3 | 1:A:94:TYR:OH | 2.00 | 0.61 |
| 3:C:486:ALA:HB3 | 3:C:515:TYR:OH | 2.00 | 0.61 |
| 8:I:392:ALA:HB1 | 8:I:529:MET:HA | 1.81 | 0.61 |
| 1:A:1378:THR:HG23 | 1:A:1380:ASN:H | 1.65 | 0.61 |
| 1:A:217:LEU:HD23 | 3:C:455:CYS:SG | 2.41 | 0.61 |
| 1:A:594:ARG:HG2 | 1:A:608:THR:CG2 | 2.30 | 0.61 |
| 3:P:58:LEU:HB3 | 3:P:259:PHE:HE2 | 1.66 | 0.61 |
| 1:A:445:LEU:HD22 | 1:A:479:ALA:H | 1.65 | 0.61 |
| 3:C:262:SER:O | 3:C:266:VAL:HG23 | 2.01 | 0.61 |
| 3:C:206:TRP:CZ3 | 3:C:233:PHE:CD2 | 2.88 | 0.61 |
| 9:J:397:ILE:HG22 | 9:J:398:ALA:N | 2.16 | 0.61 |
| 9:K:429:LEU:HA | 9:K:432:ILE:HG22 | 1.81 | 0.61 |
| 3:C:206:TRP:CZ3 | 3:C:233:PHE:CG | 2.88 | 0.61 |
| 8:I:269:LEU:CB | 8:I:526:LYS:HZ2 | 2.13 | 0.61 |
| 13:O:365:VAL:HG23 | 13:O:366:LYS:HD3 | 1.82 | 0.61 |
| 16:Y:222:MET:O | 16:Y:226:VAL:HG23 | 2.00 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:39:ILE:HG21 | 3:C:201:LEU:HG | 1.80 | 0.61 |
| 5:E:94:TRP:HZ3 | 6:F:564:LYS:HD2 | 1.65 | 0.61 |
| 1:A:1877:LEU:CD2 | 1:A:1881:GLN:HE22 | 2.13 | 0.61 |
| 1:A:215:HIS:ND1 | 1:A:216:PRO:HD2 | 2.16 | 0.61 |
| 9:J:193:LEU:O | 9:J:197:GLU:HB2 | 2.01 | 0.61 |
| 12:N:516:ILE:HG13 | 12:N:554:MET:HE2 | 1.83 | 0.61 |
| 13:O:348:TYR:CZ | 13:O:361:LEU:HD11 | 2.36 | 0.61 |
| 16:X:349:SER:HB2 | 16:X:358:ALA:HB2 | 1.81 | 0.61 |
| 16:Y:305:ILE:HG23 | 16:Y:340:GLU:OE1 | 2.00 | 0.61 |
| 1:A:1431:PRO:HG2 | 1:A:1434:ILE:HD12 | 1.83 | 0.60 |
| 1:A:1262:GLN:HE22 | 1:A:1582:ALA:CB | 2.14 | 0.60 |
| 1:A:664:LEU:HA | 1:A:667:MET:HB2 | 1.83 | 0.60 |
| 1:A:33:ASN:HA | 1:A:99:MET:HE3 | 1.83 | 0.60 |
| 6:F:729:LEU:HD13 | 6:F:739:VAL:HG22 | 1.82 | 0.60 |
| 13:O:274:LEU:HD11 | 13:O:306:ASN:HB3 | 1.81 | 0.60 |
| 3:C:277:ARG:NH1 | 14:R:77:ASP:OD2 | 2.30 | 0.60 |
| 1:A:188:LEU:HD12 | 1:A:211:PHE:O | 2.01 | 0.60 |
| 3:C:39:ILE:HD13 | 3:C:201:LEU:HB3 | 1.83 | 0.60 |
| 7:G:3:ARG:NH1 | 9:J:243:TYR:CD1 | 2.68 | 0.60 |
| 13:O:619:LEU:O | 13:O:623:THR:HG22 | 2.00 | 0.60 |
| 3:P:265:ILE:O | 3:P:269:ILE:HG12 | 2.01 | 0.60 |
| 1:A:1145:LEU:HD22 | 1:A:1611:VAL:CG2 | 2.28 | 0.60 |
| 1:A:79:GLY:O | 1:A:87:VAL:HG11 | 2.00 | 0.60 |
| 3:C:296:ARG:NH1 | 3:C:299:ASN:H | 1.94 | 0.60 |
| 9:J:9:ARG:O | 9:J:13:TYR:HD2 | 1.84 | 0.60 |
| 16:Y:251:ASN:O | 16:Y:255:ILE:HG22 | 2.01 | 0.60 |
| 1:A:1516:LEU:O | 1:A:1519:VAL:HG12 | 2.02 | 0.60 |
| 1:A:48:LEU:HD22 | 1:A:49:TRP:H | 1.66 | 0.60 |
| 4:D:13:THR:HG22 | 13:O:255:TYR:HE2 | 1.67 | 0.60 |
| 16:X:100:TYR:CD1 | 16:X:138:VAL:HG13 | 2.37 | 0.60 |
| 3:C:352:LEU:O | 3:C:356:ARG:HG3 | 2.01 | 0.60 |
| 9:K:77:ALA:CB | 9:K:93:LEU:HD11 | 2.31 | 0.60 |
| 6:H:656:MET:HE2 | 9:K:523:ILE:HD13 | 1.83 | 0.60 |
| 8:I:364:SER:O | 8:I:367:LYS:HB3 | 2.01 | 0.60 |
| 3:C:441:GLU:O | 3:C:445:LYS:N | 2.17 | 0.60 |
| 1:A:857:MET:CB | 1:A:858:PRO:HD3 | 2.31 | 0.60 |
| 6:F:673:CYS:O | 6:F:677:VAL:HG23 | 2.01 | 0.60 |
| 10:L:63:LEU:HD22 | 10:L:138:GLN:HE21 | 1.67 | 0.60 |
| 3:C:526:TRP:HE1 | 3:C:553:ILE:C | 2.04 | 0.60 |
| 4:D:54:ILE:HD11 | 9:J:506:LEU:HB3 | 1.83 | 0.60 |
| 13:O:361:LEU:HD13 | 13:O:384:LEU:N | 2.17 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:178:VAL:O | 3:C:182:LEU:HD22 | 2.02 | 0.59 |
| 8:I:73:TRP:CE2 | 8:I:80:LEU:HD22 | 2.36 | 0.59 |
| 1:A:97:GLY:O | 1:A:123:VAL:HG23 | 2.02 | 0.59 |
| 1:A:213:MET:HE1 | 1:A:216:PRO:HA | 1.84 | 0.59 |
| 1:A:460:SER:HB3 | 1:A:467:ILE:HD11 | 1.83 | 0.59 |
| 6:H:481:CYS:CB | 6:H:512:LEU:HD13 | 2.32 | 0.59 |
| 9:J:337:TRP:HB3 | 9:J:360:ALA:HB2 | 1.84 | 0.59 |
| 16:X:294:PHE:CE2 | 16:X:311:TYR:HB2 | 2.37 | 0.59 |
| 8:I:349:ILE:HG23 | 8:I:404:LEU:HD11 | 1.83 | 0.59 |
| 8:I:46:LEU:HD22 | 8:I:56:TRP:NE1 | 2.17 | 0.59 |
| 9:J:223:SER:HB3 | 9:J:228:GLN:HE21 | 1.54 | 0.59 |
| 9:K:441:VAL:HG13 | 9:K:474:LEU:HD22 | 1.84 | 0.59 |
| 12:N:531:PHE:CB | 12:N:534:SER:HB2 | 2.32 | 0.59 |
| 12:N:704:VAL:HG23 | 12:N:705:LEU:HD22 | 1.85 | 0.59 |
| 13:O:727:THR:O | 13:O:730:ARG:HB2 | 2.02 | 0.59 |
| 8:I:497:TRP:HE3 | 13:O:492:HIS:CD2 | 2.19 | 0.59 |
| 1:A:1638:TYR:HD1 | 1:A:1638:TYR:H | 1.49 | 0.59 |
| 1:A:210:MET:HB2 | 1:A:239:VAL:HG21 | 1.83 | 0.59 |
| 3:C:101:ARG:CG | 3:C:101:ARG:NH1 | 2.57 | 0.59 |
| 3:C:151:LEU:HD22 | 3:C:178:VAL:HG13 | 1.84 | 0.59 |
| 12:N:619:LEU:HG | 12:N:637:TRP:CH2 | 2.38 | 0.59 |
| 16:X:159:LEU:HD22 | 16:X:171:ILE:HG23 | 1.83 | 0.59 |
| 16:Y:42:ARG:CG | 16:Y:82:TYR:OH | 2.46 | 0.59 |
| 1:A:93:LEU:HD22 | 1:A:128:TRP:CE2 | 2.38 | 0.59 |
| 3:C:510:SER:O | 3:C:512:ALA:N | 2.35 | 0.59 |
| 3:C:535:LYS:O | 3:C:539:PHE:HD1 | 1.86 | 0.59 |
| 12:N:393:THR:O | 12:N:395:ASP:HB3 | 2.02 | 0.59 |
| 12:N:435:VAL:HA | 12:N:438:ILE:HD12 | 1.83 | 0.59 |
| 3:P:389:ARG:HA | 3:P:392:ILE:HG23 | 1.84 | 0.59 |
| 16:X:363:ALA:HB2 | 16:X:379:LYS:NZ | 2.17 | 0.59 |
| 16:X:52:ASN:ND2 | 16:Y:202:ALA:HB1 | 2.18 | 0.59 |
| 10:L:113:LEU:HD13 | 10:L:120:ILE:HD13 | 1.85 | 0.59 |
| 10:L:44:GLN:HA | 10:L:47:ASP:OD2 | 2.03 | 0.59 |
| 11:M:2:ASP:CG | 11:M:3:SER:H | 2.06 | 0.59 |
| 16:Y:159:LEU:HD22 | 16:Y:171:ILE:HG23 | 1.84 | 0.59 |
| 16:Y:294:PHE:CE2 | 16:Y:311:TYR:HB2 | 2.36 | 0.59 |
| 2:B:14:TRP:HA | 2:B:15:LEU:CB | 2.32 | 0.59 |
| 16:Y:45:ALA:HB2 | 16:Y:82:TYR:CD2 | 2.37 | 0.59 |
| 16:X:270:ASN:HA | 16:Y:62:THR:HG21 | 1.84 | 0.59 |
| 16:Y:100:TYR:HD1 | 16:Y:138:VAL:HG13 | 1.68 | 0.59 |
| 9:J:354:MET:HE3 | 9:J:354:MET:HA | 1.85 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:Y:452:LEU:HD21 | 16:Y:460:LYS:HB2 | 1.85 | 0.58 |
| 6:F:130:ARG:CG | 16:Y:506:GLN:HE21 | 2.16 | 0.58 |
| 1:A:1469:CYS:SG | 1:A:1519:VAL:HA | 2.43 | 0.58 |
| 10:L:88:SER:HA | 10:L:145:HIS:O | 2.03 | 0.58 |
| 1:A:877:ILE:HG23 | 1:A:881:ILE:HD12 | 1.84 | 0.58 |
| 8:I:588:PHE:CE1 | 8:I:599:CYS:HB2 | 2.39 | 0.58 |
| 3:C:397:ARG:HA | 3:C:428:LEU:HD21 | 1.85 | 0.58 |
| 7:G:1:MET:HG2 | 9:J:335:PRO:HB3 | 1.86 | 0.58 |
| 9:K:185:LEU:HD13 | 9:K:209:LEU:HD11 | 1.86 | 0.58 |
| 16:X:251:ASN:O | 16:X:255:ILE:HG22 | 2.02 | 0.58 |
| 16:Y:434:TYR:HA | 16:Y:444:LEU:HD13 | 1.84 | 0.58 |
| 3:C:93:TYR:HD1 | 3:C:98:GLU:CD | 2.07 | 0.58 |
| 6:H:522:PHE:HB3 | 6:H:539:TYR:CD1 | 2.38 | 0.58 |
| 8:I:24:ILE:HG22 | 8:I:38:ALA:O | 2.04 | 0.58 |
| 13:O:262:LEU:HD13 | 13:O:270:SER:HB2 | 1.84 | 0.58 |
| 13:O:489:VAL:O | 13:O:492:HIS:N | 2.36 | 0.58 |
| 1:A:1176:LEU:HG | 1:A:1208:LEU:HG | 1.86 | 0.58 |
| 1:A:1470:LEU:HB2 | 1:A:1518:VAL:HG13 | 1.86 | 0.58 |
| 8:I:36:ALA:CB | 8:I:80:LEU:HD21 | 2.33 | 0.58 |
| 9:J:35:GLU:CD | 9:J:63:ARG:HE | 2.06 | 0.58 |
| 10:L:45:LEU:O | 10:L:155:GLN:OE1 | 2.21 | 0.58 |
| 12:N:350:ASP:HB2 | 12:N:351:PHE:HA | 1.86 | 0.58 |
| 12:N:368:THR:CB | 12:N:369:ASP:HA | 2.34 | 0.58 |
| 1:A:31:HIS:CD2 | 13:O:264:VAL:HG22 | 2.39 | 0.58 |
| 16:X:271:VAL:CG1 | 16:X:304:LEU:HD21 | 2.33 | 0.58 |
| 16:X:52:ASN:OD1 | 16:Y:204:ASP:HB2 | 2.03 | 0.58 |
| 1:A:1661:HIS:CE1 | 1:A:1662:LEU:HD23 | 2.38 | 0.58 |
| 3:C:134:THR:HG23 | 3:C:143:LYS:HG3 | 1.86 | 0.58 |
| 9:K:264:HIS:HD2 | 9:K:267:CYS:H | 1.50 | 0.58 |
| 16:X:77:TYR:CE1 | 16:X:107:LYS:HB2 | 2.39 | 0.58 |
| 1:A:1409:LEU:HA | 1:A:1471:SER:HB2 | 1.86 | 0.58 |
| 6:F:145:ASN:HB2 | 6:F:146:PRO:C | 2.24 | 0.58 |
| 8:I:81:ALA:HA | 8:I:92:LEU:HA | 1.85 | 0.58 |
| 9:K:403:PHE:O | 9:K:407:GLU:HG2 | 2.02 | 0.58 |
| 4:D:47:LYS:HD2 | 3:P:355:GLN:HE22 | 1.67 | 0.58 |
| 16:X:203:LEU:HD21 | 16:Y:55:LEU:HD23 | 1.86 | 0.58 |
| 16:X:452:LEU:HD21 | 16:X:460:LYS:HB2 | 1.85 | 0.58 |
| 1:A:852:LEU:HD11 | 1:A:1819:GLU:HB3 | 1.86 | 0.58 |
| 1:A:1465:ILE:HB | 1:A:1491:PHE:HE2 | 1.69 | 0.58 |
| 1:A:1896:ALA:HB3 | 1:A:1897:PRO:HD3 | 1.86 | 0.58 |
| 3:C:101:ARG:HB2 | 3:P:295:TYR:HB2 | 1.86 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:184:LEU:HB3 | 3:C:187:GLU:HG3 | 1.86 | 0.58 |
| 3:C:46:ARG:CZ | 3:C:170:PHE:CG | 2.87 | 0.58 |
| 9:J:332:THR:HA | 9:J:363:LEU:CD2 | 2.27 | 0.58 |
| 9:J:77:ALA:CB | 9:J:93:LEU:HD11 | 2.33 | 0.58 |
| 12:N:281:TYR:CZ | 12:N:356:PRO:HB2 | 2.38 | 0.58 |
| 12:N:546:LYS:HA | 12:N:550:GLY:CA | 2.34 | 0.58 |
| 13:O:308:ALA:HA | 13:O:323:ALA:HB3 | 1.86 | 0.58 |
| 4:D:9:PHE:HD2 | 13:O:346:TRP:CH2 | 2.21 | 0.58 |
| 3:P:252:GLN:O | 3:P:255:ILE:HG22 | 2.04 | 0.58 |
| 3:C:309:VAL:HG23 | 14:R:78:ARG:CG | 2.32 | 0.58 |
| 16:X:282:PHE:HE1 | 16:X:313:TYR:HD2 | 1.52 | 0.58 |
| 1:A:125:GLN:NE2 | 1:A:179:ASN:HA | 2.19 | 0.57 |
| 1:A:213:MET:CE | 1:A:216:PRO:HA | 2.34 | 0.57 |
| 3:C:526:TRP:HE1 | 3:C:553:ILE:CA | 2.15 | 0.57 |
| 6:F:507:ARG:HH11 | 6:F:538:ILE:HD13 | 1.69 | 0.57 |
| 3:P:238:TYR:HB3 | 3:P:247:ALA:HB2 | 1.86 | 0.57 |
| 1:A:1089:LEU:HD12 | 1:A:1145:LEU:HB3 | 1.85 | 0.57 |
| 3:C:106:LEU:HD12 | 3:C:106:LEU:H | 1.68 | 0.57 |
| 3:C:119:MET:HA | 3:C:122:ARG:CD | 2.34 | 0.57 |
| 3:C:381:THR:HG21 | 3:C:412:LEU:HD21 | 1.86 | 0.57 |
| 12:N:73:GLU:O | 12:N:74:TRP:HB3 | 2.04 | 0.57 |
| 3:P:276:ILE:CG2 | 3:P:277:ARG:N | 2.67 | 0.57 |
| 3:C:89:LEU:HD11 | 3:C:105:PHE:CD2 | 2.39 | 0.57 |
| 6:H:145:ASN:HB2 | 6:H:146:PRO:C | 2.25 | 0.57 |
| 1:A:1376:LEU:HD23 | 1:A:1377:LYS:HG3 | 1.85 | 0.57 |
| 1:A:1399:VAL:HG11 | 1:A:1404:LEU:HG | 1.86 | 0.57 |
| 1:A:667:MET:O | 1:A:755:LEU:O | 2.23 | 0.57 |
| 8:I:730:VAL:HG22 | 8:I:731:SER:N | 2.19 | 0.57 |
| 9:J:445:GLU:HA | 9:J:474:LEU:HD23 | 1.85 | 0.57 |
| 12:N:527:LEU:HD21 | 12:N:561:LEU:HD22 | 1.85 | 0.57 |
| 12:N:676:TRP:O | 12:N:713:PHE:HB2 | 2.05 | 0.57 |
| 3:P:441:GLU:HG2 | 3:P:472:LYS:CE | 2.34 | 0.57 |
| 1:A:1252:ALA:O | 1:A:1256:GLY:N | 2.36 | 0.57 |
| 1:A:44:PRO:HB2 | 3:C:181:LYS:HD3 | 1.84 | 0.57 |
| 3:C:93:TYR:CD1 | 3:C:98:GLU:CD | 2.78 | 0.57 |
| 9:J:270:VAL:O | 9:J:274:THR:HG22 | 2.05 | 0.57 |
| 3:C:120:TYR:CE2 | 3:C:124:LEU:HD11 | 2.39 | 0.57 |
| 6:F:684:LYS:HD3 | 6:F:687:LYS:HD2 | 1.86 | 0.57 |
| 10:L:153:MET:HG2 | 10:L:156:ILE:HD11 | 1.85 | 0.57 |
| 12:N:277:CYS:HA | 12:N:285:PHE:CE2 | 2.38 | 0.57 |
| 13:O:231:LEU:HD23 | 13:O:236:LEU:CA | 2.34 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:O:381:ILE:HG21 | 13:O:405:SER:HB2 | 1.85 | 0.57 |
| 13:O:578:GLU:HA | 13:O:616:LEU:CD1 | 2.31 | 0.57 |
| 3:P:48:LEU:HD21 | 3:P:116:PHE:CZ | 2.39 | 0.57 |
| 9:K:373:TYR:CE1 | 7:W:4:ARG:HG2 | 2.39 | 0.57 |
| 16:X:215:LYS:O | 16:X:219:VAL:HG23 | 2.04 | 0.57 |
| 16:Y:215:LYS:O | 16:Y:219:VAL:HG23 | 2.04 | 0.57 |
| 1:A:1433:ILE:H | 1:A:1433:ILE:CD1 | 1.98 | 0.57 |
| 3:C:301:ASP:OD1 | 3:C:335:CYS:HB3 | 2.05 | 0.57 |
| 8:I:79:LEU:HD11 | 8:I:168:LEU:HD23 | 1.86 | 0.57 |
| 9:J:264:HIS:HD2 | 9:J:267:CYS:H | 1.51 | 0.57 |
| 9:J:439:VAL:HG21 | 9:J:448:LEU:HD21 | 1.86 | 0.57 |
| 4:D:5:PHE:CZ | 13:O:390:PHE:HZ | 2.23 | 0.57 |
| 1:A:1032:LEU:HD12 | 1:A:1035:GLN:HB3 | 1.86 | 0.57 |
| 12:N:293:ILE:O | 12:N:297:VAL:HG23 | 2.05 | 0.57 |
| 12:N:456:LEU:HA | 12:N:548:ARG:HH21 | 1.69 | 0.57 |
| 13:O:386:GLN:HB2 | 13:O:424:GLN:HE22 | 1.70 | 0.57 |
| 3:C:238:TYR:HB3 | 3:C:247:ALA:HB2 | 1.87 | 0.57 |
| 8:I:17:LYS:CE | 8:I:51:SER:O | 2.53 | 0.57 |
| 8:I:32:ARG:HB2 | 8:I:34:LEU:CD2 | 2.35 | 0.57 |
| 12:N:164:SER:H | 12:N:165:THR:HA | 1.69 | 0.57 |
| 3:C:416:PHE:H | 13:O:326:GLU:CD | 2.07 | 0.56 |
| 16:X:40:HIS:HB3 | 16:Y:201:LEU:HD13 | 1.87 | 0.56 |
| 1:A:1079:ALA:HB1 | 1:A:1556:LEU:HA | 1.87 | 0.56 |
| 1:A:667:MET:O | 1:A:756:PHE:N | 2.37 | 0.56 |
| 8:I:166:LYS:O | 8:I:170:ASP:HB2 | 2.05 | 0.56 |
| 13:O:490:LEU:O | 13:O:494:LYS:HB2 | 2.04 | 0.56 |
| 1:A:93:LEU:HB2 | 1:A:128:TRP:CH2 | 2.39 | 0.56 |
| 1:A:48:LEU:HD13 | 1:A:50:SER:CA | 2.36 | 0.56 |
| 9:J:245:CYS:HA | 9:J:247:PHE:CE1 | 2.39 | 0.56 |
| 13:O:530:SER:O | 13:O:533:THR:HG23 | 2.04 | 0.56 |
| 3:P:276:ILE:CG2 | 3:P:277:ARG:H | 2.17 | 0.56 |
| 16:Y:96:ALA:O | 16:Y:100:TYR:HD2 | 1.88 | 0.56 |
| 3:C:48:LEU:HD21 | 3:C:116:PHE:CZ | 2.39 | 0.56 |
| 3:C:353:TYR:CZ | 3:C:356:ARG:NH1 | 2.73 | 0.56 |
| 16:Y:45:ALA:HB3 | 16:Y:82:TYR:HE2 | 1.71 | 0.56 |
| 1:A:248:PHE:CD1 | 1:A:430:VAL:O | 2.58 | 0.56 |
| 6:H:689:LEU:HD21 | 6:H:713:LEU:HG | 1.85 | 0.56 |
| 13:O:576:ASN:ND2 | 13:O:579:MET:HB2 | 2.20 | 0.56 |
| 4:D:9:PHE:CD2 | 13:O:346:TRP:CZ3 | 2.81 | 0.56 |
| 1:A:1236:LEU:HD21 | 1:A:1243:LEU:HD13 | 1.86 | 0.56 |
| 3:C:202:HIS:CE1 | 3:C:205:ALA:H | 2.23 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:X:434:TYR:HA | 16:X:444:LEU:HD13 | 1.86 | 0.56 |
| 1:A:1251:VAL:O | 1:A:1255:VAL:HG23 | 2.06 | 0.56 |
| 1:A:257:MET:HG2 | 1:A:430:VAL:HG11 | 1.86 | 0.56 |
| 6:H:146:PRO:HG3 | 6:H:167:THR:HA | 1.88 | 0.56 |
| 9:K:376:LEU:HG | 9:K:407:GLU:OE1 | 2.06 | 0.56 |
| 9:K:418:TRP:HB3 | 9:K:458:LEU:HD12 | 1.87 | 0.56 |
| 13:O:605:LEU:HD23 | 13:O:608:LEU:HD12 | 1.87 | 0.56 |
| 3:P:296:ARG:HD2 | 3:P:298:GLU:HB3 | 1.87 | 0.56 |
| 3:C:47:GLY:HA3 | 3:C:94:PHE:HE2 | 1.70 | 0.56 |
| 6:F:59:ARG:HH22 | 6:H:562:MET:HB2 | 1.69 | 0.56 |
| 8:I:56:TRP:CZ3 | 8:I:58:PHE:HB2 | 2.31 | 0.56 |
| 13:O:104:GLU:N | 13:O:107:ASP:OD2 | 2.39 | 0.56 |
| 1:A:79:GLY:O | 1:A:87:VAL:CG1 | 2.53 | 0.56 |
| 4:D:10:PRO:HG3 | 13:O:345:SER:HB3 | 1.88 | 0.56 |
| 4:D:53:PRO:HB3 | 3:P:385:ILE:HD13 | 1.88 | 0.56 |
| 9:J:20:GLN:HB2 | 9:K:165:GLU:CD | 2.26 | 0.56 |
| 9:J:495:PHE:CZ | 9:J:525:MET:HG2 | 2.40 | 0.56 |
| 6:F:125:TYR:HD1 | 6:F:130:ARG:HE | 1.50 | 0.56 |
| 5:E:92:ASP:HB3 | 6:H:592:ARG:NH2 | 2.21 | 0.56 |
| 16:X:77:TYR:N | 16:X:106:GLN:HE21 | 2.04 | 0.56 |
| 1:A:1644:TYR:O | 1:A:1645:GLU:HG2 | 2.06 | 0.55 |
| 3:C:376:MET:O | 14:R:130:ILE:HG21 | 2.06 | 0.55 |
| 6:F:125:TYR:CD1 | 6:F:130:ARG:NE | 2.69 | 0.55 |
| 9:K:272:ILE:HG23 | 9:K:307:CYS:SG | 2.47 | 0.55 |
| 13:O:244:LEU:HD22 | 13:O:248:PRO:HA | 1.88 | 0.55 |
| 3:C:379:LYS:HE2 | 14:R:94:LEU:HB3 | 1.86 | 0.55 |
| 6:F:666:PRO:O | 6:F:667:GLN:HG3 | 2.07 | 0.55 |
| 6:F:696:ILE:HG12 | 6:F:705:CYS:SG | 2.46 | 0.55 |
| 1:A:118:THR:OG1 | 13:O:266:ASP:OD1 | 2.24 | 0.55 |
| 3:C:170:PHE:O | 3:C:173:TYR:N | 2.40 | 0.55 |
| 13:O:123:GLU:N | 13:O:124:PRO:HA | 2.20 | 0.55 |
| 16:Y:269:ASP:HB3 | 16:Y:300:LEU:HD21 | 1.89 | 0.55 |
| 6:F:611:PHE:CB | 6:F:620:ALA:HB2 | 2.36 | 0.55 |
| 6:H:128:THR:HG21 | 6:H:130:ARG:HH12 | 1.71 | 0.55 |
| 9:K:167:PHE:CE1 | 9:K:171:THR:HG21 | 2.42 | 0.55 |
| 12:N:519:TYR:O | 12:N:523:LEU:HG | 2.07 | 0.55 |
| 13:O:504:ALA:HA | 13:O:507:TRP:NE1 | 2.21 | 0.55 |
| 16:Y:168:THR:HB | 16:Y:169:PRO:HD2 | 1.88 | 0.55 |
| 1:A:39:LEU:HD12 | 1:A:40:ARG:HG2 | 1.87 | 0.55 |
| 1:A:762:ILE:O | 1:A:765:VAL:HG12 | 2.06 | 0.55 |
| 6:F:522:PHE:HB3 | 6:F:539:TYR:CD1 | 2.42 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 6:F:611:PHE:HB3 | 6:F:620:ALA:HB2 | 1.87 | 0.55 |
| 9:J:178:ALA:HB1 | 9:J:213:ASN:HD22 | 1.71 | 0.55 |
| 9:J:53:TYR:O | 9:J:79:CYS:SG | 2.65 | 0.55 |
| 10:L:50:LEU:HD21 | 10:L:119:TRP:HZ2 | 1.72 | 0.55 |
| 12:N:289:PHE:HA | 12:N:292:TRP:CB | 2.33 | 0.55 |
| 2:B:8:TRP:HD1 | 12:N:644:VAL:HG12 | 1.71 | 0.55 |
| 3:P:48:LEU:HD21 | 3:P:116:PHE:CE2 | 2.41 | 0.55 |
| 14:R:388[A]:CYS:HG | 14:R:389:SER:N | 2.04 | 0.55 |
| 1:A:1165:HIS:HD2 | 1:A:1167:GLU:HB2 | 1.71 | 0.55 |
| 1:A:1751:ALA:HA | 1:A:1755:CYS:SG | 2.47 | 0.55 |
| 1:A:189:PHE:HB2 | 1:A:211:PHE:HB2 | 1.88 | 0.55 |
| 1:A:48:LEU:HD13 | 1:A:50:SER:CB | 2.37 | 0.55 |
| 3:C:217:GLU:HA | 3:C:220:LYS:HD2 | 1.88 | 0.55 |
| 3:C:397:ARG:O | 3:C:428:LEU:CD2 | 2.55 | 0.55 |
| 6:F:739:VAL:O | 6:F:743:ILE:HG13 | 2.06 | 0.55 |
| 6:H:611:PHE:CB | 6:H:620:ALA:HB2 | 2.37 | 0.55 |
| 9:J:25:TRP:NE1 | 9:K:162:TYR:O | 2.31 | 0.55 |
| 12:N:289:PHE:O | 12:N:291:LYS:N | 2.38 | 0.55 |
| 13:O:536:THR:HA | 13:O:543:GLY:HA3 | 1.87 | 0.55 |
| 13:O:688:GLU:O | 13:O:691:ILE:HG22 | 2.06 | 0.55 |
| 14:R:177:ASP:OD1 | 15:S:834:ILE:CD1 | 2.50 | 0.55 |
| 16:Y:83:HIS:O | 16:Y:86:SER:OG | 2.19 | 0.55 |
| 1:A:1333:HIS:HB2 | 1:A:1357:THR:HA | 1.89 | 0.55 |
| 1:A:1621:PRO:HA | 1:A:1697:LEU:O | 2.07 | 0.55 |
| 3:C:313:LYS:HG2 | 3:C:343:LEU:HD13 | 1.87 | 0.55 |
| 8:I:353:GLN:NE2 | 8:I:353:GLN:HA | 2.22 | 0.55 |
| 8:I:197:ARG:O | 8:I:545:GLY:HA3 | 2.06 | 0.55 |
| 6:H:611:PHE:HB3 | 6:H:620:ALA:HB2 | 1.89 | 0.55 |
| 8:I:28:TRP:CD1 | 8:I:723:ALA:HB1 | 2.42 | 0.55 |
| 9:J:37:PRO:HA | 9:J:65:LEU:HD11 | 1.88 | 0.55 |
| 16:Y:70:LEU:HD12 | 16:Y:71:PHE:CE2 | 2.42 | 0.55 |
| 1:A:1502:PRO:O | 1:A:1503:ASN:HB3 | 2.07 | 0.55 |
| 3:C:416:PHE:CD2 | 13:O:323:ALA:HB2 | 2.42 | 0.55 |
| 8:I:52:PHE:CD1 | 8:I:743:VAL:HG21 | 2.42 | 0.55 |
| 6:H:86:ALA:HB2 | 9:K:473:VAL:O | 2.07 | 0.55 |
| 12:N:559:VAL:HA | 12:N:562:LYS:HG2 | 1.89 | 0.55 |
| 16:Y:423:ILE:HG13 | 16:Y:424:ARG:N | 2.22 | 0.55 |
| 1:A:1573:SER:HB2 | 1:A:1617:ARG:NH2 | 2.19 | 0.55 |
| 1:A:77:ARG:HG2 | 1:A:78:LYS:O | 2.07 | 0.55 |
| 4:D:42:GLN:O | 4:D:46:GLU:HG2 | 2.07 | 0.55 |
| 6:F:104:ASP:OD1 | 6:F:104:ASP:N | 2.37 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:I:536:CYS:O | 8:I:540:PRO:HD3 | 2.07 | 0.55 |
| 9:K:495:PHE:CZ | 9:K:525:MET:HG2 | 2.41 | 0.55 |
| 13:O:356:ASP:HA | 13:O:357:SER:HB2 | 1.88 | 0.55 |
| 1:A:1137:PHE:O | 1:A:1141:VAL:HG23 | 2.07 | 0.54 |
| 3:C:554:LEU:HD13 | 9:K:386:LEU:HD11 | 1.88 | 0.54 |
| 3:C:93:TYR:CE1 | 3:C:98:GLU:OE2 | 2.60 | 0.54 |
| 8:I:115:TRP:CZ3 | 8:I:176:LEU:HD22 | 2.42 | 0.54 |
| 1:A:1094:PRO:HG2 | 1:A:1147:ILE:HG12 | 1.90 | 0.54 |
| 1:A:1251:VAL:HG12 | 1:A:1294:TYR:HA | 1.88 | 0.54 |
| 3:C:173:TYR:CD1 | 3:C:202:HIS:CE1 | 2.93 | 0.54 |
| 9:J:185:LEU:HD13 | 9:J:206:GLU:OE1 | 2.08 | 0.54 |
| 6:H:653:LEU:HD22 | 9:K:523:ILE:CG2 | 2.36 | 0.54 |
| 12:N:542:VAL:HG11 | 12:N:558:GLU:HG2 | 1.89 | 0.54 |
| 13:O:119:PHE:CE1 | 13:O:136:LEU:HD11 | 2.42 | 0.54 |
| 16:X:168:THR:HB | 16:X:169:PRO:HD2 | 1.89 | 0.54 |
| 16:Y:42:ARG:CA | 16:Y:82:TYR:CE2 | 2.70 | 0.54 |
| 1:A:1332:GLY:O | 1:A:1358:ILE:HG13 | 2.08 | 0.54 |
| 6:H:689:LEU:HD11 | 6:H:712:VAL:CG1 | 2.37 | 0.54 |
| 8:I:195:ILE:HD11 | 8:I:251:MET:HE3 | 1.88 | 0.54 |
| 9:J:319:ALA:O | 9:J:323:LEU:HD22 | 2.08 | 0.54 |
| 9:J:322:TYR:HE1 | 11:M:36:LEU:HD11 | 1.72 | 0.54 |
| 9:K:355:ALA:O | 9:K:359:THR:HG22 | 2.07 | 0.54 |
| 2:B:15:LEU:HD12 | 12:N:633:ARG:HG2 | 1.90 | 0.54 |
| 13:O:119:PHE:HE1 | 13:O:136:LEU:HD21 | 1.72 | 0.54 |
| 9:J:69:TYR:O | 9:J:70:GLU:CB | 2.56 | 0.54 |
| 12:N:425:ARG:CG | 12:N:425:ARG:HH11 | 2.10 | 0.54 |
| 1:A:181:TRP:HB2 | 1:A:188:LEU:HB3 | 1.90 | 0.54 |
| 3:C:41:GLY:O | 3:C:45:GLU:HG2 | 2.07 | 0.54 |
| 6:F:164:PRO:CG | 6:F:471:LYS:HG3 | 2.38 | 0.54 |
| 6:H:553:SER:HA | 6:H:576:CYS:SG | 2.48 | 0.54 |
| 6:H:739:VAL:O | 6:H:743:ILE:HG13 | 2.07 | 0.54 |
| 8:I:138:LEU:CD1 | 8:I:253:ARG:HA | 2.37 | 0.54 |
| 8:I:195:ILE:HD11 | 8:I:251:MET:CE | 2.37 | 0.54 |
| 13:O:76:SER:HB2 | 13:O:165:GLY:HA2 | 1.89 | 0.54 |
| 3:P:361:ASN:HD22 | 3:P:363:ARG:N | 2.05 | 0.54 |
| 1:A:1019:MET:HB2 | 1:A:1021:HIS:CE1 | 2.42 | 0.54 |
| 1:A:1412:CYS:HB2 | 1:A:1471:SER:OG | 2.08 | 0.54 |
| 1:A:1877:LEU:CD1 | 1:A:1885:LEU:CD1 | 2.85 | 0.54 |
| 3:C:244:ILE:HD13 | 3:C:276:ILE:HG12 | 1.89 | 0.54 |
| 3:C:493:TYR:CE2 | 3:C:497:ILE:HD11 | 2.43 | 0.54 |
| 6:F:146:PRO:HG3 | 6:F:167:THR:HA | 1.89 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:H:638:TRP:CZ3 | 6:H:660:LYS:HD2 | 2.43 | 0.54 |
| 16:Y:200:PRO:O | 16:Y:202:ALA:N | 2.28 | 0.54 |
| 3:C:46:ARG:HB3 | 3:C:116:PHE:CE2 | 2.43 | 0.54 |
| 9:K:391:PHE:CE2 | 9:K:411:VAL:HG21 | 2.42 | 0.54 |
| 3:P:238:TYR:CB | 3:P:247:ALA:HB2 | 2.38 | 0.54 |
| 1:A:456:LYS:HB3 | 1:A:469:GLY:HA3 | 1.90 | 0.54 |
| 6:F:59:ARG:HH12 | 6:H:562:MET:HG3 | 1.73 | 0.54 |
| 1:A:1431:PRO:HG2 | 1:A:1434:ILE:CD1 | 2.38 | 0.54 |
| 1:A:1595:HIS:CE1 | 1:A:1598:ASP:HB2 | 2.43 | 0.54 |
| 1:A:250:ASN:HD22 | 1:A:251:THR:N | 2.06 | 0.53 |
| 1:A:34:ALA:O | 13:O:237:GLN:NE2 | 2.41 | 0.53 |
| 13:O:354:ARG:CD | 13:O:573:LYS:O | 2.57 | 0.53 |
| 3:P:117:LEU:O | 3:P:117:LEU:HD23 | 2.07 | 0.53 |
| 3:P:270:ALA:HB2 | 3:P:285:ILE:HG22 | 1.90 | 0.53 |
| 16:X:269:ASP:HB3 | 16:X:300:LEU:HD21 | 1.91 | 0.53 |
| 1:A:1306:CYS:HB2 | 1:A:1374:ILE:HG12 | 1.88 | 0.53 |
| 1:A:1750:PHE:HD2 | 1:A:1775:LEU:HD12 | 1.73 | 0.53 |
| 8:I:218:SER:OG | 8:I:584:HIS:ND1 | 2.41 | 0.53 |
| 9:J:253:LEU:O | 9:J:256:VAL:HG22 | 2.08 | 0.53 |
| 12:N:165:THR:N | 12:N:166:PRO:CA | 2.71 | 0.53 |
| 16:X:192:TYR:HA | 16:X:195:VAL:HG22 | 1.90 | 0.53 |
| 1:A:776:ASN:O | 1:A:777:THR:HB | 2.07 | 0.53 |
| 1:A:1794:ASP:HA | 1:A:1797:ILE:HG12 | 1.91 | 0.53 |
| 1:A:189:PHE:N | 1:A:211:PHE:O | 2.39 | 0.53 |
| 3:C:238:TYR:CD1 | 3:C:243:LEU:HD12 | 2.44 | 0.53 |
| 3:C:79:GLU:OE1 | 3:C:79:GLU:N | 2.39 | 0.53 |
| 6:H:762:TRP:HA | 6:H:765:ASP:HB2 | 1.89 | 0.53 |
| 8:I:370:ALA:HB1 | 8:I:383:ALA:HA | 1.91 | 0.53 |
| 8:I:360:LEU:HD21 | 8:I:390:ILE:HG23 | 1.90 | 0.53 |
| 9:K:258:MET:HG3 | 9:K:271:HIS:CD2 | 2.43 | 0.53 |
| 3:P:120:TYR:CZ | 3:P:124:LEU:HD11 | 2.43 | 0.53 |
| 1:A:1243:LEU:O | 1:A:1245:VAL:N | 2.41 | 0.53 |
| 1:A:1329:MET:HE2 | 1:A:1368:THR:HG22 | 1.90 | 0.53 |
| 3:C:206:TRP:CE3 | 3:C:233:PHE:CG | 2.96 | 0.53 |
| 13:O:236:LEU:HD23 | 13:O:260:ASN:HB2 | 1.90 | 0.53 |
| 13:O:351:GLY:C | 13:O:353:LYS:H | 2.12 | 0.53 |
| 16:X:76:LYS:HB3 | 16:X:106:GLN:HE22 | 1.73 | 0.53 |
| 1:A:1543:HIS:CD2 | 1:A:1559:HIS:CE1 | 2.97 | 0.53 |
| 1:A:248:PHE:CZ | 1:A:250:ASN:HB2 | 2.43 | 0.53 |
| 1:A:412:LEU:O | 1:A:468:PHE:HE2 | 1.91 | 0.53 |
| 1:A:966:PRO:HG3 | 1:A:980:ARG:HE | 1.74 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:358:LEU:HD21 | 3:C:368:TRP:NE1 | 2.23 | 0.53 |
| 7:G:15:ASP:O | 9:J:487:TYR:OH | 2.23 | 0.53 |
| 13:O:33:TYR:CE2 | 13:O:73:ILE:HG13 | 2.44 | 0.53 |
| 8:I:207:ALA:HB1 | 8:I:575:LEU:HD12 | 1.90 | 0.53 |
| 9:J:227:LEU:HD12 | 9:K:32:LEU:HG | 1.90 | 0.53 |
| 9:J:324:SER:O | 9:J:328:THR:HG23 | 2.09 | 0.53 |
| 9:K:280:LYS:CB | 9:K:283:GLU:HG2 | 2.38 | 0.53 |
| 3:P:170:PHE:O | 3:P:173:TYR:N | 2.41 | 0.53 |
| 1:A:93:LEU:HD21 | 1:A:151:ILE:HG13 | 1.90 | 0.53 |
| 1:A:1672:ARG:HD2 | 1:A:1705:GLN:HB3 | 1.91 | 0.53 |
| 1:A:31:HIS:CG | 1:A:32:PRO:HD2 | 2.43 | 0.53 |
| 1:A:48:LEU:HD22 | 1:A:48:LEU:C | 2.27 | 0.53 |
| 3:C:93:TYR:CD1 | 3:C:98:GLU:OE2 | 2.62 | 0.53 |
| 6:H:168:PHE:CB | 6:H:467:ARG:HD3 | 2.38 | 0.53 |
| 8:I:27:VAL:C | 8:I:35:ILE:HD12 | 2.28 | 0.53 |
| 10:L:63:LEU:HD22 | 10:L:138:GLN:NE2 | 2.24 | 0.53 |
| 16:X:423:ILE:HG13 | 16:X:424:ARG:N | 2.23 | 0.53 |
| 16:X:76:LYS:CB | 16:X:106:GLN:NE2 | 2.72 | 0.53 |
| 6:F:168:PHE:CB | 6:F:467:ARG:HD3 | 2.39 | 0.53 |
| 6:H:128:THR:HG21 | 6:H:130:ARG:NH1 | 2.23 | 0.53 |
| 8:I:174:ASN:OD1 | 8:I:190:TYR:HA | 2.08 | 0.53 |
| 9:J:406:HIS:HE1 | 9:J:450:ASN:HD22 | 1.55 | 0.53 |
| 9:J:442:ASP:OD1 | 9:J:475:ILE:HG22 | 2.09 | 0.53 |
| 12:N:503:SER:O | 12:N:507:SER:HB3 | 2.09 | 0.53 |
| 12:N:612:PRO:HG2 | 12:N:615:ILE:HG12 | 1.91 | 0.53 |
| 12:N:78:VAL:O | 12:N:81:ASN:N | 2.42 | 0.53 |
| 13:O:83:GLU:HG3 | 13:O:90:ALA:CB | 2.39 | 0.53 |
| 14:R:91:ALA:O | 14:R:92:SER:C | 2.46 | 0.53 |
| 1:A:1153:ILE:HD11 | 1:A:1184:HIS:HB3 | 1.91 | 0.53 |
| 3:C:152:ARG:HG3 | 3:C:153:GLU:N | 2.23 | 0.53 |
| 8:I:639:LEU:HB2 | 8:I:652:VAL:HG12 | 1.91 | 0.53 |
| 10:L:126:ASP:OD2 | 10:L:130:LYS:O | 2.27 | 0.53 |
| 2:B:11:VAL:HG13 | 12:N:642:GLY:HA2 | 1.90 | 0.53 |
| 4:D:48:ASP:OD2 | 3:P:386:GLN:HG2 | 2.09 | 0.53 |
| 16:X:203:LEU:CD2 | 16:Y:55:LEU:HD23 | 2.39 | 0.53 |
| 1:A:1078:MET:HB2 | 1:A:1552:TYR:CE1 | 2.44 | 0.52 |
| 1:A:476:ALA:HB3 | 1:A:492:GLU:HA | 1.91 | 0.52 |
| 1:A:641:TRP:CD1 | 1:A:663:CYS:CB | 2.92 | 0.52 |
| 3:C:141:LEU:HD22 | 3:C:368:TRP:HZ2 | 1.73 | 0.52 |
| 6:F:498:THR:HG21 | 6:H:33:ALA:HB2 | 1.90 | 0.52 |
| 8:I:207:ALA:CB | 8:I:575:LEU:HD12 | 2.38 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:K:46:CYS:O | 9:K:50:THR:OG1 | 2.23 | 0.52 |
| 3:C:416:PHE:CE2 | 13:O:323:ALA:HB2 | 2.43 | 0.52 |
| 7:G:4:ARG:HD2 | 9:J:373:TYR:CD1 | 2.44 | 0.52 |
| 1:A:1165:HIS:CD2 | 1:A:1167:GLU:HB2 | 2.45 | 0.52 |
| 1:A:506:VAL:HA | 1:A:639:VAL:HG23 | 1.91 | 0.52 |
| 9:K:324:SER:O | 9:K:328:THR:HG23 | 2.09 | 0.52 |
| 16:X:282:PHE:HE1 | 16:X:313:TYR:CD2 | 2.28 | 0.52 |
| 3:C:202:HIS:CE1 | 3:C:205:ALA:N | 2.78 | 0.52 |
| 8:I:65:GLY:HA3 | 8:I:84:LEU:HB3 | 1.91 | 0.52 |
| 8:I:64:THR:HG22 | 8:I:84:LEU:HD11 | 1.90 | 0.52 |
| 9:K:429:LEU:O | 9:K:433:LYS:HG3 | 2.10 | 0.52 |
| 12:N:202:GLU:O | 12:N:204:ASP:N | 2.42 | 0.52 |
| 13:O:608:LEU:HD22 | 13:O:612:LYS:HE2 | 1.91 | 0.52 |
| 14:R:175:ILE:O | 15:S:833:ASP:O | 2.28 | 0.52 |
| 3:C:304:SER:HB2 | 3:C:336:VAL:HG22 | 1.91 | 0.52 |
| 8:I:23:ILE:HD12 | 8:I:37:LEU:HD23 | 1.91 | 0.52 |
| 9:J:514:PHE:O | 9:J:518:MET:HB2 | 2.10 | 0.52 |
| 12:N:249:ARG:HB3 | 12:N:250:LEU:HD23 | 1.91 | 0.52 |
| 13:O:355:SER:O | 13:O:357:SER:HB2 | 2.10 | 0.52 |
| 16:Y:192:TYR:HA | 16:Y:195:VAL:HG22 | 1.91 | 0.52 |
| 16:Y:308:MET:HG3 | 16:Y:331:LEU:HD21 | 1.91 | 0.52 |
| 1:A:1041:LEU:HD13 | 1:A:1084:ARG:HA | 1.91 | 0.52 |
| 1:A:1658:PRO:HG2 | 1:A:1663:LEU:HD13 | 1.91 | 0.52 |
| 1:A:1767:ILE:HA | 1:A:1798:ARG:NH2 | 2.25 | 0.52 |
| 2:B:47:VAL:HG21 | 2:B:60:ILE:HG21 | 1.90 | 0.52 |
| 8:I:269:LEU:HD11 | 8:I:522:LEU:HD13 | 1.91 | 0.52 |
| 7:G:4:ARG:HB2 | 9:J:373:TYR:HE1 | 1.73 | 0.52 |
| 9:J:28:LYS:HD3 | 9:K:230:ASN:HD21 | 1.75 | 0.52 |
| 1:A:791:VAL:O | 1:A:793:LEU:N | 2.42 | 0.52 |
| 6:F:553:SER:HA | 6:F:576:CYS:SG | 2.49 | 0.52 |
| 8:I:116:MET:HE1 | 8:I:211:SER:O | 2.10 | 0.52 |
| 9:J:305:VAL:HG11 | 11:M:31:ILE:CD1 | 2.40 | 0.52 |
| 12:N:577:GLU:HB3 | 12:N:625:LYS:HE3 | 1.91 | 0.52 |
| 3:P:296:ARG:HH11 | 3:P:299:ASN:HD21 | 1.57 | 0.52 |
| 14:R:206:VAL:HG23 | 14:R:229:ILE:HD13 | 1.92 | 0.52 |
| 16:X:149:LEU:O | 16:X:150:LYS:HB2 | 2.10 | 0.52 |
| 16:X:203:LEU:C | 16:X:203:LEU:HD23 | 2.30 | 0.52 |
| 3:C:327:ASP:OD2 | 3:C:330:ARG:HD3 | 2.09 | 0.52 |
| 8:I:355:GLY:O | 8:I:359:LEU:HB2 | 2.10 | 0.52 |
| 3:C:76:ILE:HD13 | 3:P:70:LEU:HD23 | 1.92 | 0.52 |
| 3:C:60:PHE:HB2 | 3:P:89:LEU:HD12 | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1797:ILE:HG22 | 1:A:1852:ILE:HD11 | 1.91 | 0.52 |
| 3:C:365:LEU:HD11 | 3:C:395:ASN:HB2 | 1.92 | 0.52 |
| 6:F:130:ARG:HD2 | 6:F:133:LYS:HD3 | 1.90 | 0.52 |
| 7:G:3:ARG:HB2 | 9:J:443:LYS:NZ | 2.25 | 0.52 |
| 8:I:381:LEU:HD12 | 8:I:386:ILE:HD11 | 1.91 | 0.52 |
| 14:R:110:LYS:HZ2 | 14:R:114:LYS:HB2 | 1.75 | 0.52 |
| 1:A:246:ILE:HD11 | 1:A:249:LEU:CD2 | 2.40 | 0.52 |
| 1:A:252:ASP:HB3 | 1:A:253:PRO:CD | 2.34 | 0.52 |
| 6:F:544:TRP:CE3 | 14:R:499:ARG:HD3 | 2.45 | 0.52 |
| 1:A:1556:LEU:HD11 | 1:A:1607:ARG:HG2 | 1.92 | 0.51 |
| 1:A:1853:ASP:O | 1:A:1857:ASP:HB2 | 2.10 | 0.51 |
| 1:A:246:ILE:HD11 | 1:A:249:LEU:HD22 | 1.91 | 0.51 |
| 4:D:4:LEU:HB3 | 13:O:468:VAL:HG12 | 1.92 | 0.51 |
| 9:J:355:ALA:O | 9:J:359:THR:HG23 | 2.11 | 0.51 |
| 1:A:125:GLN:NE2 | 1:A:180:VAL:H | 2.07 | 0.51 |
| 1:A:1799:ARG:HD3 | 1:A:1805:MET:HB2 | 1.92 | 0.51 |
| 1:A:191:ARG:HG2 | 1:A:192:SER:H | 1.75 | 0.51 |
| 1:A:439:GLN:OE1 | 1:A:456:LYS:HG2 | 2.11 | 0.51 |
| 1:A:668:MET:SD | 1:A:668:MET:N | 2.83 | 0.51 |
| 9:K:154:LYS:HE2 | 9:K:184:LEU:HD22 | 1.92 | 0.51 |
| 16:Y:330:ARG:O | 16:Y:334:ILE:HG23 | 2.10 | 0.51 |
| 16:Y:452:LEU:CD2 | 16:Y:460:LYS:HB2 | 2.41 | 0.51 |
| 1:A:1134:TRP:HD1 | 1:A:1597:THR:HA | 1.75 | 0.51 |
| 1:A:1232:ILE:HG13 | 1:A:1235:LEU:HB3 | 1.91 | 0.51 |
| 1:A:811:PRO:HG3 | 1:A:1806:SER:O | 2.11 | 0.51 |
| 6:F:150:SER:HB3 | 6:H:23:ASP:HB3 | 1.92 | 0.51 |
| 12:N:331:PHE:CE2 | 12:N:335:ILE:HD11 | 2.45 | 0.51 |
| 14:R:95:LEU:HG | 14:R:130:ILE:HD11 | 1.93 | 0.51 |
| 1:A:36:ASN:H | 1:A:36:ASN:HD22 | 1.58 | 0.51 |
| 3:C:93:TYR:CE2 | 3:C:101:ARG:CZ | 2.94 | 0.51 |
| 3:C:414:MET:HG2 | 13:O:330:ILE:CG1 | 2.36 | 0.51 |
| 9:K:9:ARG:O | 9:K:13:TYR:HD1 | 1.94 | 0.51 |
| 10:L:90:THR:HB | 10:L:145:HIS:ND1 | 2.25 | 0.51 |
| 13:O:146:LEU:HB2 | 13:O:151:VAL:CG2 | 2.40 | 0.51 |
| 8:I:497:TRP:CE3 | 13:O:492:HIS:CD2 | 2.99 | 0.51 |
| 1:A:1177:MET:HB2 | 1:A:1207:GLY:C | 2.31 | 0.51 |
| 8:I:218:SER:HA | 8:I:235:GLN:HA | 1.92 | 0.51 |
| 9:K:37:PRO:HB3 | 9:K:69:TYR:CE2 | 2.46 | 0.51 |
| 16:X:437:LEU:HB2 | 16:X:444:LEU:HD11 | 1.93 | 0.51 |
| 16:X:83:HIS:O | 16:X:86:SER:OG | 2.19 | 0.51 |
| 1:A:1509:PRO:O | 1:A:1513:GLU:HG2 | 2.11 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:F:571:CYS:SG | 6:F:606:LEU:HD12 | 2.51 | 0.51 |
| 8:I:279:ILE:HD11 | 8:I:337:ILE:CA | 2.28 | 0.51 |
| 8:I:396:PHE:HA | 8:I:525:VAL:HG11 | 1.93 | 0.51 |
| 13:O:114:ASP:CA | 13:O:117:ASP:OD1 | 2.59 | 0.51 |
| 1:A:1078:MET:HB3 | 1:A:1135:ALA:HB2 | 1.92 | 0.51 |
| 9:J:376:LEU:CD2 | 9:J:407:GLU:HG2 | 2.41 | 0.51 |
| 9:K:272:ILE:CG2 | 9:K:307:CYS:SG | 2.98 | 0.51 |
| 3:P:310:ARG:HB3 | 3:P:312:MET:HE2 | 1.93 | 0.51 |
| 6:H:527:ARG:HB3 | 16:Y:302:PRO:HG3 | 1.92 | 0.51 |
| 1:A:45:ALA:O | 3:C:180:ARG:NH1 | 2.42 | 0.51 |
| 3:C:188:ALA:HA | 3:C:191:VAL:HG22 | 1.92 | 0.51 |
| 8:I:224:SER:HB3 | 8:I:229:SER:HA | 1.90 | 0.51 |
| 9:K:185:LEU:HD11 | 9:K:205:PHE:HB3 | 1.93 | 0.51 |
| 3:P:389:ARG:O | 3:P:392:ILE:HG23 | 2.10 | 0.51 |
| 1:A:1092:TYR:O | 1:A:1147:ILE:HA | 2.10 | 0.51 |
| 1:A:1409:LEU:HD23 | 1:A:1471:SER:CA | 2.41 | 0.51 |
| 1:A:1637:THR:O | 1:A:1664:LYS:N | 2.40 | 0.51 |
| 8:I:52:PHE:HD1 | 8:I:743:VAL:HG21 | 1.75 | 0.51 |
| 12:N:406:ALA:O | 12:N:409:VAL:HB | 2.11 | 0.51 |
| 16:Y:149:LEU:O | 16:Y:150:LYS:HB2 | 2.10 | 0.51 |
| 16:Y:294:PHE:CD1 | 16:Y:294:PHE:C | 2.85 | 0.51 |
| 4:D:10:PRO:CG | 13:O:345:SER:HB3 | 2.40 | 0.51 |
| 6:F:26:PHE:O | 6:F:30:ARG:HG2 | 2.11 | 0.51 |
| 6:F:636:ASN:H | 6:F:636:ASN:HD22 | 1.59 | 0.51 |
| 6:F:758:MET:HG2 | 6:F:762:TRP:CZ2 | 2.46 | 0.51 |
| 1:A:89:TYR:HB3 | 13:O:536:THR:HG23 | 1.93 | 0.51 |
| 16:X:452:LEU:CD2 | 16:X:460:LYS:HB2 | 2.41 | 0.51 |
| 1:A:1396:LEU:HD11 | 1:A:1434:ILE:HD11 | 1.93 | 0.50 |
| 1:A:1617:ARG:HH11 | 1:A:1659:GLU:HA | 1.77 | 0.50 |
| 1:A:434:SER:HA | 1:A:439:GLN:O | 2.11 | 0.50 |
| 1:A:87:VAL:HG12 | 1:A:88:ASP:H | 1.73 | 0.50 |
| 8:I:358:SER:O | 8:I:362:HIS:HD2 | 1.94 | 0.50 |
| 9:J:465:LEU:HA | 9:J:488:ILE:CD1 | 2.40 | 0.50 |
| 12:N:362:LYS:HB2 | 12:N:410:LEU:CD2 | 2.22 | 0.50 |
| 12:N:409:VAL:O | 12:N:410:LEU:HB2 | 2.11 | 0.50 |
| 13:O:427:ALA:O | 13:O:430:ARG:HB3 | 2.10 | 0.50 |
| 13:O:580:VAL:HA | 13:O:583:VAL:HG12 | 1.93 | 0.50 |
| 3:P:361:ASN:HD22 | 3:P:363:ARG:H | 1.57 | 0.50 |
| 1:A:1278:GLY:HA3 | 1:A:1328:TYR:CE1 | 2.46 | 0.50 |
| 1:A:1672:ARG:HB2 | 1:A:1673:TYR:CD1 | 2.47 | 0.50 |
| 1:A:172:SER:OG | 3:C:427:GLN:HG2 | 2.12 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1774:VAL:HG13 | 1:A:1790:TYR:HB3 | 1.93 | 0.50 |
| 2:B:11:VAL:HB | 12:N:594:VAL:CG1 | 2.41 | 0.50 |
| 6:H:26:PHE:O | 6:H:30:ARG:HG2 | 2.11 | 0.50 |
| 9:K:23:LEU:HA | 9:K:46:CYS:SG | 2.52 | 0.50 |
| 9:K:509:ARG:HG3 | 9:K:509:ARG:O | 2.11 | 0.50 |
| 9:K:513:THR:O | 9:K:517:THR:HG22 | 2.11 | 0.50 |
| 13:O:631:GLN:HB3 | 13:O:640:ALA:HB2 | 1.92 | 0.50 |
| 1:A:1573:SER:HG | 1:A:1656:LEU:HD22 | 1.76 | 0.50 |
| 1:A:1704:GLY:H | 1:A:1742:THR:HG21 | 1.76 | 0.50 |
| 3:C:323:LEU:HD12 | 3:C:336:VAL:HG11 | 1.92 | 0.50 |
| 3:C:402:TRP:HB3 | 3:C:425:ALA:HB2 | 1.92 | 0.50 |
| 6:H:73:TYR:CD1 | 6:H:117:THR:HG22 | 2.45 | 0.50 |
| 9:J:24:PHE:O | 9:J:28:LYS:HG2 | 2.11 | 0.50 |
| 13:O:68:LEU:HD23 | 13:O:131:VAL:HG12 | 1.92 | 0.50 |
| 13:O:113:ASP:CG | 3:P:344:ARG:HH22 | 2.12 | 0.50 |
| 16:Y:77:TYR:CE1 | 16:Y:107:LYS:HB2 | 2.46 | 0.50 |
| 16:Y:235:TRP:CE3 | 16:Y:236:LEU:HA | 2.46 | 0.50 |
| 1:A:1209:LEU:HD22 | 1:A:1228:LEU:CD2 | 2.39 | 0.50 |
| 3:C:106:LEU:HD13 | 3:C:118:TYR:HB2 | 1.93 | 0.50 |
| 3:C:295:TYR:HD1 | 3:C:326:ILE:HG12 | 1.76 | 0.50 |
| 6:F:103:HIS:HA | 6:F:106:ILE:HD12 | 1.93 | 0.50 |
| 10:L:119:TRP:HH2 | 10:L:155:GLN:HG2 | 1.76 | 0.50 |
| 12:N:212:TYR:HA | 12:N:215:LEU:HB2 | 1.93 | 0.50 |
| 12:N:609:LEU:HD22 | 12:N:639:HIS:CD2 | 2.46 | 0.50 |
| 13:O:35:ILE:CG2 | 13:O:158:LEU:HD13 | 2.40 | 0.50 |
| 14:R:216:ILE:HG12 | 15:S:831:LEU:HB2 | 1.93 | 0.50 |
| 1:A:1097:THR:HG23 | 13:O:340:LEU:HB3 | 1.93 | 0.50 |
| 1:A:1250:GLN:O | 1:A:1254:VAL:HG23 | 2.12 | 0.50 |
| 1:A:213:MET:HE3 | 1:A:220:ILE:HG22 | 1.93 | 0.50 |
| 3:C:449:LEU:HD22 | 3:C:476:LEU:HD22 | 1.88 | 0.50 |
| 13:O:657:ILE:HA | 13:O:660:LYS:CB | 2.41 | 0.50 |
| 16:X:203:LEU:HD22 | 16:Y:55:LEU:CD2 | 2.42 | 0.50 |
| 5:E:76:VAL:O | 5:E:80:GLU:HB2 | 2.12 | 0.50 |
| 13:O:113:ASP:OD2 | 3:P:344:ARG:NH2 | 2.26 | 0.50 |
| 13:O:33:TYR:CE1 | 13:O:37:VAL:HG21 | 2.47 | 0.50 |
| 1:A:1032:LEU:HD12 | 1:A:1035:GLN:CB | 2.41 | 0.50 |
| 1:A:99:MET:HB3 | 1:A:118:THR:HG23 | 1.94 | 0.50 |
| 1:A:1579:SER:O | 1:A:1582:ALA:HB3 | 2.12 | 0.50 |
| 1:A:23:PHE:O | 1:A:26:ASP:HB3 | 2.12 | 0.50 |
| 10:L:53:TYR:HE2 | 10:L:152:HIS:CE1 | 2.29 | 0.50 |
| 1:A:1519:VAL:CG1 | 1:A:1520:LEU:N | 2.74 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:250:ASN:HD22 | 1:A:251:THR:H | 1.58 | 0.50 |
| 1:A:433:THR:HG21 | 1:A:481:PRO:HB3 | 1.90 | 0.50 |
| 1:A:487:THR:HG22 | 1:A:501:THR:HA | 1.94 | 0.50 |
| 1:A:770:TYR:HB2 | 1:A:786:LEU:HD22 | 1.93 | 0.50 |
| 1:A:33:ASN:HA | 1:A:99:MET:CE | 2.42 | 0.50 |
| 9:J:58:HIS:CD2 | 9:K:262:PRO:HD3 | 2.47 | 0.50 |
| 9:K:263:PHE:HZ | 9:K:290:LYS:CG | 2.14 | 0.50 |
| 10:L:40:PHE:HA | 10:L:44:GLN:OE1 | 2.12 | 0.50 |
| 11:M:32:PRO:O | 11:M:33:LEU:HB2 | 2.12 | 0.50 |
| 12:N:580:LYS:HB3 | 12:N:582:PRO:HD2 | 1.94 | 0.50 |
| 3:P:310:ARG:HB3 | 3:P:312:MET:CE | 2.41 | 0.50 |
| 16:X:363:ALA:HB2 | 16:X:379:LYS:HZ3 | 1.75 | 0.50 |
| 16:Y:271:VAL:CG1 | 16:Y:304:LEU:HD21 | 2.40 | 0.50 |
| 1:A:1236:LEU:HD11 | 1:A:1243:LEU:HD22 | 1.93 | 0.49 |
| 8:I:116:MET:SD | 8:I:210:LEU:HB3 | 2.52 | 0.49 |
| 9:J:245:CYS:SG | 9:J:443:LYS:HD3 | 2.52 | 0.49 |
| 13:O:114:ASP:C | 13:O:117:ASP:OD1 | 2.50 | 0.49 |
| 16:X:99:LYS:HD3 | 16:X:102:MET:CE | 2.42 | 0.49 |
| 16:Y:437:LEU:HB2 | 16:Y:444:LEU:HD11 | 1.94 | 0.49 |
| 6:F:656:MET:HG3 | 16:Y:526:GLN:HB2 | 1.94 | 0.49 |
| 1:A:1196:TYR:HB2 | 1:A:1208:LEU:CD1 | 2.41 | 0.49 |
| 6:F:529:GLU:OE1 | 6:F:532:ARG:HB2 | 2.12 | 0.49 |
| 8:I:49:LEU:HD13 | 8:I:730:VAL:HG21 | 1.95 | 0.49 |
| 9:K:410:VAL:HG13 | 7:W:9:LEU:HD21 | 1.93 | 0.49 |
| 9:K:458:LEU:HB3 | 9:K:460:LYS:HG3 | 1.93 | 0.49 |
| 10:L:50:LEU:HD21 | 10:L:119:TRP:CZ2 | 2.47 | 0.49 |
| 10:L:83:TYR:CD1 | 10:L:115:GLU:HA | 2.47 | 0.49 |
| 12:N:76:VAL:C | 12:N:78:VAL:H | 2.15 | 0.49 |
| 13:O:258:TYR:O | 13:O:262:LEU:HB2 | 2.12 | 0.49 |
| 13:O:36:ALA:O | 13:O:39:VAL:HG12 | 2.12 | 0.49 |
| 3:P:178:VAL:O | 3:P:182:LEU:HD22 | 2.13 | 0.49 |
| 16:Y:186:ARG:O | 16:Y:189:VAL:HG12 | 2.12 | 0.49 |
| 1:A:126:ALA:HA | 1:A:152:CYS:O | 2.12 | 0.49 |
| 3:C:308:TYR:CD1 | 3:C:343:LEU:HG | 2.47 | 0.49 |
| 6:F:19:TYR:HE1 | 6:H:50:ARG:HE | 1.59 | 0.49 |
| 3:P:36:LEU:HD21 | 3:P:58:LEU:HB2 | 1.93 | 0.49 |
| 16:Y:485:LEU:O | 16:Y:489:GLU:HG2 | 2.12 | 0.49 |
| 1:A:1691:LEU:HA | 1:A:1695:GLY:HA2 | 1.93 | 0.49 |
| 1:A:442:LEU:O | 1:A:455:VAL:HG12 | 2.13 | 0.49 |
| 3:C:403:TYR:CD2 | 3:C:435:MET:SD | 2.97 | 0.49 |
| 3:C:531:THR:O | 3:C:535:LYS:HG2 | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:F:537:GLU:HG3 | 6:F:538:ILE:N | 2.27 | 0.49 |
| 8:I:399:LYS:HE3 | 8:I:478:TYR:HE1 | 1.77 | 0.49 |
| 13:O:580:VAL:O | 13:O:583:VAL:HG12 | 2.12 | 0.49 |
| 3:P:531:THR:O | 3:P:535:LYS:HG2 | 2.12 | 0.49 |
| 16:X:349:SER:CB | 16:X:358:ALA:HB2 | 2.43 | 0.49 |
| 16:X:384:ARG:HH22 | 16:X:415:GLU:HB3 | 1.77 | 0.49 |
| 16:Y:349:SER:CB | 16:Y:358:ALA:HB2 | 2.42 | 0.49 |
| 1:A:1140:GLY:HA3 | 1:A:1171:GLU:O | 2.13 | 0.49 |
| 1:A:1860:LEU:O | 1:A:1865:ASP:HB2 | 2.12 | 0.49 |
| 1:A:44:PRO:CA | 1:A:45:ALA:CB | 2.91 | 0.49 |
| 1:A:594:ARG:HG2 | 1:A:608:THR:HG23 | 1.94 | 0.49 |
| 2:B:23:CYS:HA | 2:B:30:PHE:CZ | 2.48 | 0.49 |
| 3:C:239:THR:HG21 | 3:C:268:GLN:HE21 | 1.76 | 0.49 |
| 12:N:546:LYS:HA | 12:N:550:GLY:HA2 | 1.93 | 0.49 |
| 1:A:661:VAL:HG12 | 1:A:789:LEU:HD12 | 1.93 | 0.49 |
| 3:C:329:TYR:OH | 11:M:20:ARG:HB2 | 2.13 | 0.49 |
| 8:I:224:SER:HB2 | 8:I:230:GLU:H | 1.77 | 0.49 |
| 8:I:618:ILE:HD12 | 8:I:705:MET:HE1 | 1.94 | 0.49 |
| 8:I:48:ARG:HG2 | 12:N:390:GLY:HA2 | 1.95 | 0.49 |
| 13:O:433:GLY:HA2 | 13:O:618:TYR:HD2 | 1.77 | 0.49 |
| 13:O:91:ASN:O | 13:O:95:ILE:HG12 | 2.13 | 0.49 |
| 16:X:203:LEU:HD13 | 16:Y:55:LEU:HB3 | 1.93 | 0.49 |
| 1:A:1047:VAL:O | 1:A:1109:GLY:HA2 | 2.13 | 0.49 |
| 1:A:39:LEU:HD12 | 1:A:40:ARG:H | 1.77 | 0.49 |
| 1:A:872:LEU:HD12 | 1:A:937:VAL:HG11 | 1.94 | 0.49 |
| 3:C:151:LEU:HD11 | 3:C:181:LYS:CB | 2.42 | 0.49 |
| 8:I:219:VAL:N | 8:I:234:PHE:O | 2.44 | 0.49 |
| 12:N:267:GLN:HG3 | 12:N:268:VAL:N | 2.27 | 0.49 |
| 13:O:240:LEU:HD11 | 13:O:256:LEU:HB3 | 1.93 | 0.49 |
| 3:P:487:ALA:HB1 | 3:P:519:TYR:CE1 | 2.46 | 0.49 |
| 3:C:370:LEU:CG | 14:R:79:TYR:HE1 | 2.23 | 0.49 |
| 16:X:330:ARG:O | 16:X:334:ILE:HG23 | 2.13 | 0.49 |
| 3:C:244:ILE:HD12 | 3:C:245:GLU:N | 2.27 | 0.49 |
| 9:K:256:VAL:O | 9:K:259:GLU:HG2 | 2.13 | 0.49 |
| 10:L:74:VAL:HG21 | 10:L:137:ILE:HD11 | 1.93 | 0.49 |
| 3:P:332:GLU:O | 3:P:333:THR:C | 2.51 | 0.49 |
| 14:R:493:LEU:O | 14:R:494:ILE:HB | 2.12 | 0.49 |
| 1:A:1611:VAL:CG1 | 1:A:1612:LEU:N | 2.75 | 0.49 |
| 9:K:337:TRP:HB3 | 9:K:360:ALA:HB2 | 1.94 | 0.49 |
| 9:K:36:GLU:HG2 | 9:K:37:PRO:HD2 | 1.95 | 0.49 |
| 13:O:215:PHE:HD2 | 13:O:216:LEU:HD23 | 1.78 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:O:39:VAL:HG11 | 13:O:97:ILE:HG13 | 1.95 | 0.49 |
| 16:X:321:LEU:HD21 | 16:X:351:TYR:HB2 | 1.94 | 0.49 |
| 16:X:485:LEU:O | 16:X:489:GLU:HG2 | 2.13 | 0.49 |
| 16:Y:226:VAL:HG22 | 16:Y:236:LEU:HD23 | 1.94 | 0.49 |
| 1:A:1777:GLU:O | 1:A:1781:GLN:HG2 | 2.13 | 0.49 |
| 1:A:629:LEU:HB2 | 1:A:630:PRO:CD | 2.42 | 0.49 |
| 3:C:119:MET:HA | 3:C:122:ARG:HG2 | 1.95 | 0.49 |
| 3:C:234:LEU:HB3 | 3:C:250:LYS:CE | 2.42 | 0.49 |
| 6:H:150:SER:N | 6:H:151:PRO:HD2 | 2.28 | 0.49 |
| 8:I:56:TRP:CD2 | 8:I:98:PRO:HB3 | 2.43 | 0.49 |
| 9:J:45:GLN:O | 9:J:49:LEU:HG | 2.13 | 0.49 |
| 9:K:391:PHE:CZ | 9:K:411:VAL:HG21 | 2.48 | 0.49 |
| 16:X:59:LEU:HD22 | 16:Y:270:ASN:ND2 | 2.27 | 0.49 |
| 1:A:1196:TYR:CB | 1:A:1208:LEU:HD11 | 2.42 | 0.48 |
| 9:J:451:LEU:O | 9:J:454:VAL:HG22 | 2.13 | 0.48 |
| 9:J:513:THR:O | 9:J:517:THR:HG22 | 2.13 | 0.48 |
| 9:K:320:ARG:HB2 | 9:K:340:TYR:HE1 | 1.78 | 0.48 |
| 3:C:115:TYR:CZ | 3:C:161:LYS:HD3 | 2.48 | 0.48 |
| 3:C:238:TYR:CB | 3:C:247:ALA:HB2 | 2.43 | 0.48 |
| 3:C:270:ALA:HB2 | 3:C:285:ILE:HG22 | 1.94 | 0.48 |
| 8:I:673:LEU:HA | 8:I:676:ASN:HB2 | 1.95 | 0.48 |
| 9:J:320:ARG:HB3 | 9:J:340:TYR:HE1 | 1.78 | 0.48 |
| 12:N:211:ARG:O | 12:N:215:LEU:CG | 2.50 | 0.48 |
| 14:R:110:LYS:NZ | 14:R:114:LYS:HB2 | 2.28 | 0.48 |
| 14:R:420:PHE:HA | 14:R:421:ALA:HA | 1.65 | 0.48 |
| 16:X:146:TYR:CD1 | 16:X:154:ASP:HB2 | 2.48 | 0.48 |
| 16:X:204:ASP:HB2 | 16:Y:52:ASN:OD1 | 2.13 | 0.48 |
| 1:A:1377:LYS:HE2 | 1:A:1416:TRP:CE2 | 2.48 | 0.48 |
| 3:C:180:ARG:HG3 | 3:C:212:LEU:HD21 | 1.95 | 0.48 |
| 5:E:60:SER:O | 5:E:63:VAL:HG12 | 2.13 | 0.48 |
| 8:I:571:LYS:HE2 | 8:I:571:LYS:HB3 | 1.65 | 0.48 |
| 9:K:277:GLU:HB3 | 9:K:443:LYS:NZ | 2.28 | 0.48 |
| 13:O:672:VAL:HG13 | 13:O:687:LEU:HD11 | 1.96 | 0.48 |
| 1:A:1308:GLY:N | 1:A:1373:MET:O | 2.46 | 0.48 |
| 1:A:1781:GLN:HB2 | 1:A:1783:THR:HG22 | 1.95 | 0.48 |
| 1:A:90:ASP:HB3 | 1:A:591:VAL:HG21 | 1.94 | 0.48 |
| 2:B:36:ASP:OD1 | 2:B:36:ASP:N | 2.46 | 0.48 |
| 6:H:130:ARG:HD2 | 6:H:133:LYS:HD3 | 1.95 | 0.48 |
| 6:H:158:ILE:HG22 | 6:H:159:GLY:N | 2.29 | 0.48 |
| 1:A:1401:PRO:HD3 | 10:L:135:PHE:CE2 | 2.48 | 0.48 |
| 4:D:4:LEU:HD21 | 13:O:506:LEU:HB2 | 1.94 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1313:LEU:HD13 | 1:A:1316:MET:HB2 | 1.95 | 0.48 |
| 1:A:1375:TYR:HB3 | 1:A:1378:THR:HG21 | 1.96 | 0.48 |
| 1:A:1672:ARG:HB2 | 1:A:1673:TYR:CE1 | 2.47 | 0.48 |
| 1:A:266:HIS:CE1 | 1:A:427:ALA:HB2 | 2.49 | 0.48 |
| 1:A:43:GLN:HG3 | 3:C:142:GLU:O | 2.13 | 0.48 |
| 1:A:945:GLU:HG3 | 13:O:599:ILE:HG23 | 1.95 | 0.48 |
| 3:C:370:LEU:CG | 14:R:79:TYR:CE1 | 2.96 | 0.48 |
| 13:O:405:SER:O | 13:O:409:HIS:CD2 | 2.66 | 0.48 |
| 9:K:242:TYR:O | 7:W:3:ARG:NH2 | 2.45 | 0.48 |
| 16:X:87:LEU:HD22 | 16:X:95:ASN:HD22 | 1.79 | 0.48 |
| 16:Y:491:LYS:O | 16:Y:494:ASP:OD1 | 2.32 | 0.48 |
| 1:A:1454:LEU:O | 1:A:1458:SER:HB2 | 2.14 | 0.48 |
| 1:A:1589:TYR:CE2 | 1:A:1591:HIS:HB2 | 2.48 | 0.48 |
| 1:A:1636:VAL:HG22 | 1:A:1651:LEU:HD11 | 1.95 | 0.48 |
| 3:C:332:GLU:O | 3:C:333:THR:C | 2.50 | 0.48 |
| 6:F:653:LEU:O | 6:F:656:MET:HG2 | 2.14 | 0.48 |
| 6:H:529:GLU:OE1 | 6:H:532:ARG:HB2 | 2.12 | 0.48 |
| 9:J:36:GLU:HG2 | 9:J:37:PRO:HD2 | 1.96 | 0.48 |
| 11:M:19:TRP:CD1 | 11:M:19:TRP:C | 2.87 | 0.48 |
| 12:N:179:CYS:HA | 12:N:182:ARG:HB2 | 1.95 | 0.48 |
| 12:N:550:GLY:HA2 | 12:N:551:GLU:HB2 | 1.94 | 0.48 |
| 1:A:942:ARG:HG2 | 13:O:565:GLN:HG2 | 1.95 | 0.48 |
| 3:P:441:GLU:HG2 | 3:P:472:LYS:NZ | 2.28 | 0.48 |
| 3:P:490:TYR:CD1 | 3:P:515:TYR:HB3 | 2.49 | 0.48 |
| 1:A:1543:HIS:CD2 | 1:A:1559:HIS:HE1 | 2.31 | 0.48 |
| 1:A:72:GLU:HB2 | 1:A:96:ALA:HA | 1.95 | 0.48 |
| 1:A:982:ASP:OD1 | 1:A:983:LEU:N | 2.46 | 0.48 |
| 3:C:296:ARG:HA | 3:P:101:ARG:NH1 | 2.28 | 0.48 |
| 9:J:129:LYS:O | 9:J:132:ILE:HG22 | 2.14 | 0.48 |
| 9:J:445:GLU:N | 9:J:446:PRO:HD2 | 2.29 | 0.48 |
| 9:K:320:ARG:HB2 | 9:K:340:TYR:CE1 | 2.49 | 0.48 |
| 10:L:111:LEU:HD11 | 10:L:122:VAL:HG22 | 1.96 | 0.48 |
| 3:P:120:TYR:CE2 | 3:P:124:LEU:HD11 | 2.48 | 0.48 |
| 6:F:544:TRP:CD2 | 14:R:499:ARG:HD3 | 2.48 | 0.48 |
| 16:Y:146:TYR:CD1 | 16:Y:154:ASP:HB2 | 2.48 | 0.48 |
| 1:A:125:GLN:HG3 | 1:A:154:LEU:HD23 | 1.96 | 0.48 |
| 3:C:206:TRP:HE3 | 3:C:233:PHE:CD1 | 2.31 | 0.48 |
| 3:C:28:ASP:OD1 | 3:C:29:LEU:N | 2.46 | 0.48 |
| 3:C:389:ARG:HG2 | 13:O:279:ASP:CB | 2.44 | 0.48 |
| 7:G:4:ARG:HD3 | 9:J:376:LEU:HD12 | 1.95 | 0.48 |
| 8:I:17:LYS:HE3 | 8:I:51:SER:O | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:I:138:LEU:HD12 | 8:I:253:ARG:HA | 1.96 | 0.48 |
| 12:N:395:ASP:HB2 | 12:N:397:ILE:H | 1.79 | 0.48 |
| 3:P:87:TYR:CZ | 3:P:113:LYS:HE2 | 2.48 | 0.48 |
| 16:X:100:TYR:HD1 | 16:X:138:VAL:HG13 | 1.78 | 0.48 |
| 16:Y:321:LEU:HD21 | 16:Y:351:TYR:HB2 | 1.95 | 0.48 |
| 16:Y:50:HIS:ND1 | 16:Y:86:SER:HA | 2.28 | 0.48 |
| 1:A:1102:ILE:HG21 | 1:A:1171:GLU:OE1 | 2.13 | 0.48 |
| 1:A:105:GLY:O | 1:A:111:LEU:HD23 | 2.14 | 0.48 |
| 1:A:1640:GLY:HA3 | 1:A:1645:GLU:O | 2.13 | 0.48 |
| 1:A:1849:LYS:O | 1:A:1852:ILE:HB | 2.14 | 0.48 |
| 8:I:47:HIS:CE1 | 8:I:54:ARG:NH1 | 2.82 | 0.48 |
| 1:A:1475:ARG:HG2 | 1:A:1476:PHE:CE2 | 2.49 | 0.48 |
| 1:A:173:LEU:HD22 | 1:A:177:VAL:HG11 | 1.95 | 0.48 |
| 2:B:39:VAL:CB | 2:B:43:ASP:CB | 2.87 | 0.48 |
| 3:C:252:GLN:HA | 3:C:255:ILE:HD12 | 1.96 | 0.48 |
| 6:F:152:PHE:CE1 | 6:F:162:PRO:HG2 | 2.48 | 0.48 |
| 8:I:74:ARG:HD2 | 8:I:174:ASN:HD22 | 1.78 | 0.48 |
| 9:J:242:TYR:HB2 | 9:J:250:CYS:SG | 2.54 | 0.48 |
| 9:K:185:LEU:HA | 9:K:188:LEU:CD2 | 2.43 | 0.48 |
| 9:K:227:LEU:O | 9:K:230:ASN:N | 2.46 | 0.48 |
| 16:X:40:HIS:HB3 | 16:Y:201:LEU:CD1 | 2.44 | 0.48 |
| 1:A:1253:ALA:O | 1:A:1257:ILE:N | 2.40 | 0.47 |
| 1:A:1502:PRO:O | 1:A:1503:ASN:CB | 2.62 | 0.47 |
| 1:A:1536:LEU:HD23 | 1:A:1562:LEU:CD2 | 2.44 | 0.47 |
| 1:A:32:PRO:HD3 | 13:O:233:PRO:HB3 | 1.95 | 0.47 |
| 7:G:13:LEU:HA | 7:G:16:ILE:HD12 | 1.96 | 0.47 |
| 7:G:3:ARG:HH22 | 9:J:243:TYR:HA | 1.78 | 0.47 |
| 8:I:17:LYS:NZ | 8:I:51:SER:O | 2.44 | 0.47 |
| 9:J:447:LEU:O | 9:J:451:LEU:HD23 | 2.14 | 0.47 |
| 9:K:445:GLU:N | 9:K:446:PRO:HD2 | 2.29 | 0.47 |
| 12:N:270:ARG:O | 12:N:274:GLU:HB2 | 2.14 | 0.47 |
| 12:N:397:ILE:O | 12:N:401:ILE:HG13 | 2.13 | 0.47 |
| 12:N:560:MET:HA | 12:N:560:MET:CE | 2.44 | 0.47 |
| 13:O:425:LYS:HB3 | 13:O:441:GLN:HG2 | 1.95 | 0.47 |
| 3:P:224:LEU:HB2 | 3:P:230:LYS:HD2 | 1.96 | 0.47 |
| 16:X:491:LYS:O | 16:X:494:ASP:OD1 | 2.32 | 0.47 |
| 1:A:1771:PHE:O | 1:A:1774:VAL:HB | 2.13 | 0.47 |
| 2:B:83:LYS:O | 2:B:84:GLU:HB2 | 2.14 | 0.47 |
| 3:C:412:LEU:O | 3:C:414:MET:HG3 | 2.14 | 0.47 |
| 5:E:92:ASP:HB3 | 6:H:592:ARG:HH22 | 1.79 | 0.47 |
| 9:J:210:LYS:HE2 | 9:J:213:ASN:HB3 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:O:477:HIS:CB | 13:O:486:ALA:HB2 | 2.44 | 0.47 |
| 3:P:170:PHE:O | 3:P:173:TYR:HB3 | 2.13 | 0.47 |
| 3:P:233:PHE:O | 3:P:237:ILE:HG13 | 2.13 | 0.47 |
| 16:X:235:TRP:CE3 | 16:X:236:LEU:HA | 2.48 | 0.47 |
| 1:A:1078:MET:HB2 | 1:A:1552:TYR:HE1 | 1.78 | 0.47 |
| 1:A:1871:TYR:HB2 | 1:A:1877:LEU:HD11 | 1.96 | 0.47 |
| 3:C:303:PHE:C | 3:C:303:PHE:HD1 | 2.18 | 0.47 |
| 6:F:150:SER:N | 6:F:151:PRO:HD2 | 2.29 | 0.47 |
| 8:I:139:LEU:HD21 | 8:I:192:MET:CE | 2.44 | 0.47 |
| 8:I:44:VAL:C | 8:I:45:LEU:HD12 | 2.35 | 0.47 |
| 8:I:45:LEU:HG | 8:I:57:SER:HA | 1.96 | 0.47 |
| 9:J:441:VAL:CG2 | 9:J:444:TRP:HD1 | 2.19 | 0.47 |
| 13:O:280:ARG:HA | 13:O:280:ARG:HD2 | 1.67 | 0.47 |
| 13:O:411:LYS:HE2 | 13:O:412:HIS:CE1 | 2.48 | 0.47 |
| 13:O:467:ALA:HB1 | 13:O:506:LEU:CD1 | 2.43 | 0.47 |
| 3:P:94:PHE:O | 3:P:97:LYS:HB2 | 2.14 | 0.47 |
| 16:X:226:VAL:HG22 | 16:X:236:LEU:HD23 | 1.95 | 0.47 |
| 6:F:692:LEU:HD13 | 6:F:709:ARG:HA | 1.95 | 0.47 |
| 6:H:103:HIS:HA | 6:H:106:ILE:HD12 | 1.96 | 0.47 |
| 9:J:212:TYR:HB3 | 9:J:243:TYR:CD1 | 2.50 | 0.47 |
| 13:O:146:LEU:CB | 13:O:151:VAL:HG23 | 2.44 | 0.47 |
| 1:A:1380:ASN:HD22 | 1:A:1383:ILE:HD12 | 1.79 | 0.47 |
| 1:A:247:VAL:HG11 | 1:A:427:ALA:HB3 | 1.97 | 0.47 |
| 1:A:481:PRO:HA | 1:A:488:MET:HA | 1.97 | 0.47 |
| 2:B:16:TRP:CD1 | 2:B:46:LEU:HG | 2.50 | 0.47 |
| 8:I:12:ARG:O | 8:I:744:PHE:HA | 2.14 | 0.47 |
| 9:K:167:PHE:O | 9:K:171:THR:HG22 | 2.14 | 0.47 |
| 9:K:496:GLU:HB2 | 9:K:526:TYR:HE1 | 1.78 | 0.47 |
| 13:O:445:LEU:O | 13:O:448:MET:HB2 | 2.14 | 0.47 |
| 3:P:402:TRP:HB3 | 3:P:425:ALA:HB2 | 1.96 | 0.47 |
| 1:A:582:THR:N | 1:A:583:TYR:HA | 2.29 | 0.47 |
| 1:A:770:TYR:CD1 | 1:A:783:ILE:HD11 | 2.49 | 0.47 |
| 3:C:526:TRP:NE1 | 3:C:553:ILE:HB | 2.30 | 0.47 |
| 6:F:481:CYS:O | 6:F:485:ILE:HG12 | 2.15 | 0.47 |
| 9:K:384:SER:HB3 | 9:K:415:ASN:OD1 | 2.15 | 0.47 |
| 12:N:387:LEU:HD21 | 12:N:424:ILE:HG12 | 1.96 | 0.47 |
| 13:O:421:SER:O | 13:O:424:GLN:HB3 | 2.15 | 0.47 |
| 1:A:15:ARG:HE | 13:O:526:HIS:CB | 2.26 | 0.47 |
| 1:A:269:TRP:HA | 1:A:411:HIS:HA | 1.96 | 0.47 |
| 3:C:134:THR:OG1 | 3:C:146:VAL:HG21 | 2.15 | 0.47 |
| 3:C:303:PHE:CE1 | 3:C:307:LEU:HD12 | 2.49 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:F:554:VAL:HG22 | 9:K:285:PHE:HD2 | 1.77 | 0.47 |
| 7:G:4:ARG:HD2 | 9:J:373:TYR:HD1 | 1.80 | 0.47 |
| 9:J:21:SER:N | 9:K:165:GLU:HG2 | 2.29 | 0.47 |
| 9:J:23:LEU:HA | 9:J:46:CYS:SG | 2.54 | 0.47 |
| 13:O:515:GLN:HB3 | 13:O:531:LEU:HD11 | 1.96 | 0.47 |
| 14:R:181:ILE:HG22 | 14:R:465:GLU:HG2 | 1.96 | 0.47 |
| 1:A:489:LEU:HD22 | 1:A:497:LEU:HD22 | 1.96 | 0.47 |
| 1:A:591:VAL:HG22 | 1:A:606:ARG:NH2 | 2.29 | 0.47 |
| 3:C:114:ALA:C | 3:C:116:PHE:N | 2.68 | 0.47 |
| 8:I:166:LYS:O | 8:I:170:ASP:N | 2.45 | 0.47 |
| 9:J:469:ARG:O | 9:J:473:VAL:HG23 | 2.14 | 0.47 |
| 9:K:42:TRP:HA | 9:K:42:TRP:CE3 | 2.49 | 0.47 |
| 9:K:45:GLN:O | 9:K:49:LEU:HG | 2.14 | 0.47 |
| 12:N:533:PHE:CZ | 12:N:564:MET:HB3 | 2.50 | 0.47 |
| 16:X:203:LEU:CD2 | 16:Y:55:LEU:CD2 | 2.92 | 0.47 |
| 1:A:273:ARG:O | 1:A:274:VAL:HB | 2.14 | 0.47 |
| 4:D:27:GLU:HG3 | 13:O:134:LEU:HD21 | 1.97 | 0.47 |
| 6:F:73:TYR:CD1 | 6:F:117:THR:HG22 | 2.49 | 0.47 |
| 6:F:554:VAL:O | 6:F:558:ASP:HB2 | 2.15 | 0.47 |
| 8:I:561:ARG:NH2 | 8:I:589:THR:O | 2.47 | 0.47 |
| 9:J:55:ARG:NH1 | 9:K:265:ALA:H | 2.12 | 0.47 |
| 9:K:93:LEU:HD12 | 9:K:93:LEU:N | 2.30 | 0.47 |
| 13:O:707:LYS:HA | 13:O:710:ILE:HG22 | 1.95 | 0.47 |
| 16:X:54:ARG:NH2 | 16:X:90:ASP:OD2 | 2.48 | 0.47 |
| 16:X:87:LEU:HD22 | 16:X:95:ASN:ND2 | 2.30 | 0.47 |
| 3:C:296:ARG:HG2 | 3:C:296:ARG:HH11 | 1.74 | 0.47 |
| 8:I:27:VAL:O | 8:I:35:ILE:HD12 | 2.14 | 0.47 |
| 12:N:362:LYS:HA | 12:N:410:LEU:CD2 | 2.44 | 0.47 |
| 13:O:247:ASN:HD21 | 13:O:250:PHE:HB2 | 1.79 | 0.47 |
| 8:I:514:PHE:CD2 | 13:O:443:GLN:HG3 | 2.50 | 0.47 |
| 13:O:539:ASN:HD22 | 13:O:542:GLU:HB2 | 1.79 | 0.47 |
| 13:O:40:LEU:HD22 | 13:O:82:ILE:HD12 | 1.96 | 0.47 |
| 3:P:384:ALA:O | 3:P:388:TYR:CD2 | 2.68 | 0.47 |
| 16:X:76:LYS:HB2 | 16:X:106:GLN:NE2 | 2.29 | 0.47 |
| 1:A:240:VAL:H | 1:A:241:ASP:CB | 2.28 | 0.47 |
| 12:N:397:ILE:HA | 12:N:400:TYR:HB3 | 1.97 | 0.47 |
| 13:O:641:LEU:HD11 | 13:O:671:GLN:HG2 | 1.97 | 0.47 |
| 3:P:251:TYR:HB3 | 3:P:269:ILE:HD11 | 1.95 | 0.47 |
| 3:P:308:TYR:CD1 | 3:P:343:LEU:HG | 2.50 | 0.47 |
| 1:A:430:VAL:HA | 1:A:443:CYS:O | 2.15 | 0.46 |
| 3:C:233:PHE:O | 3:C:237:ILE:HG12 | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:493:TYR:CZ | 3:C:497:ILE:HD11 | 2.50 | 0.46 |
| 9:J:320:ARG:HB3 | 9:J:340:TYR:CE1 | 2.51 | 0.46 |
| 12:N:550:GLY:HA2 | 12:N:551:GLU:CB | 2.45 | 0.46 |
| 13:O:296:TYR:HE1 | 14:R:95:LEU:HB3 | 1.80 | 0.46 |
| 13:O:621:SER:HB3 | 13:O:651:ILE:HG12 | 1.97 | 0.46 |
| 13:O:665:PHE:CD1 | 13:O:713:VAL:HG23 | 2.50 | 0.46 |
| 16:X:294:PHE:CD1 | 16:X:294:PHE:C | 2.88 | 0.46 |
| 16:Y:99:LYS:HD3 | 16:Y:102:MET:CE | 2.45 | 0.46 |
| 1:A:1274:LEU:HG | 1:A:1302:LEU:HD11 | 1.97 | 0.46 |
| 1:A:263:GLN:HB2 | 1:A:265:VAL:HG11 | 1.96 | 0.46 |
| 2:B:16:TRP:HB3 | 2:B:31:ASN:HA | 1.97 | 0.46 |
| 6:F:164:PRO:HG3 | 6:F:471:LYS:HG3 | 1.98 | 0.46 |
| 5:E:94:TRP:HE1 | 6:F:595:GLN:NE2 | 2.13 | 0.46 |
| 9:K:243:TYR:OH | 7:W:1:MET:HG2 | 2.15 | 0.46 |
| 4:D:10:PRO:HD2 | 13:O:346:TRP:CZ3 | 2.50 | 0.46 |
| 1:A:1145:LEU:HD13 | 1:A:1610:TYR:OH | 2.15 | 0.46 |
| 1:A:1153:ILE:HG12 | 1:A:1184:HIS:CD2 | 2.50 | 0.46 |
| 1:A:181:TRP:CZ2 | 1:A:246:ILE:O | 2.69 | 0.46 |
| 1:A:183:THR:OG1 | 1:A:184:LYS:O | 2.25 | 0.46 |
| 6:F:149:TRP:HH2 | 6:F:470:GLY:HA2 | 1.80 | 0.46 |
| 6:H:121:LEU:HG | 6:H:125:TYR:CE1 | 2.50 | 0.46 |
| 6:H:522:PHE:CB | 6:H:539:TYR:CD1 | 2.98 | 0.46 |
| 5:E:102:LEU:HD13 | 6:H:594:ILE:HG22 | 1.98 | 0.46 |
| 9:J:445:GLU:OE1 | 9:J:475:ILE:HG21 | 2.14 | 0.46 |
| 12:N:149:LEU:HB3 | 12:N:150:ARG:H | 1.46 | 0.46 |
| 12:N:213:TYR:H | 12:N:214:ARG:N | 2.12 | 0.46 |
| 13:O:546:ARG:HA | 13:O:549:VAL:HG12 | 1.96 | 0.46 |
| 16:X:346:GLY:HA3 | 16:X:378:LEU:HD21 | 1.97 | 0.46 |
| 1:A:1351:GLN:HG3 | 10:L:36:CYS:SG | 2.56 | 0.46 |
| 3:C:303:PHE:C | 3:C:303:PHE:CD1 | 2.88 | 0.46 |
| 6:H:494:HIS:CD2 | 6:H:495:HIS:CD2 | 3.04 | 0.46 |
| 8:I:262:LEU:HA | 8:I:265:ILE:HG22 | 1.98 | 0.46 |
| 9:K:37:PRO:HB3 | 9:K:69:TYR:CZ | 2.50 | 0.46 |
| 12:N:74:TRP:CZ3 | 12:N:76:VAL:HG13 | 2.50 | 0.46 |
| 13:O:105:LEU:HD13 | 13:O:155:TYR:HB2 | 1.97 | 0.46 |
| 13:O:591:TYR:HE2 | 13:O:603:MET:HG3 | 1.79 | 0.46 |
| 7:W:13:LEU:HA | 7:W:16:ILE:HD12 | 1.96 | 0.46 |
| 16:Y:281:TYR:CE1 | 16:Y:289:ASN:HB3 | 2.50 | 0.46 |
| 16:Y:60:LEU:HB3 | 16:Y:79:LEU:HD11 | 1.97 | 0.46 |
| 1:A:215:HIS:CG | 1:A:216:PRO:HD2 | 2.50 | 0.46 |
| 6:F:145:ASN:HB2 | 6:F:146:PRO:O | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:I:36:ALA:HB2 | 8:I:80:LEU:HD21 | 1.97 | 0.46 |
| 9:J:211:LYS:O | 9:J:212:TYR:CD2 | 2.67 | 0.46 |
| 9:K:35:GLU:HB3 | 9:K:40:ILE:HD11 | 1.98 | 0.46 |
| 1:A:165:GLU:O | 13:O:316:HIS:HB3 | 2.15 | 0.46 |
| 13:O:361:LEU:HD12 | 13:O:387:GLN:NE2 | 2.30 | 0.46 |
| 3:P:296:ARG:NH1 | 3:P:299:ASN:HD21 | 2.13 | 0.46 |
| 14:R:430:TYR:HA | 14:R:431:PRO:HA | 1.77 | 0.46 |
| 1:A:1177:MET:HB2 | 1:A:1207:GLY:O | 2.15 | 0.46 |
| 1:A:1469:CYS:HB2 | 1:A:1488:LEU:CD2 | 2.45 | 0.46 |
| 3:C:384:ALA:O | 3:C:388:TYR:CD2 | 2.68 | 0.46 |
| 6:F:131:LEU:HD11 | 6:F:158:ILE:HG12 | 1.98 | 0.46 |
| 6:F:541:THR:HG23 | 14:R:499:ARG:CG | 2.46 | 0.46 |
| 8:I:685:PHE:HA | 8:I:701:PRO:HD3 | 1.98 | 0.46 |
| 9:J:165:GLU:HG3 | 9:K:20:GLN:HB2 | 1.98 | 0.46 |
| 9:J:55:ARG:HD2 | 9:K:261:ASP:OD1 | 2.15 | 0.46 |
| 9:J:93:LEU:HD12 | 9:J:93:LEU:N | 2.31 | 0.46 |
| 9:K:181:GLU:HB3 | 9:K:209:LEU:HD13 | 1.98 | 0.46 |
| 13:O:146:LEU:HD12 | 13:O:151:VAL:HG22 | 1.98 | 0.46 |
| 13:O:321:GLU:HG3 | 13:O:350:LEU:HD22 | 1.98 | 0.46 |
| 1:A:1659:GLU:O | 1:A:1662:LEU:HG | 2.15 | 0.46 |
| 3:C:328:LYS:HB3 | 3:C:329:TYR:CE2 | 2.50 | 0.46 |
| 3:C:48:LEU:HD21 | 3:C:116:PHE:HZ | 1.81 | 0.46 |
| 4:D:5:PHE:CE1 | 13:O:390:PHE:CZ | 2.98 | 0.46 |
| 8:I:74:ARG:HD2 | 8:I:174:ASN:ND2 | 2.31 | 0.46 |
| 13:O:727:THR:HG22 | 13:O:730:ARG:HD2 | 1.97 | 0.46 |
| 3:P:274:HIS:ND1 | 3:P:306:LEU:HB3 | 2.30 | 0.46 |
| 3:P:405:LEU:HD23 | 3:P:405:LEU:HA | 1.78 | 0.46 |
| 3:C:441:GLU:HB2 | 3:C:445:LYS:HE3 | 1.97 | 0.46 |
| 6:F:59:ARG:NH1 | 6:H:562:MET:HG3 | 2.30 | 0.46 |
| 9:J:454:VAL:C | 9:J:458:LEU:HD12 | 2.31 | 0.46 |
| 3:C:321:HIS:HA | 11:M:24:LEU:CD1 | 2.45 | 0.46 |
| 13:O:361:LEU:HD13 | 13:O:384:LEU:CA | 2.46 | 0.46 |
| 16:Y:466:ASP:OD1 | 16:Y:482:LYS:CE | 2.62 | 0.46 |
| 16:X:267:LEU:CD1 | 16:Y:59:LEU:CD1 | 2.89 | 0.46 |
| 1:A:1894:VAL:HA | 1:A:1895:PRO:HD3 | 1.69 | 0.46 |
| 3:C:112:LYS:HD2 | 3:C:112:LYS:H | 1.81 | 0.46 |
| 3:C:300:MET:HG3 | 3:C:319:LEU:HD11 | 1.98 | 0.46 |
| 3:C:465:VAL:HG23 | 3:C:466:GLU:H | 1.81 | 0.46 |
| 6:H:145:ASN:HB2 | 6:H:146:PRO:O | 2.16 | 0.46 |
| 8:I:213:ASP:OD1 | 8:I:215:LYS:N | 2.29 | 0.46 |
| 9:J:35:GLU:HB3 | 9:J:40:ILE:HD11 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 9:J:481:THR:O | 9:J:485:ILE:HG12 | 2.16 | 0.46 |
| 12:N:212:TYR:C | 12:N:215:LEU:HB2 | 2.37 | 0.46 |
| 13:O:136:LEU:HD12 | 13:O:136:LEU:C | 2.36 | 0.46 |
| 16:Y:233:LEU:HD22 | 16:Y:235:TRP:CZ2 | 2.51 | 0.46 |
| 16:Y:301:ASP:HA | 16:Y:302:PRO:HD2 | 1.76 | 0.46 |
| 16:X:203:LEU:HD22 | 16:Y:55:LEU:HB3 | 1.96 | 0.46 |
| 1:A:1321:VAL:HG23 | 1:A:1322:PRO:HD3 | 1.97 | 0.46 |
| 3:C:209:LEU:O | 3:C:213:ILE:HG12 | 2.16 | 0.46 |
| 3:C:234:LEU:CD2 | 3:C:250:LYS:HE3 | 2.37 | 0.46 |
| 3:C:422:TYR:CE2 | 3:C:438:ALA:HB1 | 2.51 | 0.46 |
| 3:C:46:ARG:CZ | 3:C:170:PHE:CD2 | 2.99 | 0.46 |
| 6:H:488:LEU:HD22 | 6:H:501:VAL:HG13 | 1.98 | 0.46 |
| 6:H:502:LEU:HB2 | 6:H:525:VAL:HG22 | 1.98 | 0.46 |
| 6:H:499:GLY:O | 6:H:503:CYS:HB2 | 2.16 | 0.46 |
| 9:J:262:PRO:HD3 | 9:K:58:HIS:CD2 | 2.51 | 0.46 |
| 9:J:272:ILE:O | 9:J:276:VAL:HG23 | 2.16 | 0.46 |
| 6:F:762:TRP:CE2 | 9:J:362:GLN:HB2 | 2.51 | 0.46 |
| 9:J:46:CYS:O | 9:J:50:THR:OG1 | 2.22 | 0.46 |
| 9:J:493:GLY:HA2 | 9:J:495:PHE:CE1 | 2.51 | 0.46 |
| 9:J:9:ARG:O | 9:J:13:TYR:CD2 | 2.67 | 0.46 |
| 9:K:386:LEU:CD1 | 9:K:386:LEU:H | 2.29 | 0.46 |
| 12:N:268:VAL:HA | 12:N:271:GLU:CD | 2.36 | 0.46 |
| 13:O:99:LEU:C | 13:O:99:LEU:HD12 | 2.36 | 0.46 |
| 3:P:251:TYR:HA | 3:P:254:LEU:HD12 | 1.98 | 0.46 |
| 1:A:168:ASP:OD1 | 1:A:168:ASP:N | 2.49 | 0.45 |
| 6:F:459:ALA:HB2 | 6:H:7:PRO:HG2 | 1.97 | 0.45 |
| 8:I:203:GLY:HA3 | 8:I:223:VAL:HG22 | 1.98 | 0.45 |
| 8:I:237:GLU:CG | 8:I:607:ILE:HD13 | 2.47 | 0.45 |
| 8:I:67:GLU:HB2 | 8:I:85:ALA:HB3 | 1.98 | 0.45 |
| 13:O:585:LEU:HD21 | 13:O:623:THR:HB | 1.98 | 0.45 |
| 13:O:715:TYR:HE1 | 13:O:719:ARG:HE | 1.64 | 0.45 |
| 3:P:45:GLU:O | 3:P:87:TYR:OH | 2.33 | 0.45 |
| 16:Y:168:THR:OG1 | 16:Y:171:ILE:CD1 | 2.64 | 0.45 |
| 1:A:1201:HIS:HE1 | 1:A:1203:MET:HB2 | 1.81 | 0.45 |
| 6:H:12:ILE:CG2 | 6:H:43:LEU:HD21 | 2.46 | 0.45 |
| 6:H:149:TRP:HH2 | 6:H:470:GLY:HA2 | 1.81 | 0.45 |
| 8:I:115:TRP:CE3 | 8:I:176:LEU:HD22 | 2.50 | 0.45 |
| 12:N:659:VAL:HG22 | 12:N:660:THR:H | 1.82 | 0.45 |
| 16:X:281:TYR:CE1 | 16:X:289:ASN:HB3 | 2.51 | 0.45 |
| 3:C:206:TRP:O | 3:C:209:LEU:HB2 | 2.16 | 0.45 |
| 3:C:255:ILE:O | 3:C:260:SER:OG | 2.34 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:F:699:ASP:HB3 | 6:F:702:ASN:OD1 | 2.16 | 0.45 |
| 7:G:3:ARG:HB2 | 9:J:443:LYS:HZ1 | 1.81 | 0.45 |
| 6:H:656:MET:HE3 | 6:H:660:LYS:HE2 | 1.99 | 0.45 |
| 6:H:658:PHE:HB3 | 6:H:675:ILE:HG12 | 1.98 | 0.45 |
| 9:J:397:ILE:O | 9:J:398:ALA:C | 2.55 | 0.45 |
| 12:N:542:VAL:HG11 | 12:N:558:GLU:CG | 2.46 | 0.45 |
| 16:Y:346:GLY:HA3 | 16:Y:378:LEU:HD21 | 1.98 | 0.45 |
| 16:Y:517:ASP:O | 16:Y:520:VAL:HG22 | 2.16 | 0.45 |
| 1:A:1177:MET:CB | 1:A:1207:GLY:HA2 | 2.42 | 0.45 |
| 1:A:173:LEU:HD22 | 1:A:177:VAL:CG1 | 2.46 | 0.45 |
| 1:A:1819:GLU:O | 1:A:1823:SER:HB3 | 2.16 | 0.45 |
| 1:A:256:VAL:HG23 | 1:A:271:LEU:HD22 | 1.98 | 0.45 |
| 1:A:584:ILE:O | 1:A:598:GLU:O | 2.33 | 0.45 |
| 2:B:20:ASP:O | 2:B:30:PHE:CD2 | 2.69 | 0.45 |
| 3:C:389:ARG:HD3 | 3:C:389:ARG:HA | 1.52 | 0.45 |
| 9:J:290:LYS:HA | 9:J:290:LYS:HE3 | 1.98 | 0.45 |
| 9:J:47:LEU:HD21 | 9:J:55:ARG:HH21 | 1.80 | 0.45 |
| 9:J:58:HIS:CG | 9:K:262:PRO:HD3 | 2.51 | 0.45 |
| 10:L:62:HIS:CD2 | 10:L:62:HIS:H | 2.35 | 0.45 |
| 3:C:416:PHE:CB | 13:O:326:GLU:HG2 | 2.45 | 0.45 |
| 3:C:441:GLU:OE2 | 14:R:83:ARG:NH1 | 2.50 | 0.45 |
| 16:Y:394:ILE:HA | 16:Y:397:ARG:HD3 | 1.97 | 0.45 |
| 1:A:1304:MET:O | 1:A:1307:LEU:HB2 | 2.17 | 0.45 |
| 1:A:451:GLN:HA | 1:A:475:PRO:O | 2.16 | 0.45 |
| 1:A:810:TYR:HA | 1:A:811:PRO:HD2 | 1.68 | 0.45 |
| 6:F:12:ILE:CG2 | 6:F:43:LEU:HD21 | 2.47 | 0.45 |
| 9:J:468:HIS:HB3 | 9:J:485:ILE:HG23 | 1.99 | 0.45 |
| 1:A:1354:GLU:HA | 10:L:30:VAL:HG12 | 1.99 | 0.45 |
| 13:O:423:ALA:HA | 13:O:426:THR:HG22 | 1.98 | 0.45 |
| 13:O:608:LEU:HD23 | 13:O:624:VAL:HG22 | 1.97 | 0.45 |
| 16:X:168:THR:OG1 | 16:X:171:ILE:CD1 | 2.65 | 0.45 |
| 16:X:54:ARG:CZ | 16:X:90:ASP:OD2 | 2.64 | 0.45 |
| 1:A:1274:LEU:O | 1:A:1277:ILE:HG22 | 2.16 | 0.45 |
| 3:C:285:ILE:HA | 3:C:288:GLU:CD | 2.37 | 0.45 |
| 3:C:96:VAL:N | 3:C:97:LYS:HA | 2.31 | 0.45 |
| 6:F:33:ALA:HB2 | 6:H:498:THR:HG21 | 1.99 | 0.45 |
| 9:K:272:ILE:O | 9:K:276:VAL:HG23 | 2.16 | 0.45 |
| 12:N:241:HIS:NE2 | 12:N:302:LYS:HE2 | 2.31 | 0.45 |
| 13:O:127:HIS:O | 13:O:128:LYS:HB3 | 2.17 | 0.45 |
| 14:R:128:ALA:HB1 | 14:R:129:LYS:CA | 2.27 | 0.45 |
| 16:X:517:ASP:O | 16:X:520:VAL:HG22 | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:Y:294:PHE:CD1 | 16:Y:294:PHE:O | 2.69 | 0.45 |
| 1:A:1485:PHE:CD1 | 1:A:1523:LEU:HD21 | 2.52 | 0.45 |
| 1:A:1572:TYR:CE2 | 1:A:1616:PRO:HB3 | 2.52 | 0.45 |
| 1:A:1638:TYR:N | 1:A:1638:TYR:HD1 | 2.10 | 0.45 |
| 3:C:122:ARG:HG3 | 3:C:154:LEU:HD11 | 1.98 | 0.45 |
| 6:F:59:ARG:NH2 | 6:H:562:MET:HB2 | 2.32 | 0.45 |
| 9:K:236:SER:O | 9:K:240:ARG:HG3 | 2.16 | 0.45 |
| 9:K:464:ALA:HB1 | 9:K:488:ILE:HD12 | 1.99 | 0.45 |
| 13:O:402:LEU:HD23 | 13:O:402:LEU:HA | 1.89 | 0.45 |
| 10:L:125:THR:HA | 10:L:126:ASP:HB3 | 1.98 | 0.45 |
| 12:N:233:CYS:O | 12:N:235:GLN:N | 2.49 | 0.45 |
| 3:P:201:LEU:HA | 3:P:229:MET:SD | 2.57 | 0.45 |
| 16:Y:506:GLN:HG3 | 16:Y:508:ASP:OD1 | 2.17 | 0.45 |
| 1:A:1640:GLY:N | 1:A:1645:GLU:O | 2.50 | 0.45 |
| 2:B:33:CYS:HB3 | 2:B:39:VAL:O | 2.17 | 0.45 |
| 3:C:277:ARG:O | 3:C:279:ILE:CD1 | 2.65 | 0.45 |
| 8:I:116:MET:SD | 8:I:210:LEU:CG | 3.05 | 0.45 |
| 8:I:269:LEU:HD22 | 8:I:526:LYS:HD2 | 1.99 | 0.45 |
| 8:I:262:LEU:HD21 | 8:I:533:ILE:HD13 | 1.99 | 0.45 |
| 9:K:38:GLN:HE21 | 9:K:38:GLN:HB2 | 1.68 | 0.45 |
| 6:H:656:MET:HE3 | 9:K:526:TYR:CD2 | 2.51 | 0.45 |
| 3:P:151:LEU:HD23 | 3:P:151:LEU:HA | 1.85 | 0.45 |
| 9:J:476:PRO:HB3 | 3:P:182:LEU:HB3 | 1.98 | 0.45 |
| 3:P:209:LEU:O | 3:P:213:ILE:HG12 | 2.17 | 0.45 |
| 3:P:405:LEU:HA | 3:P:408:THR:HG22 | 1.97 | 0.45 |
| 3:P:61:SER:HB2 | 3:P:262:SER:CB | 2.43 | 0.45 |
| 16:X:60:LEU:HB3 | 16:X:79:LEU:HD11 | 1.98 | 0.45 |
| 1:A:1189:ALA:O | 1:A:1191:LEU:N | 2.50 | 0.45 |
| 1:A:1262:GLN:HE22 | 1:A:1582:ALA:HB1 | 1.82 | 0.45 |
| 1:A:1480:GLU:HA | 1:A:1527:MET:HA | 1.98 | 0.45 |
| 6:H:554:VAL:O | 6:H:558:ASP:HB2 | 2.17 | 0.45 |
| 8:I:167:LEU:HD12 | 8:I:168:LEU:N | 2.32 | 0.45 |
| 13:O:262:LEU:HD13 | 13:O:270:SER:CB | 2.47 | 0.45 |
| 13:O:581:ILE:HG22 | 13:O:610:LEU:HD23 | 1.99 | 0.45 |
| 16:X:168:THR:OG1 | 16:X:171:ILE:HD12 | 2.17 | 0.45 |
| 16:X:173:MET:SD | 16:Y:49:LEU:HB3 | 2.57 | 0.45 |
| 1:A:1417:ASP:HA | 1:A:1643:TRP:CZ2 | 2.51 | 0.44 |
| 3:C:405:LEU:HA | 3:C:408:THR:HG22 | 1.99 | 0.44 |
| 3:C:48:LEU:HD21 | 3:C:116:PHE:CE2 | 2.52 | 0.44 |
| 5:E:63:VAL:HA | 5:E:66:THR:HG22 | 1.98 | 0.44 |
| 9:J:52:GLN:HG2 | 9:K:295:TYR:HE2 | 1.82 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:J:69:TYR:O | 9:J:70:GLU:HB3 | 2.16 | 0.44 |
| 9:K:78:ARG:HG3 | 9:K:135:LEU:HD22 | 1.98 | 0.44 |
| 9:K:284:LEU:HD13 | 9:K:308:TYR:HB2 | 2.00 | 0.44 |
| 2:B:15:LEU:HD12 | 12:N:626:TYR:HE2 | 1.82 | 0.44 |
| 12:N:659:VAL:HG22 | 12:N:660:THR:N | 2.32 | 0.44 |
| 6:F:639:TYR:CZ | 14:R:498:ILE:HG13 | 2.52 | 0.44 |
| 16:Y:270:ASN:HB2 | 16:Y:273:LEU:HB3 | 1.99 | 0.44 |
| 1:A:1637:THR:HA | 1:A:1647:THR:O | 2.17 | 0.44 |
| 1:A:260:ASP:OD1 | 1:A:262:VAL:HG22 | 2.17 | 0.44 |
| 1:A:872:LEU:HA | 1:A:933:TRP:HH2 | 1.82 | 0.44 |
| 6:H:130:ARG:HH12 | 9:K:473:VAL:CG2 | 2.26 | 0.44 |
| 9:J:512:ASP:O | 9:J:516:VAL:HG23 | 2.17 | 0.44 |
| 9:K:222:GLU:O | 9:K:225:ASP:O | 2.35 | 0.44 |
| 9:K:413:PHE:HD1 | 9:K:454:VAL:HG23 | 1.82 | 0.44 |
| 12:N:197:PRO:HA | 12:N:198:GLU:HA | 1.77 | 0.44 |
| 12:N:350:ASP:HB3 | 12:N:351:PHE:HA | 1.96 | 0.44 |
| 13:O:219:GLN:O | 13:O:222:LEU:HB2 | 2.17 | 0.44 |
| 13:O:350:LEU:HD23 | 13:O:350:LEU:HA | 1.76 | 0.44 |
| 8:I:371:SER:HB3 | 13:O:652:LEU:HB3 | 1.99 | 0.44 |
| 1:A:1642:GLN:HG3 | 1:A:1643:TRP:CE2 | 2.52 | 0.44 |
| 1:A:1675:GLU:HG3 | 1:A:1676:LEU:N | 2.31 | 0.44 |
| 3:C:170:PHE:O | 3:C:173:TYR:HB3 | 2.16 | 0.44 |
| 6:F:522:PHE:CB | 6:F:539:TYR:CD1 | 2.99 | 0.44 |
| 6:F:539:TYR:O | 6:F:542:THR:HB | 2.17 | 0.44 |
| 8:I:287:LEU:HD22 | 8:I:300:VAL:HG11 | 2.00 | 0.44 |
| 8:I:38:ALA:HB2 | 8:I:71:LEU:HD11 | 1.99 | 0.44 |
| 9:J:337:TRP:CZ3 | 9:J:340:TYR:HD2 | 2.36 | 0.44 |
| 9:K:192:LYS:HG2 | 9:K:198:GLN:HE21 | 1.82 | 0.44 |
| 12:N:330:ARG:HB2 | 12:N:334:ARG:NH2 | 2.32 | 0.44 |
| 1:A:131:PHE:CE1 | 1:A:216:PRO:HD3 | 2.52 | 0.44 |
| 1:A:38:GLN:HG3 | 3:C:396:LYS:H | 1.82 | 0.44 |
| 3:C:112:LYS:HB2 | 3:C:113:LYS:NZ | 2.32 | 0.44 |
| 3:C:286:PHE:HB3 | 3:C:303:PHE:CE2 | 2.53 | 0.44 |
| 6:F:18:HIS:O | 6:H:73:TYR:OH | 2.18 | 0.44 |
| 6:F:488:LEU:HD22 | 6:F:501:VAL:HG13 | 2.00 | 0.44 |
| 8:I:186:GLU:OE2 | 8:I:197:ARG:CZ | 2.62 | 0.44 |
| 9:J:206:GLU:HA | 9:J:209:LEU:HG | 1.98 | 0.44 |
| 12:N:281:TYR:HB3 | 12:N:282:GLU:H | 1.55 | 0.44 |
| 12:N:574:ILE:HD12 | 12:N:625:LYS:HG2 | 1.99 | 0.44 |
| 13:O:668:ALA:CB | 13:O:694:LEU:HD23 | 2.47 | 0.44 |
| 3:P:323:LEU:HD12 | 3:P:336:VAL:HG11 | 2.00 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 3:P:475:LYS:O | 3:P:479:GLN:NE2 | 2.50 | 0.44 |
| 3:P:54:TRP:CH2 | 3:P:58:LEU:HD11 | 2.53 | 0.44 |
| 1:A:191:ARG:HG2 | 1:A:192:SER:N | 2.32 | 0.44 |
| 1:A:880:TYR:HB2 | 1:A:930:LEU:HD22 | 1.98 | 0.44 |
| 3:C:235:ALA:H | 3:C:250:LYS:HZ2 | 1.62 | 0.44 |
| 8:I:399:LYS:HG2 | 8:I:525:VAL:HG21 | 1.98 | 0.44 |
| 9:J:342:HIS:CD2 | 9:J:357:TYR:OH | 2.70 | 0.44 |
| 9:J:506:LEU:HD21 | 9:J:516:VAL:HA | 1.98 | 0.44 |
| 9:K:406:HIS:CE1 | 7:W:6:PRO:HB3 | 2.53 | 0.44 |
| 12:N:400:TYR:CZ | 12:N:404:ILE:HD11 | 2.53 | 0.44 |
| 14:R:406:LEU:HD13 | 14:R:451[B]:MET:HB2 | 1.99 | 0.44 |
| 16:X:134:SER:O | 16:X:138:VAL:HG23 | 2.17 | 0.44 |
| 16:Y:384:ARG:HH22 | 16:Y:415:GLU:HB3 | 1.82 | 0.44 |
| 1:A:91:GLU:CD | 1:A:102:TRP:HE1 | 2.20 | 0.44 |
| 1:A:1478:GLY:O | 1:A:1617:ARG:NH2 | 2.50 | 0.44 |
| 1:A:1589:TYR:HE2 | 1:A:1591:HIS:HB2 | 1.82 | 0.44 |
| 1:A:1674:TRP:HD1 | 1:A:1674:TRP:H | 1.65 | 0.44 |
| 1:A:632:GLU:O | 1:A:635:VAL:HB | 2.17 | 0.44 |
| 2:B:23:CYS:HA | 2:B:30:PHE:CE1 | 2.53 | 0.44 |
| 6:F:15:ALA:HA | 6:H:116:PHE:CE1 | 2.52 | 0.44 |
| 6:H:121:LEU:O | 6:H:125:TYR:CD1 | 2.70 | 0.44 |
| 9:J:37:PRO:HB3 | 9:J:69:TYR:CZ | 2.52 | 0.44 |
| 9:K:290:LYS:HA | 9:K:290:LYS:HE3 | 1.99 | 0.44 |
| 9:K:369:LEU:O | 9:K:373:TYR:CD2 | 2.71 | 0.44 |
| 12:N:180:PHE:CD1 | 12:N:299:TRP:HZ3 | 2.35 | 0.44 |
| 12:N:411:ASP:O | 12:N:412:PRO:C | 2.56 | 0.44 |
| 3:P:399:TYR:HB3 | 3:P:428:LEU:HD22 | 1.99 | 0.44 |
| 16:X:229:THR:HG21 | 16:X:233:LEU:HD12 | 1.99 | 0.44 |
| 16:X:394:ILE:HA | 16:X:397:ARG:HD3 | 2.00 | 0.44 |
| 16:X:201:LEU:CD1 | 16:Y:40:HIS:HB3 | 2.36 | 0.44 |
| 1:A:1070:LEU:HA | 1:A:1073:LEU:HD12 | 1.99 | 0.44 |
| 1:A:100:VAL:HG23 | 1:A:123:VAL:HG21 | 1.98 | 0.44 |
| 1:A:1821:PHE:CD1 | 1:A:1845:LEU:HD13 | 2.53 | 0.44 |
| 3:C:39:ILE:CG2 | 3:C:201:LEU:HG | 2.47 | 0.44 |
| 3:C:311:SER:OG | 3:C:311:SER:O | 2.34 | 0.44 |
| 3:C:488:GLN:O | 3:C:491:ILE:HG13 | 2.17 | 0.44 |
| 6:F:499:GLY:O | 6:F:503:CYS:HB2 | 2.18 | 0.44 |
| 8:I:189:ALA:N | 8:I:193:PHE:O | 2.50 | 0.44 |
| 8:I:396:PHE:CE1 | 8:I:522:LEU:HD22 | 2.53 | 0.44 |
| 8:I:586:LEU:HD12 | 8:I:587:LEU:N | 2.32 | 0.44 |
| 8:I:69:THR:HG23 | 8:I:85:ALA:HB2 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:J:465:LEU:CA | 9:J:488:ILE:HD12 | 2.44 | 0.44 |
| 12:N:264:THR:HA | 12:N:267:GLN:HG2 | 2.00 | 0.44 |
| 13:O:129:THR:O | 13:O:130:SER:CB | 2.65 | 0.44 |
| 13:O:78:LEU:HD12 | 13:O:78:LEU:O | 2.17 | 0.44 |
| 14:R:74:PRO:HA | 14:R:75:GLY:HA2 | 1.79 | 0.44 |
| 16:Y:134:SER:O | 16:Y:138:VAL:HG23 | 2.18 | 0.44 |
| 16:Y:474:ASP:OD1 | 16:Y:502:ALA:HA | 2.18 | 0.44 |
| 1:A:1265:ALA:HB2 | 1:A:1309:HIS:CD2 | 2.53 | 0.44 |
| 1:A:1477:ALA:HB1 | 1:A:1574:LEU:HD12 | 2.00 | 0.44 |
| 1:A:435:ASP:HB2 | 1:A:501:THR:HG22 | 2.00 | 0.44 |
| 6:F:25:VAL:HG22 | 6:F:47:CYS:HB3 | 2.00 | 0.44 |
| 6:F:502:LEU:HB2 | 6:F:525:VAL:HG22 | 1.99 | 0.44 |
| 9:K:40:ILE:CD1 | 9:K:65:LEU:HD21 | 2.48 | 0.44 |
| 10:L:33:LEU:HD12 | 10:L:42:VAL:HG22 | 2.00 | 0.44 |
| 12:N:477:PRO:HA | 12:N:478:GLU:HA | 1.72 | 0.44 |
| 12:N:676:TRP:HE3 | 12:N:680:GLU:HB3 | 1.83 | 0.44 |
| 3:P:185:VAL:HG13 | 3:P:212:LEU:HD22 | 2.00 | 0.44 |
| 14:R:107:PRO:HA | 14:R:110:LYS:HB3 | 2.00 | 0.44 |
| 16:X:506:GLN:HG3 | 16:X:508:ASP:OD1 | 2.17 | 0.44 |
| 16:Y:168:THR:OG1 | 16:Y:171:ILE:HD12 | 2.18 | 0.44 |
| 16:Y:70:LEU:HD13 | 16:Y:70:LEU:O | 2.17 | 0.44 |
| 1:A:1466:ALA:HB2 | 1:A:1515:CYS:HB2 | 2.00 | 0.44 |
| 1:A:269:TRP:CD2 | 1:A:411:HIS:HB3 | 2.53 | 0.44 |
| 1:A:93:LEU:HD11 | 1:A:151:ILE:CD1 | 2.48 | 0.44 |
| 6:F:56:LYS:HE3 | 6:H:532:ARG:HA | 1.98 | 0.44 |
| 8:I:231:VAL:HG12 | 8:I:232:SER:N | 2.33 | 0.44 |
| 8:I:70:CYS:C | 8:I:71:LEU:HD12 | 2.38 | 0.44 |
| 12:N:284:SER:HA | 12:N:285:PHE:CG | 2.53 | 0.44 |
| 13:O:402:LEU:HD13 | 13:O:425:LYS:HG3 | 2.00 | 0.44 |
| 7:W:14:ASP:O | 7:W:17:GLU:HB2 | 2.18 | 0.44 |
| 16:Y:229:THR:HG21 | 16:Y:233:LEU:HD12 | 2.00 | 0.44 |
| 1:A:941:LEU:HD12 | 1:A:977:LEU:O | 2.18 | 0.43 |
| 2:B:16:TRP:NE1 | 2:B:46:LEU:HG | 2.32 | 0.43 |
| 3:C:370:LEU:HD23 | 3:C:370:LEU:HA | 1.91 | 0.43 |
| 6:F:639:TYR:CD2 | 14:R:498:ILE:HG21 | 2.53 | 0.43 |
| 9:J:164:PHE:CZ | 9:J:168:ASP:HB2 | 2.53 | 0.43 |
| 12:N:519:TYR:CE1 | 12:N:523:LEU:HD21 | 2.53 | 0.43 |
| 12:N:577:GLU:HG2 | 12:N:583:ALA:HB2 | 1.99 | 0.43 |
| 16:X:233:LEU:HD22 | 16:X:235:TRP:CZ2 | 2.53 | 0.43 |
| 16:X:474:ASP:OD1 | 16:X:502:ALA:HA | 2.18 | 0.43 |
| 16:X:204:ASP:OD1 | 16:Y:55:LEU:HB2 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:104:LYS:HE2 | 1:A:114:TYR:CD1 | 2.53 | 0.43 |
| 1:A:1473:GLY:HA2 | 1:A:1526:VAL:CG1 | 2.48 | 0.43 |
| 2:B:20:ASP:CB | 2:B:30:PHE:HE2 | 2.30 | 0.43 |
| 1:A:40:ARG:HD3 | 3:C:142:GLU:HG3 | 2.00 | 0.43 |
| 3:C:60:PHE:CB | 3:P:89:LEU:HD12 | 2.47 | 0.43 |
| 6:F:61:LEU:HD23 | 6:F:61:LEU:HA | 1.94 | 0.43 |
| 8:I:449:ALA:HB2 | 13:O:65:LEU:HD21 | 1.99 | 0.43 |
| 6:F:765:ASP:OD2 | 9:J:359:THR:HG22 | 2.19 | 0.43 |
| 9:J:475:ILE:HG13 | 9:J:475:ILE:O | 2.17 | 0.43 |
| 16:Y:39:ASP:N | 16:Y:39:ASP:OD1 | 2.51 | 0.43 |
| 1:A:1198:THR:O | 1:A:1200:GLY:N | 2.51 | 0.43 |
| 1:A:160:ASN:OD1 | 1:A:170:ILE:HG23 | 2.18 | 0.43 |
| 3:C:36:LEU:HD21 | 3:C:58:LEU:HB2 | 1.98 | 0.43 |
| 6:F:658:PHE:HB3 | 6:F:675:ILE:HG12 | 1.99 | 0.43 |
| 6:H:707:PHE:CE2 | 6:H:738:LEU:HG | 2.53 | 0.43 |
| 8:I:202:ALA:O | 8:I:223:VAL:CG2 | 2.66 | 0.43 |
| 8:I:413:ASN:HB3 | 8:I:451:PHE:CE1 | 2.53 | 0.43 |
| 8:I:74:ARG:HH21 | 8:I:78:LYS:HB2 | 1.83 | 0.43 |
| 9:J:211:LYS:O | 9:J:212:TYR:CG | 2.71 | 0.43 |
| 9:J:369:LEU:O | 9:J:373:TYR:CD2 | 2.72 | 0.43 |
| 9:K:45:GLN:NE2 | 9:K:45:GLN:HA | 2.27 | 0.43 |
| 12:N:392:ASN:O | 12:N:395:ASP:HA | 2.18 | 0.43 |
| 13:O:596:SER:OG | 13:O:599:ILE:HD12 | 2.18 | 0.43 |
| 16:X:355:TYR:CE1 | 16:X:385:ASN:HB2 | 2.51 | 0.43 |
| 16:X:50:HIS:HA | 16:X:53:VAL:HG22 | 2.00 | 0.43 |
| 16:Y:355:TYR:CZ | 16:Y:385:ASN:HB3 | 2.53 | 0.43 |
| 1:A:269:TRP:CE3 | 1:A:411:HIS:HB3 | 2.52 | 0.43 |
| 3:C:234:LEU:HB3 | 3:C:250:LYS:HE3 | 2.00 | 0.43 |
| 3:C:353:TYR:HA | 3:C:356:ARG:HD2 | 2.00 | 0.43 |
| 6:H:121:LEU:CD1 | 6:H:125:TYR:HE1 | 2.32 | 0.43 |
| 6:H:689:LEU:CD2 | 6:H:713:LEU:HG | 2.48 | 0.43 |
| 8:I:501:LEU:HD23 | 8:I:516:TYR:HE2 | 1.83 | 0.43 |
| 9:K:371:MET:HA | 9:K:374:ILE:HD12 | 1.99 | 0.43 |
| 12:N:157:LEU:O | 12:N:161:LEU:HG | 2.17 | 0.43 |
| 1:A:1230:ILE:HD13 | 1:A:1236:LEU:HD13 | 2.00 | 0.43 |
| 1:A:1230:ILE:HA | 1:A:1236:LEU:HB3 | 2.01 | 0.43 |
| 1:A:776:ASN:HA | 1:A:869:ARG:NE | 2.33 | 0.43 |
| 3:C:321:HIS:HA | 11:M:24:LEU:HD13 | 1.99 | 0.43 |
| 6:F:46:THR:HG23 | 6:H:19:TYR:OH | 2.18 | 0.43 |
| 6:H:164:PRO:HB2 | 6:H:467:ARG:HG3 | 2.01 | 0.43 |
| 8:I:184:PHE:HB2 | 8:I:198:VAL:O | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:N:520:ARG:HD3 | 12:N:556:PHE:HB3 | 2.00 | 0.43 |
| 3:C:416:PHE:HA | 3:C:446:LEU:HD11 | 2.01 | 0.43 |
| 6:H:539:TYR:O | 6:H:542:THR:HB | 2.18 | 0.43 |
| 9:J:247:PHE:CD2 | 9:J:277:GLU:HB3 | 2.53 | 0.43 |
| 9:J:506:LEU:HA | 9:J:506:LEU:HD12 | 1.79 | 0.43 |
| 6:F:554:VAL:HG21 | 9:K:286:TYR:HD1 | 1.83 | 0.43 |
| 6:F:550:VAL:HG21 | 9:K:289:HIS:HB3 | 2.01 | 0.43 |
| 9:K:349:GLU:HB3 | 9:K:352:GLN:HE21 | 1.84 | 0.43 |
| 10:L:61:PRO:HB3 | 10:L:142:LEU:HA | 2.00 | 0.43 |
| 9:J:305:VAL:CG1 | 11:M:31:ILE:HD11 | 2.46 | 0.43 |
| 8:I:32:ARG:HG2 | 12:N:388:HIS:CE1 | 2.54 | 0.43 |
| 12:N:693:ARG:HA | 12:N:696:MET:HB3 | 2.00 | 0.43 |
| 12:N:699:TRP:CE3 | 12:N:699:TRP:HA | 2.53 | 0.43 |
| 3:C:414:MET:HA | 13:O:326:GLU:OE1 | 2.19 | 0.43 |
| 16:X:39:ASP:OD1 | 16:X:39:ASP:N | 2.51 | 0.43 |
| 16:Y:475:TYR:O | 16:Y:479:VAL:HG23 | 2.19 | 0.43 |
| 1:A:1405:LEU:C | 1:A:1405:LEU:HD12 | 2.38 | 0.43 |
| 3:C:150:ALA:O | 3:C:154:LEU:HD13 | 2.18 | 0.43 |
| 6:F:554:VAL:HG21 | 9:K:286:TYR:CD1 | 2.53 | 0.43 |
| 3:P:389:ARG:HA | 3:P:392:ILE:CG2 | 2.49 | 0.43 |
| 16:X:408:ASP:O | 16:X:411:GLU:HG2 | 2.19 | 0.43 |
| 1:A:114:TYR:O | 1:A:115:LYS:HG3 | 2.18 | 0.43 |
| 1:A:412:LEU:HD12 | 1:A:468:PHE:CZ | 2.54 | 0.43 |
| 1:A:248:PHE:CB | 1:A:430:VAL:HG21 | 2.44 | 0.43 |
| 1:A:876:SER:HB2 | 1:A:930:LEU:HD11 | 2.00 | 0.43 |
| 5:E:105:PHE:HA | 9:K:510:ARG:HG2 | 2.00 | 0.43 |
| 6:H:121:LEU:HD11 | 6:H:125:TYR:HE1 | 1.83 | 0.43 |
| 8:I:11:PHE:HD1 | 8:I:746:MET:HA | 1.84 | 0.43 |
| 13:O:319:GLN:O | 13:O:322:LEU:HB2 | 2.19 | 0.43 |
| 16:X:270:ASN:HB2 | 16:X:273:LEU:HB3 | 2.01 | 0.43 |
| 1:A:1660:LEU:HD21 | 1:A:1687:LEU:HB3 | 2.01 | 0.43 |
| 1:A:183:THR:HG22 | 1:A:249:LEU:HG | 2.00 | 0.43 |
| 1:A:755:LEU:HA | 1:A:756:PHE:HA | 1.74 | 0.43 |
| 3:C:446:LEU:HD23 | 3:C:448:GLN:OE1 | 2.19 | 0.43 |
| 6:F:157:GLU:HG2 | 6:F:477:CYS:SG | 2.57 | 0.43 |
| 8:I:619:LYS:HE3 | 8:I:704:THR:HG23 | 2.01 | 0.43 |
| 9:J:354:MET:HA | 9:J:354:MET:HE2 | 1.98 | 0.43 |
| 9:K:296:PRO:HB2 | 11:M:55:MET:HG3 | 2.00 | 0.43 |
| 12:N:268:VAL:HA | 12:N:271:GLU:CG | 2.48 | 0.43 |
| 12:N:523:LEU:O | 12:N:527:LEU:HG | 2.19 | 0.43 |
| 13:O:610:LEU:HD12 | 13:O:614:TYR:HE1 | 1.83 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:P:523:CYS:O | 3:P:524:LYS:HG3 | 2.18 | 0.43 |
| 16:Y:71:PHE:O | 16:Y:76:LYS:HE3 | 2.19 | 0.43 |
| 16:Y:45:ALA:CB | 16:Y:82:TYR:CD2 | 3.00 | 0.43 |
| 1:A:1364:CYS:N | 1:A:1365:PRO:HD2 | 2.34 | 0.43 |
| 1:A:949:PHE:N | 1:A:1813:GLN:HE21 | 2.16 | 0.43 |
| 3:C:102:ALA:O | 3:C:106:LEU:HD12 | 2.18 | 0.43 |
| 3:C:248:LEU:HD21 | 3:C:276:ILE:HD11 | 2.01 | 0.43 |
| 3:C:296:ARG:NH1 | 3:C:296:ARG:CG | 2.53 | 0.43 |
| 6:F:120:LEU:O | 6:F:124:VAL:HG23 | 2.19 | 0.43 |
| 6:H:702:ASN:HA | 6:H:703:PRO:HD3 | 1.92 | 0.43 |
| 8:I:556:LEU:HD11 | 8:I:586:LEU:HD21 | 1.99 | 0.43 |
| 9:J:180:GLU:OE1 | 9:J:180:GLU:CA | 2.67 | 0.43 |
| 9:J:456:ARG:CG | 9:J:488:ILE:HG22 | 2.49 | 0.43 |
| 9:K:231:LEU:HA | 9:K:234:VAL:HG22 | 2.00 | 0.43 |
| 10:L:80:TYR:HD2 | 10:L:154:ARG:HB2 | 1.84 | 0.43 |
| 11:M:32:PRO:C | 11:M:34:ASN:H | 2.22 | 0.43 |
| 12:N:151:GLU:O | 12:N:155:THR:HG23 | 2.19 | 0.43 |
| 8:I:497:TRP:HB3 | 13:O:460:GLN:NE2 | 2.34 | 0.43 |
| 9:K:406:HIS:ND1 | 7:W:6:PRO:HB3 | 2.32 | 0.43 |
| 6:F:65:SER:N | 16:Y:296:GLN:HE22 | 2.17 | 0.43 |
| 16:Y:508:ASP:HB3 | 16:Y:509:CYS:H | 1.65 | 0.43 |
| 1:A:1110:ARG:HG2 | 1:A:1117:THR:HG22 | 2.01 | 0.42 |
| 1:A:1774:VAL:CG1 | 1:A:1790:TYR:HB3 | 2.49 | 0.42 |
| 2:B:41:GLY:O | 2:B:45:PRO:HA | 2.19 | 0.42 |
| 6:F:164:PRO:HG2 | 6:F:471:LYS:HG3 | 2.01 | 0.42 |
| 8:I:202:ALA:C | 8:I:223:VAL:HG22 | 2.39 | 0.42 |
| 9:J:320:ARG:HG2 | 9:J:340:TYR:CE1 | 2.54 | 0.42 |
| 13:O:539:ASN:ND2 | 13:O:542:GLU:CB | 2.71 | 0.42 |
| 3:P:460:TYR:CE1 | 3:P:470:LEU:HD11 | 2.53 | 0.42 |
| 16:Y:203:LEU:HA | 16:Y:206:ILE:HD12 | 2.01 | 0.42 |
| 16:Y:73:PRO:O | 16:Y:106:GLN:OE1 | 2.37 | 0.42 |
| 1:A:1377:LYS:HG2 | 1:A:1416:TRP:CG | 2.54 | 0.42 |
| 1:A:591:VAL:O | 1:A:591:VAL:HG23 | 2.19 | 0.42 |
| 3:C:112:LYS:H | 3:C:112:LYS:CD | 2.32 | 0.42 |
| 3:C:523:CYS:O | 3:C:524:LYS:HG3 | 2.19 | 0.42 |
| 8:I:640:ASP:OD1 | 8:I:641:ALA:N | 2.52 | 0.42 |
| 9:J:472:LEU:O | 9:J:476:PRO:HA | 2.19 | 0.42 |
| 10:L:24:GLU:HA | 10:L:158:ILE:O | 2.19 | 0.42 |
| 13:O:584:LEU:HD13 | 13:O:607:ALA:HB2 | 2.01 | 0.42 |
| 16:X:304:LEU:HD23 | 16:X:304:LEU:HA | 1.87 | 0.42 |
| 16:Y:294:PHE:HD1 | 16:Y:294:PHE:C | 2.21 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1262:GLN:NE2 | 1:A:1582:ALA:CB | 2.81 | 0.42 |
| 1:A:15:ARG:HH21 | 13:O:526:HIS:HB3 | 1.84 | 0.42 |
| 3:C:215:ASP:HB3 | 3:C:218:MET:HG3 | 2.01 | 0.42 |
| 3:C:61:SER:CB | 3:C:262:SER:HB2 | 2.42 | 0.42 |
| 8:I:25:PHE:CD1 | 8:I:71:LEU:HD13 | 2.54 | 0.42 |
| 9:J:214:LYS:HE2 | 9:J:216:SER:OG | 2.20 | 0.42 |
| 9:K:178:ALA:HA | 9:K:181:GLU:CD | 2.40 | 0.42 |
| 9:K:203:PHE:HE1 | 9:K:218:THR:HB | 1.84 | 0.42 |
| 12:N:333:TYR:HD1 | 12:N:364:CYS:SG | 2.41 | 0.42 |
| 1:A:31:HIS:CD2 | 13:O:264:VAL:CG2 | 3.01 | 0.42 |
| 13:O:322:LEU:O | 13:O:325:GLN:HB2 | 2.19 | 0.42 |
| 13:O:394:THR:HG22 | 13:O:615:ARG:HH12 | 1.84 | 0.42 |
| 13:O:382:GLN:HG3 | 13:O:417:LEU:HD13 | 2.02 | 0.42 |
| 3:P:414:MET:HA | 3:P:415:PRO:HD3 | 1.86 | 0.42 |
| 3:P:96:VAL:N | 3:P:97:LYS:HA | 2.34 | 0.42 |
| 16:X:246:VAL:HG13 | 16:X:280:LEU:HD21 | 2.01 | 0.42 |
| 1:A:584:ILE:HG13 | 1:A:599:LEU:HD23 | 2.02 | 0.42 |
| 3:C:279:ILE:HD11 | 14:R:77:ASP:OD1 | 2.19 | 0.42 |
| 6:H:12:ILE:HG21 | 6:H:43:LEU:CD2 | 2.50 | 0.42 |
| 8:I:345:GLN:HB2 | 8:I:407:ILE:HG21 | 2.00 | 0.42 |
| 8:I:514:PHE:HE2 | 13:O:440:GLN:CA | 2.20 | 0.42 |
| 9:J:342:HIS:HD2 | 9:J:357:TYR:OH | 2.01 | 0.42 |
| 9:J:495:PHE:HD2 | 9:J:522:CYS:SG | 2.39 | 0.42 |
| 13:O:361:LEU:HD13 | 13:O:384:LEU:HA | 2.01 | 0.42 |
| 13:O:672:VAL:HG21 | 13:O:720:LEU:HD21 | 2.01 | 0.42 |
| 13:O:730:ARG:O | 13:O:733:CYS:HB2 | 2.20 | 0.42 |
| 3:P:293:ASP:HA | 3:P:294:PRO:HD3 | 1.96 | 0.42 |
| 16:X:242:ALA:O | 16:X:246:VAL:HG23 | 2.20 | 0.42 |
| 16:X:281:TYR:HB3 | 16:X:290:SER:OG | 2.19 | 0.42 |
| 16:Y:84:ALA:HB1 | 16:Y:100:TYR:CZ | 2.54 | 0.42 |
| 1:A:1632:ALA:H | 1:A:1653:ALA:HB3 | 1.84 | 0.42 |
| 3:C:365:LEU:HD23 | 3:C:365:LEU:HA | 1.84 | 0.42 |
| 3:C:403:TYR:C | 3:C:403:TYR:CD1 | 2.93 | 0.42 |
| 3:C:526:TRP:NE1 | 3:C:553:ILE:O | 2.49 | 0.42 |
| 3:C:58:LEU:O | 3:C:61:SER:HB3 | 2.20 | 0.42 |
| 6:H:32:TYR:CE1 | 6:H:41:LEU:HB2 | 2.54 | 0.42 |
| 6:H:481:CYS:O | 6:H:485:ILE:HG12 | 2.20 | 0.42 |
| 9:J:220:ILE:HG22 | 9:J:222:GLU:H | 1.85 | 0.42 |
| 9:J:443:LYS:O | 9:J:446:PRO:HD2 | 2.19 | 0.42 |
| 12:N:150:ARG:HA | 12:N:153:VAL:HG23 | 2.01 | 0.42 |
| 12:N:73:GLU:O | 12:N:74:TRP:CB | 2.67 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:O:581:ILE:HD13 | 13:O:611:SER:HB3 | 2.02 | 0.42 |
| 16:X:203:LEU:HA | 16:X:206:ILE:HD12 | 2.01 | 0.42 |
| 16:Y:145:CYS:O | 16:Y:149:LEU:HG | 2.20 | 0.42 |
| 16:Y:281:TYR:HB3 | 16:Y:290:SER:OG | 2.19 | 0.42 |
| 16:Y:42:ARG:HG3 | 16:Y:82:TYR:HH | 1.79 | 0.42 |
| 1:A:1329:MET:CE | 1:A:1371:LEU:HD12 | 2.50 | 0.42 |
| 1:A:1403:PHE:O | 1:A:1407:ARG:HB2 | 2.19 | 0.42 |
| 1:A:1790:TYR:O | 1:A:1793:MET:HB2 | 2.19 | 0.42 |
| 1:A:247:VAL:HG12 | 1:A:257:MET:O | 2.20 | 0.42 |
| 3:C:244:ILE:HD12 | 3:C:245:GLU:H | 1.85 | 0.42 |
| 3:C:46:ARG:NH2 | 3:C:48:LEU:HD11 | 2.21 | 0.42 |
| 6:H:532:ARG:HG3 | 6:H:534:GLU:H | 1.84 | 0.42 |
| 8:I:269:LEU:HD23 | 8:I:523:HIS:CE1 | 2.55 | 0.42 |
| 9:J:300:VAL:HG22 | 9:J:333:TYR:OH | 2.19 | 0.42 |
| 6:F:762:TRP:NE1 | 9:J:362:GLN:HB2 | 2.34 | 0.42 |
| 9:J:445:GLU:CA | 9:J:474:LEU:HD23 | 2.48 | 0.42 |
| 10:L:33:LEU:HD13 | 10:L:54:TRP:CD2 | 2.55 | 0.42 |
| 12:N:520:ARG:HD2 | 12:N:556:PHE:CD1 | 2.55 | 0.42 |
| 1:A:1329:MET:HE1 | 1:A:1371:LEU:HD12 | 2.02 | 0.42 |
| 1:A:1611:VAL:CG1 | 1:A:1612:LEU:HD12 | 2.50 | 0.42 |
| 1:A:980:ARG:NH2 | 1:A:1674:TRP:O | 2.52 | 0.42 |
| 1:A:612:ILE:O | 1:A:641:TRP:CH2 | 2.73 | 0.42 |
| 6:H:465:LEU:HD22 | 6:H:495:HIS:CE1 | 2.55 | 0.42 |
| 9:J:167:PHE:HA | 9:J:170:LEU:HD21 | 2.01 | 0.42 |
| 9:J:323:LEU:O | 9:J:327:THR:HG22 | 2.20 | 0.42 |
| 12:N:523:LEU:HD22 | 12:N:538:GLU:OE1 | 2.20 | 0.42 |
| 13:O:439:LEU:HG | 13:O:476:LEU:HD13 | 2.02 | 0.42 |
| 13:O:657:ILE:HG13 | 13:O:658:LEU:N | 2.35 | 0.42 |
| 14:R:202:LEU:HD12 | 14:R:207:TYR:CD2 | 2.55 | 0.42 |
| 6:F:704:LEU:HD13 | 14:R:494:ILE:H | 1.84 | 0.42 |
| 16:Y:465:LEU:HD23 | 16:Y:485:LEU:HD11 | 2.02 | 0.42 |
| 1:A:1586:CYS:HB3 | 1:A:1606:LEU:HD22 | 2.01 | 0.42 |
| 1:A:871:ARG:HG3 | 1:A:872:LEU:N | 2.34 | 0.42 |
| 2:B:20:ASP:O | 2:B:30:PHE:HD2 | 2.03 | 0.42 |
| 9:J:180:GLU:O | 9:J:184:LEU:N | 2.37 | 0.42 |
| 9:K:404:VAL:O | 9:K:408:VAL:HG23 | 2.20 | 0.42 |
| 10:L:12:ASP:HA | 10:L:13:PRO:HD2 | 1.84 | 0.42 |
| 16:X:475:TYR:O | 16:X:479:VAL:HG23 | 2.19 | 0.42 |
| 16:Y:291:VAL:HG22 | 16:Y:314:LEU:HB3 | 2.01 | 0.42 |
| 1:A:1350:TYR:O | 10:L:42:VAL:HG23 | 2.20 | 0.42 |
| 1:A:93:LEU:HD11 | 1:A:151:ILE:HD11 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1531:GLY:HA3 | 1:A:1566:PHE:CE2 | 2.55 | 0.42 |
| 3:C:115:TYR:CZ | 3:C:161:LYS:CD | 3.03 | 0.42 |
| 3:C:395:ASN:HB3 | 3:C:398:ASP:H | 1.85 | 0.42 |
| 3:C:413:LYS:C | 3:C:415:PRO:CD | 2.86 | 0.42 |
| 8:I:72:ALA:C | 8:I:80:LEU:HD12 | 2.40 | 0.42 |
| 9:J:84:LYS:HD3 | 9:J:86:HIS:NE2 | 2.34 | 0.42 |
| 9:K:509:ARG:HG3 | 9:K:512:ASP:HB2 | 2.02 | 0.42 |
| 12:N:213:TYR:C | 12:N:214:ARG:HA | 2.40 | 0.42 |
| 12:N:347:ILE:HG21 | 12:N:358:ILE:HG23 | 2.02 | 0.42 |
| 2:B:11:VAL:HB | 12:N:594:VAL:HG12 | 2.00 | 0.42 |
| 12:N:681:LEU:HD23 | 12:N:692:LEU:HD21 | 2.01 | 0.42 |
| 13:O:360:LEU:O | 13:O:364:SER:HB2 | 2.19 | 0.42 |
| 16:Y:42:ARG:HA | 16:Y:82:TYR:OH | 2.17 | 0.42 |
| 1:A:1198:THR:C | 1:A:1200:GLY:N | 2.73 | 0.42 |
| 1:A:425:SER:N | 1:A:448:SER:HG | 2.17 | 0.42 |
| 3:C:153:GLU:O | 3:C:157:GLU:OE1 | 2.38 | 0.42 |
| 3:C:306:LEU:HD12 | 3:C:307:LEU:N | 2.35 | 0.42 |
| 6:H:550:VAL:O | 6:H:554:VAL:HG23 | 2.20 | 0.42 |
| 8:I:188:TYR:HA | 8:I:193:PHE:O | 2.20 | 0.42 |
| 12:N:156:MET:O | 12:N:160:VAL:HG23 | 2.20 | 0.42 |
| 12:N:210:ARG:HB3 | 12:N:214:ARG:CZ | 2.50 | 0.42 |
| 12:N:22:VAL:CB | 12:N:58:ALA:HA | 2.50 | 0.42 |
| 12:N:700:LEU:HD13 | 12:N:707:GLU:HG3 | 2.01 | 0.42 |
| 3:P:58:LEU:O | 3:P:61:SER:HB3 | 2.20 | 0.42 |
| 14:R:110:LYS:O | 14:R:113:GLN:HB2 | 2.19 | 0.42 |
| 9:K:514:PHE:CZ | 7:W:11:LEU:HD22 | 2.55 | 0.42 |
| 16:X:393:ILE:HG22 | 16:X:397:ARG:HH11 | 1.85 | 0.42 |
| 16:X:87:LEU:HD11 | 16:X:99:LYS:HG3 | 2.01 | 0.42 |
| 16:Y:294:PHE:HD1 | 16:Y:294:PHE:O | 2.03 | 0.42 |
| 3:C:297:ILE:O | 3:C:297:ILE:HG12 | 2.18 | 0.41 |
| 6:H:120:LEU:O | 6:H:124:VAL:HG23 | 2.20 | 0.41 |
| 8:I:497:TRP:CD1 | 13:O:446:LEU:O | 2.73 | 0.41 |
| 10:L:109:ARG:NH2 | 10:L:123:PRO:HD2 | 2.35 | 0.41 |
| 6:H:704:LEU:HA | 10:L:177:PHE:CZ | 2.55 | 0.41 |
| 12:N:281:TYR:HE1 | 12:N:357:ALA:HA | 1.83 | 0.41 |
| 12:N:331:PHE:CZ | 12:N:335:ILE:HD11 | 2.55 | 0.41 |
| 8:I:349:ILE:HD13 | 13:O:410:TRP:CD1 | 2.55 | 0.41 |
| 13:O:690:ALA:O | 13:O:693:ASN:HB2 | 2.20 | 0.41 |
| 16:X:508:ASP:HB3 | 16:X:509:CYS:H | 1.65 | 0.41 |
| 1:A:23:PHE:HE2 | 1:A:113:VAL:HB | 1.84 | 0.41 |
| 1:A:101:ILE:HG23 | 1:A:113:VAL:HG23 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1560:MET:O | 1:A:1564:LEU:HD22 | 2.20 | 0.41 |
| 1:A:1584:LEU:HD22 | 1:A:1588:LEU:CD2 | 2.50 | 0.41 |
| 1:A:1672:ARG:O | 1:A:1701:LEU:HA | 2.20 | 0.41 |
| 3:C:119:MET:HA | 3:C:122:ARG:CG | 2.50 | 0.41 |
| 3:C:526:TRP:HE1 | 3:C:553:ILE:HA | 1.85 | 0.41 |
| 6:F:705:CYS:SG | 6:F:706:LYS:N | 2.92 | 0.41 |
| 8:I:206:LEU:HD22 | 8:I:570:PHE:CD2 | 2.55 | 0.41 |
| 8:I:34:LEU:HA | 8:I:47:HIS:O | 2.20 | 0.41 |
| 9:J:450:ASN:O | 9:J:454:VAL:HG13 | 2.20 | 0.41 |
| 9:J:489:HIS:HB3 | 9:J:498:ALA:HB2 | 2.02 | 0.41 |
| 9:K:369:LEU:O | 9:K:373:TYR:HD2 | 2.03 | 0.41 |
| 9:K:495:PHE:CE2 | 9:K:525:MET:HG2 | 2.56 | 0.41 |
| 13:O:247:ASN:HA | 13:O:248:PRO:HD3 | 1.82 | 0.41 |
| 13:O:225:ASN:O | 13:O:461:ASN:O | 2.38 | 0.41 |
| 3:P:92:ALA:O | 3:P:96:VAL:HG23 | 2.20 | 0.41 |
| 16:X:145:CYS:O | 16:X:149:LEU:HG | 2.20 | 0.41 |
| 16:X:206:ILE:O | 16:X:210:LEU:HG | 2.20 | 0.41 |
| 16:X:270:ASN:HB2 | 16:X:273:LEU:CB | 2.50 | 0.41 |
| 16:X:71:PHE:O | 16:X:76:LYS:HE3 | 2.20 | 0.41 |
| 1:A:1093:HIS:CD2 | 1:A:1093:HIS:N | 2.88 | 0.41 |
| 1:A:1521:LEU:O | 1:A:1525:MET:HB2 | 2.21 | 0.41 |
| 1:A:594:ARG:HG2 | 1:A:608:THR:HG22 | 2.02 | 0.41 |
| 6:H:25:VAL:HG22 | 6:H:47:CYS:HB3 | 2.02 | 0.41 |
| 6:H:692:LEU:HD13 | 6:H:709:ARG:HA | 2.02 | 0.41 |
| 8:I:25:PHE:CE1 | 8:I:27:VAL:HG23 | 2.55 | 0.41 |
| 9:J:386:LEU:H | 9:J:386:LEU:CD1 | 2.30 | 0.41 |
| 6:F:550:VAL:CG2 | 9:K:289:HIS:CG | 3.03 | 0.41 |
| 3:P:106:LEU:CB | 3:P:118:TYR:HB2 | 2.50 | 0.41 |
| 3:P:355:GLN:HG3 | 3:P:371:MET:HE1 | 2.01 | 0.41 |
| 3:P:464:ASP:OD2 | 3:P:469:ALA:HB3 | 2.20 | 0.41 |
| 3:C:305:ASN:OD1 | 14:R:78:ARG:HD3 | 2.19 | 0.41 |
| 16:X:167:ARG:HB3 | 16:X:172:ASN:OD1 | 2.20 | 0.41 |
| 16:X:339:ALA:HB2 | 16:X:369:ASN:HB2 | 2.01 | 0.41 |
| 16:Y:242:ALA:O | 16:Y:246:VAL:HG23 | 2.19 | 0.41 |
| 1:A:248:PHE:CE1 | 1:A:430:VAL:O | 2.73 | 0.41 |
| 6:F:128:THR:O | 6:F:129:ASP:HB3 | 2.20 | 0.41 |
| 6:F:32:TYR:CE1 | 6:F:41:LEU:HB2 | 2.55 | 0.41 |
| 6:H:12:ILE:HG21 | 6:H:43:LEU:HD21 | 2.01 | 0.41 |
| 6:F:5:GLN:HA | 6:H:455:GLN:HG3 | 2.02 | 0.41 |
| 9:J:334:GLY:N | 9:J:335:PRO:CD | 2.84 | 0.41 |
| 12:N:177:TYR:O | 12:N:180:PHE:HB3 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:O:79:TYR:HA | 13:O:82:ILE:HG22 | 2.03 | 0.41 |
| 3:P:311:SER:HA | 3:P:343:LEU:HD11 | 2.03 | 0.41 |
| 16:X:465:LEU:HD23 | 16:X:485:LEU:HD11 | 2.02 | 0.41 |
| 16:Y:270:ASN:HB2 | 16:Y:273:LEU:CB | 2.50 | 0.41 |
| 1:A:119:VAL:O | 1:A:121:SER:N | 2.50 | 0.41 |
| 1:A:485:ILE:HG12 | 1:A:611:GLU:HA | 2.03 | 0.41 |
| 3:C:377:GLU:HA | 14:R:130:ILE:HG22 | 2.02 | 0.41 |
| 6:F:486:ASN:O | 6:F:490:HIS:ND1 | 2.52 | 0.41 |
| 6:F:15:ALA:HA | 6:H:116:PHE:CZ | 2.56 | 0.41 |
| 6:H:61:LEU:HD12 | 6:H:61:LEU:HA | 1.85 | 0.41 |
| 8:I:414:PHE:HZ | 8:I:472:VAL:HG13 | 1.85 | 0.41 |
| 8:I:655:ASP:OD1 | 8:I:657:VAL:HG22 | 2.20 | 0.41 |
| 9:K:337:TRP:CZ3 | 9:K:340:TYR:HD2 | 2.39 | 0.41 |
| 10:L:68:PHE:HE1 | 10:L:137:ILE:HD12 | 1.84 | 0.41 |
| 10:L:53:TYR:CE2 | 10:L:152:HIS:CE1 | 3.08 | 0.41 |
| 12:N:343:GLU:O | 12:N:347:ILE:N | 2.52 | 0.41 |
| 12:N:386:LEU:HD23 | 12:N:399:LEU:HD13 | 2.00 | 0.41 |
| 13:O:483:PHE:O | 13:O:487:SER:N | 2.46 | 0.41 |
| 13:O:668:ALA:HB3 | 13:O:694:LEU:HD23 | 2.02 | 0.41 |
| 14:R:364:CYS:HA | 14:R:365:PRO:HD3 | 1.89 | 0.41 |
| 16:Y:408:ASP:O | 16:Y:411:GLU:HG2 | 2.20 | 0.41 |
| 1:A:1408:THR:HG21 | 1:A:1468:ALA:HB2 | 2.02 | 0.41 |
| 1:A:1519:VAL:CG1 | 1:A:1520:LEU:H | 2.34 | 0.41 |
| 3:C:26:PHE:O | 3:C:27:SER:OG | 2.31 | 0.41 |
| 3:C:92:ALA:O | 3:C:96:VAL:HG23 | 2.21 | 0.41 |
| 8:I:231:VAL:HG11 | 8:I:556:LEU:HD12 | 2.02 | 0.41 |
| 8:I:578:ASN:OD1 | 8:I:578:ASN:C | 2.59 | 0.41 |
| 9:J:42:TRP:HA | 9:J:42:TRP:CE3 | 2.55 | 0.41 |
| 13:O:215:PHE:CD2 | 13:O:216:LEU:HD23 | 2.55 | 0.41 |
| 13:O:35:ILE:HG21 | 13:O:158:LEU:CD1 | 2.44 | 0.41 |
| 13:O:532:VAL:HG21 | 13:O:547:LYS:HA | 2.02 | 0.41 |
| 13:O:657:ILE:HG22 | 13:O:660:LYS:HE2 | 2.01 | 0.41 |
| 14:R:177:ASP:CG | 15:S:834:ILE:HD12 | 2.31 | 0.41 |
| 6:F:639:TYR:CE2 | 14:R:498:ILE:HG13 | 2.56 | 0.41 |
| 16:X:154:ASP:N | 16:X:154:ASP:OD1 | 2.53 | 0.41 |
| 1:A:1434:ILE:CG2 | 1:A:1461:HIS:HB2 | 2.51 | 0.41 |
| 1:A:240:VAL:HG13 | 1:A:241:ASP:CB | 2.50 | 0.41 |
| 1:A:88:ASP:O | 1:A:594:ARG:NH2 | 2.54 | 0.41 |
| 6:F:146:PRO:CG | 6:F:167:THR:HA | 2.50 | 0.41 |
| 6:H:164:PRO:HG3 | 6:H:471:LYS:HG3 | 2.03 | 0.41 |
| 9:J:475:ILE:HA | 9:J:476:PRO:HD3 | 1.88 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:N:607:GLU:HG2 | 12:N:688:PRO:HG2 | 2.03 | 0.41 |
| 12:N:663:GLN:HB3 | 12:N:699:TRP:CZ2 | 2.55 | 0.41 |
| 13:O:608:LEU:CD2 | 13:O:612:LYS:HE2 | 2.50 | 0.41 |
| 3:P:242:GLN:NE2 | 3:P:429:ARG:HG3 | 2.31 | 0.41 |
| 16:Y:186:ARG:HA | 16:Y:189:VAL:HG12 | 2.01 | 0.41 |
| 1:A:1575:SER:O | 1:A:1580:SER:OG | 2.36 | 0.41 |
| 1:A:1743:SER:HA | 1:A:1748:LEU:HD22 | 2.03 | 0.41 |
| 1:A:27:HIS:CE1 | 1:A:31:HIS:CD2 | 3.09 | 0.41 |
| 3:C:46:ARG:HB3 | 3:C:116:PHE:HE2 | 1.84 | 0.41 |
| 6:F:12:ILE:HG21 | 6:F:43:LEU:CD2 | 2.50 | 0.41 |
| 6:F:465:LEU:HD22 | 6:F:495:HIS:CE1 | 2.56 | 0.41 |
| 6:F:550:VAL:O | 6:F:554:VAL:HG23 | 2.21 | 0.41 |
| 6:H:682:LEU:HD13 | 6:H:684:LYS:HE3 | 2.02 | 0.41 |
| 9:J:215:PRO:HG2 | 9:J:402:PRO:HG2 | 2.02 | 0.41 |
| 9:J:19:TYR:CE1 | 9:J:49:LEU:HD13 | 2.55 | 0.41 |
| 1:A:1453:ASN:ND2 | 10:L:133:ARG:HD2 | 2.36 | 0.41 |
| 3:P:307:LEU:HD12 | 3:P:307:LEU:HA | 1.84 | 0.41 |
| 1:A:1236:LEU:H | 1:A:1236:LEU:HD23 | 1.85 | 0.41 |
| 1:A:1325:LEU:HD23 | 1:A:1371:LEU:HG | 2.03 | 0.41 |
| 1:A:1602:HIS:O | 1:A:1603:LEU:HB3 | 2.20 | 0.41 |
| 1:A:245:LYS:O | 1:A:258:THR:HA | 2.21 | 0.41 |
| 1:A:628:ILE:HG22 | 1:A:629:LEU:N | 2.36 | 0.41 |
| 6:H:146:PRO:CG | 6:H:167:THR:HA | 2.50 | 0.41 |
| 8:I:118:VAL:HG12 | 8:I:173:LEU:O | 2.21 | 0.41 |
| 8:I:618:ILE:HD12 | 8:I:705:MET:CE | 2.51 | 0.41 |
| 8:I:737:ASN:OD1 | 8:I:738:LEU:N | 2.54 | 0.41 |
| 9:J:276:VAL:HA | 9:J:311:MET:SD | 2.60 | 0.41 |
| 9:J:289:HIS:CD2 | 9:J:289:HIS:C | 2.93 | 0.41 |
| 9:J:485:ILE:HG22 | 9:J:488:ILE:HD11 | 2.02 | 0.41 |
| 9:K:418:TRP:HB3 | 9:K:458:LEU:CD1 | 2.50 | 0.41 |
| 9:K:42:TRP:HE3 | 9:K:42:TRP:HA | 1.84 | 0.41 |
| 10:L:68:PHE:CE1 | 10:L:137:ILE:HD12 | 2.56 | 0.41 |
| 12:N:527:LEU:HD22 | 12:N:564:MET:CG | 2.51 | 0.41 |
| 13:O:75:LEU:HB2 | 13:O:161:TYR:CE2 | 2.56 | 0.41 |
| 4:D:53:PRO:HD3 | 3:P:382:SER:OG | 2.21 | 0.41 |
| 16:X:199:CYS:SG | 16:Y:44:MET:CG | 3.04 | 0.41 |
| 1:A:1209:LEU:HA | 1:A:1209:LEU:HD23 | 1.85 | 0.41 |
| 1:A:1237:PRO:CB | 1:A:1238:PRO:CD | 2.95 | 0.41 |
| 1:A:1673:TYR:CZ | 1:A:1701:LEU:HD13 | 2.56 | 0.41 |
| 1:A:1739:SER:CA | 1:A:1740:ALA:CB | 2.98 | 0.41 |
| 1:A:87:VAL:CG1 | 1:A:88:ASP:N | 2.73 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:15:LEU:HD21 | 12:N:635:LEU:HA | 2.02 | 0.41 |
| 3:C:261:LYS:HA | 3:C:261:LYS:HD2 | 1.89 | 0.41 |
| 4:D:15:THR:HB | 4:D:19:ASN:HD22 | 1.86 | 0.41 |
| 5:E:63:VAL:HG11 | 16:Y:364:LYS:NZ | 2.36 | 0.41 |
| 6:F:18:HIS:NE2 | 6:H:113:SER:HB2 | 2.35 | 0.41 |
| 8:I:349:ILE:HD13 | 13:O:410:TRP:HD1 | 1.86 | 0.41 |
| 7:G:1:MET:CG | 9:J:335:PRO:HB3 | 2.51 | 0.41 |
| 9:K:351:ASP:OD1 | 9:K:351:ASP:N | 2.46 | 0.41 |
| 10:L:88:SER:O | 10:L:144:ASN:HB3 | 2.21 | 0.41 |
| 12:N:601:TRP:HA | 12:N:602:PRO:HD2 | 1.97 | 0.41 |
| 13:O:119:PHE:CZ | 13:O:136:LEU:HD11 | 2.55 | 0.41 |
| 8:I:397:ILE:HD12 | 13:O:440:GLN:HG3 | 2.03 | 0.41 |
| 13:O:40:LEU:HD11 | 13:O:60:LEU:HD21 | 2.03 | 0.41 |
| 3:P:235:ALA:HB1 | 3:P:251:TYR:CE2 | 2.55 | 0.41 |
| 3:P:402:TRP:CE2 | 3:P:424:ARG:HG2 | 2.56 | 0.41 |
| 16:Y:154:ASP:N | 16:Y:154:ASP:OD1 | 2.53 | 0.41 |
| 16:Y:84:ALA:HB1 | 16:Y:100:TYR:CD2 | 2.55 | 0.41 |
| 1:A:1409:LEU:HD23 | 1:A:1471:SER:CB | 2.51 | 0.41 |
| 1:A:23:PHE:O | 1:A:26:ASP:N | 2.50 | 0.41 |
| 1:A:794:ALA:HB1 | 1:A:797:LEU:HB3 | 2.02 | 0.41 |
| 1:A:860:TYR:HA | 1:A:861:PRO:HD3 | 1.98 | 0.41 |
| 3:C:93:TYR:CZ | 3:C:101:ARG:NE | 2.90 | 0.41 |
| 3:C:235:ALA:HB1 | 3:C:251:TYR:CE2 | 2.56 | 0.41 |
| 6:F:550:VAL:HG21 | 9:K:289:HIS:CB | 2.50 | 0.41 |
| 6:F:636:ASN:N | 6:F:636:ASN:HD22 | 2.18 | 0.41 |
| 6:F:707:PHE:CE1 | 6:F:742:LEU:HD13 | 2.56 | 0.41 |
| 9:K:484:ALA:O | 9:K:488:ILE:HG12 | 2.20 | 0.41 |
| 10:L:64:VAL:HB | 10:L:139:ILE:HB | 2.03 | 0.41 |
| 6:H:515:TYR:HD1 | 10:L:179:MET:HE2 | 1.86 | 0.41 |
| 12:N:456:LEU:HA | 12:N:548:ARG:NH2 | 2.36 | 0.41 |
| 13:O:467:ALA:CB | 13:O:506:LEU:HD11 | 2.49 | 0.41 |
| 3:P:306:LEU:HD12 | 3:P:307:LEU:N | 2.36 | 0.41 |
| 1:A:89:TYR:HB3 | 13:O:536:THR:CG2 | 2.51 | 0.40 |
| 3:C:397:ARG:O | 3:C:428:LEU:HD21 | 2.21 | 0.40 |
| 6:H:128:THR:O | 6:H:129:ASP:HB3 | 2.21 | 0.40 |
| 6:H:634:HIS:CE1 | 6:H:636:ASN:HB2 | 2.56 | 0.40 |
| 8:I:231:VAL:HG21 | 8:I:557:TYR:CE2 | 2.55 | 0.40 |
| 9:K:214:LYS:HA | 9:K:215:PRO:HD2 | 1.84 | 0.40 |
| 12:N:281:TYR:CE2 | 12:N:356:PRO:HB2 | 2.56 | 0.40 |
| 13:O:119:PHE:CE1 | 13:O:136:LEU:HD21 | 2.53 | 0.40 |
| 13:O:275:LEU:HD12 | 13:O:275:LEU:N | 2.36 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:O:539:ASN:ND2 | 13:O:542:GLU:HB2 | 2.35 | 0.40 |
| 13:O:649:GLU:HB3 | 13:O:650:PRO:HD3 | 2.02 | 0.40 |
| 3:P:170:PHE:O | 3:P:171:GLY:C | 2.59 | 0.40 |
| 3:P:297:ILE:HD11 | 3:P:333:THR:HB | 2.03 | 0.40 |
| 3:P:370:LEU:HA | 3:P:370:LEU:HD23 | 1.89 | 0.40 |
| 3:P:403:TYR:CD1 | 3:P:422:TYR:HE1 | 2.39 | 0.40 |
| 16:X:325:GLU:HG3 | 16:X:348:HIS:CD2 | 2.56 | 0.40 |
| 16:X:475:TYR:HB3 | 16:X:478:ALA:HB3 | 2.03 | 0.40 |
| 16:Y:366:ILE:HG13 | 16:Y:366:ILE:H | 1.72 | 0.40 |
| 1:A:1611:VAL:HG13 | 1:A:1612:LEU:N | 2.36 | 0.40 |
| 1:A:213:MET:HE3 | 1:A:220:ILE:CG2 | 2.51 | 0.40 |
| 1:A:657:TRP:HA | 1:A:660:PHE:HB3 | 2.02 | 0.40 |
| 3:C:46:ARG:NH2 | 3:C:170:PHE:CD1 | 2.89 | 0.40 |
| 5:E:89:LEU:HD22 | 6:H:588:LYS:HB3 | 2.03 | 0.40 |
| 6:F:138:TYR:O | 6:F:141:SER:OG | 2.33 | 0.40 |
| 6:F:548:LYS:HB3 | 6:F:551:ALA:HB3 | 2.03 | 0.40 |
| 8:I:28:TRP:HZ3 | 8:I:33:ASP:O | 2.04 | 0.40 |
| 8:I:406:VAL:O | 8:I:410:SER:HB2 | 2.21 | 0.40 |
| 9:J:204:LEU:HD22 | 9:K:28:LYS:NZ | 2.36 | 0.40 |
| 3:C:322:ASN:N | 9:J:282:ASN:ND2 | 2.69 | 0.40 |
| 9:J:489:HIS:CB | 9:J:498:ALA:HB2 | 2.51 | 0.40 |
| 4:D:54:ILE:CD1 | 9:J:506:LEU:HB3 | 2.48 | 0.40 |
| 9:K:40:ILE:HD13 | 9:K:65:LEU:HD21 | 2.03 | 0.40 |
| 10:L:40:PHE:O | 10:L:54:TRP:HA | 2.21 | 0.40 |
| 12:N:501:ILE:O | 12:N:504:LEU:HB2 | 2.22 | 0.40 |
| 13:O:666:LEU:HG | 13:O:666:LEU:O | 2.20 | 0.40 |
| 1:A:23:PHE:CE2 | 1:A:113:VAL:HB | 2.57 | 0.40 |
| 1:A:1040:LEU:HG | 1:A:1543:HIS:CE1 | 2.57 | 0.40 |
| 3:C:117:LEU:HD23 | 3:C:117:LEU:O | 2.21 | 0.40 |
| 3:C:397:ARG:CA | 3:C:428:LEU:HD21 | 2.50 | 0.40 |
| 3:C:460:TYR:CE1 | 3:C:470:LEU:HD11 | 2.57 | 0.40 |
| 6:F:42:PHE:HB2 | 6:F:71:CYS:SG | 2.61 | 0.40 |
| 12:N:386:LEU:HD13 | 12:N:396:ILE:HG23 | 2.02 | 0.40 |
| 13:O:536:THR:O | 13:O:540:SER:HA | 2.21 | 0.40 |
| 13:O:435:SER:HB2 | 13:O:618:TYR:HE2 | 1.86 | 0.40 |
| 13:O:637:PRO:HB2 | 13:O:674:SER:HB3 | 2.03 | 0.40 |
| 13:O:689:ALA:O | 13:O:692:GLU:HB2 | 2.22 | 0.40 |
| 3:P:49:LEU:H | 3:P:49:LEU:HD12 | 1.86 | 0.40 |
| 14:R:193:SER:O | 14:R:453:PRO:HG3 | 2.20 | 0.40 |
| 14:R:83:ARG:HA | 14:R:83:ARG:HE | 1.86 | 0.40 |
| 16:X:164:SER:HA | 16:X:167:ARG:NE | 2.37 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:Y:87:LEU:HD11 | 16:Y:99:LYS:HG3 | 2.04 | 0.40 |
| 1:A:1462:VAL:O | 1:A:1465:ILE:HG13 | 2.21 | 0.40 |
| 1:A:1473:GLY:HA2 | 1:A:1526:VAL:HG13 | 2.03 | 0.40 |
| 1:A:1673:TYR:CE2 | 1:A:1701:LEU:HD13 | 2.56 | 0.40 |
| 1:A:244:MET:SD | 1:A:244:MET:N | 2.94 | 0.40 |
| 1:A:188:LEU:HD23 | 1:A:249:LEU:HD21 | 2.03 | 0.40 |
| 1:A:433:THR:HG22 | 1:A:481:PRO:CB | 2.39 | 0.40 |
| 3:C:26:PHE:CD2 | 3:C:257:VAL:HG21 | 2.56 | 0.40 |
| 3:C:65:LEU:HD13 | 3:C:66:PRO:HD2 | 2.03 | 0.40 |
| 6:H:464:SER:O | 6:H:468:GLU:HG2 | 2.21 | 0.40 |
| 6:H:592:ARG:HA | 6:H:592:ARG:HD3 | 1.77 | 0.40 |
| 8:I:14:VAL:N | 8:I:743:VAL:O | 2.55 | 0.40 |
| 9:J:441:VAL:O | 9:J:442:ASP:CB | 2.69 | 0.40 |
| 12:N:386:LEU:HD21 | 12:N:399:LEU:HD22 | 2.03 | 0.40 |
| 14:R:209:TRP:HD1 | 14:R:216:ILE:HG13 | 1.87 | 0.40 |
| 16:X:203:LEU:HD22 | 16:Y:55:LEU:CB | 2.52 | 0.40 |
| 16:Y:246:VAL:HG13 | 16:Y:280:LEU:HD21 | 2.03 | 0.40 |
| 1:A:1420:LEU:HA | 1:A:1421:PRO:HD3 | 1.91 | 0.40 |
| 1:A:1640:GLY:CA | 1:A:1645:GLU:O | 2.70 | 0.40 |
| 3:C:151:LEU:CD1 | 3:C:181:LYS:CB | 2.99 | 0.40 |
| 3:C:312:MET:HG2 | 3:C:312:MET:H | 1.67 | 0.40 |
| 4:D:48:ASP:OD1 | 4:D:48:ASP:N | 2.54 | 0.40 |
| 6:H:128:THR:HG21 | 9:K:473:VAL:HG22 | 2.03 | 0.40 |
| 6:H:692:LEU:HB3 | 6:H:709:ARG:HG3 | 2.04 | 0.40 |
| 8:I:245:LEU:HB3 | 8:I:246:PRO:HD3 | 2.03 | 0.40 |
| 8:I:279:ILE:HD12 | 8:I:279:ILE:HA | 1.83 | 0.40 |
| 8:I:495:ASN:HA | 13:O:459:GLN:HA | 2.03 | 0.40 |
| 8:I:648:THR:HG22 | 8:I:670:PRO:HA | 2.02 | 0.40 |
| 9:J:376:LEU:HD23 | 9:J:407:GLU:HG2 | 2.03 | 0.40 |
| 9:J:56:ALA:HB3 | 9:J:79:CYS:SG | 2.61 | 0.40 |
| 11:M:1:MET:SD | 11:M:4:GLU:HB2 | 2.62 | 0.40 |
| 12:N:210:ARG:O | 12:N:214:ARG:N | 2.55 | 0.40 |
| 8:I:32:ARG:HG2 | 12:N:388:HIS:HE1 | 1.85 | 0.40 |
| 12:N:401:ILE:HG22 | 12:N:405:LYS:HE3 | 2.04 | 0.40 |
| 13:O:381:ILE:CG2 | 13:O:405:SER:HB2 | 2.50 | 0.40 |
| 16:X:311:TYR:HA | 16:X:314:LEU:HD12 | 2.04 | 0.40 |
| 16:Y:100:TYR:CD1 | 16:Y:138:VAL:HG13 | 2.51 | 0.40 |
| 16:X:232:ASN:O | 16:Y:63:MET:HE1 | 2.22 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|------------------|------------|-----------|----------|-------------|-----|
| 1 | A | 1393/1944 (72%) | 1186 (85%) | 149 (11%) | 58 (4%) | 3 | 30 |
| 2 | B | 83/84 (99%) | 72 (87%) | 7 (8%) | 4 (5%) | 2 | 27 |
| 3 | C | 520/597 (87%) | 489 (94%) | 23 (4%) | 8 (2%) | 11 | 51 |
| 3 | P | 485/597 (81%) | 460 (95%) | 20 (4%) | 5 (1%) | 17 | 58 |
| 4 | D | 53/121 (44%) | 45 (85%) | 7 (13%) | 1 (2%) | 9 | 46 |
| 5 | E | 54/110 (49%) | 54 (100%) | 0 | 0 | 100 | 100 |
| 6 | F | 494/824 (60%) | 461 (93%) | 25 (5%) | 8 (2%) | 11 | 50 |
| 6 | H | 477/824 (58%) | 448 (94%) | 22 (5%) | 7 (2%) | 11 | 51 |
| 7 | G | 23/85 (27%) | 23 (100%) | 0 | 0 | 100 | 100 |
| 7 | W | 23/85 (27%) | 23 (100%) | 0 | 0 | 100 | 100 |
| 8 | I | 722/808 (89%) | 683 (95%) | 34 (5%) | 5 (1%) | 24 | 66 |
| 9 | J | 500/620 (81%) | 467 (93%) | 29 (6%) | 4 (1%) | 21 | 63 |
| 9 | K | 489/620 (79%) | 459 (94%) | 24 (5%) | 6 (1%) | 14 | 55 |
| 10 | L | 180/184 (98%) | 165 (92%) | 11 (6%) | 4 (2%) | 7 | 43 |
| 11 | M | 55/74 (74%) | 42 (76%) | 10 (18%) | 3 (6%) | 2 | 25 |
| 12 | N | 601/822 (73%) | 497 (83%) | 58 (10%) | 46 (8%) | 1 | 17 |
| 13 | O | 677/755 (90%) | 619 (91%) | 46 (7%) | 12 (2%) | 9 | 47 |
| 14 | R | 361/499 (72%) | 338 (94%) | 20 (6%) | 3 (1%) | 21 | 63 |
| 15 | S | 8/206 (4%) | 6 (75%) | 0 | 2 (25%) | 0 | 1 |
| 16 | X | 478/599 (80%) | 463 (97%) | 12 (2%) | 3 (1%) | 27 | 68 |
| 16 | Y | 492/599 (82%) | 474 (96%) | 14 (3%) | 4 (1%) | 21 | 63 |
| All | All | 8168/11057 (74%) | 7474 (92%) | 511 (6%) | 183 (2%) | 11 | 43 |

All (183) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 45 | ALA |
| 1 | A | 241 | ASP |
| 1 | A | 274 | VAL |
| 1 | A | 411 | HIS |
| 1 | A | 413 | TRP |
| 1 | A | 414 | THR |
| 1 | A | 430 | VAL |
| 1 | A | 475 | PRO |
| 1 | A | 672 | THR |
| 1 | A | 857 | MET |
| 1 | A | 1099 | PRO |
| 1 | A | 1190 | THR |
| 1 | A | 1237 | PRO |
| 1 | A | 1358 | ILE |
| 1 | A | 1924 | MET |
| 2 | B | 15 | LEU |
| 3 | C | 361 | ASN |
| 3 | C | 441 | GLU |
| 3 | C | 511 | THR |
| 4 | D | 23 | PRO |
| 6 | F | 103 | HIS |
| 6 | F | 165 | ASP |
| 8 | I | 483 | ASP |
| 8 | I | 487 | VAL |
| 8 | I | 489 | PRO |
| 9 | J | 221 | PRO |
| 9 | K | 211 | LYS |
| 9 | K | 215 | PRO |
| 10 | L | 71 | LYS |
| 10 | L | 171 | PRO |
| 11 | M | 2 | ASP |
| 12 | N | 16 | PRO |
| 12 | N | 63 | ARG |
| 12 | N | 74 | TRP |
| 12 | N | 91 | PHE |
| 12 | N | 126 | LEU |
| 12 | N | 144 | THR |
| 12 | N | 203 | LEU |
| 12 | N | 219 | PRO |
| 12 | N | 368 | THR |
| 12 | N | 395 | ASP |
| 12 | N | 412 | PRO |
| 12 | N | 477 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 12 | N | 481 | VAL |
| 12 | N | 488 | ASP |
| 12 | N | 489 | PRO |
| 12 | N | 496 | ARG |
| 12 | N | 497 | ARG |
| 12 | N | 530 | GLN |
| 12 | N | 674 | ALA |
| 12 | N | 716 | ILE |
| 13 | O | 555 | ASN |
| 3 | P | 361 | ASN |
| 3 | P | 365 | LEU |
| 3 | P | 464 | ASP |
| 14 | R | 494 | ILE |
| 15 | S | 834 | ILE |
| 16 | Y | 201 | LEU |
| 1 | A | 120 | ASP |
| 1 | A | 265 | VAL |
| 1 | A | 584 | ILE |
| 1 | A | 592 | HIS |
| 1 | A | 630 | PRO |
| 1 | A | 758 | HIS |
| 1 | A | 1125 | ILE |
| 1 | A | 1199 | LYS |
| 1 | A | 1238 | PRO |
| 1 | A | 1242 | GLU |
| 1 | A | 1244 | ASP |
| 1 | A | 1314 | ILE |
| 3 | C | 27 | SER |
| 6 | F | 147 | PHE |
| 6 | H | 147 | PHE |
| 8 | I | 503 | ASN |
| 9 | J | 70 | GLU |
| 9 | J | 397 | ILE |
| 9 | K | 86 | HIS |
| 9 | K | 129 | LYS |
| 9 | K | 228 | GLN |
| 10 | L | 167 | ILE |
| 11 | M | 4 | GLU |
| 12 | N | 76 | VAL |
| 12 | N | 78 | VAL |
| 12 | N | 99 | GLU |
| 12 | N | 234 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 12 | N | 290 | HIS |
| 12 | N | 350 | ASP |
| 12 | N | 500 | ASP |
| 12 | N | 531 | PHE |
| 12 | N | 595 | ILE |
| 12 | N | 606 | ASP |
| 13 | O | 462 | ASN |
| 13 | O | 657 | ILE |
| 14 | R | 498 | ILE |
| 16 | X | 202 | ALA |
| 16 | X | 213 | SER |
| 16 | Y | 213 | SER |
| 1 | A | 30 | HIS |
| 1 | A | 757 | THR |
| 1 | A | 777 | THR |
| 1 | A | 790 | LEU |
| 1 | A | 1100 | LEU |
| 1 | A | 1217 | LEU |
| 1 | A | 1284 | GLU |
| 1 | A | 1307 | LEU |
| 1 | A | 1740 | ALA |
| 1 | A | 1758 | THR |
| 2 | B | 16 | TRP |
| 3 | C | 510 | SER |
| 6 | F | 493 | SER |
| 6 | H | 493 | SER |
| 8 | I | 490 | PRO |
| 12 | N | 77 | GLU |
| 12 | N | 278 | ARG |
| 12 | N | 289 | PHE |
| 12 | N | 410 | LEU |
| 12 | N | 413 | SER |
| 12 | N | 480 | TRP |
| 12 | N | 487 | ALA |
| 12 | N | 491 | LYS |
| 12 | N | 672 | ASP |
| 13 | O | 126 | VAL |
| 13 | O | 149 | SER |
| 13 | O | 284 | THR |
| 13 | O | 345 | SER |
| 13 | O | 352 | GLN |
| 13 | O | 682 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 13 | O | 707 | LYS |
| 16 | X | 456 | VAL |
| 16 | Y | 202 | ALA |
| 16 | Y | 456 | VAL |
| 1 | A | 87 | VAL |
| 1 | A | 486 | ASP |
| 1 | A | 585 | HIS |
| 1 | A | 652 | SER |
| 1 | A | 793 | LEU |
| 1 | A | 811 | PRO |
| 1 | A | 1055 | PRO |
| 1 | A | 1164 | LYS |
| 2 | B | 69 | VAL |
| 3 | C | 414 | MET |
| 6 | F | 145 | ASN |
| 6 | H | 145 | ASN |
| 10 | L | 131 | PRO |
| 12 | N | 354 | SER |
| 12 | N | 490 | GLY |
| 12 | N | 535 | PRO |
| 12 | N | 629 | LEU |
| 13 | O | 540 | SER |
| 14 | R | 84 | SER |
| 15 | S | 833 | ASP |
| 1 | A | 242 | HIS |
| 1 | A | 860 | TYR |
| 1 | A | 1056 | GLU |
| 1 | A | 1896 | ALA |
| 1 | A | 1933 | ALA |
| 6 | F | 96 | VAL |
| 6 | H | 97 | PHE |
| 9 | J | 442 | ASP |
| 11 | M | 66 | HIS |
| 12 | N | 252 | LEU |
| 12 | N | 287 | ARG |
| 3 | P | 66 | PRO |
| 1 | A | 184 | LYS |
| 1 | A | 648 | PRO |
| 1 | A | 759 | ILE |
| 1 | A | 792 | GLN |
| 2 | B | 40 | PRO |
| 3 | C | 66 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 6 | H | 96 | VAL |
| 12 | N | 551 | GLU |
| 3 | P | 415 | PRO |
| 1 | A | 861 | PRO |
| 1 | A | 1348 | PRO |
| 3 | C | 415 | PRO |
| 6 | F | 492 | PRO |
| 6 | H | 492 | PRO |
| 1 | A | 502 | GLY |
| 1 | A | 1283 | PRO |
| 9 | K | 399 | PRO |
| 6 | F | 146 | PRO |
| 6 | H | 146 | PRO |
| 13 | O | 124 | PRO |

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 PDB entries followed by that with respect to all EM entries.

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|-----------|-----------|-------------|----|
| 1 | A | 1150/1720 (67%) | 970 (84%) | 180 (16%) | 3 | 20 |
| 2 | B | 65/75 (87%) | 54 (83%) | 11 (17%) | 2 | 17 |
| 3 | C | 452/520 (87%) | 357 (79%) | 95 (21%) | 1 | 8 |
| 3 | P | 421/520 (81%) | 363 (86%) | 58 (14%) | 4 | 24 |
| 4 | D | 46/115 (40%) | 37 (80%) | 9 (20%) | 1 | 11 |
| 5 | E | 47/89 (53%) | 37 (79%) | 10 (21%) | 1 | 8 |
| 6 | F | 407/727 (56%) | 369 (91%) | 38 (9%) | 10 | 37 |
| 6 | H | 408/727 (56%) | 374 (92%) | 34 (8%) | 12 | 44 |
| 7 | G | 23/77 (30%) | 22 (96%) | 1 (4%) | 32 | 63 |
| 7 | W | 23/77 (30%) | 22 (96%) | 1 (4%) | 32 | 63 |
| 8 | I | 620/730 (85%) | 584 (94%) | 36 (6%) | 22 | 55 |
| 9 | J | 424/548 (77%) | 382 (90%) | 42 (10%) | 8 | 35 |
| 9 | K | 423/548 (77%) | 379 (90%) | 44 (10%) | 8 | 33 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|-------------|-----|
| 10 | L | 155/169 (92%) | 136 (88%) | 19 (12%) | 5 | 27 |
| 11 | M | 55/67 (82%) | 42 (76%) | 13 (24%) | 1 | 6 |
| 12 | N | 460/724 (64%) | 398 (86%) | 62 (14%) | 4 | 25 |
| 13 | O | 576/650 (89%) | 478 (83%) | 98 (17%) | 2 | 17 |
| 14 | R | 304/411 (74%) | 290 (95%) | 14 (5%) | 29 | 62 |
| 15 | S | 8/195 (4%) | 8 (100%) | 0 | 100 | 100 |
| 16 | X | 406/513 (79%) | 373 (92%) | 33 (8%) | 13 | 45 |
| 16 | Y | 416/513 (81%) | 375 (90%) | 41 (10%) | 8 | 35 |
| All | All | 6889/9715 (71%) | 6050 (88%) | 839 (12%) | 9 | 28 |

All (839) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 25 | ARG |
| 1 | A | 26 | ASP |
| 1 | A | 29 | LYS |
| 1 | A | 31 | HIS |
| 1 | A | 35 | LEU |
| 1 | A | 36 | ASN |
| 1 | A | 37 | LEU |
| 1 | A | 39 | LEU |
| 1 | A | 40 | ARG |
| 1 | A | 42 | LEU |
| 1 | A | 43 | GLN |
| 1 | A | 47 | GLU |
| 1 | A | 48 | LEU |
| 1 | A | 80 | VAL |
| 1 | A | 90 | ASP |
| 1 | A | 99 | MET |
| 1 | A | 103 | SER |
| 1 | A | 118 | THR |
| 1 | A | 124 | GLN |
| 1 | A | 127 | LEU |
| 1 | A | 129 | CYS |
| 1 | A | 133 | ILE |
| 1 | A | 149 | LYS |
| 1 | A | 167 | LYS |
| 1 | A | 168 | ASP |
| 1 | A | 170 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 173 | LEU |
| 1 | A | 183 | THR |
| 1 | A | 185 | TYR |
| 1 | A | 188 | LEU |
| 1 | A | 192 | SER |
| 1 | A | 210 | MET |
| 1 | A | 214 | LEU |
| 1 | A | 220 | ILE |
| 1 | A | 221 | THR |
| 1 | A | 223 | LEU |
| 1 | A | 240 | VAL |
| 1 | A | 242 | HIS |
| 1 | A | 249 | LEU |
| 1 | A | 250 | ASN |
| 1 | A | 252 | ASP |
| 1 | A | 269 | TRP |
| 1 | A | 411 | HIS |
| 1 | A | 412 | LEU |
| 1 | A | 430 | VAL |
| 1 | A | 433 | THR |
| 1 | A | 439 | GLN |
| 1 | A | 440 | LYS |
| 1 | A | 442 | LEU |
| 1 | A | 444 | PHE |
| 1 | A | 450 | LEU |
| 1 | A | 452 | LEU |
| 1 | A | 453 | ARG |
| 1 | A | 467 | ILE |
| 1 | A | 482 | VAL |
| 1 | A | 483 | GLU |
| 1 | A | 497 | LEU |
| 1 | A | 508 | LYS |
| 1 | A | 584 | ILE |
| 1 | A | 611 | GLU |
| 1 | A | 616 | GLU |
| 1 | A | 617 | LEU |
| 1 | A | 636 | GLN |
| 1 | A | 637 | MET |
| 1 | A | 638 | LEU |
| 1 | A | 655 | SER |
| 1 | A | 659 | LEU |
| 1 | A | 663 | CYS |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 665 | MET |
| 1 | A | 668 | MET |
| 1 | A | 758 | HIS |
| 1 | A | 759 | ILE |
| 1 | A | 766 | LEU |
| 1 | A | 774 | LYS |
| 1 | A | 781 | GLU |
| 1 | A | 792 | GLN |
| 1 | A | 795 | ARG |
| 1 | A | 796 | ASP |
| 1 | A | 798 | LYS |
| 1 | A | 808 | ARG |
| 1 | A | 813 | LEU |
| 1 | A | 871 | ARG |
| 1 | A | 937 | VAL |
| 1 | A | 942 | ARG |
| 1 | A | 953 | LEU |
| 1 | A | 964 | GLU |
| 1 | A | 976 | LEU |
| 1 | A | 1075 | GLN |
| 1 | A | 1088 | THR |
| 1 | A | 1100 | LEU |
| 1 | A | 1107 | LEU |
| 1 | A | 1118 | VAL |
| 1 | A | 1131 | MET |
| 1 | A | 1133 | SER |
| 1 | A | 1136 | SER |
| 1 | A | 1146 | LYS |
| 1 | A | 1168 | LEU |
| 1 | A | 1170 | ASN |
| 1 | A | 1176 | LEU |
| 1 | A | 1177 | MET |
| 1 | A | 1179 | LEU |
| 1 | A | 1191 | LEU |
| 1 | A | 1195 | ASP |
| 1 | A | 1202 | GLU |
| 1 | A | 1204 | THR |
| 1 | A | 1216 | LYS |
| 1 | A | 1217 | LEU |
| 1 | A | 1220 | MET |
| 1 | A | 1230 | ILE |
| 1 | A | 1232 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1239 | THR |
| 1 | A | 1241 | THR |
| 1 | A | 1243 | LEU |
| 1 | A | 1250 | GLN |
| 1 | A | 1257 | ILE |
| 1 | A | 1273 | LEU |
| 1 | A | 1279 | ARG |
| 1 | A | 1292 | GLU |
| 1 | A | 1312 | ASN |
| 1 | A | 1313 | LEU |
| 1 | A | 1319 | LEU |
| 1 | A | 1323 | GLU |
| 1 | A | 1325 | LEU |
| 1 | A | 1329 | MET |
| 1 | A | 1330 | VAL |
| 1 | A | 1359 | ASN |
| 1 | A | 1376 | LEU |
| 1 | A | 1386 | TRP |
| 1 | A | 1396 | LEU |
| 1 | A | 1405 | LEU |
| 1 | A | 1409 | LEU |
| 1 | A | 1411 | ARG |
| 1 | A | 1415 | LEU |
| 1 | A | 1424 | LYS |
| 1 | A | 1433 | ILE |
| 1 | A | 1469 | CYS |
| 1 | A | 1470 | LEU |
| 1 | A | 1482 | LEU |
| 1 | A | 1487 | CYS |
| 1 | A | 1498 | TYR |
| 1 | A | 1520 | LEU |
| 1 | A | 1523 | LEU |
| 1 | A | 1536 | LEU |
| 1 | A | 1538 | LEU |
| 1 | A | 1539 | CYS |
| 1 | A | 1540 | ARG |
| 1 | A | 1562 | LEU |
| 1 | A | 1564 | LEU |
| 1 | A | 1573 | SER |
| 1 | A | 1574 | LEU |
| 1 | A | 1588 | LEU |
| 1 | A | 1597 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1603 | LEU |
| 1 | A | 1607 | ARG |
| 1 | A | 1609 | LEU |
| 1 | A | 1611 | VAL |
| 1 | A | 1638 | TYR |
| 1 | A | 1646 | GLN |
| 1 | A | 1651 | LEU |
| 1 | A | 1652 | MET |
| 1 | A | 1666 | ILE |
| 1 | A | 1667 | LYS |
| 1 | A | 1672 | ARG |
| 1 | A | 1674 | TRP |
| 1 | A | 1679 | ASP |
| 1 | A | 1687 | LEU |
| 1 | A | 1688 | LYS |
| 1 | A | 1706 | LEU |
| 1 | A | 1731 | ARG |
| 1 | A | 1742 | THR |
| 1 | A | 1749 | SER |
| 1 | A | 1770 | LEU |
| 1 | A | 1798 | ARG |
| 1 | A | 1805 | MET |
| 1 | A | 1811 | LEU |
| 1 | A | 1825 | SER |
| 1 | A | 1851 | THR |
| 1 | A | 1882 | LEU |
| 1 | A | 1893 | SER |
| 1 | A | 1894 | VAL |
| 2 | B | 11 | VAL |
| 2 | B | 14 | TRP |
| 2 | B | 15 | LEU |
| 2 | B | 16 | TRP |
| 2 | B | 28 | MET |
| 2 | B | 34 | CYS |
| 2 | B | 36 | ASP |
| 2 | B | 50 | GLN |
| 2 | B | 61 | LEU |
| 2 | B | 83 | LYS |
| 2 | B | 84 | GLU |
| 3 | C | 27 | SER |
| 3 | C | 31 | GLU |
| 3 | C | 37 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | C | 38 | LEU |
| 3 | C | 39 | ILE |
| 3 | C | 46 | ARG |
| 3 | C | 49 | LEU |
| 3 | C | 55 | SER |
| 3 | C | 57 | GLU |
| 3 | C | 65 | LEU |
| 3 | C | 70 | LEU |
| 3 | C | 79 | GLU |
| 3 | C | 82 | GLN |
| 3 | C | 83 | ASP |
| 3 | C | 89 | LEU |
| 3 | C | 91 | LYS |
| 3 | C | 97 | LYS |
| 3 | C | 98 | GLU |
| 3 | C | 101 | ARG |
| 3 | C | 105 | PHE |
| 3 | C | 106 | LEU |
| 3 | C | 112 | LYS |
| 3 | C | 113 | LYS |
| 3 | C | 119 | MET |
| 3 | C | 122 | ARG |
| 3 | C | 128 | LYS |
| 3 | C | 132 | ASP |
| 3 | C | 136 | ASP |
| 3 | C | 141 | LEU |
| 3 | C | 143 | LYS |
| 3 | C | 146 | VAL |
| 3 | C | 152 | ARG |
| 3 | C | 157 | GLU |
| 3 | C | 172 | LEU |
| 3 | C | 179 | LEU |
| 3 | C | 182 | LEU |
| 3 | C | 187 | GLU |
| 3 | C | 203 | TRP |
| 3 | C | 216 | LYS |
| 3 | C | 243 | LEU |
| 3 | C | 254 | LEU |
| 3 | C | 286 | PHE |
| 3 | C | 288 | GLU |
| 3 | C | 291 | LYS |
| 3 | C | 296 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | C | 298 | GLU |
| 3 | C | 300 | MET |
| 3 | C | 302 | THR |
| 3 | C | 303 | PHE |
| 3 | C | 306 | LEU |
| 3 | C | 309 | VAL |
| 3 | C | 312 | MET |
| 3 | C | 313 | LYS |
| 3 | C | 324 | CYS |
| 3 | C | 325 | GLU |
| 3 | C | 328 | LYS |
| 3 | C | 330 | ARG |
| 3 | C | 335 | CYS |
| 3 | C | 343 | LEU |
| 3 | C | 344 | ARG |
| 3 | C | 346 | GLN |
| 3 | C | 348 | GLU |
| 3 | C | 349 | LYS |
| 3 | C | 352 | LEU |
| 3 | C | 358 | LEU |
| 3 | C | 359 | LYS |
| 3 | C | 360 | LEU |
| 3 | C | 361 | ASN |
| 3 | C | 365 | LEU |
| 3 | C | 374 | GLU |
| 3 | C | 378 | MET |
| 3 | C | 389 | ARG |
| 3 | C | 395 | ASN |
| 3 | C | 413 | LYS |
| 3 | C | 414 | MET |
| 3 | C | 424 | ARG |
| 3 | C | 427 | GLN |
| 3 | C | 428 | LEU |
| 3 | C | 429 | ARG |
| 3 | C | 434 | ARG |
| 3 | C | 451 | GLU |
| 3 | C | 455 | CYS |
| 3 | C | 458 | ARG |
| 3 | C | 464 | ASP |
| 3 | C | 465 | VAL |
| 3 | C | 466 | GLU |
| 3 | C | 467 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | C | 468 | MET |
| 3 | C | 475 | LYS |
| 3 | C | 518 | GLN |
| 3 | C | 524 | LYS |
| 3 | C | 526 | TRP |
| 3 | C | 527 | ASP |
| 3 | C | 547 | LYS |
| 3 | C | 557 | ARG |
| 4 | D | 4 | LEU |
| 4 | D | 11 | ARG |
| 4 | D | 12 | VAL |
| 4 | D | 15 | THR |
| 4 | D | 16 | LEU |
| 4 | D | 20 | LEU |
| 4 | D | 32 | GLN |
| 4 | D | 36 | GLN |
| 4 | D | 49 | ASN |
| 5 | E | 58 | VAL |
| 5 | E | 61 | TYR |
| 5 | E | 63 | VAL |
| 5 | E | 69 | GLN |
| 5 | E | 87 | GLU |
| 5 | E | 88 | GLU |
| 5 | E | 89 | LEU |
| 5 | E | 90 | GLU |
| 5 | E | 99 | ILE |
| 5 | E | 106 | THR |
| 6 | F | 14 | GLN |
| 6 | F | 27 | LEU |
| 6 | F | 62 | LYS |
| 6 | F | 90 | GLN |
| 6 | F | 98 | ASN |
| 6 | F | 104 | ASP |
| 6 | F | 118 | LEU |
| 6 | F | 121 | LEU |
| 6 | F | 141 | SER |
| 6 | F | 144 | LEU |
| 6 | F | 145 | ASN |
| 6 | F | 163 | ASP |
| 6 | F | 466 | LEU |
| 6 | F | 474 | LEU |
| 6 | F | 477 | CYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | F | 494 | HIS |
| 6 | F | 520 | ARG |
| 6 | F | 521 | ILE |
| 6 | F | 527 | ARG |
| 6 | F | 530 | ASN |
| 6 | F | 538 | ILE |
| 6 | F | 562 | MET |
| 6 | F | 576 | CYS |
| 6 | F | 578 | SER |
| 6 | F | 595 | GLN |
| 6 | F | 614 | THR |
| 6 | F | 617 | LEU |
| 6 | F | 618 | ASP |
| 6 | F | 625 | ARG |
| 6 | F | 655 | GLU |
| 6 | F | 667 | GLN |
| 6 | F | 701 | LYS |
| 6 | F | 702 | ASN |
| 6 | F | 705 | CYS |
| 6 | F | 720 | LYS |
| 6 | F | 721 | SER |
| 6 | F | 729 | LEU |
| 6 | F | 742 | LEU |
| 7 | G | 5 | LYS |
| 6 | H | 27 | LEU |
| 6 | H | 61 | LEU |
| 6 | H | 90 | GLN |
| 6 | H | 98 | ASN |
| 6 | H | 118 | LEU |
| 6 | H | 130 | ARG |
| 6 | H | 144 | LEU |
| 6 | H | 145 | ASN |
| 6 | H | 163 | ASP |
| 6 | H | 165 | ASP |
| 6 | H | 466 | LEU |
| 6 | H | 480 | ASN |
| 6 | H | 520 | ARG |
| 6 | H | 521 | ILE |
| 6 | H | 530 | ASN |
| 6 | H | 562 | MET |
| 6 | H | 568 | GLU |
| 6 | H | 571 | CYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | H | 576 | CYS |
| 6 | H | 588 | LYS |
| 6 | H | 592 | ARG |
| 6 | H | 599 | ASN |
| 6 | H | 614 | THR |
| 6 | H | 618 | ASP |
| 6 | H | 633 | ARG |
| 6 | H | 655 | GLU |
| 6 | H | 667 | GLN |
| 6 | H | 694 | LYS |
| 6 | H | 702 | ASN |
| 6 | H | 720 | LYS |
| 6 | H | 729 | LEU |
| 6 | H | 742 | LEU |
| 6 | H | 762 | TRP |
| 6 | H | 765 | ASP |
| 8 | I | 26 | LEU |
| 8 | I | 34 | LEU |
| 8 | I | 37 | LEU |
| 8 | I | 71 | LEU |
| 8 | I | 89 | LYS |
| 8 | I | 92 | LEU |
| 8 | I | 218 | SER |
| 8 | I | 224 | SER |
| 8 | I | 232 | SER |
| 8 | I | 266 | ASN |
| 8 | I | 269 | LEU |
| 8 | I | 284 | ASP |
| 8 | I | 333 | LEU |
| 8 | I | 340 | SER |
| 8 | I | 349 | ILE |
| 8 | I | 353 | GLN |
| 8 | I | 359 | LEU |
| 8 | I | 360 | LEU |
| 8 | I | 371 | SER |
| 8 | I | 372 | TRP |
| 8 | I | 381 | LEU |
| 8 | I | 387 | GLU |
| 8 | I | 399 | LYS |
| 8 | I | 401 | ASN |
| 8 | I | 404 | LEU |
| 8 | I | 473 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | I | 492 | THR |
| 8 | I | 496 | GLN |
| 8 | I | 512 | LEU |
| 8 | I | 522 | LEU |
| 8 | I | 537 | LEU |
| 8 | I | 539 | LYS |
| 8 | I | 564 | ASP |
| 8 | I | 688 | THR |
| 8 | I | 718 | LYS |
| 8 | I | 736 | SER |
| 9 | J | 15 | ASP |
| 9 | J | 23 | LEU |
| 9 | J | 38 | GLN |
| 9 | J | 46 | CYS |
| 9 | J | 61 | ARG |
| 9 | J | 141 | ASP |
| 9 | J | 157 | LEU |
| 9 | J | 163 | CYS |
| 9 | J | 169 | LEU |
| 9 | J | 170 | LEU |
| 9 | J | 180 | GLU |
| 9 | J | 185 | LEU |
| 9 | J | 188 | LEU |
| 9 | J | 202 | ARG |
| 9 | J | 206 | GLU |
| 9 | J | 248 | LYS |
| 9 | J | 254 | THR |
| 9 | J | 259 | GLU |
| 9 | J | 267 | CYS |
| 9 | J | 287 | LEU |
| 9 | J | 290 | LYS |
| 9 | J | 298 | ASN |
| 9 | J | 317 | GLU |
| 9 | J | 323 | LEU |
| 9 | J | 329 | LEU |
| 9 | J | 343 | SER |
| 9 | J | 351 | ASP |
| 9 | J | 354 | MET |
| 9 | J | 363 | LEU |
| 9 | J | 385 | LYS |
| 9 | J | 395 | LEU |
| 9 | J | 429 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | J | 439 | VAL |
| 9 | J | 445 | GLU |
| 9 | J | 451 | LEU |
| 9 | J | 472 | LEU |
| 9 | J | 475 | ILE |
| 9 | J | 485 | ILE |
| 9 | J | 506 | LEU |
| 9 | J | 515 | SER |
| 9 | J | 518 | MET |
| 9 | J | 523 | ILE |
| 9 | K | 15 | ASP |
| 9 | K | 20 | GLN |
| 9 | K | 38 | GLN |
| 9 | K | 45 | GLN |
| 9 | K | 46 | CYS |
| 9 | K | 63 | ARG |
| 9 | K | 78 | ARG |
| 9 | K | 128 | ILE |
| 9 | K | 129 | LYS |
| 9 | K | 134 | LEU |
| 9 | K | 141 | ASP |
| 9 | K | 146 | ARG |
| 9 | K | 157 | LEU |
| 9 | K | 163 | CYS |
| 9 | K | 169 | LEU |
| 9 | K | 173 | HIS |
| 9 | K | 184 | LEU |
| 9 | K | 188 | LEU |
| 9 | K | 190 | LEU |
| 9 | K | 206 | GLU |
| 9 | K | 231 | LEU |
| 9 | K | 254 | THR |
| 9 | K | 267 | CYS |
| 9 | K | 284 | LEU |
| 9 | K | 287 | LEU |
| 9 | K | 289 | HIS |
| 9 | K | 290 | LYS |
| 9 | K | 342 | HIS |
| 9 | K | 343 | SER |
| 9 | K | 351 | ASP |
| 9 | K | 359 | THR |
| 9 | K | 363 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | K | 376 | LEU |
| 9 | K | 385 | LYS |
| 9 | K | 386 | LEU |
| 9 | K | 429 | LEU |
| 9 | K | 432 | ILE |
| 9 | K | 438 | GLU |
| 9 | K | 454 | VAL |
| 9 | K | 506 | LEU |
| 9 | K | 509 | ARG |
| 9 | K | 510 | ARG |
| 9 | K | 515 | SER |
| 9 | K | 523 | ILE |
| 10 | L | 7 | THR |
| 10 | L | 12 | ASP |
| 10 | L | 23 | ARG |
| 10 | L | 25 | ILE |
| 10 | L | 32 | SER |
| 10 | L | 49 | ASN |
| 10 | L | 65 | ASN |
| 10 | L | 67 | GLN |
| 10 | L | 74 | VAL |
| 10 | L | 77 | LEU |
| 10 | L | 84 | LYS |
| 10 | L | 101 | ASN |
| 10 | L | 103 | HIS |
| 10 | L | 113 | LEU |
| 10 | L | 132 | THR |
| 10 | L | 151 | THR |
| 10 | L | 162 | VAL |
| 10 | L | 182 | SER |
| 10 | L | 184 | ARG |
| 11 | M | 1 | MET |
| 11 | M | 6 | GLN |
| 11 | M | 10 | ARG |
| 11 | M | 12 | LEU |
| 11 | M | 17 | ASP |
| 11 | M | 19 | TRP |
| 11 | M | 20 | ARG |
| 11 | M | 31 | ILE |
| 11 | M | 33 | LEU |
| 11 | M | 51 | LYS |
| 11 | M | 55 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11 | M | 64 | TYR |
| 11 | M | 65 | LEU |
| 12 | N | 74 | TRP |
| 12 | N | 75 | PHE |
| 12 | N | 76 | VAL |
| 12 | N | 77 | GLU |
| 12 | N | 80 | GLN |
| 12 | N | 150 | ARG |
| 12 | N | 162 | PHE |
| 12 | N | 180 | PHE |
| 12 | N | 202 | GLU |
| 12 | N | 214 | ARG |
| 12 | N | 233 | CYS |
| 12 | N | 241 | HIS |
| 12 | N | 243 | LEU |
| 12 | N | 250 | LEU |
| 12 | N | 256 | VAL |
| 12 | N | 271 | GLU |
| 12 | N | 274 | GLU |
| 12 | N | 280 | GLU |
| 12 | N | 281 | TYR |
| 12 | N | 285 | PHE |
| 12 | N | 299 | TRP |
| 12 | N | 322 | ARG |
| 12 | N | 323 | ARG |
| 12 | N | 334 | ARG |
| 12 | N | 364 | CYS |
| 12 | N | 365 | LEU |
| 12 | N | 366 | GLU |
| 12 | N | 373 | GLN |
| 12 | N | 374 | LEU |
| 12 | N | 378 | LEU |
| 12 | N | 386 | LEU |
| 12 | N | 388 | HIS |
| 12 | N | 392 | ASN |
| 12 | N | 398 | THR |
| 12 | N | 425 | ARG |
| 12 | N | 435 | VAL |
| 12 | N | 503 | SER |
| 12 | N | 504 | LEU |
| 12 | N | 505 | LEU |
| 12 | N | 517 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12 | N | 531 | PHE |
| 12 | N | 544 | LEU |
| 12 | N | 547 | LEU |
| 12 | N | 557 | CYS |
| 12 | N | 561 | LEU |
| 12 | N | 566 | ASP |
| 12 | N | 571 | ASN |
| 12 | N | 584 | GLU |
| 12 | N | 592 | TYR |
| 12 | N | 594 | VAL |
| 12 | N | 609 | LEU |
| 12 | N | 619 | LEU |
| 12 | N | 622 | TYR |
| 12 | N | 625 | LYS |
| 12 | N | 626 | TYR |
| 12 | N | 633 | ARG |
| 12 | N | 638 | LYS |
| 12 | N | 640 | THR |
| 12 | N | 670 | PHE |
| 12 | N | 678 | LEU |
| 12 | N | 695 | ARG |
| 12 | N | 699 | TRP |
| 13 | O | 28 | ASP |
| 13 | O | 29 | TRP |
| 13 | O | 38 | LEU |
| 13 | O | 40 | LEU |
| 13 | O | 43 | GLU |
| 13 | O | 59 | ARG |
| 13 | O | 62 | GLN |
| 13 | O | 63 | LEU |
| 13 | O | 73 | ILE |
| 13 | O | 78 | LEU |
| 13 | O | 89 | LEU |
| 13 | O | 96 | ARG |
| 13 | O | 98 | LYS |
| 13 | O | 99 | LEU |
| 13 | O | 104 | GLU |
| 13 | O | 106 | LYS |
| 13 | O | 129 | THR |
| 13 | O | 136 | LEU |
| 13 | O | 160 | GLN |
| 13 | O | 207 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13 | O | 218 | GLN |
| 13 | O | 228 | THR |
| 13 | O | 237 | GLN |
| 13 | O | 249 | ASP |
| 13 | O | 256 | LEU |
| 13 | O | 257 | SER |
| 13 | O | 264 | VAL |
| 13 | O | 265 | GLN |
| 13 | O | 266 | ASP |
| 13 | O | 267 | VAL |
| 13 | O | 280 | ARG |
| 13 | O | 283 | LEU |
| 13 | O | 299 | SER |
| 13 | O | 328 | ILE |
| 13 | O | 330 | ILE |
| 13 | O | 344 | LEU |
| 13 | O | 345 | SER |
| 13 | O | 352 | GLN |
| 13 | O | 358 | TYR |
| 13 | O | 363 | HIS |
| 13 | O | 364 | SER |
| 13 | O | 383 | SER |
| 13 | O | 387 | GLN |
| 13 | O | 396 | ASN |
| 13 | O | 408 | LEU |
| 13 | O | 414 | LEU |
| 13 | O | 417 | LEU |
| 13 | O | 420 | ILE |
| 13 | O | 429 | TRP |
| 13 | O | 434 | ARG |
| 13 | O | 465 | SER |
| 13 | O | 468 | VAL |
| 13 | O | 491 | LYS |
| 13 | O | 495 | GLU |
| 13 | O | 501 | SER |
| 13 | O | 510 | CYS |
| 13 | O | 511 | ASP |
| 13 | O | 512 | GLN |
| 13 | O | 518 | ARG |
| 13 | O | 531 | LEU |
| 13 | O | 532 | VAL |
| 13 | O | 533 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13 | O | 535 | ILE |
| 13 | O | 563 | LEU |
| 13 | O | 581 | ILE |
| 13 | O | 586 | SER |
| 13 | O | 598 | THR |
| 13 | O | 608 | LEU |
| 13 | O | 616 | LEU |
| 13 | O | 617 | GLN |
| 13 | O | 618 | TYR |
| 13 | O | 619 | LEU |
| 13 | O | 622 | GLU |
| 13 | O | 623 | THR |
| 13 | O | 625 | LEU |
| 13 | O | 632 | LEU |
| 13 | O | 633 | ILE |
| 13 | O | 634 | LEU |
| 13 | O | 636 | ILE |
| 13 | O | 641 | LEU |
| 13 | O | 646 | MET |
| 13 | O | 657 | ILE |
| 13 | O | 670 | CYS |
| 13 | O | 680 | GLN |
| 13 | O | 683 | LYS |
| 13 | O | 693 | ASN |
| 13 | O | 694 | LEU |
| 13 | O | 695 | ASN |
| 13 | O | 706 | CYS |
| 13 | O | 707 | LYS |
| 13 | O | 713 | VAL |
| 13 | O | 715 | TYR |
| 13 | O | 723 | THR |
| 13 | O | 730 | ARG |
| 13 | O | 735 | MET |
| 13 | O | 751 | LEU |
| 13 | O | 752 | ILE |
| 13 | O | 755 | LEU |
| 3 | P | 37 | LEU |
| 3 | P | 38 | LEU |
| 3 | P | 39 | ILE |
| 3 | P | 42 | LEU |
| 3 | P | 49 | LEU |
| 3 | P | 70 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | P | 78 | GLU |
| 3 | P | 83 | ASP |
| 3 | P | 89 | LEU |
| 3 | P | 97 | LYS |
| 3 | P | 119 | MET |
| 3 | P | 131 | ASP |
| 3 | P | 147 | LYS |
| 3 | P | 154 | LEU |
| 3 | P | 172 | LEU |
| 3 | P | 179 | LEU |
| 3 | P | 182 | LEU |
| 3 | P | 201 | LEU |
| 3 | P | 234 | LEU |
| 3 | P | 244 | ILE |
| 3 | P | 288 | GLU |
| 3 | P | 291 | LYS |
| 3 | P | 299 | ASN |
| 3 | P | 300 | MET |
| 3 | P | 302 | THR |
| 3 | P | 303 | PHE |
| 3 | P | 306 | LEU |
| 3 | P | 309 | VAL |
| 3 | P | 310 | ARG |
| 3 | P | 312 | MET |
| 3 | P | 313 | LYS |
| 3 | P | 316 | LEU |
| 3 | P | 321 | HIS |
| 3 | P | 324 | CYS |
| 3 | P | 328 | LYS |
| 3 | P | 335 | CYS |
| 3 | P | 343 | LEU |
| 3 | P | 348 | GLU |
| 3 | P | 352 | LEU |
| 3 | P | 358 | LEU |
| 3 | P | 359 | LYS |
| 3 | P | 365 | LEU |
| 3 | P | 378 | MET |
| 3 | P | 382 | SER |
| 3 | P | 386 | GLN |
| 3 | P | 392 | ILE |
| 3 | P | 395 | ASN |
| 3 | P | 400 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | P | 428 | LEU |
| 3 | P | 429 | ARG |
| 3 | P | 435 | MET |
| 3 | P | 451 | GLU |
| 3 | P | 455 | CYS |
| 3 | P | 468 | MET |
| 3 | P | 472 | LYS |
| 3 | P | 479 | GLN |
| 3 | P | 518 | GLN |
| 3 | P | 524 | LYS |
| 14 | R | 73 | LYS |
| 14 | R | 83 | ARG |
| 14 | R | 109 | LYS |
| 14 | R | 110 | LYS |
| 14 | R | 114 | LYS |
| 14 | R | 118 | LEU |
| 14 | R | 125 | VAL |
| 14 | R | 129 | LYS |
| 14 | R | 132 | ARG |
| 14 | R | 252 | LEU |
| 14 | R | 316 | ARG |
| 14 | R | 411 | TYR |
| 14 | R | 496 | GLN |
| 14 | R | 499 | ARG |
| 7 | W | 5 | LYS |
| 16 | X | 39 | ASP |
| 16 | X | 49 | LEU |
| 16 | X | 79 | LEU |
| 16 | X | 106 | GLN |
| 16 | X | 110 | LEU |
| 16 | X | 154 | ASP |
| 16 | X | 184 | GLN |
| 16 | X | 193 | LYS |
| 16 | X | 201 | LEU |
| 16 | X | 204 | ASP |
| 16 | X | 253 | ARG |
| 16 | X | 255 | ILE |
| 16 | X | 276 | SER |
| 16 | X | 289 | ASN |
| 16 | X | 295 | GLU |
| 16 | X | 303 | TYR |
| 16 | X | 306 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16 | X | 323 | ASP |
| 16 | X | 334 | ILE |
| 16 | X | 366 | ILE |
| 16 | X | 371 | ASN |
| 16 | X | 372 | SER |
| 16 | X | 401 | ARG |
| 16 | X | 407 | LEU |
| 16 | X | 414 | ILE |
| 16 | X | 423 | ILE |
| 16 | X | 452 | LEU |
| 16 | X | 453 | GLU |
| 16 | X | 457 | THR |
| 16 | X | 465 | LEU |
| 16 | X | 487 | SER |
| 16 | X | 506 | GLN |
| 16 | X | 515 | LEU |
| 16 | Y | 39 | ASP |
| 16 | Y | 49 | LEU |
| 16 | Y | 54 | ARG |
| 16 | Y | 63 | MET |
| 16 | Y | 79 | LEU |
| 16 | Y | 94 | ARG |
| 16 | Y | 95 | ASN |
| 16 | Y | 154 | ASP |
| 16 | Y | 184 | GLN |
| 16 | Y | 193 | LYS |
| 16 | Y | 199 | CYS |
| 16 | Y | 201 | LEU |
| 16 | Y | 204 | ASP |
| 16 | Y | 253 | ARG |
| 16 | Y | 255 | ILE |
| 16 | Y | 276 | SER |
| 16 | Y | 289 | ASN |
| 16 | Y | 294 | PHE |
| 16 | Y | 295 | GLU |
| 16 | Y | 300 | LEU |
| 16 | Y | 303 | TYR |
| 16 | Y | 323 | ASP |
| 16 | Y | 334 | ILE |
| 16 | Y | 364 | LYS |
| 16 | Y | 366 | ILE |
| 16 | Y | 371 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16 | Y | 372 | SER |
| 16 | Y | 401 | ARG |
| 16 | Y | 407 | LEU |
| 16 | Y | 414 | ILE |
| 16 | Y | 423 | ILE |
| 16 | Y | 452 | LEU |
| 16 | Y | 453 | GLU |
| 16 | Y | 457 | THR |
| 16 | Y | 465 | LEU |
| 16 | Y | 487 | SER |
| 16 | Y | 503 | LEU |
| 16 | Y | 506 | GLN |
| 16 | Y | 515 | LEU |
| 16 | Y | 551 | LYS |
| 16 | Y | 552 | MET |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (145) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 27 | HIS |
| 1 | A | 36 | ASN |
| 1 | A | 38 | GLN |
| 1 | A | 124 | GLN |
| 1 | A | 125 | GLN |
| 1 | A | 162 | HIS |
| 1 | A | 250 | ASN |
| 1 | A | 263 | GLN |
| 1 | A | 593 | ASN |
| 1 | A | 658 | ASN |
| 1 | A | 666 | ASN |
| 1 | A | 776 | ASN |
| 1 | A | 936 | ASN |
| 1 | A | 1021 | HIS |
| 1 | A | 1161 | ASN |
| 1 | A | 1165 | HIS |
| 1 | A | 1184 | HIS |
| 1 | A | 1201 | HIS |
| 1 | A | 1262 | GLN |
| 1 | A | 1266 | HIS |
| 1 | A | 1327 | GLN |
| 1 | A | 1380 | ASN |
| 1 | A | 1543 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1559 | HIS |
| 1 | A | 1604 | GLN |
| 1 | A | 1813 | GLN |
| 2 | B | 9 | ASN |
| 2 | B | 50 | GLN |
| 3 | C | 202 | HIS |
| 3 | C | 236 | HIS |
| 3 | C | 249 | GLN |
| 3 | C | 287 | ASN |
| 3 | C | 373 | HIS |
| 3 | C | 386 | GLN |
| 4 | D | 36 | GLN |
| 4 | D | 37 | HIS |
| 4 | D | 38 | GLN |
| 4 | D | 49 | ASN |
| 5 | E | 75 | GLN |
| 6 | F | 100 | GLN |
| 6 | F | 495 | HIS |
| 6 | F | 583 | HIS |
| 6 | F | 595 | GLN |
| 6 | F | 634 | HIS |
| 6 | F | 636 | ASN |
| 6 | F | 754 | HIS |
| 6 | H | 14 | GLN |
| 6 | H | 480 | ASN |
| 6 | H | 494 | HIS |
| 6 | H | 495 | HIS |
| 6 | H | 545 | HIS |
| 6 | H | 634 | HIS |
| 6 | H | 648 | GLN |
| 6 | H | 680 | HIS |
| 6 | H | 708 | HIS |
| 8 | I | 18 | GLN |
| 8 | I | 266 | ASN |
| 8 | I | 323 | ASN |
| 8 | I | 345 | GLN |
| 8 | I | 351 | HIS |
| 8 | I | 353 | GLN |
| 8 | I | 362 | HIS |
| 8 | I | 471 | ASN |
| 8 | I | 523 | HIS |
| 9 | J | 17 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | J | 38 | GLN |
| 9 | J | 45 | GLN |
| 9 | J | 58 | HIS |
| 9 | J | 173 | HIS |
| 9 | J | 228 | GLN |
| 9 | J | 271 | HIS |
| 9 | J | 289 | HIS |
| 9 | J | 316 | ASN |
| 9 | J | 342 | HIS |
| 9 | J | 352 | GLN |
| 9 | J | 382 | ASN |
| 9 | J | 406 | HIS |
| 9 | K | 17 | GLN |
| 9 | K | 20 | GLN |
| 9 | K | 38 | GLN |
| 9 | K | 45 | GLN |
| 9 | K | 198 | GLN |
| 9 | K | 271 | HIS |
| 9 | K | 316 | ASN |
| 9 | K | 352 | GLN |
| 9 | K | 382 | ASN |
| 10 | L | 49 | ASN |
| 10 | L | 103 | HIS |
| 10 | L | 128 | HIS |
| 10 | L | 138 | GLN |
| 10 | L | 152 | HIS |
| 12 | N | 370 | GLN |
| 12 | N | 388 | HIS |
| 12 | N | 571 | ASN |
| 12 | N | 639 | HIS |
| 12 | N | 663 | GLN |
| 12 | N | 702 | GLN |
| 12 | N | 726 | ASN |
| 13 | O | 62 | GLN |
| 13 | O | 69 | GLN |
| 13 | O | 91 | ASN |
| 13 | O | 211 | GLN |
| 13 | O | 219 | GLN |
| 13 | O | 237 | GLN |
| 13 | O | 242 | ASN |
| 13 | O | 247 | ASN |
| 13 | O | 319 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13 | O | 387 | GLN |
| 13 | O | 412 | HIS |
| 13 | O | 424 | GLN |
| 13 | O | 443 | GLN |
| 13 | O | 460 | GLN |
| 13 | O | 462 | ASN |
| 13 | O | 492 | HIS |
| 13 | O | 539 | ASN |
| 13 | O | 556 | GLN |
| 13 | O | 565 | GLN |
| 13 | O | 576 | ASN |
| 13 | O | 717 | GLN |
| 13 | O | 753 | ASN |
| 3 | P | 236 | HIS |
| 3 | P | 242 | GLN |
| 3 | P | 249 | GLN |
| 3 | P | 287 | ASN |
| 3 | P | 305 | ASN |
| 3 | P | 321 | HIS |
| 14 | R | 87 | GLN |
| 14 | R | 99 | ASN |
| 16 | X | 50 | HIS |
| 16 | X | 89 | HIS |
| 16 | X | 95 | ASN |
| 16 | X | 106 | GLN |
| 16 | X | 298 | GLN |
| 16 | X | 337 | GLN |
| 16 | X | 371 | ASN |
| 16 | X | 395 | HIS |
| 16 | X | 506 | GLN |
| 16 | Y | 270 | ASN |
| 16 | Y | 296 | GLN |
| 16 | Y | 298 | GLN |
| 16 | Y | 337 | GLN |
| 16 | Y | 371 | ASN |
| 16 | Y | 395 | HIS |
| 16 | Y | 505 | ASN |
| 16 | Y | 506 | GLN |

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 12 | N | 6 |
| 14 | R | 2 |
| 16 | X | 1 |
| 6 | H | 1 |
| 1 | A | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | N | 510:GLY | C | 511:SER | N | 3.32 |
| 1 | N | 213:TYR | C | 214:ARG | N | 3.24 |
| 1 | X | 386:MET | C | 387:GLY | N | 3.24 |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|------------|--------|-----------|--------|--------------|
| 1 | N | 92:TRP | C | 93:ASN | N | 3.21 |
| 1 | R | 388[A]:CYS | C | 389:SER | N | 3.09 |
| 1 | N | 166:PRO | C | 167:ARG | N | 2.97 |
| 1 | N | 549:PHE | C | 550:GLY | N | 2.95 |
| 1 | R | 388[B]:CYS | C | 389:SER | N | 2.94 |
| 1 | A | 1228:LEU | C | 1229:SER | N | 2.89 |
| 1 | N | 563:ASP | C | 564:MET | N | 2.82 |
| 1 | H | 479:TYR | C | 480:ASN | N | 2.09 |