



Full wwPDB EM Validation Report ⓘ

Dec 1, 2021 – 05:13 am GMT

PDB ID : 7P3X
EMDB ID : EMD-13187
Title : Homology model of the full-length AP-3 complex in a compact open conformation
Authors : Schubert, E.; Raunser, S.
Deposited on : 2021-07-09
Resolution : 9.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

EMDB validation analysis : 0.0.0.dev97
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

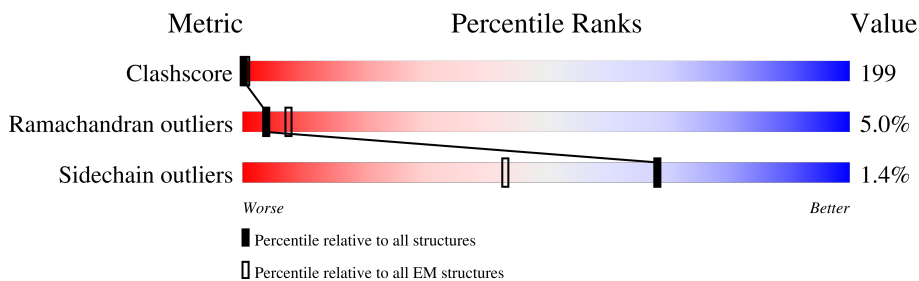
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 9.10 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 | 158937 | 4297 |
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 964 | |
| 2 | B | 809 | |
| 3 | S | 194 | |
| 4 | M | 483 | |

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14104 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 AP-3 complex subunit delta.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 1 | A | 576 | 4625 | 2978 | 738 | 881 | 28 | 0 | 0 |

There are 32 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|----------------|
| A | 933 | ARG | - | expression tag | UNP A0A7I9C4X2 |
| A | 934 | THR | - | expression tag | UNP A0A7I9C4X2 |
| A | 935 | LEU | - | expression tag | UNP A0A7I9C4X2 |
| A | 936 | GLN | - | expression tag | UNP A0A7I9C4X2 |
| A | 937 | VAL | - | expression tag | UNP A0A7I9C4X2 |
| A | 938 | ASP | - | expression tag | UNP A0A7I9C4X2 |
| A | 939 | GLY | - | expression tag | UNP A0A7I9C4X2 |
| A | 940 | SER | - | expression tag | UNP A0A7I9C4X2 |
| A | 941 | ASP | - | expression tag | UNP A0A7I9C4X2 |
| A | 942 | TYR | - | expression tag | UNP A0A7I9C4X2 |
| A | 943 | LYS | - | expression tag | UNP A0A7I9C4X2 |
| A | 944 | ASP | - | expression tag | UNP A0A7I9C4X2 |
| A | 945 | ASP | - | expression tag | UNP A0A7I9C4X2 |
| A | 946 | ASP | - | expression tag | UNP A0A7I9C4X2 |
| A | 947 | ASP | - | expression tag | UNP A0A7I9C4X2 |
| A | 948 | LYS | - | expression tag | UNP A0A7I9C4X2 |
| A | 949 | ASP | - | expression tag | UNP A0A7I9C4X2 |
| A | 950 | TYR | - | expression tag | UNP A0A7I9C4X2 |
| A | 951 | LYS | - | expression tag | UNP A0A7I9C4X2 |
| A | 952 | ASP | - | expression tag | UNP A0A7I9C4X2 |
| A | 953 | ASP | - | expression tag | UNP A0A7I9C4X2 |
| A | 954 | ASP | - | expression tag | UNP A0A7I9C4X2 |
| A | 955 | ASP | - | expression tag | UNP A0A7I9C4X2 |
| A | 956 | LYS | - | expression tag | UNP A0A7I9C4X2 |
| A | 957 | ASP | - | expression tag | UNP A0A7I9C4X2 |
| A | 958 | TYR | - | expression tag | UNP A0A7I9C4X2 |
| A | 959 | LYS | - | expression tag | UNP A0A7I9C4X2 |
| A | 960 | ASP | - | expression tag | UNP A0A7I9C4X2 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|----------------|
| A | 961 | ASP | - | expression tag | UNP A0A7I9C4X2 |
| A | 962 | ASP | - | expression tag | UNP A0A7I9C4X2 |
| A | 963 | ASP | - | expression tag | UNP A0A7I9C4X2 |
| A | 964 | LYS | - | expression tag | UNP A0A7I9C4X2 |

- Molecule 2 is a protein called Y55_G0035830.mRNA.1.CDS.1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 2 | B | 621 | 4963 | 3168 | 830 | 937 | 28 | 0 | 0 |

- Molecule 3 is a protein called AP complex subunit sigma.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 3 | S | 168 | 1358 | 867 | 215 | 272 | 4 | 0 | 0 |

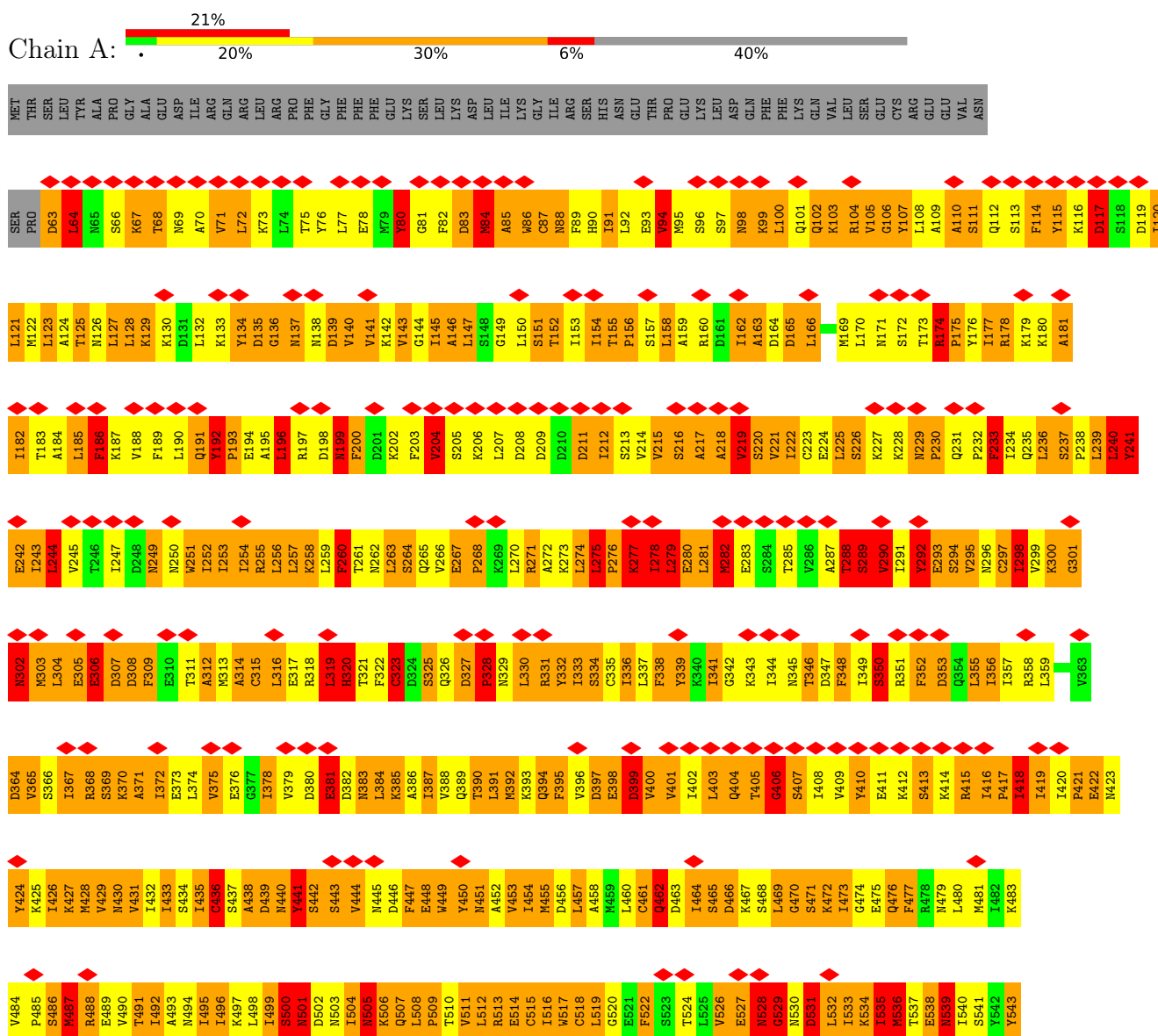
- Molecule 4 is a protein called AP-3 complex subunit mu.

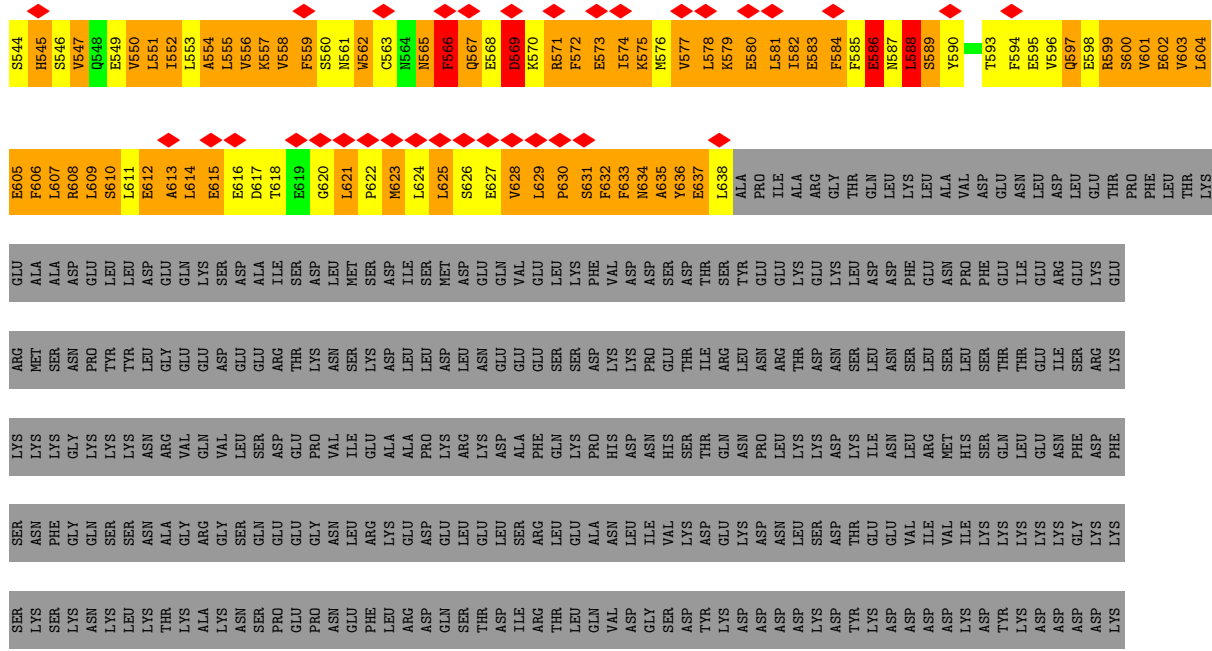
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 4 | M | 397 | 3158 | 2018 | 516 | 612 | 12 | 0 | 0 |

3 Residue-property plots

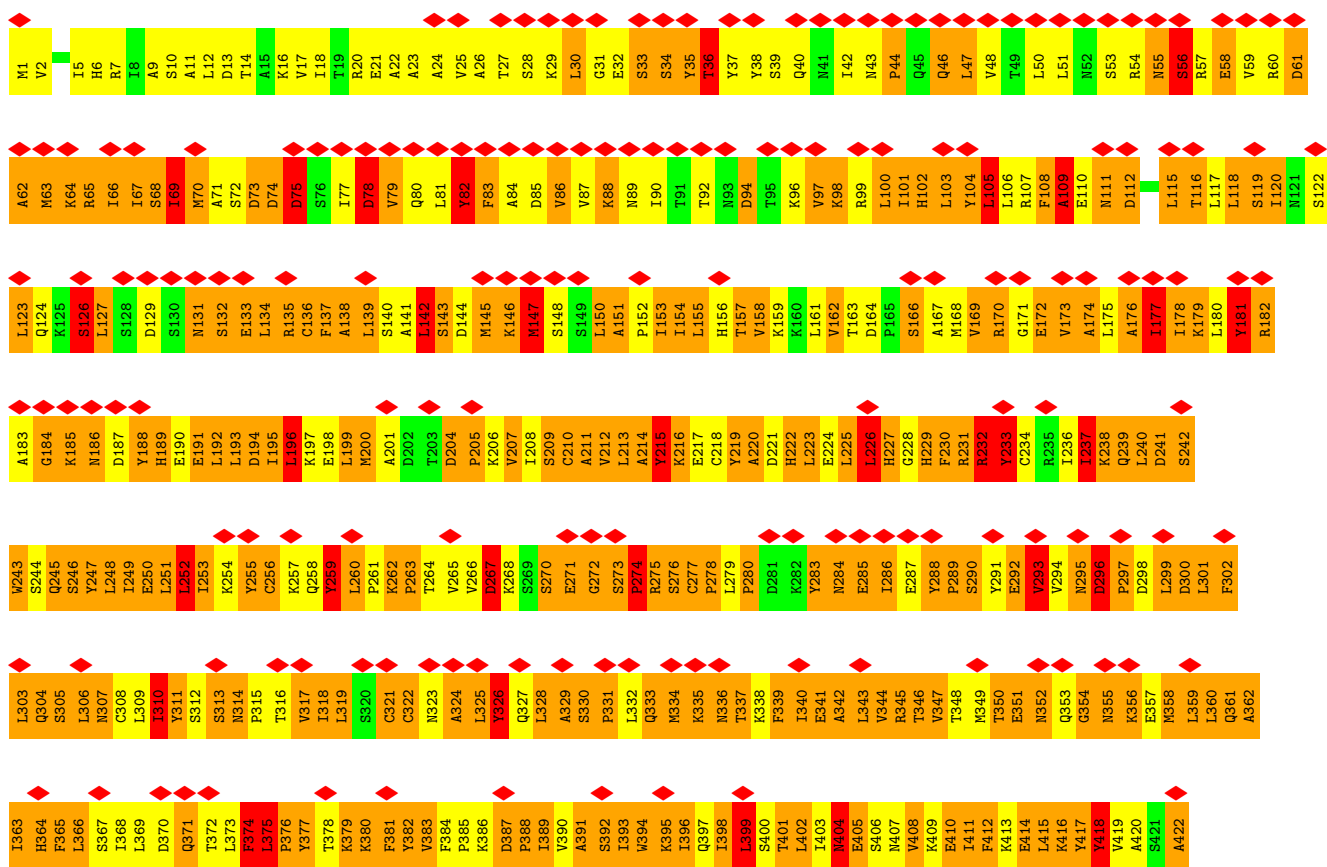
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

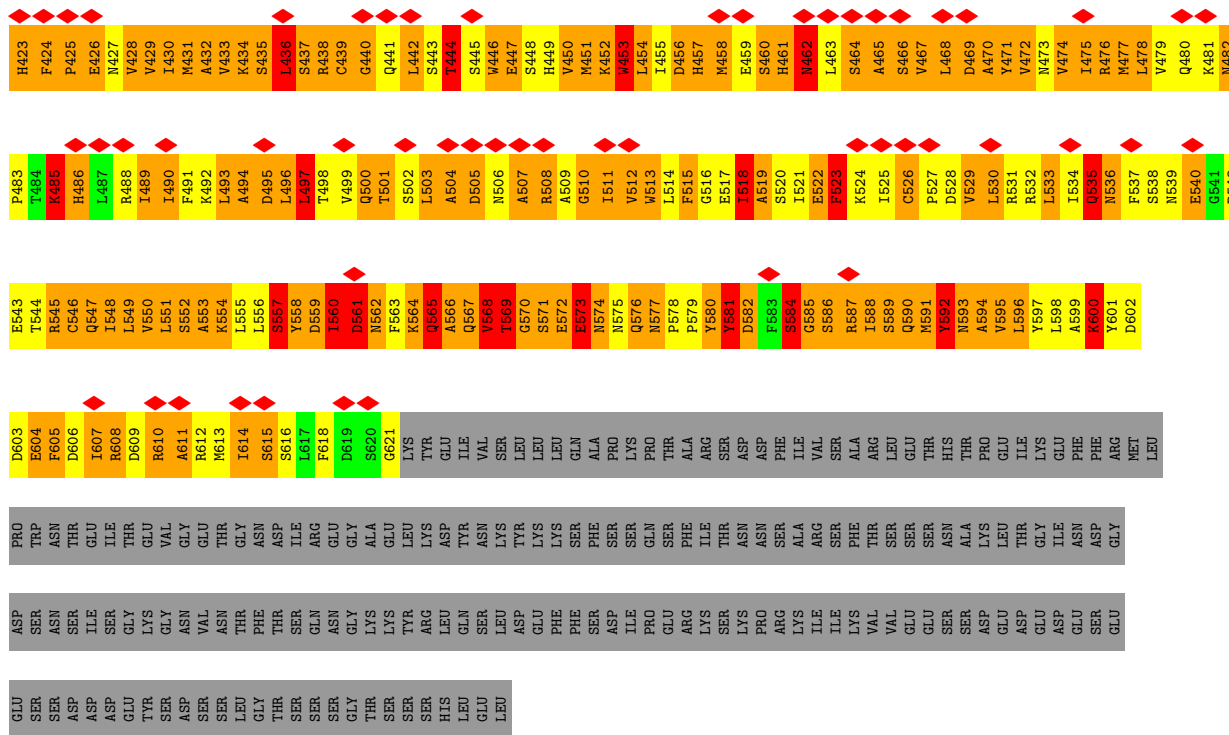
- Molecule 1: AP-3 complex subunit delta



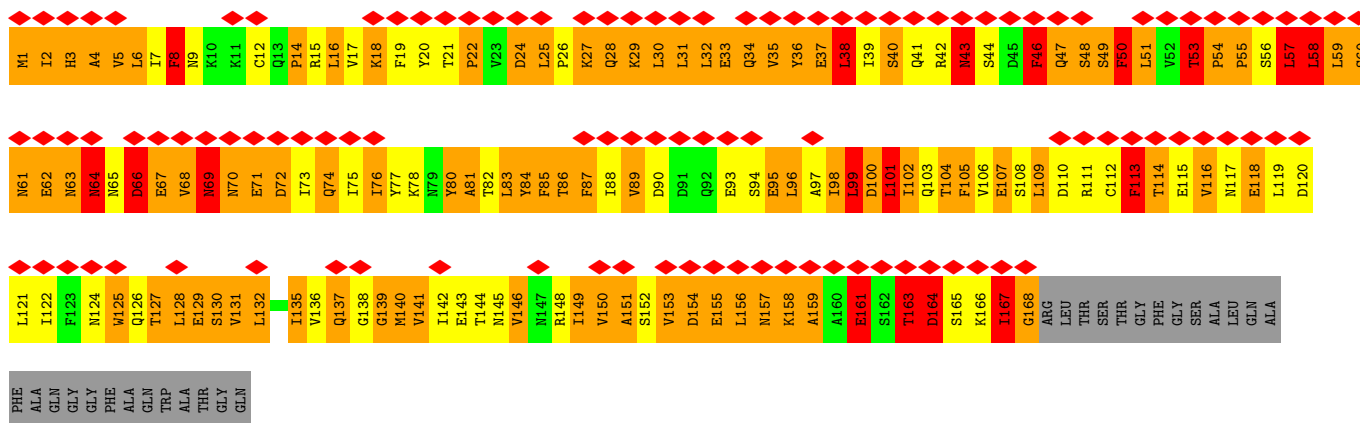


• Molecule 2: Y55_G0035830.mRNA.1.CDS.1

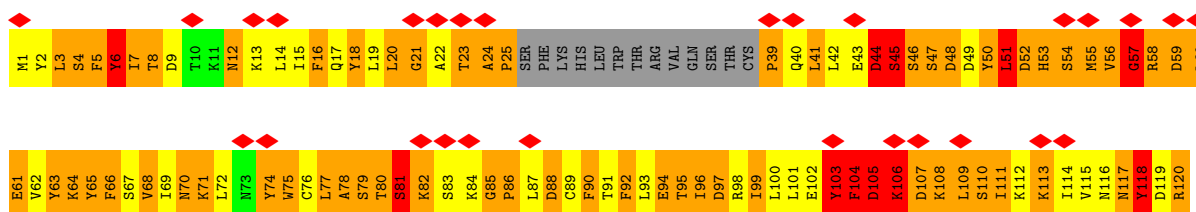
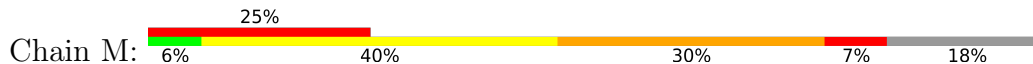




• Molecule 3: AP complex subunit sigma



• Molecule 4: AP-3 complex subunit mu



| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|
| I121 | I122 | L123 | I124 | F125 | C126 | C127 | C128 | V129 | E130 | A131 | G132 | E133 | P134 | N135 | V136 | S137 | D138 | MET | LEU | TYR | VAL | ASN | ASN | LYS | LYS | LYS | LYS | GLU | GLU | ALA | ALA | VAL | PRO | PRO | GLU | ARG | SER | ASP | LEU | SER | LYS | PHE | ILE | SER | THR | ALA | HIS | ASN | LEU | GLN | GLN | ALA | VAL | GLN | VAL | GLN | LEU | PRO | GLN | GLN | ARG | GLN | GLN | LEU |
| H241 | G242 | I243 | V244 | D245 | V246 | R247 | S248 | Y249 | L250 | N251 | D252 | N253 | P254 | L255 | V256 | A257 | V258 | K259 | L260 | N261 | T262 | M263 | G264 | N265 | D266 | I267 | G268 | I269 | P270 | S271 | L272 | H273 | D274 | C275 | V276 | E277 | I278 | N279 | D280 | G281 | V282 | F283 | S284 | P285 | S286 | N287 | I288 | T289 | F290 | I291 | P292 | P293 | D294 | G295 | K296 | F297 | R298 | L299 | L300 | | | | | |
| E301 | Y302 | S303 | V304 | D305 | L306 | S307 | S308 | Q309 | V310 | K311 | Q312 | S313 | G314 | V315 | R316 | M317 | N318 | S319 | L320 | N321 | L322 | M323 | S324 | L325 | H326 | F327 | Q328 | N329 | G330 | L331 | G332 | K333 | D334 | S335 | D336 | E337 | F338 | E339 | L340 | S341 | L342 | N343 | I344 | E345 | N346 | F347 | K348 | K349 | V350 | S351 | Q352 | V353 | D354 | D355 | L356 | K357 | I358 | D359 | L360 | | | | | |
| G361 | F362 | N363 | V364 | E365 | N366 | A367 | D368 | P369 | N370 | E371 | I372 | A373 | Y374 | K375 | I376 | K377 | I378 | R380 | N381 | T382 | H383 | G384 | R385 | F386 | E387 | N388 | S389 | I390 | I391 | M392 | G393 | Q394 | G395 | Q396 | W397 | I398 | F399 | D400 | K401 | S402 | T403 | A404 | T405 | G406 | T407 | V408 | P409 | V410 | L411 | R412 | G413 | C414 | I415 | E416 | Y417 | E418 | N419 | T420 | | | | | | |
| G421 | P422 | M423 | F424 | T425 | K426 | K427 | V428 | D429 | L430 | Q431 | T432 | V433 | S434 | L435 | E436 | Y437 | S438 | V439 | L440 | G441 | Q442 | S443 | A444 | S445 | G446 | T447 | Y448 | V449 | E450 | A451 | L452 | D453 | T454 | V455 | S456 | G457 | L458 | T459 | L460 | G461 | K462 | M463 | T464 | K465 | L466 | Y467 | K468 | G469 | A470 | K471 | Y472 | K473 | T474 | Q475 | T476 | G477 | M478 | F479 | Q480 | | | | | |
| V481 | R482 | L483 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |

4 Experimental information

| Property | Value | Source |
|--------------------------------------|---------------------------|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 23039 | Depositor |
| Resolution determination method | FSC 0.5 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING ONLY | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 81 | Depositor |
| Minimum defocus (nm) | 1500 | Depositor |
| Maximum defocus (nm) | 3600 | Depositor |
| Magnification | 130000 | Depositor |
| Image detector | GATAN K2 SUMMIT (4k x 4k) | Depositor |
| Maximum map value | 0.049 | Depositor |
| Minimum map value | -0.014 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.002 | Depositor |
| Recommended contour level | 0.015 | Depositor |
| Map size (\AA) | 282.48, 282.48, 282.48 | wwPDB |
| Map dimensions | 264, 264, 264 | wwPDB |
| Map angles ($^\circ$) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (\AA) | 1.07, 1.07, 1.07 | Depositor |

5 Model quality i

5.1 Standard geometry i

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|-------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | A | 1.85 | 106/4699 (2.3%) | 2.69 | 616/6358 (9.7%) |
| 2 | B | 1.71 | 91/5057 (1.8%) | 2.45 | 596/6855 (8.7%) |
| 3 | S | 2.51 | 75/1379 (5.4%) | 2.79 | 167/1874 (8.9%) |
| 4 | M | 2.39 | 156/3217 (4.8%) | 2.55 | 283/4346 (6.5%) |
| All | All | 2.01 | 428/14352 (3.0%) | 2.59 | 1662/19433 (8.6%) |

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 | 54 |
| 2 | B | 0 | 31 |
| 3 | S | 1 | 18 |
| 4 | M | 1 | 24 |
| All | All | 2 | 127 |

All (428) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 4 | M | 104 | PHE | N-CA | -22.48 | 1.01 | 1.46 |
| 4 | M | 64 | LYS | N-CA | -18.25 | 1.09 | 1.46 |
| 4 | M | 135 | ASN | C-N | -17.55 | 0.93 | 1.34 |
| 4 | M | 132 | GLY | CA-C | -17.17 | 1.24 | 1.51 |
| 4 | M | 281 | GLY | CA-C | 16.88 | 1.78 | 1.51 |
| 4 | M | 107 | ASP | N-CA | -15.73 | 1.14 | 1.46 |
| 4 | M | 136 | VAL | N-CA | -15.49 | 1.15 | 1.46 |
| 1 | A | 438 | ALA | CA-CB | -15.46 | 1.20 | 1.52 |
| 3 | S | 49 | SER | N-CA | -15.21 | 1.16 | 1.46 |
| 4 | M | 133 | GLU | N-CA | -14.60 | 1.17 | 1.46 |
| 3 | S | 53 | THR | N-CA | -14.44 | 1.17 | 1.46 |
| 3 | S | 68 | VAL | C-N | 14.43 | 1.67 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 4 | M | 132 | GLY | N-CA | -13.97 | 1.25 | 1.46 |
| 4 | M | 65 | TYR | CA-C | -13.82 | 1.17 | 1.52 |
| 4 | M | 63 | TYR | CA-C | -13.76 | 1.17 | 1.52 |
| 3 | S | 48 | SER | C-N | -13.29 | 1.03 | 1.34 |
| 4 | M | 131 | ALA | CA-CB | 13.14 | 1.80 | 1.52 |
| 4 | M | 293 | PRO | N-CD | 12.65 | 1.65 | 1.47 |
| 4 | M | 131 | ALA | CA-C | -12.47 | 1.20 | 1.52 |
| 4 | M | 66 | PHE | N-CA | -11.96 | 1.22 | 1.46 |
| 3 | S | 48 | SER | CA-C | -11.71 | 1.22 | 1.52 |
| 1 | A | 406 | GLY | CA-C | 11.69 | 1.70 | 1.51 |
| 2 | B | 581 | TYR | N-CA | -11.65 | 1.23 | 1.46 |
| 3 | S | 163 | THR | CA-C | 11.62 | 1.83 | 1.52 |
| 4 | M | 282 | VAL | N-CA | 11.60 | 1.69 | 1.46 |
| 4 | M | 3 | LEU | C-N | -11.30 | 1.08 | 1.34 |
| 3 | S | 46 | PHE | CA-C | -11.12 | 1.24 | 1.52 |
| 4 | M | 81 | SER | C-N | -11.06 | 1.08 | 1.34 |
| 4 | M | 137 | SER | N-CA | -11.02 | 1.24 | 1.46 |
| 4 | M | 295 | GLY | CA-C | 10.85 | 1.69 | 1.51 |
| 4 | M | 63 | TYR | N-CA | -10.82 | 1.24 | 1.46 |
| 4 | M | 61 | GLU | CA-C | -10.75 | 1.25 | 1.52 |
| 4 | M | 20 | LEU | C-N | -10.60 | 1.14 | 1.33 |
| 3 | S | 64 | ASN | CA-C | 10.50 | 1.80 | 1.52 |
| 3 | S | 55 | PRO | N-CA | 10.50 | 1.65 | 1.47 |
| 4 | M | 56 | VAL | CA-C | -10.34 | 1.26 | 1.52 |
| 4 | M | 105 | ASP | C-N | -10.33 | 1.10 | 1.34 |
| 4 | M | 135 | ASN | CA-C | -10.24 | 1.26 | 1.52 |
| 3 | S | 58 | LEU | CA-C | -10.13 | 1.26 | 1.52 |
| 4 | M | 80 | THR | C-N | -9.95 | 1.11 | 1.34 |
| 3 | S | 124 | ASN | N-CA | -9.89 | 1.26 | 1.46 |
| 1 | A | 218 | ALA | CA-C | -9.82 | 1.27 | 1.52 |
| 3 | S | 50 | PHE | CA-C | -9.82 | 1.27 | 1.52 |
| 3 | S | 49 | SER | C-N | 9.81 | 1.56 | 1.34 |
| 4 | M | 65 | TYR | N-CA | -9.77 | 1.26 | 1.46 |
| 4 | M | 131 | ALA | N-CA | -9.65 | 1.27 | 1.46 |
| 1 | A | 404 | GLN | N-CA | -9.64 | 1.27 | 1.46 |
| 2 | B | 274 | PRO | N-CD | 9.59 | 1.61 | 1.47 |
| 4 | M | 62 | VAL | N-CA | -9.57 | 1.27 | 1.46 |
| 1 | A | 407 | SER | N-CA | 9.57 | 1.65 | 1.46 |
| 3 | S | 71 | GLU | N-CA | -9.57 | 1.27 | 1.46 |
| 1 | A | 509 | PRO | N-CD | 9.36 | 1.60 | 1.47 |
| 4 | M | 62 | VAL | CA-C | -9.34 | 1.28 | 1.52 |
| 4 | M | 130 | GLU | C-N | -9.29 | 1.12 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3 | S | 51 | LEU | N-CA | -9.27 | 1.27 | 1.46 |
| 3 | S | 54 | PRO | N-CA | 9.26 | 1.62 | 1.47 |
| 2 | B | 284 | ASN | C-N | -9.13 | 1.13 | 1.34 |
| 1 | A | 175 | PRO | N-CD | 9.12 | 1.60 | 1.47 |
| 2 | B | 293 | VAL | C-N | -9.08 | 1.13 | 1.34 |
| 4 | M | 21 | GLY | N-CA | -9.03 | 1.32 | 1.46 |
| 2 | B | 337 | THR | N-CA | -8.98 | 1.28 | 1.46 |
| 4 | M | 41 | LEU | CA-C | -8.95 | 1.29 | 1.52 |
| 4 | M | 63 | TYR | C-N | -8.92 | 1.13 | 1.34 |
| 4 | M | 21 | GLY | C-N | -8.91 | 1.13 | 1.34 |
| 3 | S | 4 | ALA | CA-CB | 8.84 | 1.71 | 1.52 |
| 1 | A | 467 | LYS | N-CA | -8.79 | 1.28 | 1.46 |
| 3 | S | 67 | GLU | N-CA | -8.68 | 1.28 | 1.46 |
| 4 | M | 61 | GLU | C-N | -8.67 | 1.14 | 1.34 |
| 4 | M | 351 | SER | C-N | -8.63 | 1.14 | 1.34 |
| 2 | B | 289 | PRO | CA-C | -8.54 | 1.35 | 1.52 |
| 1 | A | 138 | ASN | CA-C | -8.50 | 1.30 | 1.52 |
| 3 | S | 144 | THR | N-CA | -8.48 | 1.29 | 1.46 |
| 4 | M | 349 | LYS | N-CA | 8.48 | 1.63 | 1.46 |
| 2 | B | 501 | THR | N-CA | -8.41 | 1.29 | 1.46 |
| 3 | S | 72 | ASP | N-CA | -8.40 | 1.29 | 1.46 |
| 3 | S | 63 | ASN | CA-C | -8.39 | 1.31 | 1.52 |
| 4 | M | 231 | SER | N-CA | 8.39 | 1.63 | 1.46 |
| 2 | B | 342 | ALA | N-CA | -8.34 | 1.29 | 1.46 |
| 2 | B | 581 | TYR | C-N | -8.32 | 1.15 | 1.34 |
| 4 | M | 52 | ASP | C-N | -8.31 | 1.15 | 1.34 |
| 4 | M | 64 | LYS | CA-C | -8.29 | 1.31 | 1.52 |
| 2 | B | 260 | LEU | N-CA | -8.26 | 1.29 | 1.46 |
| 4 | M | 106 | LYS | C-N | -8.25 | 1.15 | 1.34 |
| 4 | M | 281 | GLY | C-N | 8.24 | 1.53 | 1.34 |
| 1 | A | 508 | LEU | C-N | -8.21 | 1.18 | 1.34 |
| 4 | M | 406 | GLY | N-CA | -8.20 | 1.33 | 1.46 |
| 1 | A | 87 | CYS | N-CA | -8.20 | 1.29 | 1.46 |
| 4 | M | 59 | ASP | N-CA | 8.17 | 1.62 | 1.46 |
| 3 | S | 60 | SER | N-CA | -8.11 | 1.30 | 1.46 |
| 1 | A | 513 | ARG | N-CA | -8.10 | 1.30 | 1.46 |
| 3 | S | 167 | ILE | C-N | 8.10 | 1.47 | 1.33 |
| 4 | M | 348 | LYS | C-N | 8.10 | 1.52 | 1.34 |
| 1 | A | 477 | PHE | N-CA | -8.06 | 1.30 | 1.46 |
| 3 | S | 83 | LEU | CA-C | 8.05 | 1.73 | 1.52 |
| 1 | A | 394 | GLN | CA-C | -8.02 | 1.32 | 1.52 |
| 4 | M | 56 | VAL | C-N | -7.99 | 1.18 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2 | B | 185 | LYS | N-CA | -7.99 | 1.30 | 1.46 |
| 4 | M | 225 | VAL | CA-C | -7.98 | 1.32 | 1.52 |
| 1 | A | 440 | ASN | N-CA | -7.97 | 1.30 | 1.46 |
| 1 | A | 139 | ASP | N-CA | -7.93 | 1.30 | 1.46 |
| 1 | A | 217 | ALA | C-N | 7.90 | 1.52 | 1.34 |
| 4 | M | 138 | ASP | N-CA | -7.89 | 1.30 | 1.46 |
| 2 | B | 212 | VAL | C-O | 7.88 | 1.38 | 1.23 |
| 4 | M | 294 | ASP | N-CA | -7.88 | 1.30 | 1.46 |
| 4 | M | 348 | LYS | CA-C | 7.87 | 1.73 | 1.52 |
| 2 | B | 183 | ALA | CA-CB | -7.84 | 1.35 | 1.52 |
| 4 | M | 335 | SER | CA-C | -7.83 | 1.32 | 1.52 |
| 4 | M | 239 | SER | N-CA | -7.80 | 1.30 | 1.46 |
| 4 | M | 352 | GLN | C-N | -7.75 | 1.16 | 1.34 |
| 2 | B | 522 | GLU | CD-OE2 | -7.74 | 1.17 | 1.25 |
| 4 | M | 354 | ASP | CA-C | 7.74 | 1.73 | 1.52 |
| 1 | A | 616 | GLU | CD-OE1 | -7.72 | 1.17 | 1.25 |
| 3 | S | 8 | PHE | C-N | -7.71 | 1.16 | 1.34 |
| 4 | M | 44 | ASP | C-N | 7.71 | 1.51 | 1.34 |
| 4 | M | 453 | ASP | C-N | -7.67 | 1.16 | 1.34 |
| 4 | M | 279 | ASN | C-N | -7.67 | 1.16 | 1.34 |
| 1 | A | 405 | THR | CA-C | -7.62 | 1.33 | 1.52 |
| 4 | M | 136 | VAL | CA-C | -7.62 | 1.33 | 1.52 |
| 1 | A | 406 | GLY | C-N | 7.54 | 1.51 | 1.34 |
| 4 | M | 134 | PRO | C-N | -7.51 | 1.16 | 1.34 |
| 2 | B | 464 | SER | CA-CB | -7.50 | 1.41 | 1.52 |
| 1 | A | 515 | CYS | CA-C | -7.49 | 1.33 | 1.52 |
| 4 | M | 103 | TYR | CA-C | 7.48 | 1.72 | 1.52 |
| 3 | S | 62 | GLU | CD-OE2 | -7.46 | 1.17 | 1.25 |
| 4 | M | 283 | PHE | N-CA | -7.46 | 1.31 | 1.46 |
| 4 | M | 319 | SER | C-N | -7.45 | 1.17 | 1.34 |
| 3 | S | 55 | PRO | CA-C | -7.44 | 1.38 | 1.52 |
| 3 | S | 140 | MET | N-CA | -7.44 | 1.31 | 1.46 |
| 4 | M | 91 | THR | CA-C | -7.42 | 1.33 | 1.52 |
| 4 | M | 293 | PRO | CA-C | -7.42 | 1.38 | 1.52 |
| 4 | M | 45 | SER | CA-C | 7.41 | 1.72 | 1.52 |
| 2 | B | 466 | SER | CA-CB | -7.38 | 1.41 | 1.52 |
| 1 | A | 218 | ALA | CA-CB | -7.35 | 1.37 | 1.52 |
| 1 | A | 507 | GLN | C-N | -7.34 | 1.17 | 1.34 |
| 1 | A | 534 | LYS | CA-C | -7.29 | 1.33 | 1.52 |
| 4 | M | 62 | VAL | C-N | -7.27 | 1.17 | 1.34 |
| 3 | S | 116 | VAL | CA-C | -7.27 | 1.34 | 1.52 |
| 3 | S | 103 | GLN | CA-C | -7.25 | 1.34 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4 | M | 280 | ASP | C-N | -7.22 | 1.20 | 1.33 |
| 3 | S | 70 | ASN | C-N | -7.21 | 1.17 | 1.34 |
| 3 | S | 129 | GLU | CG-CD | -7.18 | 1.41 | 1.51 |
| 2 | B | 330 | SER | N-CA | -7.18 | 1.31 | 1.46 |
| 1 | A | 287 | ALA | CA-CB | -7.17 | 1.37 | 1.52 |
| 4 | M | 109 | LEU | N-CA | -7.15 | 1.32 | 1.46 |
| 4 | M | 450 | GLU | C-N | -7.12 | 1.17 | 1.34 |
| 4 | M | 403 | THR | C-N | -7.11 | 1.17 | 1.34 |
| 4 | M | 55 | MET | C-N | 7.08 | 1.50 | 1.34 |
| 4 | M | 230 | LYS | CA-C | 7.05 | 1.71 | 1.52 |
| 4 | M | 442 | GLN | N-CA | -7.05 | 1.32 | 1.46 |
| 1 | A | 125 | THR | N-CA | -7.03 | 1.32 | 1.46 |
| 2 | B | 311 | TYR | CD2-CE2 | -7.02 | 1.28 | 1.39 |
| 4 | M | 70 | ASN | C-N | -7.01 | 1.18 | 1.34 |
| 1 | A | 136 | GLY | CA-C | -7.00 | 1.40 | 1.51 |
| 4 | M | 136 | VAL | C-N | -6.99 | 1.18 | 1.34 |
| 3 | S | 115 | GLU | CA-C | -6.98 | 1.34 | 1.52 |
| 2 | B | 307 | ASN | N-CA | -6.98 | 1.32 | 1.46 |
| 1 | A | 289 | SER | C-N | -6.97 | 1.18 | 1.34 |
| 3 | S | 22 | PRO | C-N | -6.97 | 1.18 | 1.34 |
| 3 | S | 55 | PRO | N-CD | 6.96 | 1.57 | 1.47 |
| 2 | B | 285 | GLU | N-CA | -6.96 | 1.32 | 1.46 |
| 4 | M | 420 | THR | N-CA | -6.94 | 1.32 | 1.46 |
| 4 | M | 81 | SER | N-CA | -6.92 | 1.32 | 1.46 |
| 1 | A | 529 | GLY | N-CA | -6.90 | 1.35 | 1.46 |
| 1 | A | 509 | PRO | CA-C | -6.89 | 1.39 | 1.52 |
| 4 | M | 322 | LEU | C-O | 6.88 | 1.36 | 1.23 |
| 4 | M | 307 | SER | CB-OG | -6.87 | 1.33 | 1.42 |
| 3 | S | 6 | LEU | C-N | -6.84 | 1.18 | 1.34 |
| 2 | B | 334 | MET | N-CA | 6.83 | 1.60 | 1.46 |
| 2 | B | 329 | ALA | CA-C | -6.82 | 1.35 | 1.52 |
| 4 | M | 441 | GLY | N-CA | -6.81 | 1.35 | 1.46 |
| 4 | M | 441 | GLY | CA-C | -6.81 | 1.41 | 1.51 |
| 3 | S | 22 | PRO | N-CA | -6.80 | 1.35 | 1.47 |
| 4 | M | 64 | LYS | C-N | -6.78 | 1.18 | 1.34 |
| 4 | M | 95 | THR | N-CA | 6.78 | 1.59 | 1.46 |
| 2 | B | 330 | SER | C-N | -6.74 | 1.21 | 1.34 |
| 2 | B | 458 | MET | C-O | 6.73 | 1.36 | 1.23 |
| 3 | S | 120 | ASP | N-CA | -6.70 | 1.32 | 1.46 |
| 4 | M | 392 | MET | N-CA | -6.70 | 1.32 | 1.46 |
| 4 | M | 379 | LEU | C-N | -6.68 | 1.18 | 1.34 |
| 3 | S | 81 | ALA | CA-CB | -6.67 | 1.38 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 4 | M | 451 | ALA | CA-CB | 6.66 | 1.66 | 1.52 |
| 1 | A | 243 | ILE | N-CA | -6.64 | 1.33 | 1.46 |
| 3 | S | 62 | GLU | CD-OE1 | -6.64 | 1.18 | 1.25 |
| 2 | B | 363 | ILE | N-CA | -6.64 | 1.33 | 1.46 |
| 3 | S | 114 | THR | C-N | -6.60 | 1.18 | 1.34 |
| 4 | M | 55 | MET | N-CA | -6.60 | 1.33 | 1.46 |
| 1 | A | 552 | ILE | CA-C | -6.60 | 1.35 | 1.52 |
| 4 | M | 440 | ILE | C-N | -6.59 | 1.21 | 1.33 |
| 2 | B | 582 | ASP | N-CA | -6.59 | 1.33 | 1.46 |
| 4 | M | 440 | ILE | N-CA | -6.58 | 1.33 | 1.46 |
| 1 | A | 298 | ILE | C-O | 6.58 | 1.35 | 1.23 |
| 4 | M | 288 | ILE | N-CA | 6.57 | 1.59 | 1.46 |
| 3 | S | 138 | GLY | C-N | 6.55 | 1.44 | 1.33 |
| 2 | B | 382 | TYR | N-CA | -6.51 | 1.33 | 1.46 |
| 4 | M | 105 | ASP | N-CA | -6.47 | 1.33 | 1.46 |
| 1 | A | 288 | THR | N-CA | 6.47 | 1.59 | 1.46 |
| 4 | M | 439 | TYR | CA-C | -6.46 | 1.36 | 1.52 |
| 2 | B | 334 | MET | C-N | -6.44 | 1.19 | 1.34 |
| 4 | M | 25 | PRO | CA-C | -6.44 | 1.40 | 1.52 |
| 1 | A | 378 | ILE | C-N | -6.43 | 1.19 | 1.34 |
| 3 | S | 113 | PHE | C-N | -6.43 | 1.19 | 1.34 |
| 4 | M | 282 | VAL | CA-C | -6.43 | 1.36 | 1.52 |
| 4 | M | 323 | MET | N-CA | -6.42 | 1.33 | 1.46 |
| 1 | A | 278 | ILE | N-CA | -6.39 | 1.33 | 1.46 |
| 2 | B | 184 | GLY | C-N | -6.37 | 1.19 | 1.34 |
| 3 | S | 108 | SER | N-CA | -6.37 | 1.33 | 1.46 |
| 1 | A | 71 | VAL | CA-C | -6.36 | 1.36 | 1.52 |
| 4 | M | 82 | LYS | C-N | -6.35 | 1.19 | 1.34 |
| 2 | B | 585 | GLY | N-CA | -6.35 | 1.36 | 1.46 |
| 4 | M | 320 | ILE | N-CA | -6.34 | 1.33 | 1.46 |
| 1 | A | 533 | ILE | N-CA | -6.33 | 1.33 | 1.46 |
| 1 | A | 221 | VAL | N-CA | 6.32 | 1.58 | 1.46 |
| 1 | A | 439 | ASP | C-N | -6.30 | 1.19 | 1.34 |
| 4 | M | 377 | LYS | C-N | -6.28 | 1.19 | 1.34 |
| 1 | A | 230 | PRO | N-CD | -6.27 | 1.39 | 1.47 |
| 3 | S | 143 | GLU | CA-C | -6.25 | 1.36 | 1.52 |
| 3 | S | 116 | VAL | N-CA | -6.25 | 1.33 | 1.46 |
| 4 | M | 212 | ASN | N-CA | -6.25 | 1.33 | 1.46 |
| 3 | S | 159 | ALA | CA-CB | 6.25 | 1.65 | 1.52 |
| 3 | S | 3 | HIS | N-CA | -6.25 | 1.33 | 1.46 |
| 1 | A | 387 | ILE | CA-C | -6.24 | 1.36 | 1.52 |
| 1 | A | 465 | SER | N-CA | -6.24 | 1.33 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 4 | M | 23 | THR | C-N | -6.24 | 1.19 | 1.34 |
| 4 | M | 97 | ASP | CA-C | -6.23 | 1.36 | 1.52 |
| 1 | A | 535 | ILE | C-N | -6.22 | 1.19 | 1.34 |
| 4 | M | 288 | ILE | C-N | -6.20 | 1.19 | 1.34 |
| 2 | B | 345 | ARG | CD-NE | -6.19 | 1.35 | 1.46 |
| 1 | A | 441 | TYR | C-O | -6.19 | 1.11 | 1.23 |
| 2 | B | 326 | TYR | N-CA | -6.17 | 1.34 | 1.46 |
| 1 | A | 281 | LEU | N-CA | 6.17 | 1.58 | 1.46 |
| 4 | M | 402 | SER | C-N | 6.16 | 1.48 | 1.34 |
| 4 | M | 404 | ALA | N-CA | -6.15 | 1.34 | 1.46 |
| 2 | B | 329 | ALA | N-CA | -6.11 | 1.34 | 1.46 |
| 1 | A | 589 | SER | N-CA | -6.11 | 1.34 | 1.46 |
| 4 | M | 6 | TYR | C-N | -6.10 | 1.20 | 1.34 |
| 3 | S | 60 | SER | C-N | -6.09 | 1.20 | 1.34 |
| 3 | S | 62 | GLU | C-N | -6.09 | 1.20 | 1.34 |
| 4 | M | 60 | LEU | CA-C | -6.08 | 1.37 | 1.52 |
| 2 | B | 259 | TYR | C-N | -6.07 | 1.20 | 1.34 |
| 3 | S | 48 | SER | N-CA | -6.07 | 1.34 | 1.46 |
| 2 | B | 382 | TYR | CA-C | -6.06 | 1.37 | 1.52 |
| 1 | A | 464 | ILE | C-N | -6.06 | 1.20 | 1.34 |
| 2 | B | 153 | ILE | CA-C | -6.05 | 1.37 | 1.52 |
| 2 | B | 568 | VAL | N-CA | -6.04 | 1.34 | 1.46 |
| 4 | M | 252 | ASP | C-N | -6.04 | 1.20 | 1.34 |
| 1 | A | 444 | VAL | N-CA | -6.03 | 1.34 | 1.46 |
| 1 | A | 394 | GLN | N-CA | -6.00 | 1.34 | 1.46 |
| 1 | A | 302 | ASN | CA-C | -5.97 | 1.37 | 1.52 |
| 2 | B | 82 | TYR | N-CA | -5.97 | 1.34 | 1.46 |
| 3 | S | 57 | LEU | CA-C | -5.96 | 1.37 | 1.52 |
| 1 | A | 348 | PHE | CA-C | -5.96 | 1.37 | 1.52 |
| 2 | B | 301 | LEU | N-CA | -5.95 | 1.34 | 1.46 |
| 1 | A | 244 | LEU | C-N | -5.95 | 1.20 | 1.34 |
| 3 | S | 144 | THR | C-N | -5.94 | 1.20 | 1.34 |
| 2 | B | 187 | ASP | CA-C | -5.93 | 1.37 | 1.52 |
| 4 | M | 288 | ILE | CA-C | -5.93 | 1.37 | 1.52 |
| 1 | A | 277 | LYS | C-N | -5.93 | 1.20 | 1.34 |
| 2 | B | 259 | TYR | CA-C | -5.92 | 1.37 | 1.52 |
| 1 | A | 263 | LEU | N-CA | -5.92 | 1.34 | 1.46 |
| 1 | A | 242 | GLU | CA-C | -5.92 | 1.37 | 1.52 |
| 4 | M | 22 | ALA | N-CA | -5.92 | 1.34 | 1.46 |
| 3 | S | 139 | GLY | CA-C | -5.92 | 1.42 | 1.51 |
| 1 | A | 531 | ASP | CA-C | -5.90 | 1.37 | 1.52 |
| 4 | M | 263 | MET | N-CA | -5.90 | 1.34 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2 | B | 222 | HIS | N-CA | 5.89 | 1.58 | 1.46 |
| 4 | M | 96 | ILE | C-N | 5.89 | 1.47 | 1.34 |
| 4 | M | 18 | TYR | N-CA | -5.88 | 1.34 | 1.46 |
| 4 | M | 262 | THR | CA-C | -5.88 | 1.37 | 1.52 |
| 2 | B | 293 | VAL | CA-C | -5.87 | 1.37 | 1.52 |
| 1 | A | 566 | PHE | CA-C | -5.86 | 1.37 | 1.52 |
| 2 | B | 543 | GLU | CD-OE2 | -5.86 | 1.19 | 1.25 |
| 2 | B | 334 | MET | CA-C | -5.85 | 1.37 | 1.52 |
| 1 | A | 401 | VAL | CA-C | -5.85 | 1.37 | 1.52 |
| 4 | M | 407 | THR | N-CA | -5.85 | 1.34 | 1.46 |
| 2 | B | 184 | GLY | N-CA | 5.84 | 1.54 | 1.46 |
| 1 | A | 466 | ASP | C-N | -5.83 | 1.20 | 1.34 |
| 1 | A | 387 | ILE | N-CA | -5.83 | 1.34 | 1.46 |
| 4 | M | 68 | VAL | N-CA | -5.83 | 1.34 | 1.46 |
| 2 | B | 395 | LYS | CA-C | -5.82 | 1.37 | 1.52 |
| 1 | A | 588 | LEU | C-N | -5.78 | 1.20 | 1.34 |
| 2 | B | 363 | ILE | CA-C | -5.78 | 1.38 | 1.52 |
| 3 | S | 35 | VAL | N-CA | -5.77 | 1.34 | 1.46 |
| 3 | S | 59 | LEU | N-CA | -5.77 | 1.34 | 1.46 |
| 4 | M | 50 | TYR | C-N | -5.77 | 1.20 | 1.34 |
| 1 | A | 418 | ILE | C-N | 5.75 | 1.47 | 1.34 |
| 1 | A | 407 | SER | CB-OG | -5.75 | 1.34 | 1.42 |
| 4 | M | 287 | ASN | CA-C | 5.75 | 1.67 | 1.52 |
| 4 | M | 336 | ASP | N-CA | -5.75 | 1.34 | 1.46 |
| 3 | S | 158 | LYS | CA-C | -5.73 | 1.38 | 1.52 |
| 1 | A | 301 | GLY | CA-C | -5.73 | 1.42 | 1.51 |
| 1 | A | 448 | GLU | CD-OE1 | -5.73 | 1.19 | 1.25 |
| 1 | A | 410 | TYR | N-CA | -5.72 | 1.34 | 1.46 |
| 4 | M | 278 | ILE | CA-C | -5.72 | 1.38 | 1.52 |
| 2 | B | 219 | TYR | C-N | -5.71 | 1.21 | 1.34 |
| 1 | A | 381 | GLU | CD-OE1 | -5.70 | 1.19 | 1.25 |
| 2 | B | 567 | GLN | CA-C | -5.70 | 1.38 | 1.52 |
| 2 | B | 150 | LEU | N-CA | -5.69 | 1.34 | 1.46 |
| 2 | B | 326 | TYR | CG-CD2 | -5.67 | 1.31 | 1.39 |
| 1 | A | 550 | VAL | CA-C | -5.67 | 1.38 | 1.52 |
| 3 | S | 95 | GLU | CD-OE1 | -5.67 | 1.19 | 1.25 |
| 2 | B | 522 | GLU | CA-C | -5.66 | 1.38 | 1.52 |
| 4 | M | 457 | GLY | CA-C | -5.65 | 1.42 | 1.51 |
| 3 | S | 47 | GLN | N-CA | -5.65 | 1.35 | 1.46 |
| 2 | B | 83 | PHE | C-N | 5.65 | 1.47 | 1.34 |
| 2 | B | 290 | SER | N-CA | -5.65 | 1.35 | 1.46 |
| 2 | B | 352 | ASN | C-N | -5.65 | 1.21 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2 | B | 576 | GLN | C-N | -5.64 | 1.21 | 1.34 |
| 1 | A | 499 | ILE | C-O | -5.64 | 1.12 | 1.23 |
| 2 | B | 304 | GLN | CA-C | -5.64 | 1.38 | 1.52 |
| 4 | M | 462 | LYS | C-N | -5.64 | 1.21 | 1.34 |
| 3 | S | 14 | PRO | C-N | -5.62 | 1.21 | 1.34 |
| 1 | A | 293 | GLU | CD-OE1 | -5.61 | 1.19 | 1.25 |
| 3 | S | 84 | TYR | C-N | -5.60 | 1.21 | 1.34 |
| 3 | S | 83 | LEU | C-N | -5.59 | 1.21 | 1.34 |
| 1 | A | 216 | SER | C-N | 5.59 | 1.47 | 1.34 |
| 2 | B | 584 | SER | C-N | -5.59 | 1.23 | 1.33 |
| 4 | M | 118 | TYR | CA-C | -5.58 | 1.38 | 1.52 |
| 2 | B | 500 | GLN | C-N | -5.58 | 1.21 | 1.34 |
| 1 | A | 84 | MET | N-CA | -5.58 | 1.35 | 1.46 |
| 1 | A | 615 | GLU | N-CA | -5.58 | 1.35 | 1.46 |
| 3 | S | 64 | ASN | C-N | 5.57 | 1.46 | 1.34 |
| 4 | M | 223 | HIS | C-N | -5.56 | 1.21 | 1.34 |
| 1 | A | 535 | ILE | N-CA | -5.55 | 1.35 | 1.46 |
| 1 | A | 93 | GLU | CD-OE1 | -5.54 | 1.19 | 1.25 |
| 1 | A | 464 | ILE | CA-C | -5.54 | 1.38 | 1.52 |
| 3 | S | 80 | TYR | N-CA | -5.53 | 1.35 | 1.46 |
| 4 | M | 24 | ALA | N-CA | -5.53 | 1.35 | 1.46 |
| 3 | S | 83 | LEU | N-CA | -5.51 | 1.35 | 1.46 |
| 2 | B | 515 | PHE | CA-C | 5.51 | 1.67 | 1.52 |
| 4 | M | 262 | THR | N-CA | -5.50 | 1.35 | 1.46 |
| 1 | A | 303 | MET | N-CA | -5.50 | 1.35 | 1.46 |
| 4 | M | 446 | GLY | CA-C | 5.50 | 1.60 | 1.51 |
| 3 | S | 5 | VAL | CA-C | 5.50 | 1.67 | 1.52 |
| 4 | M | 83 | SER | N-CA | -5.49 | 1.35 | 1.46 |
| 4 | M | 41 | LEU | C-N | 5.47 | 1.46 | 1.34 |
| 1 | A | 623 | MET | CA-C | -5.46 | 1.38 | 1.52 |
| 1 | A | 138 | ASN | C-N | -5.46 | 1.21 | 1.34 |
| 4 | M | 296 | LYS | CA-C | -5.46 | 1.38 | 1.52 |
| 1 | A | 511 | VAL | N-CA | -5.45 | 1.35 | 1.46 |
| 2 | B | 172 | GLU | CD-OE2 | -5.43 | 1.19 | 1.25 |
| 1 | A | 634 | ASN | CA-C | -5.43 | 1.38 | 1.52 |
| 4 | M | 128 | CYS | C-O | 5.42 | 1.33 | 1.23 |
| 2 | B | 526 | CYS | N-CA | -5.41 | 1.35 | 1.46 |
| 1 | A | 308 | ASP | N-CA | -5.41 | 1.35 | 1.46 |
| 2 | B | 344 | VAL | CA-CB | -5.41 | 1.43 | 1.54 |
| 4 | M | 228 | LYS | C-N | -5.40 | 1.21 | 1.34 |
| 2 | B | 273 | SER | N-CA | -5.39 | 1.35 | 1.46 |
| 1 | A | 388 | VAL | CA-C | -5.38 | 1.39 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 4 | M | 367 | ALA | CA-CB | -5.38 | 1.41 | 1.52 |
| 2 | B | 557 | SER | C-N | -5.37 | 1.21 | 1.34 |
| 3 | S | 119 | LEU | C-N | 5.37 | 1.46 | 1.34 |
| 3 | S | 129 | GLU | CD-OE1 | -5.37 | 1.19 | 1.25 |
| 1 | A | 147 | LEU | CA-C | -5.36 | 1.39 | 1.52 |
| 1 | A | 392 | MET | N-CA | -5.36 | 1.35 | 1.46 |
| 2 | B | 561 | ASP | CG-OD1 | -5.35 | 1.13 | 1.25 |
| 3 | S | 105 | PHE | N-CA | -5.35 | 1.35 | 1.46 |
| 4 | M | 296 | LYS | N-CA | 5.35 | 1.57 | 1.46 |
| 1 | A | 406 | GLY | N-CA | -5.34 | 1.38 | 1.46 |
| 4 | M | 78 | ALA | C-N | -5.33 | 1.21 | 1.34 |
| 4 | M | 71 | LYS | N-CA | -5.33 | 1.35 | 1.46 |
| 2 | B | 381 | PHE | CE2-CZ | -5.33 | 1.27 | 1.37 |
| 4 | M | 253 | ASN | N-CA | -5.33 | 1.35 | 1.46 |
| 1 | A | 134 | TYR | CB-CG | -5.32 | 1.43 | 1.51 |
| 3 | S | 70 | ASN | CA-C | -5.32 | 1.39 | 1.52 |
| 4 | M | 257 | ALA | N-CA | -5.32 | 1.35 | 1.46 |
| 2 | B | 276 | SER | N-CA | -5.32 | 1.35 | 1.46 |
| 2 | B | 485 | LYS | CA-C | -5.31 | 1.39 | 1.52 |
| 4 | M | 61 | GLU | N-CA | -5.30 | 1.35 | 1.46 |
| 2 | B | 380 | LYS | C-O | -5.30 | 1.13 | 1.23 |
| 4 | M | 65 | TYR | C-N | -5.30 | 1.21 | 1.34 |
| 4 | M | 387 | GLU | CD-OE1 | -5.30 | 1.19 | 1.25 |
| 2 | B | 256 | CYS | N-CA | -5.29 | 1.35 | 1.46 |
| 2 | B | 381 | PHE | C-N | -5.28 | 1.21 | 1.34 |
| 1 | A | 633 | PHE | CA-C | -5.28 | 1.39 | 1.52 |
| 2 | B | 289 | PRO | C-N | -5.27 | 1.22 | 1.34 |
| 4 | M | 354 | ASP | C-N | -5.27 | 1.22 | 1.34 |
| 1 | A | 489 | GLU | CA-C | -5.27 | 1.39 | 1.52 |
| 1 | A | 435 | ILE | N-CA | -5.26 | 1.35 | 1.46 |
| 1 | A | 445 | ASN | CA-C | -5.26 | 1.39 | 1.52 |
| 4 | M | 113 | LYS | CA-C | -5.26 | 1.39 | 1.52 |
| 1 | A | 534 | LYS | N-CA | -5.25 | 1.35 | 1.46 |
| 3 | S | 40 | SER | CA-CB | -5.22 | 1.45 | 1.52 |
| 1 | A | 399 | ASP | N-CA | -5.21 | 1.35 | 1.46 |
| 3 | S | 161 | GLU | CD-OE2 | -5.21 | 1.20 | 1.25 |
| 2 | B | 580 | TYR | CA-C | -5.21 | 1.39 | 1.52 |
| 4 | M | 280 | ASP | CA-C | -5.21 | 1.39 | 1.52 |
| 1 | A | 192 | TYR | CA-C | -5.20 | 1.39 | 1.52 |
| 4 | M | 284 | SER | C-N | -5.20 | 1.24 | 1.34 |
| 2 | B | 35 | TYR | CA-C | -5.19 | 1.39 | 1.52 |
| 4 | M | 426 | LYS | C-N | -5.19 | 1.22 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 4 | M | 130 | GLU | CA-C | 5.18 | 1.66 | 1.52 |
| 4 | M | 75 | TRP | C-N | -5.18 | 1.22 | 1.34 |
| 2 | B | 443 | SER | CA-C | -5.17 | 1.39 | 1.52 |
| 2 | B | 290 | SER | CA-C | -5.17 | 1.39 | 1.52 |
| 1 | A | 403 | LEU | C-O | -5.16 | 1.13 | 1.23 |
| 2 | B | 579 | PRO | N-CD | -5.15 | 1.40 | 1.47 |
| 1 | A | 522 | PHE | CA-C | -5.14 | 1.39 | 1.52 |
| 2 | B | 424 | PHE | N-CA | -5.13 | 1.36 | 1.46 |
| 4 | M | 51 | LEU | N-CA | 5.12 | 1.56 | 1.46 |
| 1 | A | 281 | LEU | C-N | -5.12 | 1.22 | 1.34 |
| 1 | A | 302 | ASN | N-CA | -5.10 | 1.36 | 1.46 |
| 4 | M | 126 | ASN | CA-C | -5.10 | 1.39 | 1.52 |
| 2 | B | 75 | ASP | C-N | -5.09 | 1.22 | 1.34 |
| 4 | M | 250 | LEU | N-CA | -5.09 | 1.36 | 1.46 |
| 3 | S | 67 | GLU | CA-C | -5.09 | 1.39 | 1.52 |
| 4 | M | 129 | VAL | C-O | -5.08 | 1.13 | 1.23 |
| 1 | A | 388 | VAL | N-CA | -5.08 | 1.36 | 1.46 |
| 1 | A | 630 | PRO | N-CD | -5.08 | 1.40 | 1.47 |
| 3 | S | 143 | GLU | C-N | -5.07 | 1.22 | 1.34 |
| 3 | S | 2 | ILE | CA-C | -5.07 | 1.39 | 1.52 |
| 1 | A | 111 | SER | CA-CB | -5.06 | 1.45 | 1.52 |
| 1 | A | 225 | LEU | N-CA | -5.05 | 1.36 | 1.46 |
| 4 | M | 253 | ASN | C-N | -5.05 | 1.24 | 1.34 |
| 2 | B | 582 | ASP | C-N | -5.05 | 1.22 | 1.34 |
| 2 | B | 422 | ALA | CA-C | -5.05 | 1.39 | 1.52 |
| 2 | B | 540 | GLU | CD-OE1 | -5.05 | 1.20 | 1.25 |
| 1 | A | 304 | LEU | N-CA | -5.04 | 1.36 | 1.46 |
| 2 | B | 325 | LEU | C-N | -5.03 | 1.22 | 1.34 |
| 1 | A | 120 | ILE | CA-C | -5.03 | 1.39 | 1.52 |
| 2 | B | 109 | ALA | CA-CB | -5.03 | 1.41 | 1.52 |
| 2 | B | 407 | ASN | N-CA | -5.02 | 1.36 | 1.46 |
| 2 | B | 574 | ASN | N-CA | -5.02 | 1.36 | 1.46 |
| 2 | B | 405 | GLU | CD-OE2 | -5.02 | 1.20 | 1.25 |
| 2 | B | 331 | PRO | N-CA | -5.02 | 1.38 | 1.47 |
| 2 | B | 272 | GLY | CA-C | -5.01 | 1.43 | 1.51 |
| 4 | M | 477 | GLY | N-CA | -5.01 | 1.38 | 1.46 |
| 1 | A | 567 | GLN | CA-C | -5.01 | 1.40 | 1.52 |
| 4 | M | 66 | PHE | C-N | -5.00 | 1.22 | 1.34 |

All (1662) bond angle outliers are listed below:

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 4 | M | 404 | ALA | CB-CA-C | 24.95 | 147.53 | 110.10 |
| 3 | S | 69 | ASN | N-CA-C | 23.29 | 173.89 | 111.00 |
| 1 | A | 242 | GLU | C-N-CA | 22.94 | 179.05 | 121.70 |
| 4 | M | 130 | GLU | N-CA-C | -19.38 | 58.67 | 111.00 |
| 1 | A | 265 | GLN | N-CA-C | -19.25 | 59.04 | 111.00 |
| 4 | M | 404 | ALA | N-CA-CB | -18.91 | 83.63 | 110.10 |
| 3 | S | 69 | ASN | CA-C-N | -18.82 | 75.79 | 117.20 |
| 3 | S | 69 | ASN | O-C-N | 18.81 | 152.80 | 122.70 |
| 1 | A | 80 | TYR | N-CA-C | -18.32 | 61.54 | 111.00 |
| 3 | S | 69 | ASN | CA-C-O | -17.85 | 82.61 | 120.10 |
| 3 | S | 58 | LEU | N-CA-C | -17.79 | 62.98 | 111.00 |
| 4 | M | 45 | SER | C-N-CA | -17.35 | 78.33 | 121.70 |
| 4 | M | 82 | LYS | C-N-CA | 16.95 | 164.08 | 121.70 |
| 4 | M | 103 | TYR | N-CA-C | -16.88 | 65.42 | 111.00 |
| 3 | S | 69 | ASN | CB-CA-C | -16.71 | 76.99 | 110.40 |
| 1 | A | 277 | LYS | C-N-CA | 16.59 | 163.18 | 121.70 |
| 4 | M | 354 | ASP | N-CA-C | -16.56 | 66.30 | 111.00 |
| 4 | M | 354 | ASP | C-N-CA | 16.38 | 162.66 | 121.70 |
| 1 | A | 444 | VAL | N-CA-C | -16.20 | 67.25 | 111.00 |
| 1 | A | 439 | ASP | N-CA-C | -16.11 | 67.51 | 111.00 |
| 4 | M | 403 | THR | C-N-CA | 16.03 | 161.77 | 121.70 |
| 4 | M | 373 | ALA | CB-CA-C | 15.54 | 133.40 | 110.10 |
| 2 | B | 580 | TYR | C-N-CA | -15.41 | 83.18 | 121.70 |
| 1 | A | 98 | ASN | C-N-CA | 15.19 | 159.67 | 121.70 |
| 1 | A | 534 | LYS | CA-C-N | 15.18 | 150.60 | 117.20 |
| 4 | M | 280 | ASP | N-CA-C | 15.14 | 151.89 | 111.00 |
| 2 | B | 584 | SER | N-CA-C | 15.04 | 151.61 | 111.00 |
| 2 | B | 275 | ARG | N-CA-C | -14.98 | 70.56 | 111.00 |
| 1 | A | 304 | LEU | C-N-CA | -14.94 | 84.35 | 121.70 |
| 4 | M | 21 | GLY | C-N-CA | 14.89 | 158.91 | 121.70 |
| 4 | M | 103 | TYR | O-C-N | -14.66 | 99.24 | 122.70 |
| 2 | B | 263 | PRO | C-N-CA | 14.64 | 158.29 | 121.70 |
| 2 | B | 290 | SER | C-N-CA | -14.63 | 85.12 | 121.70 |
| 4 | M | 131 | ALA | CA-C-N | -14.62 | 86.95 | 116.20 |
| 1 | A | 534 | LYS | C-N-CA | 14.54 | 158.05 | 121.70 |
| 4 | M | 135 | ASN | N-CA-C | -14.31 | 72.36 | 111.00 |
| 4 | M | 294 | ASP | N-CA-C | -13.97 | 73.28 | 111.00 |
| 1 | A | 543 | TYR | CB-CG-CD2 | 13.89 | 129.34 | 121.00 |
| 4 | M | 103 | TYR | C-N-CA | 13.82 | 156.26 | 121.70 |
| 1 | A | 418 | ILE | C-N-CA | -13.80 | 87.20 | 121.70 |
| 2 | B | 600 | LYS | C-N-CA | -13.41 | 88.18 | 121.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1 | A | 532 | LEU | C-N-CA | -13.36 | 88.30 | 121.70 |
| 2 | B | 579 | PRO | C-N-CA | -13.34 | 88.35 | 121.70 |
| 4 | M | 80 | THR | N-CA-C | 13.27 | 146.83 | 111.00 |
| 2 | B | 78 | ASP | C-N-CA | -13.22 | 88.65 | 121.70 |
| 1 | A | 98 | ASN | N-CA-C | -13.12 | 75.59 | 111.00 |
| 1 | A | 80 | TYR | O-C-N | -13.10 | 100.93 | 123.20 |
| 1 | A | 405 | THR | C-N-CA | -12.96 | 95.09 | 122.30 |
| 4 | M | 293 | PRO | CA-N-CD | -12.91 | 93.42 | 111.50 |
| 4 | M | 59 | ASP | C-N-CA | -12.82 | 89.65 | 121.70 |
| 1 | A | 536 | MET | O-C-N | -12.76 | 102.29 | 122.70 |
| 1 | A | 302 | ASN | N-CA-C | -12.70 | 76.72 | 111.00 |
| 1 | A | 64 | LEU | O-C-N | -12.69 | 102.39 | 122.70 |
| 4 | M | 51 | LEU | N-CA-C | 12.65 | 145.15 | 111.00 |
| 4 | M | 130 | GLU | C-N-CA | 12.64 | 153.30 | 121.70 |
| 1 | A | 464 | ILE | C-N-CA | -12.63 | 90.11 | 121.70 |
| 1 | A | 260 | PHE | O-C-N | -12.55 | 102.63 | 122.70 |
| 3 | S | 46 | PHE | C-N-CA | -12.54 | 90.34 | 121.70 |
| 3 | S | 168 | GLY | N-CA-C | 12.40 | 144.09 | 113.10 |
| 1 | A | 151 | SER | C-N-CA | -12.35 | 90.82 | 121.70 |
| 4 | M | 133 | GLU | C-N-CD | 12.31 | 154.26 | 128.40 |
| 4 | M | 405 | THR | N-CA-C | 12.24 | 144.04 | 111.00 |
| 2 | B | 581 | TYR | C-N-CA | 12.23 | 152.28 | 121.70 |
| 4 | M | 61 | GLU | N-CA-C | -12.17 | 78.15 | 111.00 |
| 4 | M | 54 | SER | N-CA-C | 12.15 | 143.81 | 111.00 |
| 1 | A | 469 | LEU | C-N-CA | -12.11 | 96.88 | 122.30 |
| 4 | M | 82 | LYS | N-CA-C | -12.03 | 78.53 | 111.00 |
| 4 | M | 132 | GLY | CA-C-N | -12.02 | 90.77 | 117.20 |
| 4 | M | 351 | SER | N-CA-C | 11.96 | 143.28 | 111.00 |
| 4 | M | 22 | ALA | CB-CA-C | 11.92 | 127.97 | 110.10 |
| 4 | M | 50 | TYR | N-CA-C | 11.87 | 143.05 | 111.00 |
| 1 | A | 289 | SER | O-C-N | -11.78 | 103.85 | 122.70 |
| 1 | A | 135 | ASP | C-N-CA | -11.74 | 97.64 | 122.30 |
| 2 | B | 330 | SER | N-CA-C | -11.74 | 79.30 | 111.00 |
| 1 | A | 323 | CYS | C-N-CA | 11.69 | 150.91 | 121.70 |
| 1 | A | 233 | PHE | C-N-CA | -11.63 | 92.62 | 121.70 |
| 2 | B | 336 | ASN | C-N-CA | 11.61 | 150.72 | 121.70 |
| 2 | B | 185 | LYS | C-N-CA | -11.61 | 92.69 | 121.70 |
| 1 | A | 265 | GLN | CA-C-N | 11.48 | 142.45 | 117.20 |
| 2 | B | 286 | ILE | N-CA-C | -11.42 | 80.16 | 111.00 |
| 1 | A | 536 | MET | C-N-CA | -11.38 | 93.24 | 121.70 |
| 1 | A | 136 | GLY | C-N-CA | -11.36 | 93.30 | 121.70 |
| 3 | S | 53 | THR | C-N-CD | 11.34 | 152.22 | 128.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 2 | B | 329 | ALA | CB-CA-C | -11.32 | 93.11 | 110.10 |
| 4 | M | 458 | LEU | O-C-N | 11.27 | 140.74 | 122.70 |
| 4 | M | 23 | THR | N-CA-C | -11.26 | 80.61 | 111.00 |
| 2 | B | 404 | ASN | C-N-CA | -11.21 | 93.68 | 121.70 |
| 4 | M | 462 | LYS | N-CA-C | -11.19 | 80.79 | 111.00 |
| 4 | M | 52 | ASP | N-CA-C | 11.15 | 141.11 | 111.00 |
| 3 | S | 63 | ASN | N-CA-C | -11.10 | 81.03 | 111.00 |
| 2 | B | 260 | LEU | N-CA-C | -11.08 | 81.07 | 111.00 |
| 1 | A | 242 | GLU | CA-C-N | 11.08 | 141.57 | 117.20 |
| 3 | S | 54 | PRO | CA-N-CD | -11.04 | 96.05 | 111.50 |
| 2 | B | 310 | ILE | C-N-CA | -10.90 | 94.44 | 121.70 |
| 1 | A | 204 | VAL | O-C-N | -10.84 | 105.36 | 122.70 |
| 3 | S | 109 | LEU | O-C-N | -10.76 | 105.48 | 122.70 |
| 1 | A | 80 | TYR | CA-C-N | 10.73 | 137.66 | 116.20 |
| 1 | A | 416 | ILE | C-N-CD | 10.73 | 150.93 | 128.40 |
| 3 | S | 43 | ASN | O-C-N | -10.70 | 105.58 | 122.70 |
| 1 | A | 287 | ALA | C-N-CA | 10.70 | 148.45 | 121.70 |
| 4 | M | 46 | SER | C-N-CA | -10.70 | 94.94 | 121.70 |
| 3 | S | 163 | THR | C-N-CA | 10.61 | 148.23 | 121.70 |
| 1 | A | 84 | MET | C-N-CA | -10.50 | 95.44 | 121.70 |
| 2 | B | 428 | VAL | O-C-N | 10.47 | 139.46 | 122.70 |
| 1 | A | 586 | GLU | C-N-CA | -10.47 | 95.52 | 121.70 |
| 2 | B | 497 | LEU | O-C-N | -10.44 | 106.00 | 122.70 |
| 2 | B | 287 | GLU | C-N-CA | 10.39 | 147.68 | 121.70 |
| 2 | B | 82 | TYR | C-N-CA | -10.38 | 95.74 | 121.70 |
| 2 | B | 292 | GLU | C-N-CA | 10.38 | 147.64 | 121.70 |
| 4 | M | 80 | THR | C-N-CA | 10.37 | 147.62 | 121.70 |
| 3 | S | 164 | ASP | C-N-CA | -10.32 | 95.89 | 121.70 |
| 4 | M | 279 | ASN | N-CA-C | 10.29 | 138.79 | 111.00 |
| 1 | A | 621 | LEU | C-N-CD | 10.29 | 150.01 | 128.40 |
| 2 | B | 335 | LYS | N-CA-C | -10.29 | 83.22 | 111.00 |
| 2 | B | 584 | SER | C-N-CA | -10.29 | 100.70 | 122.30 |
| 1 | A | 629 | LEU | C-N-CD | 10.27 | 149.97 | 128.40 |
| 1 | A | 519 | LEU | C-N-CA | -10.27 | 100.73 | 122.30 |
| 1 | A | 543 | TYR | CB-CG-CD1 | -10.21 | 114.88 | 121.00 |
| 1 | A | 534 | LYS | CA-C-O | -10.14 | 98.81 | 120.10 |
| 1 | A | 244 | LEU | O-C-N | -10.12 | 106.50 | 122.70 |
| 2 | B | 577 | ASN | C-N-CD | 10.12 | 149.66 | 128.40 |
| 2 | B | 571 | SER | N-CA-C | -10.10 | 83.73 | 111.00 |
| 2 | B | 162 | VAL | C-N-CA | -10.03 | 96.63 | 121.70 |
| 2 | B | 289 | PRO | C-N-CA | -10.01 | 96.67 | 121.70 |
| 4 | M | 402 | SER | C-N-CA | -9.99 | 96.72 | 121.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | A | 504 | ILE | O-C-N | -9.99 | 106.72 | 122.70 |
| 1 | A | 534 | LYS | N-CA-C | -9.98 | 84.04 | 111.00 |
| 2 | B | 262 | LYS | C-N-CD | 9.94 | 149.28 | 128.40 |
| 1 | A | 586 | GLU | O-C-N | -9.90 | 106.85 | 122.70 |
| 4 | M | 83 | SER | C-N-CA | 9.90 | 146.46 | 121.70 |
| 1 | A | 569 | ASP | C-N-CA | -9.89 | 96.97 | 121.70 |
| 3 | S | 57 | LEU | CA-C-N | -9.89 | 95.44 | 117.20 |
| 2 | B | 584 | SER | N-CA-CB | -9.80 | 95.80 | 110.50 |
| 1 | A | 380 | ASP | N-CA-C | -9.79 | 84.58 | 111.00 |
| 1 | A | 440 | ASN | C-N-CA | 9.78 | 146.15 | 121.70 |
| 2 | B | 576 | GLN | N-CA-C | -9.78 | 84.60 | 111.00 |
| 2 | B | 570 | GLY | N-CA-C | -9.75 | 88.72 | 113.10 |
| 1 | A | 320 | HIS | O-C-N | -9.75 | 107.11 | 122.70 |
| 4 | M | 268 | GLY | C-N-CA | -9.75 | 97.34 | 121.70 |
| 2 | B | 187 | ASP | C-N-CA | -9.72 | 97.40 | 121.70 |
| 4 | M | 306 | LEU | O-C-N | -9.70 | 107.18 | 122.70 |
| 1 | A | 84 | MET | O-C-N | -9.69 | 107.19 | 122.70 |
| 1 | A | 282 | MET | O-C-N | -9.64 | 107.27 | 122.70 |
| 4 | M | 3 | LEU | O-C-N | -9.64 | 107.27 | 122.70 |
| 4 | M | 57 | GLY | C-N-CA | 9.63 | 145.77 | 121.70 |
| 1 | A | 346 | THR | C-N-CA | -9.60 | 97.70 | 121.70 |
| 1 | A | 462 | GLN | O-C-N | -9.60 | 107.34 | 122.70 |
| 3 | S | 21 | THR | C-N-CD | 9.60 | 148.56 | 128.40 |
| 1 | A | 365 | VAL | C-N-CA | -9.58 | 97.76 | 121.70 |
| 1 | A | 212 | ILE | C-N-CA | -9.53 | 97.88 | 121.70 |
| 3 | S | 68 | VAL | N-CA-C | 9.52 | 136.72 | 111.00 |
| 1 | A | 403 | LEU | C-N-CA | -9.52 | 97.90 | 121.70 |
| 4 | M | 279 | ASN | C-N-CA | 9.50 | 145.44 | 121.70 |
| 2 | B | 325 | LEU | O-C-N | -9.46 | 107.56 | 122.70 |
| 2 | B | 230 | PHE | C-N-CA | -9.46 | 98.06 | 121.70 |
| 3 | S | 6 | LEU | O-C-N | -9.46 | 107.57 | 122.70 |
| 1 | A | 80 | TYR | C-N-CA | 9.45 | 142.13 | 122.30 |
| 1 | A | 465 | SER | C-N-CA | 9.44 | 145.29 | 121.70 |
| 2 | B | 212 | VAL | CA-C-O | 9.39 | 139.82 | 120.10 |
| 1 | A | 569 | ASP | N-CA-C | -9.39 | 85.65 | 111.00 |
| 1 | A | 319 | LEU | O-C-N | -9.39 | 107.68 | 122.70 |
| 2 | B | 577 | ASN | N-CA-C | 9.38 | 136.34 | 111.00 |
| 4 | M | 379 | LEU | O-C-N | -9.38 | 107.69 | 122.70 |
| 4 | M | 134 | PRO | N-CA-C | -9.38 | 87.72 | 112.10 |
| 3 | S | 116 | VAL | CA-C-N | -9.37 | 96.60 | 117.20 |
| 1 | A | 465 | SER | CA-C-N | -9.36 | 96.61 | 117.20 |
| 1 | A | 305 | GLU | N-CA-C | 9.35 | 136.24 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2 | B | 535 | GLN | C-N-CA | -9.34 | 98.34 | 121.70 |
| 4 | M | 6 | TYR | O-C-N | -9.32 | 107.78 | 122.70 |
| 3 | S | 58 | LEU | CA-C-N | -9.32 | 96.70 | 117.20 |
| 1 | A | 381 | GLU | C-N-CA | -9.32 | 98.41 | 121.70 |
| 2 | B | 102 | HIS | O-C-N | -9.30 | 107.82 | 122.70 |
| 1 | A | 242 | GLU | N-CA-C | -9.29 | 85.93 | 111.00 |
| 4 | M | 406 | GLY | N-CA-C | -9.27 | 89.92 | 113.10 |
| 2 | B | 366 | LEU | O-C-N | -9.26 | 107.89 | 122.70 |
| 3 | S | 143 | GLU | N-CA-C | -9.26 | 86.01 | 111.00 |
| 4 | M | 136 | VAL | CA-C-N | -9.25 | 96.85 | 117.20 |
| 1 | A | 275 | LEU | C-N-CD | 9.25 | 147.82 | 128.40 |
| 4 | M | 252 | ASP | N-CA-C | -9.20 | 86.16 | 111.00 |
| 1 | A | 240 | LEU | C-N-CA | -9.19 | 98.72 | 121.70 |
| 2 | B | 505 | ASP | C-N-CA | -9.15 | 98.82 | 121.70 |
| 2 | B | 580 | TYR | N-CA-C | -9.14 | 86.31 | 111.00 |
| 2 | B | 461 | HIS | C-N-CA | -9.14 | 98.85 | 121.70 |
| 4 | M | 59 | ASP | CA-C-N | 9.13 | 137.28 | 117.20 |
| 2 | B | 560 | ILE | C-N-CA | -9.09 | 98.98 | 121.70 |
| 1 | A | 504 | ILE | C-N-CA | -9.09 | 98.98 | 121.70 |
| 4 | M | 41 | LEU | O-C-N | 9.09 | 137.24 | 122.70 |
| 2 | B | 211 | ALA | O-C-N | 9.07 | 137.21 | 122.70 |
| 1 | A | 163 | ALA | C-N-CA | -9.06 | 99.04 | 121.70 |
| 2 | B | 497 | LEU | C-N-CA | -9.05 | 99.06 | 121.70 |
| 1 | A | 100 | LEU | C-N-CA | -9.05 | 99.07 | 121.70 |
| 2 | B | 223 | LEU | C-N-CA | -9.05 | 99.08 | 121.70 |
| 2 | B | 205 | PRO | C-N-CA | -9.04 | 99.09 | 121.70 |
| 2 | B | 568 | VAL | CA-C-N | -9.03 | 97.33 | 117.20 |
| 1 | A | 350 | SER | O-C-N | -8.99 | 108.31 | 122.70 |
| 3 | S | 100 | ASP | O-C-N | 8.98 | 137.06 | 122.70 |
| 1 | A | 86 | TRP | C-N-CA | -8.97 | 99.26 | 121.70 |
| 4 | M | 92 | PHE | O-C-N | 8.97 | 137.06 | 122.70 |
| 3 | S | 161 | GLU | O-C-N | -8.96 | 108.36 | 122.70 |
| 2 | B | 569 | THR | N-CA-C | 8.95 | 135.17 | 111.00 |
| 1 | A | 103 | LYS | O-C-N | -8.94 | 108.39 | 122.70 |
| 1 | A | 288 | THR | N-CA-C | 8.93 | 135.10 | 111.00 |
| 2 | B | 559 | ASP | CA-C-O | -8.93 | 101.35 | 120.10 |
| 4 | M | 477 | GLY | C-N-CA | -8.90 | 99.45 | 121.70 |
| 4 | M | 351 | SER | C-N-CA | 8.88 | 143.91 | 121.70 |
| 1 | A | 196 | LEU | C-N-CA | -8.88 | 99.49 | 121.70 |
| 2 | B | 472 | VAL | O-C-N | -8.88 | 108.49 | 122.70 |
| 1 | A | 384 | LEU | O-C-N | 8.88 | 136.90 | 122.70 |
| 4 | M | 63 | TYR | C-N-CA | -8.84 | 99.59 | 121.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | A | 529 | GLY | CA-C-O | -8.83 | 104.70 | 120.60 |
| 2 | B | 287 | GLU | N-CA-C | -8.83 | 87.17 | 111.00 |
| 4 | M | 99 | ILE | O-C-N | 8.81 | 136.80 | 122.70 |
| 3 | S | 5 | VAL | O-C-N | -8.80 | 108.62 | 122.70 |
| 1 | A | 461 | CYS | O-C-N | -8.80 | 108.62 | 122.70 |
| 2 | B | 404 | ASN | O-C-N | -8.80 | 108.62 | 122.70 |
| 3 | S | 50 | PHE | C-N-CA | -8.79 | 99.74 | 121.70 |
| 4 | M | 405 | THR | CA-C-N | -8.77 | 98.65 | 116.20 |
| 1 | A | 432 | ILE | O-C-N | 8.75 | 136.71 | 122.70 |
| 2 | B | 212 | VAL | O-C-N | -8.74 | 108.72 | 122.70 |
| 1 | A | 138 | ASN | N-CA-C | -8.74 | 87.41 | 111.00 |
| 1 | A | 110 | ALA | C-N-CA | -8.72 | 99.89 | 121.70 |
| 1 | A | 154 | ILE | N-CA-C | 8.71 | 134.52 | 111.00 |
| 2 | B | 523 | PHE | O-C-N | -8.71 | 108.76 | 122.70 |
| 3 | S | 104 | THR | O-C-N | 8.70 | 136.62 | 122.70 |
| 1 | A | 325 | SER | N-CA-C | -8.68 | 87.56 | 111.00 |
| 4 | M | 335 | SER | O-C-N | 8.67 | 136.57 | 122.70 |
| 1 | A | 88 | ASN | C-N-CA | -8.66 | 100.04 | 121.70 |
| 4 | M | 279 | ASN | CA-C-N | 8.66 | 136.24 | 117.20 |
| 1 | A | 233 | PHE | O-C-N | -8.65 | 108.86 | 122.70 |
| 4 | M | 347 | PHE | N-CA-C | -8.64 | 87.67 | 111.00 |
| 2 | B | 147 | MET | O-C-N | -8.62 | 108.91 | 122.70 |
| 1 | A | 539 | ASN | O-C-N | -8.61 | 108.92 | 122.70 |
| 4 | M | 420 | THR | C-N-CA | -8.60 | 104.24 | 122.30 |
| 3 | S | 8 | PHE | O-C-N | -8.58 | 108.97 | 122.70 |
| 3 | S | 81 | ALA | CB-CA-C | 8.58 | 122.97 | 110.10 |
| 1 | A | 545 | HIS | C-N-CA | -8.58 | 100.25 | 121.70 |
| 2 | B | 109 | ALA | C-N-CA | -8.56 | 100.31 | 121.70 |
| 4 | M | 406 | GLY | C-N-CA | -8.55 | 100.31 | 121.70 |
| 1 | A | 413 | SER | N-CA-C | -8.54 | 87.93 | 111.00 |
| 3 | S | 167 | ILE | C-N-CA | -8.54 | 104.36 | 122.30 |
| 1 | A | 94 | VAL | O-C-N | -8.54 | 109.04 | 122.70 |
| 1 | A | 461 | CYS | CA-C-O | 8.50 | 137.94 | 120.10 |
| 3 | S | 98 | ILE | O-C-N | 8.49 | 136.29 | 122.70 |
| 3 | S | 37 | GLU | O-C-N | 8.47 | 136.26 | 122.70 |
| 4 | M | 126 | ASN | O-C-N | 8.46 | 136.24 | 122.70 |
| 1 | A | 212 | ILE | O-C-N | -8.44 | 109.19 | 122.70 |
| 1 | A | 328 | PRO | C-N-CA | -8.43 | 100.63 | 121.70 |
| 2 | B | 574 | ASN | C-N-CA | -8.42 | 100.66 | 121.70 |
| 2 | B | 205 | PRO | O-C-N | -8.39 | 109.27 | 122.70 |
| 1 | A | 504 | ILE | CA-C-O | 8.38 | 137.71 | 120.10 |
| 4 | M | 292 | PRO | C-N-CA | 8.37 | 157.16 | 122.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | A | 547 | VAL | O-C-N | 8.37 | 136.09 | 122.70 |
| 1 | A | 242 | GLU | O-C-N | -8.35 | 109.34 | 122.70 |
| 1 | A | 545 | HIS | O-C-N | -8.35 | 109.34 | 122.70 |
| 1 | A | 391 | LEU | C-N-CA | -8.33 | 100.87 | 121.70 |
| 2 | B | 146 | LYS | C-N-CA | -8.31 | 100.93 | 121.70 |
| 1 | A | 431 | VAL | O-C-N | 8.30 | 135.99 | 122.70 |
| 1 | A | 281 | LEU | CA-C-O | 8.29 | 137.51 | 120.10 |
| 1 | A | 573 | GLU | O-C-N | -8.29 | 109.44 | 122.70 |
| 4 | M | 53 | HIS | CA-C-N | 8.29 | 135.44 | 117.20 |
| 4 | M | 367 | ALA | C-N-CA | 8.29 | 142.42 | 121.70 |
| 1 | A | 637 | GLU | C-N-CA | -8.28 | 101.00 | 121.70 |
| 2 | B | 444 | THR | O-C-N | -8.28 | 109.46 | 122.70 |
| 1 | A | 275 | LEU | C-N-CA | -8.26 | 87.31 | 122.00 |
| 2 | B | 366 | LEU | C-N-CA | -8.26 | 101.06 | 121.70 |
| 2 | B | 505 | ASP | O-C-N | -8.25 | 109.49 | 122.70 |
| 1 | A | 631 | SER | O-C-N | 8.25 | 135.90 | 122.70 |
| 2 | B | 339 | PHE | O-C-N | 8.24 | 135.89 | 122.70 |
| 1 | A | 215 | VAL | CA-C-O | 8.24 | 137.40 | 120.10 |
| 3 | S | 59 | LEU | CA-C-N | -8.24 | 99.08 | 117.20 |
| 2 | B | 83 | PHE | O-C-N | 8.22 | 135.85 | 122.70 |
| 4 | M | 54 | SER | O-C-N | 8.22 | 135.85 | 122.70 |
| 1 | A | 100 | LEU | O-C-N | -8.22 | 109.55 | 122.70 |
| 2 | B | 295 | ASN | C-N-CA | 8.22 | 142.24 | 121.70 |
| 2 | B | 132 | SER | C-N-CA | -8.20 | 101.21 | 121.70 |
| 4 | M | 457 | GLY | N-CA-C | -8.20 | 92.61 | 113.10 |
| 2 | B | 375 | LEU | O-C-N | -8.19 | 105.53 | 121.10 |
| 2 | B | 526 | CYS | O-C-N | 8.19 | 136.67 | 121.10 |
| 3 | S | 66 | ASP | N-CA-C | -8.19 | 88.88 | 111.00 |
| 4 | M | 105 | ASP | C-N-CA | -8.19 | 101.22 | 121.70 |
| 4 | M | 74 | TYR | CA-C-O | 8.19 | 137.30 | 120.10 |
| 1 | A | 192 | TYR | CA-C-O | -8.18 | 102.91 | 120.10 |
| 4 | M | 104 | PHE | O-C-N | -8.18 | 109.61 | 122.70 |
| 1 | A | 346 | THR | O-C-N | -8.18 | 109.61 | 122.70 |
| 1 | A | 120 | ILE | O-C-N | 8.18 | 135.78 | 122.70 |
| 3 | S | 158 | LYS | O-C-N | 8.17 | 135.77 | 122.70 |
| 4 | M | 104 | PHE | C-N-CA | 8.17 | 142.12 | 121.70 |
| 1 | A | 443 | SER | N-CA-C | 8.17 | 133.05 | 111.00 |
| 2 | B | 184 | GLY | CA-C-N | -8.16 | 99.24 | 117.20 |
| 1 | A | 424 | TYR | O-C-N | 8.16 | 135.76 | 122.70 |
| 2 | B | 108 | PHE | CA-C-O | 8.16 | 137.23 | 120.10 |
| 4 | M | 330 | GLY | C-N-CA | 8.16 | 142.09 | 121.70 |
| 2 | B | 56 | SER | O-C-N | -8.15 | 109.67 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4 | M | 51 | LEU | C-N-CA | -8.15 | 101.33 | 121.70 |
| 1 | A | 304 | LEU | O-C-N | -8.14 | 109.68 | 122.70 |
| 2 | B | 108 | PHE | O-C-N | -8.13 | 109.69 | 122.70 |
| 2 | B | 296 | ASP | CA-C-O | -8.13 | 103.03 | 120.10 |
| 2 | B | 30 | LEU | C-N-CA | 8.12 | 139.36 | 122.30 |
| 1 | A | 487 | MET | O-C-N | -8.11 | 109.72 | 122.70 |
| 2 | B | 105 | LEU | O-C-N | -8.11 | 109.72 | 122.70 |
| 1 | A | 450 | TYR | O-C-N | 8.11 | 135.67 | 122.70 |
| 1 | A | 330 | LEU | O-C-N | 8.10 | 135.66 | 122.70 |
| 4 | M | 63 | TYR | CD1-CG-CD2 | 8.10 | 126.81 | 117.90 |
| 2 | B | 486 | HIS | O-C-N | 8.10 | 135.65 | 122.70 |
| 3 | S | 108 | SER | O-C-N | 8.10 | 135.65 | 122.70 |
| 2 | B | 557 | SER | O-C-N | -8.09 | 109.75 | 122.70 |
| 2 | B | 35 | TYR | O-C-N | 8.08 | 135.63 | 122.70 |
| 1 | A | 270 | LEU | O-C-N | 8.08 | 135.63 | 122.70 |
| 1 | A | 549 | GLU | O-C-N | 8.08 | 135.63 | 122.70 |
| 4 | M | 81 | SER | O-C-N | -8.06 | 109.80 | 122.70 |
| 1 | A | 367 | ILE | O-C-N | 8.06 | 135.60 | 122.70 |
| 1 | A | 465 | SER | N-CA-C | 8.06 | 132.77 | 111.00 |
| 2 | B | 273 | SER | N-CA-C | 8.06 | 132.76 | 111.00 |
| 1 | A | 415 | ARG | N-CA-C | -8.06 | 89.25 | 111.00 |
| 4 | M | 232 | HIS | CA-C-O | 8.05 | 137.01 | 120.10 |
| 1 | A | 103 | LYS | CA-C-O | 8.05 | 137.01 | 120.10 |
| 2 | B | 336 | ASN | CA-C-N | -8.05 | 99.49 | 117.20 |
| 3 | S | 46 | PHE | CA-C-O | -8.05 | 103.20 | 120.10 |
| 3 | S | 125 | TRP | CA-C-O | -8.04 | 103.21 | 120.10 |
| 4 | M | 135 | ASN | CA-C-N | -8.04 | 99.51 | 117.20 |
| 3 | S | 103 | GLN | O-C-N | 8.03 | 135.56 | 122.70 |
| 4 | M | 63 | TYR | CB-CG-CD2 | -8.03 | 116.18 | 121.00 |
| 2 | B | 317 | VAL | O-C-N | 8.03 | 135.54 | 122.70 |
| 1 | A | 218 | ALA | CB-CA-C | 8.02 | 122.12 | 110.10 |
| 4 | M | 108 | LYS | C-N-CA | -8.01 | 101.69 | 121.70 |
| 3 | S | 16 | LEU | O-C-N | -8.00 | 109.89 | 122.70 |
| 2 | B | 274 | PRO | C-N-CA | -8.00 | 101.70 | 121.70 |
| 2 | B | 494 | ALA | O-C-N | 8.00 | 135.50 | 122.70 |
| 1 | A | 442 | SER | N-CA-C | -7.98 | 89.44 | 111.00 |
| 2 | B | 240 | LEU | N-CA-C | 7.98 | 132.53 | 111.00 |
| 2 | B | 515 | PHE | C-N-CA | -7.97 | 105.57 | 122.30 |
| 3 | S | 46 | PHE | N-CA-C | -7.96 | 89.51 | 111.00 |
| 3 | S | 139 | GLY | C-N-CA | -7.96 | 101.81 | 121.70 |
| 4 | M | 294 | ASP | C-N-CA | 7.95 | 138.99 | 122.30 |
| 4 | M | 5 | PHE | O-C-N | -7.95 | 109.99 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2 | B | 126 | SER | O-C-N | -7.94 | 110.00 | 122.70 |
| 2 | B | 299 | LEU | O-C-N | 7.94 | 135.40 | 122.70 |
| 3 | S | 74 | GLN | O-C-N | -7.93 | 110.00 | 122.70 |
| 1 | A | 328 | PRO | O-C-N | -7.93 | 110.01 | 122.70 |
| 2 | B | 174 | ALA | O-C-N | -7.93 | 110.01 | 122.70 |
| 1 | A | 158 | LEU | O-C-N | 7.92 | 135.38 | 122.70 |
| 4 | M | 262 | THR | C-N-CA | -7.92 | 101.89 | 121.70 |
| 4 | M | 55 | MET | CA-C-N | 7.92 | 134.62 | 117.20 |
| 3 | S | 113 | PHE | N-CA-C | -7.92 | 89.63 | 111.00 |
| 1 | A | 264 | SER | C-N-CA | -7.91 | 101.92 | 121.70 |
| 2 | B | 389 | ILE | O-C-N | -7.91 | 110.05 | 122.70 |
| 2 | B | 508 | ARG | O-C-N | -7.91 | 110.05 | 122.70 |
| 1 | A | 281 | LEU | C-N-CA | -7.90 | 101.96 | 121.70 |
| 2 | B | 584 | SER | O-C-N | -7.89 | 109.78 | 123.20 |
| 1 | A | 479 | ASN | O-C-N | 7.89 | 135.32 | 122.70 |
| 2 | B | 132 | SER | O-C-N | -7.89 | 110.08 | 122.70 |
| 2 | B | 293 | VAL | C-N-CA | -7.88 | 102.00 | 121.70 |
| 2 | B | 566 | ALA | C-N-CA | 7.87 | 141.38 | 121.70 |
| 1 | A | 601 | VAL | O-C-N | -7.87 | 110.11 | 122.70 |
| 1 | A | 364 | ASP | O-C-N | 7.86 | 135.28 | 122.70 |
| 4 | M | 292 | PRO | N-CA-C | -7.86 | 91.66 | 112.10 |
| 4 | M | 263 | MET | C-N-CA | 7.86 | 138.80 | 122.30 |
| 1 | A | 588 | LEU | O-C-N | -7.84 | 110.15 | 122.70 |
| 2 | B | 147 | MET | C-N-CA | -7.84 | 102.11 | 121.70 |
| 1 | A | 70 | ALA | O-C-N | 7.83 | 135.23 | 122.70 |
| 1 | A | 612 | GLU | O-C-N | 7.83 | 135.22 | 122.70 |
| 3 | S | 25 | LEU | O-C-N | -7.82 | 106.23 | 121.10 |
| 3 | S | 36 | TYR | O-C-N | 7.82 | 135.21 | 122.70 |
| 1 | A | 434 | SER | O-C-N | 7.81 | 135.20 | 122.70 |
| 2 | B | 416 | LYS | O-C-N | 7.81 | 135.19 | 122.70 |
| 1 | A | 156 | PRO | O-C-N | -7.80 | 110.22 | 122.70 |
| 4 | M | 75 | TRP | O-C-N | -7.80 | 110.22 | 122.70 |
| 1 | A | 448 | GLU | N-CA-C | -7.80 | 89.95 | 111.00 |
| 4 | M | 230 | LYS | CA-C-N | 7.79 | 134.33 | 117.20 |
| 2 | B | 237 | ILE | O-C-N | -7.78 | 110.25 | 122.70 |
| 2 | B | 142 | LEU | O-C-N | -7.78 | 110.26 | 122.70 |
| 2 | B | 220 | ALA | N-CA-C | -7.75 | 90.08 | 111.00 |
| 2 | B | 418 | TYR | C-N-CA | -7.75 | 102.33 | 121.70 |
| 3 | S | 66 | ASP | CA-C-N | -7.75 | 100.16 | 117.20 |
| 2 | B | 115 | LEU | O-C-N | 7.74 | 135.09 | 122.70 |
| 2 | B | 287 | GLU | CA-C-N | -7.74 | 100.17 | 117.20 |
| 1 | A | 461 | CYS | C-N-CA | -7.74 | 102.36 | 121.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4 | M | 97 | ASP | O-C-N | 7.74 | 135.08 | 122.70 |
| 1 | A | 279 | LEU | O-C-N | -7.73 | 110.33 | 122.70 |
| 3 | S | 62 | GLU | N-CA-C | 7.71 | 131.81 | 111.00 |
| 4 | M | 265 | ASN | N-CA-C | -7.68 | 90.25 | 111.00 |
| 3 | S | 28 | GLN | O-C-N | 7.68 | 134.99 | 122.70 |
| 1 | A | 508 | LEU | CA-C-O | -7.67 | 103.98 | 120.10 |
| 3 | S | 60 | SER | N-CA-C | -7.66 | 90.31 | 111.00 |
| 2 | B | 478 | LEU | O-C-N | -7.66 | 110.44 | 122.70 |
| 1 | A | 298 | ILE | O-C-N | -7.65 | 110.46 | 122.70 |
| 1 | A | 469 | LEU | CA-C-O | 7.65 | 136.17 | 120.10 |
| 2 | B | 585 | GLY | N-CA-C | -7.64 | 93.99 | 113.10 |
| 4 | M | 72 | LEU | C-N-CA | 7.64 | 140.81 | 121.70 |
| 1 | A | 534 | LYS | O-C-N | -7.64 | 110.48 | 122.70 |
| 1 | A | 281 | LEU | O-C-N | -7.64 | 110.48 | 122.70 |
| 1 | A | 394 | GLN | CA-C-O | -7.63 | 104.07 | 120.10 |
| 2 | B | 169 | VAL | O-C-N | 7.62 | 134.89 | 122.70 |
| 3 | S | 31 | LEU | O-C-N | 7.62 | 134.88 | 122.70 |
| 2 | B | 515 | PHE | O-C-N | -7.61 | 110.26 | 123.20 |
| 1 | A | 527 | GLU | C-N-CA | 7.60 | 140.70 | 121.70 |
| 3 | S | 132 | LEU | O-C-N | 7.60 | 134.86 | 122.70 |
| 4 | M | 104 | PHE | N-CA-CB | -7.60 | 96.92 | 110.60 |
| 2 | B | 528 | ASP | O-C-N | 7.60 | 134.86 | 122.70 |
| 3 | S | 58 | LEU | C-N-CA | -7.59 | 102.72 | 121.70 |
| 1 | A | 220 | SER | O-C-N | 7.58 | 134.83 | 122.70 |
| 4 | M | 421 | GLY | O-C-N | -7.58 | 106.69 | 121.10 |
| 2 | B | 51 | LEU | C-N-CA | -7.58 | 102.76 | 121.70 |
| 4 | M | 280 | ASP | CB-CA-C | -7.57 | 95.27 | 110.40 |
| 3 | S | 58 | LEU | CA-C-O | 7.56 | 135.98 | 120.10 |
| 1 | A | 596 | VAL | O-C-N | 7.54 | 134.76 | 122.70 |
| 3 | S | 27 | LYS | O-C-N | 7.54 | 134.76 | 122.70 |
| 1 | A | 218 | ALA | O-C-N | 7.54 | 134.76 | 122.70 |
| 4 | M | 367 | ALA | CB-CA-C | 7.53 | 121.39 | 110.10 |
| 4 | M | 450 | GLU | CA-C-O | 7.53 | 135.90 | 120.10 |
| 2 | B | 252 | LEU | O-C-N | 7.52 | 134.73 | 122.70 |
| 2 | B | 560 | ILE | O-C-N | -7.52 | 110.67 | 122.70 |
| 3 | S | 153 | VAL | O-C-N | 7.51 | 134.72 | 122.70 |
| 3 | S | 109 | LEU | CA-C-O | 7.50 | 135.84 | 120.10 |
| 2 | B | 408 | VAL | O-C-N | 7.49 | 134.68 | 122.70 |
| 4 | M | 237 | THR | C-N-CA | -7.49 | 106.57 | 122.30 |
| 1 | A | 365 | VAL | O-C-N | -7.49 | 110.72 | 122.70 |
| 4 | M | 279 | ASN | N-CA-CB | -7.48 | 97.14 | 110.60 |
| 4 | M | 105 | ASP | O-C-N | -7.48 | 110.74 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4 | M | 351 | SER | N-CA-CB | -7.47 | 99.29 | 110.50 |
| 2 | B | 442 | LEU | C-N-CA | -7.46 | 103.05 | 121.70 |
| 1 | A | 528 | ASN | CA-C-O | 7.46 | 135.76 | 120.10 |
| 1 | A | 441 | TYR | CA-C-N | -7.44 | 100.83 | 117.20 |
| 1 | A | 98 | ASN | CA-C-N | 7.44 | 133.57 | 117.20 |
| 2 | B | 554 | LYS | O-C-N | 7.43 | 134.59 | 122.70 |
| 2 | B | 237 | ILE | C-N-CA | -7.42 | 103.14 | 121.70 |
| 2 | B | 215 | TYR | O-C-N | 7.42 | 134.57 | 122.70 |
| 2 | B | 46 | GLN | O-C-N | 7.42 | 134.57 | 122.70 |
| 2 | B | 328 | LEU | C-N-CA | -7.42 | 103.15 | 121.70 |
| 1 | A | 601 | VAL | C-N-CA | -7.41 | 103.18 | 121.70 |
| 2 | B | 277 | CYS | C-N-CD | 7.41 | 143.95 | 128.40 |
| 3 | S | 25 | LEU | CA-C-O | 7.40 | 135.63 | 120.10 |
| 1 | A | 88 | ASN | CA-C-O | 7.39 | 135.62 | 120.10 |
| 2 | B | 220 | ALA | CB-CA-C | 7.39 | 121.19 | 110.10 |
| 1 | A | 311 | THR | O-C-N | 7.39 | 134.52 | 122.70 |
| 1 | A | 439 | ASP | CA-C-N | -7.39 | 100.95 | 117.20 |
| 4 | M | 407 | THR | N-CA-C | -7.38 | 91.06 | 111.00 |
| 1 | A | 260 | PHE | C-N-CA | -7.38 | 103.25 | 121.70 |
| 1 | A | 394 | GLN | O-C-N | 7.37 | 134.49 | 122.70 |
| 2 | B | 270 | SER | N-CA-C | -7.37 | 91.11 | 111.00 |
| 3 | S | 55 | PRO | CA-N-CD | -7.37 | 101.19 | 111.50 |
| 3 | S | 25 | LEU | C-N-CD | 7.36 | 143.86 | 128.40 |
| 2 | B | 488 | ARG | O-C-N | 7.36 | 134.47 | 122.70 |
| 3 | S | 54 | PRO | C-N-CD | 7.36 | 143.85 | 128.40 |
| 2 | B | 142 | LEU | C-N-CA | -7.34 | 103.35 | 121.70 |
| 1 | A | 519 | LEU | O-C-N | -7.34 | 110.72 | 123.20 |
| 3 | S | 66 | ASP | C-N-CA | 7.33 | 140.04 | 121.70 |
| 4 | M | 130 | GLU | CA-C-N | -7.33 | 101.08 | 117.20 |
| 2 | B | 183 | ALA | N-CA-C | 7.33 | 130.78 | 111.00 |
| 2 | B | 192 | LEU | O-C-N | 7.32 | 134.41 | 122.70 |
| 4 | M | 61 | GLU | O-C-N | 7.32 | 134.41 | 122.70 |
| 1 | A | 559 | PHE | O-C-N | 7.31 | 134.39 | 122.70 |
| 1 | A | 355 | LEU | O-C-N | 7.31 | 134.39 | 122.70 |
| 4 | M | 132 | GLY | CA-C-O | 7.30 | 133.74 | 120.60 |
| 3 | S | 148 | ARG | O-C-N | 7.30 | 134.38 | 122.70 |
| 3 | S | 96 | LEU | O-C-N | 7.30 | 134.38 | 122.70 |
| 1 | A | 606 | PHE | O-C-N | 7.29 | 134.36 | 122.70 |
| 2 | B | 172 | GLU | O-C-N | -7.28 | 111.05 | 122.70 |
| 1 | A | 263 | LEU | C-N-CA | -7.28 | 103.51 | 121.70 |
| 1 | A | 529 | GLY | N-CA-C | -7.27 | 94.92 | 113.10 |
| 2 | B | 243 | TRP | O-C-N | 7.26 | 134.31 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3 | S | 156 | LEU | O-C-N | 7.24 | 134.29 | 122.70 |
| 1 | A | 405 | THR | N-CA-C | 7.24 | 130.54 | 111.00 |
| 2 | B | 572 | GLU | O-C-N | 7.23 | 134.27 | 122.70 |
| 1 | A | 204 | VAL | C-N-CA | -7.22 | 103.64 | 121.70 |
| 2 | B | 531 | ARG | O-C-N | 7.22 | 134.26 | 122.70 |
| 1 | A | 511 | VAL | O-C-N | 7.21 | 134.24 | 122.70 |
| 1 | A | 107 | TYR | O-C-N | 7.21 | 134.23 | 122.70 |
| 1 | A | 302 | ASN | CA-C-N | -7.20 | 101.37 | 117.20 |
| 2 | B | 288 | TYR | N-CA-C | -7.20 | 91.57 | 111.00 |
| 2 | B | 415 | LEU | O-C-N | 7.20 | 134.21 | 122.70 |
| 1 | A | 573 | GLU | C-N-CA | -7.18 | 103.75 | 121.70 |
| 1 | A | 265 | GLN | CA-C-O | -7.18 | 105.03 | 120.10 |
| 3 | S | 167 | ILE | N-CA-C | 7.17 | 130.37 | 111.00 |
| 4 | M | 128 | CYS | C-N-CA | -7.17 | 103.77 | 121.70 |
| 1 | A | 539 | ASN | C-N-CA | -7.17 | 103.78 | 121.70 |
| 4 | M | 319 | SER | N-CA-C | -7.17 | 91.64 | 111.00 |
| 3 | S | 84 | TYR | O-C-N | -7.17 | 111.23 | 122.70 |
| 4 | M | 129 | VAL | C-N-CA | 7.16 | 139.61 | 121.70 |
| 2 | B | 153 | ILE | O-C-N | 7.16 | 134.16 | 122.70 |
| 2 | B | 213 | LEU | O-C-N | 7.16 | 134.15 | 122.70 |
| 2 | B | 323 | ASN | O-C-N | 7.16 | 134.15 | 122.70 |
| 2 | B | 493 | LEU | O-C-N | 7.16 | 134.15 | 122.70 |
| 2 | B | 325 | LEU | CA-C-O | 7.15 | 135.12 | 120.10 |
| 3 | S | 80 | TYR | CA-C-O | 7.15 | 135.12 | 120.10 |
| 4 | M | 118 | TYR | CA-C-O | -7.15 | 105.08 | 120.10 |
| 1 | A | 391 | LEU | O-C-N | -7.14 | 111.28 | 122.70 |
| 1 | A | 607 | LEU | O-C-N | 7.14 | 134.12 | 122.70 |
| 3 | S | 47 | GLN | CA-C-N | -7.14 | 101.50 | 117.20 |
| 4 | M | 460 | ILE | C-N-CA | 7.14 | 137.28 | 122.30 |
| 2 | B | 185 | LYS | O-C-N | -7.13 | 111.28 | 122.70 |
| 4 | M | 54 | SER | C-N-CA | 7.13 | 139.53 | 121.70 |
| 1 | A | 508 | LEU | N-CA-C | 7.13 | 130.25 | 111.00 |
| 3 | S | 118 | GLU | O-C-N | 7.13 | 134.11 | 122.70 |
| 1 | A | 383 | ASN | O-C-N | 7.12 | 134.09 | 122.70 |
| 2 | B | 223 | LEU | O-C-N | -7.12 | 111.31 | 122.70 |
| 2 | B | 102 | HIS | CA-C-O | 7.12 | 135.05 | 120.10 |
| 4 | M | 458 | LEU | C-N-CA | 7.12 | 139.50 | 121.70 |
| 2 | B | 478 | LEU | CA-C-O | 7.11 | 135.04 | 120.10 |
| 2 | B | 511 | ILE | O-C-N | -7.11 | 111.32 | 122.70 |
| 1 | A | 447 | PHE | O-C-N | 7.10 | 134.05 | 122.70 |
| 1 | A | 453 | VAL | O-C-N | 7.09 | 134.05 | 122.70 |
| 3 | S | 137 | GLN | CA-C-N | -7.09 | 102.02 | 116.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | A | 543 | TYR | CG-CD2-CE2 | 7.08 | 126.97 | 121.30 |
| 2 | B | 143 | SER | C-N-CA | -7.08 | 103.99 | 121.70 |
| 1 | A | 474 | GLY | O-C-N | 7.08 | 134.03 | 122.70 |
| 1 | A | 624 | LEU | O-C-N | 7.07 | 134.02 | 122.70 |
| 1 | A | 441 | TYR | CA-C-O | 7.07 | 134.95 | 120.10 |
| 1 | A | 566 | PHE | N-CA-C | 7.07 | 130.09 | 111.00 |
| 4 | M | 110 | SER | O-C-N | 7.07 | 134.01 | 122.70 |
| 4 | M | 53 | HIS | O-C-N | -7.06 | 111.40 | 122.70 |
| 4 | M | 266 | ASP | CA-C-N | -7.06 | 101.67 | 117.20 |
| 1 | A | 602 | GLU | O-C-N | 7.06 | 133.99 | 122.70 |
| 4 | M | 403 | THR | N-CA-C | -7.05 | 91.96 | 111.00 |
| 2 | B | 78 | ASP | O-C-N | -7.05 | 111.42 | 122.70 |
| 2 | B | 105 | LEU | C-N-CA | -7.04 | 104.10 | 121.70 |
| 2 | B | 355 | ASN | O-C-N | 7.04 | 133.96 | 122.70 |
| 3 | S | 99 | LEU | O-C-N | 7.04 | 133.96 | 122.70 |
| 1 | A | 488 | ARG | O-C-N | 7.03 | 133.95 | 122.70 |
| 2 | B | 56 | SER | C-N-CA | -7.03 | 104.12 | 121.70 |
| 2 | B | 226 | LEU | O-C-N | 7.02 | 133.94 | 122.70 |
| 2 | B | 475 | ILE | O-C-N | 7.02 | 133.93 | 122.70 |
| 1 | A | 256 | LEU | O-C-N | 7.01 | 133.92 | 122.70 |
| 1 | A | 300 | LYS | N-CA-C | 7.01 | 129.92 | 111.00 |
| 3 | S | 83 | LEU | CA-C-O | 7.00 | 134.81 | 120.10 |
| 4 | M | 63 | TYR | CG-CD2-CE2 | -7.00 | 115.70 | 121.30 |
| 1 | A | 581 | LEU | O-C-N | 7.00 | 133.90 | 122.70 |
| 2 | B | 267 | ASP | O-C-N | -7.00 | 111.50 | 122.70 |
| 4 | M | 63 | TYR | CA-C-N | -7.00 | 101.80 | 117.20 |
| 2 | B | 389 | ILE | C-N-CA | -7.00 | 104.21 | 121.70 |
| 2 | B | 104 | TYR | O-C-N | 7.00 | 133.89 | 122.70 |
| 4 | M | 426 | LYS | C-N-CA | 6.99 | 139.17 | 121.70 |
| 1 | A | 177 | ILE | O-C-N | 6.99 | 133.88 | 122.70 |
| 1 | A | 102 | GLN | O-C-N | 6.98 | 133.87 | 122.70 |
| 2 | B | 422 | ALA | N-CA-CB | 6.98 | 119.87 | 110.10 |
| 2 | B | 216 | LYS | C-N-CA | -6.98 | 104.26 | 121.70 |
| 2 | B | 260 | LEU | C-N-CD | 6.97 | 143.05 | 128.40 |
| 1 | A | 436 | CYS | O-C-N | -6.97 | 111.55 | 122.70 |
| 2 | B | 489 | ILE | O-C-N | 6.97 | 133.84 | 122.70 |
| 2 | B | 97 | VAL | O-C-N | 6.96 | 133.84 | 122.70 |
| 1 | A | 582 | ILE | O-C-N | 6.96 | 133.84 | 122.70 |
| 1 | A | 279 | LEU | C-N-CA | -6.95 | 104.32 | 121.70 |
| 2 | B | 474 | VAL | O-C-N | 6.95 | 133.82 | 122.70 |
| 4 | M | 106 | LYS | CA-C-N | -6.94 | 101.92 | 117.20 |
| 2 | B | 253 | ILE | O-C-N | 6.94 | 133.80 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2 | B | 395 | LYS | O-C-N | 6.94 | 133.80 | 122.70 |
| 3 | S | 33 | GLU | O-C-N | 6.94 | 133.80 | 122.70 |
| 1 | A | 182 | ILE | O-C-N | 6.93 | 133.80 | 122.70 |
| 1 | A | 517 | TRP | O-C-N | 6.93 | 133.79 | 122.70 |
| 4 | M | 63 | TYR | CB-CG-CD1 | -6.93 | 116.84 | 121.00 |
| 1 | A | 188 | VAL | O-C-N | 6.93 | 133.79 | 122.70 |
| 1 | A | 569 | ASP | O-C-N | -6.93 | 111.61 | 122.70 |
| 2 | B | 174 | ALA | C-N-CA | -6.93 | 104.37 | 121.70 |
| 3 | S | 106 | VAL | O-C-N | 6.93 | 133.79 | 122.70 |
| 3 | S | 143 | GLU | CA-C-N | -6.93 | 101.96 | 117.20 |
| 1 | A | 514 | GLU | O-C-N | 6.92 | 133.78 | 122.70 |
| 1 | A | 623 | MET | O-C-N | 6.92 | 133.77 | 122.70 |
| 1 | A | 271 | ARG | O-C-N | 6.91 | 133.76 | 122.70 |
| 2 | B | 611 | ALA | O-C-N | 6.91 | 133.76 | 122.70 |
| 1 | A | 301 | GLY | N-CA-C | -6.91 | 95.83 | 113.10 |
| 1 | A | 621 | LEU | C-N-CA | -6.91 | 93.00 | 122.00 |
| 4 | M | 91 | THR | CA-C-O | -6.91 | 105.60 | 120.10 |
| 4 | M | 425 | THR | C-N-CA | 6.91 | 138.96 | 121.70 |
| 2 | B | 521 | ILE | C-N-CA | -6.90 | 104.44 | 121.70 |
| 1 | A | 306 | GLU | O-C-N | -6.90 | 111.66 | 122.70 |
| 2 | B | 411 | ILE | O-C-N | 6.90 | 133.74 | 122.70 |
| 4 | M | 47 | SER | N-CA-C | -6.90 | 92.37 | 111.00 |
| 1 | A | 451 | ASN | O-C-N | 6.89 | 133.73 | 122.70 |
| 4 | M | 317 | MET | C-N-CA | -6.89 | 104.47 | 121.70 |
| 1 | A | 338 | PHE | O-C-N | 6.89 | 133.72 | 122.70 |
| 3 | S | 99 | LEU | CA-C-O | -6.89 | 105.64 | 120.10 |
| 1 | A | 166 | LEU | O-C-N | 6.88 | 133.71 | 122.70 |
| 1 | A | 406 | GLY | N-CA-C | -6.88 | 95.89 | 113.10 |
| 2 | B | 273 | SER | N-CA-CB | -6.88 | 100.18 | 110.50 |
| 2 | B | 271 | GLU | C-N-CA | -6.88 | 107.86 | 122.30 |
| 2 | B | 573 | GLU | C-N-CA | -6.88 | 104.51 | 121.70 |
| 3 | S | 116 | VAL | O-C-N | 6.88 | 133.70 | 122.70 |
| 3 | S | 8 | PHE | CA-C-O | 6.87 | 134.53 | 120.10 |
| 3 | S | 128 | LEU | O-C-N | 6.87 | 133.70 | 122.70 |
| 2 | B | 457 | HIS | CA-C-O | 6.87 | 134.52 | 120.10 |
| 2 | B | 552 | SER | O-C-N | 6.87 | 133.69 | 122.70 |
| 4 | M | 277 | GLU | O-C-N | -6.87 | 111.71 | 122.70 |
| 2 | B | 356 | LYS | O-C-N | 6.87 | 133.69 | 122.70 |
| 1 | A | 162 | ILE | O-C-N | 6.86 | 133.68 | 122.70 |
| 1 | A | 555 | LEU | O-C-N | 6.86 | 133.68 | 122.70 |
| 3 | S | 68 | VAL | C-N-CA | -6.86 | 104.54 | 121.70 |
| 2 | B | 158 | VAL | O-C-N | 6.86 | 133.68 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | A | 635 | ALA | O-C-N | 6.86 | 133.67 | 122.70 |
| 1 | A | 466 | ASP | O-C-N | 6.86 | 133.67 | 122.70 |
| 4 | M | 455 | VAL | C-N-CA | -6.86 | 104.56 | 121.70 |
| 2 | B | 555 | LEU | O-C-N | 6.85 | 133.66 | 122.70 |
| 1 | A | 457 | LEU | O-C-N | 6.85 | 133.66 | 122.70 |
| 1 | A | 257 | LEU | O-C-N | 6.85 | 133.66 | 122.70 |
| 1 | A | 601 | VAL | CA-C-O | 6.85 | 134.48 | 120.10 |
| 1 | A | 392 | MET | O-C-N | 6.84 | 133.65 | 122.70 |
| 2 | B | 362 | ALA | O-C-N | 6.84 | 133.65 | 122.70 |
| 3 | S | 24 | ASP | O-C-N | 6.84 | 133.65 | 122.70 |
| 4 | M | 21 | GLY | N-CA-C | -6.84 | 95.99 | 113.10 |
| 4 | M | 50 | TYR | N-CA-CB | -6.84 | 98.28 | 110.60 |
| 2 | B | 504 | ALA | O-C-N | 6.84 | 133.64 | 122.70 |
| 1 | A | 140 | VAL | CA-C-O | 6.84 | 134.46 | 120.10 |
| 1 | A | 140 | VAL | O-C-N | -6.83 | 111.76 | 122.70 |
| 2 | B | 447 | GLU | O-C-N | 6.83 | 133.63 | 122.70 |
| 1 | A | 67 | LYS | O-C-N | 6.83 | 133.62 | 122.70 |
| 1 | A | 298 | ILE | CA-C-O | 6.82 | 134.43 | 120.10 |
| 2 | B | 66 | ILE | O-C-N | 6.82 | 133.61 | 122.70 |
| 2 | B | 579 | PRO | CA-C-N | 6.82 | 132.20 | 117.20 |
| 4 | M | 394 | GLN | CA-C-O | 6.82 | 134.42 | 120.10 |
| 2 | B | 568 | VAL | C-N-CA | 6.82 | 138.74 | 121.70 |
| 1 | A | 388 | VAL | O-C-N | 6.81 | 133.59 | 122.70 |
| 2 | B | 137 | PHE | O-C-N | 6.81 | 133.59 | 122.70 |
| 2 | B | 363 | ILE | O-C-N | 6.81 | 133.59 | 122.70 |
| 1 | A | 399 | ASP | O-C-N | 6.80 | 133.59 | 122.70 |
| 1 | A | 610 | SER | O-C-N | 6.80 | 133.59 | 122.70 |
| 1 | A | 515 | CYS | O-C-N | 6.80 | 133.59 | 122.70 |
| 3 | S | 32 | LEU | O-C-N | 6.80 | 133.58 | 122.70 |
| 4 | M | 5 | PHE | CA-C-O | 6.80 | 134.38 | 120.10 |
| 3 | S | 29 | LYS | O-C-N | 6.80 | 133.58 | 122.70 |
| 2 | B | 139 | LEU | O-C-N | 6.79 | 133.57 | 122.70 |
| 2 | B | 99 | ARG | O-C-N | 6.79 | 133.57 | 122.70 |
| 1 | A | 265 | GLN | N-CA-CB | 6.79 | 122.82 | 110.60 |
| 1 | A | 225 | LEU | O-C-N | 6.78 | 133.55 | 122.70 |
| 4 | M | 60 | LEU | O-C-N | 6.78 | 133.55 | 122.70 |
| 1 | A | 105 | VAL | O-C-N | 6.78 | 134.72 | 123.20 |
| 1 | A | 599 | ARG | O-C-N | 6.78 | 133.54 | 122.70 |
| 3 | S | 157 | ASN | O-C-N | 6.78 | 133.54 | 122.70 |
| 2 | B | 267 | ASP | CA-C-O | 6.77 | 134.32 | 120.10 |
| 2 | B | 581 | TYR | N-CA-C | -6.77 | 92.72 | 111.00 |
| 2 | B | 521 | ILE | N-CA-C | -6.76 | 92.74 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2 | B | 589 | SER | O-C-N | 6.76 | 133.52 | 122.70 |
| 4 | M | 96 | ILE | O-C-N | 6.76 | 133.52 | 122.70 |
| 4 | M | 290 | PHE | C-N-CA | 6.76 | 138.60 | 121.70 |
| 2 | B | 544 | THR | O-C-N | 6.76 | 133.51 | 122.70 |
| 1 | A | 603 | VAL | O-C-N | 6.76 | 133.51 | 122.70 |
| 1 | A | 418 | ILE | N-CA-C | 6.76 | 129.24 | 111.00 |
| 2 | B | 559 | ASP | O-C-N | 6.76 | 133.51 | 122.70 |
| 4 | M | 85 | GLY | N-CA-C | -6.75 | 96.21 | 113.10 |
| 2 | B | 158 | VAL | CA-C-O | -6.75 | 105.92 | 120.10 |
| 2 | B | 150 | LEU | O-C-N | 6.75 | 133.49 | 122.70 |
| 1 | A | 156 | PRO | C-N-CA | -6.74 | 104.84 | 121.70 |
| 1 | A | 432 | ILE | CA-C-O | -6.74 | 105.94 | 120.10 |
| 1 | A | 607 | LEU | CA-C-O | -6.74 | 105.94 | 120.10 |
| 2 | B | 566 | ALA | CB-CA-C | 6.74 | 120.22 | 110.10 |
| 1 | A | 608 | ARG | O-C-N | 6.73 | 133.47 | 122.70 |
| 2 | B | 594 | ALA | O-C-N | 6.73 | 133.47 | 122.70 |
| 2 | B | 412 | PHE | O-C-N | 6.73 | 133.46 | 122.70 |
| 1 | A | 556 | VAL | O-C-N | 6.72 | 133.46 | 122.70 |
| 2 | B | 267 | ASP | C-N-CA | -6.72 | 104.89 | 121.70 |
| 1 | A | 605 | GLU | O-C-N | 6.72 | 133.46 | 122.70 |
| 1 | A | 471 | SER | O-C-N | 6.72 | 133.45 | 122.70 |
| 2 | B | 359 | LEU | O-C-N | 6.72 | 133.45 | 122.70 |
| 4 | M | 319 | SER | C-N-CA | 6.72 | 138.50 | 121.70 |
| 1 | A | 196 | LEU | CA-C-O | 6.72 | 134.20 | 120.10 |
| 1 | A | 467 | LYS | O-C-N | 6.71 | 133.44 | 122.70 |
| 3 | S | 150 | VAL | O-C-N | 6.71 | 133.43 | 122.70 |
| 4 | M | 284 | SER | O-C-N | -6.71 | 108.35 | 121.10 |
| 1 | A | 225 | LEU | CA-C-O | -6.71 | 106.02 | 120.10 |
| 1 | A | 600 | SER | O-C-N | 6.71 | 133.43 | 122.70 |
| 1 | A | 381 | GLU | O-C-N | -6.70 | 111.98 | 122.70 |
| 2 | B | 157 | THR | O-C-N | 6.70 | 133.42 | 122.70 |
| 3 | S | 30 | LEU | O-C-N | 6.69 | 133.41 | 122.70 |
| 4 | M | 54 | SER | CA-C-N | -6.69 | 102.49 | 117.20 |
| 2 | B | 123 | LEU | O-C-N | 6.68 | 133.38 | 122.70 |
| 4 | M | 4 | SER | CA-C-O | 6.67 | 134.12 | 120.10 |
| 4 | M | 59 | ASP | CB-CG-OD1 | 6.67 | 124.31 | 118.30 |
| 1 | A | 496 | ILE | O-C-N | 6.67 | 133.37 | 122.70 |
| 3 | S | 54 | PRO | N-CA-C | -6.67 | 94.76 | 112.10 |
| 2 | B | 306 | LEU | O-C-N | 6.67 | 133.37 | 122.70 |
| 2 | B | 508 | ARG | CA-C-O | 6.66 | 134.09 | 120.10 |
| 4 | M | 389 | SER | O-C-N | 6.66 | 133.36 | 122.70 |
| 2 | B | 513 | TRP | O-C-N | 6.66 | 133.36 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4 | M | 425 | THR | N-CA-C | -6.66 | 93.02 | 111.00 |
| 2 | B | 507 | ALA | O-C-N | 6.65 | 133.34 | 122.70 |
| 1 | A | 265 | GLN | O-C-N | -6.64 | 112.07 | 122.70 |
| 1 | A | 477 | PHE | O-C-N | 6.64 | 133.33 | 122.70 |
| 2 | B | 322 | CYS | O-C-N | 6.64 | 133.32 | 122.70 |
| 4 | M | 458 | LEU | N-CA-C | -6.64 | 93.07 | 111.00 |
| 1 | A | 465 | SER | O-C-N | 6.63 | 133.32 | 122.70 |
| 2 | B | 154 | ILE | CA-C-O | -6.63 | 106.17 | 120.10 |
| 1 | A | 297 | CYS | O-C-N | -6.63 | 112.09 | 122.70 |
| 1 | A | 522 | PHE | O-C-N | 6.63 | 133.31 | 122.70 |
| 4 | M | 94 | GLU | O-C-N | 6.63 | 133.31 | 122.70 |
| 2 | B | 591 | MET | O-C-N | 6.62 | 133.30 | 122.70 |
| 2 | B | 302 | PHE | O-C-N | 6.62 | 133.29 | 122.70 |
| 2 | B | 306 | LEU | CA-C-O | -6.62 | 106.19 | 120.10 |
| 4 | M | 130 | GLU | N-CA-CB | 6.62 | 122.52 | 110.60 |
| 2 | B | 361 | GLN | O-C-N | 6.61 | 133.28 | 122.70 |
| 1 | A | 388 | VAL | CA-C-O | -6.61 | 106.22 | 120.10 |
| 2 | B | 460 | SER | N-CA-C | 6.61 | 128.84 | 111.00 |
| 4 | M | 78 | ALA | CB-CA-C | 6.61 | 120.01 | 110.10 |
| 4 | M | 113 | LYS | O-C-N | 6.60 | 133.26 | 122.70 |
| 2 | B | 613 | MET | O-C-N | 6.60 | 133.26 | 122.70 |
| 2 | B | 134 | LEU | O-C-N | 6.60 | 133.26 | 122.70 |
| 4 | M | 63 | TYR | O-C-N | 6.60 | 133.26 | 122.70 |
| 4 | M | 385 | ARG | O-C-N | -6.60 | 112.15 | 122.70 |
| 1 | A | 307 | ASP | N-CA-C | -6.59 | 93.21 | 111.00 |
| 2 | B | 100 | LEU | O-C-N | 6.59 | 133.24 | 122.70 |
| 2 | B | 548 | ILE | O-C-N | 6.58 | 133.23 | 122.70 |
| 1 | A | 127 | LEU | O-C-N | 6.58 | 133.23 | 122.70 |
| 1 | A | 258 | LYS | O-C-N | 6.57 | 133.22 | 122.70 |
| 1 | A | 296 | ASN | O-C-N | 6.57 | 133.22 | 122.70 |
| 1 | A | 611 | LEU | O-C-N | 6.57 | 133.21 | 122.70 |
| 1 | A | 495 | ILE | O-C-N | 6.57 | 133.21 | 122.70 |
| 4 | M | 424 | PHE | N-CA-C | -6.57 | 93.27 | 111.00 |
| 2 | B | 343 | LEU | O-C-N | 6.57 | 133.20 | 122.70 |
| 2 | B | 154 | ILE | O-C-N | 6.56 | 133.20 | 122.70 |
| 2 | B | 604 | GLU | O-C-N | 6.56 | 133.20 | 122.70 |
| 3 | S | 18 | LYS | O-C-N | -6.56 | 112.20 | 122.70 |
| 4 | M | 125 | PHE | O-C-N | 6.56 | 133.20 | 122.70 |
| 1 | A | 240 | LEU | O-C-N | -6.56 | 112.20 | 122.70 |
| 2 | B | 301 | LEU | O-C-N | 6.55 | 133.19 | 122.70 |
| 1 | A | 146 | ALA | O-C-N | 6.55 | 133.18 | 122.70 |
| 1 | A | 297 | CYS | CA-C-O | 6.55 | 133.86 | 120.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | B | 63 | MET | O-C-N | 6.55 | 133.18 | 122.70 |
| 2 | B | 170 | ARG | O-C-N | -6.55 | 112.06 | 123.20 |
| 1 | A | 289 | SER | CA-C-O | 6.55 | 133.85 | 120.10 |
| 1 | A | 236 | LEU | O-C-N | 6.55 | 133.17 | 122.70 |
| 3 | S | 106 | VAL | CA-C-O | -6.54 | 106.36 | 120.10 |
| 2 | B | 230 | PHE | O-C-N | -6.54 | 112.23 | 122.70 |
| 2 | B | 453 | TRP | O-C-N | 6.54 | 133.16 | 122.70 |
| 2 | B | 510 | GLY | CA-C-O | -6.54 | 108.84 | 120.60 |
| 4 | M | 54 | SER | CB-CA-C | -6.53 | 97.69 | 110.10 |
| 1 | A | 91 | ILE | O-C-N | 6.53 | 133.14 | 122.70 |
| 1 | A | 87 | CYS | O-C-N | 6.53 | 133.14 | 122.70 |
| 1 | A | 475 | GLU | O-C-N | 6.52 | 133.14 | 122.70 |
| 2 | B | 146 | LYS | CA-C-N | 6.52 | 131.55 | 117.20 |
| 2 | B | 425 | PRO | O-C-N | 6.52 | 133.13 | 122.70 |
| 3 | S | 4 | ALA | O-C-N | -6.52 | 112.26 | 122.70 |
| 2 | B | 181 | TYR | C-N-CA | -6.52 | 105.40 | 121.70 |
| 2 | B | 414 | GLU | O-C-N | 6.52 | 133.13 | 122.70 |
| 4 | M | 265 | ASN | CA-C-N | 6.51 | 131.53 | 117.20 |
| 2 | B | 325 | LEU | C-N-CA | -6.51 | 105.42 | 121.70 |
| 2 | B | 337 | THR | CA-C-O | -6.51 | 106.42 | 120.10 |
| 2 | B | 607 | ILE | O-C-N | 6.51 | 133.12 | 122.70 |
| 4 | M | 281 | GLY | N-CA-C | -6.51 | 96.82 | 113.10 |
| 1 | A | 613 | ALA | O-C-N | 6.51 | 133.11 | 122.70 |
| 2 | B | 246 | SER | O-C-N | 6.51 | 133.11 | 122.70 |
| 2 | B | 256 | CYS | O-C-N | -6.51 | 112.29 | 122.70 |
| 1 | A | 522 | PHE | CA-C-O | -6.50 | 106.44 | 120.10 |
| 2 | B | 344 | VAL | O-C-N | 6.50 | 133.10 | 122.70 |
| 2 | B | 105 | LEU | CA-C-O | 6.50 | 133.75 | 120.10 |
| 3 | S | 4 | ALA | CA-C-O | 6.50 | 133.74 | 120.10 |
| 1 | A | 472 | LYS | O-C-N | 6.49 | 133.09 | 122.70 |
| 1 | A | 562 | TRP | O-C-N | 6.49 | 133.09 | 122.70 |
| 2 | B | 181 | TYR | O-C-N | -6.49 | 112.31 | 122.70 |
| 1 | A | 107 | TYR | CA-C-O | -6.49 | 106.47 | 120.10 |
| 3 | S | 101 | LEU | O-C-N | 6.49 | 133.08 | 122.70 |
| 2 | B | 135 | ARG | O-C-N | 6.49 | 133.08 | 122.70 |
| 1 | A | 487 | MET | C-N-CA | -6.49 | 105.49 | 121.70 |
| 2 | B | 116 | THR | O-C-N | 6.49 | 133.08 | 122.70 |
| 2 | B | 467 | VAL | O-C-N | 6.49 | 133.08 | 122.70 |
| 2 | B | 485 | LYS | O-C-N | 6.48 | 133.07 | 122.70 |
| 3 | S | 129 | GLU | O-C-N | 6.48 | 133.07 | 122.70 |
| 4 | M | 117 | ASN | O-C-N | 6.48 | 133.07 | 122.70 |
| 4 | M | 277 | GLU | C-N-CA | -6.48 | 105.50 | 121.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | B | 588 | ILE | O-C-N | 6.48 | 133.07 | 122.70 |
| 2 | B | 285 | GLU | N-CA-C | -6.48 | 93.51 | 111.00 |
| 2 | B | 582 | ASP | CA-C-N | 6.48 | 131.45 | 117.20 |
| 4 | M | 107 | ASP | CA-C-N | 6.48 | 131.45 | 117.20 |
| 1 | A | 609 | LEU | O-C-N | 6.47 | 133.05 | 122.70 |
| 1 | A | 462 | GLN | C-N-CA | -6.47 | 105.53 | 121.70 |
| 2 | B | 585 | GLY | O-C-N | 6.47 | 133.05 | 122.70 |
| 2 | B | 305 | SER | O-C-N | 6.46 | 133.04 | 122.70 |
| 1 | A | 385 | LYS | O-C-N | 6.46 | 133.04 | 122.70 |
| 2 | B | 151 | ALA | CA-C-O | -6.46 | 106.53 | 120.10 |
| 3 | S | 127 | THR | O-C-N | 6.46 | 133.04 | 122.70 |
| 4 | M | 124 | ILE | O-C-N | 6.46 | 133.04 | 122.70 |
| 1 | A | 145 | ILE | O-C-N | 6.46 | 133.03 | 122.70 |
| 1 | A | 386 | ALA | O-C-N | 6.46 | 133.03 | 122.70 |
| 2 | B | 102 | HIS | C-N-CA | -6.46 | 105.55 | 121.70 |
| 2 | B | 81 | LEU | C-N-CA | -6.46 | 105.56 | 121.70 |
| 4 | M | 457 | GLY | CA-C-N | -6.46 | 103.00 | 117.20 |
| 1 | A | 486 | SER | N-CA-C | -6.45 | 93.58 | 111.00 |
| 2 | B | 450 | VAL | O-C-N | 6.45 | 133.03 | 122.70 |
| 2 | B | 454 | LEU | O-C-N | 6.45 | 133.02 | 122.70 |
| 4 | M | 123 | LEU | O-C-N | 6.45 | 133.02 | 122.70 |
| 1 | A | 80 | TYR | N-CA-CB | 6.44 | 122.20 | 110.60 |
| 2 | B | 244 | SER | O-C-N | 6.44 | 133.01 | 122.70 |
| 1 | A | 407 | SER | N-CA-C | -6.44 | 93.60 | 111.00 |
| 1 | A | 200 | PHE | O-C-N | 6.44 | 133.00 | 122.70 |
| 2 | B | 62 | ALA | O-C-N | 6.44 | 133.00 | 122.70 |
| 2 | B | 65 | ARG | O-C-N | 6.44 | 133.00 | 122.70 |
| 4 | M | 105 | ASP | N-CA-C | 6.44 | 128.38 | 111.00 |
| 2 | B | 151 | ALA | O-C-N | 6.43 | 133.33 | 121.10 |
| 3 | S | 105 | PHE | O-C-N | 6.43 | 132.99 | 122.70 |
| 1 | A | 415 | ARG | C-N-CA | -6.43 | 105.62 | 121.70 |
| 2 | B | 296 | ASP | O-C-N | 6.43 | 133.31 | 121.10 |
| 1 | A | 476 | GLN | O-C-N | 6.43 | 132.98 | 122.70 |
| 1 | A | 516 | ILE | O-C-N | 6.42 | 132.98 | 122.70 |
| 2 | B | 472 | VAL | CA-C-O | 6.42 | 133.59 | 120.10 |
| 1 | A | 579 | LYS | O-C-N | 6.42 | 132.97 | 122.70 |
| 2 | B | 417 | TYR | O-C-N | 6.42 | 132.97 | 122.70 |
| 4 | M | 65 | TYR | C-N-CA | -6.42 | 105.65 | 121.70 |
| 1 | A | 348 | PHE | O-C-N | 6.42 | 132.96 | 122.70 |
| 2 | B | 229 | HIS | C-N-CA | 6.41 | 137.73 | 121.70 |
| 4 | M | 122 | SER | O-C-N | 6.41 | 132.95 | 122.70 |
| 1 | A | 159 | ALA | O-C-N | 6.41 | 132.95 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | A | 302 | ASN | CA-C-O | 6.41 | 133.55 | 120.10 |
| 1 | A | 629 | LEU | C-N-CA | -6.41 | 95.09 | 122.00 |
| 2 | B | 612 | ARG | O-C-N | 6.41 | 132.95 | 122.70 |
| 1 | A | 215 | VAL | O-C-N | -6.40 | 112.46 | 122.70 |
| 2 | B | 360 | LEU | O-C-N | 6.40 | 132.94 | 122.70 |
| 1 | A | 550 | VAL | O-C-N | 6.40 | 132.93 | 122.70 |
| 1 | A | 83 | ASP | CA-C-N | -6.39 | 103.13 | 117.20 |
| 2 | B | 145 | MET | C-N-CA | -6.39 | 105.73 | 121.70 |
| 1 | A | 425 | LYS | O-C-N | 6.38 | 132.91 | 122.70 |
| 2 | B | 191 | GLU | O-C-N | 6.38 | 132.92 | 122.70 |
| 2 | B | 399 | LEU | C-N-CA | -6.38 | 105.74 | 121.70 |
| 2 | B | 79 | VAL | CA-C-O | -6.38 | 106.70 | 120.10 |
| 1 | A | 64 | LEU | CA-C-O | 6.38 | 133.50 | 120.10 |
| 1 | A | 558 | VAL | O-C-N | 6.38 | 132.91 | 122.70 |
| 1 | A | 604 | LEU | O-C-N | 6.38 | 132.91 | 122.70 |
| 1 | A | 147 | LEU | O-C-N | 6.38 | 132.90 | 122.70 |
| 2 | B | 139 | LEU | CA-C-O | -6.37 | 106.72 | 120.10 |
| 2 | B | 342 | ALA | O-C-N | 6.37 | 132.90 | 122.70 |
| 1 | A | 554 | ALA | O-C-N | 6.37 | 132.89 | 122.70 |
| 2 | B | 452 | LYS | O-C-N | 6.37 | 132.89 | 122.70 |
| 1 | A | 290 | VAL | CA-C-O | -6.37 | 106.72 | 120.10 |
| 1 | A | 141 | VAL | O-C-N | 6.37 | 132.89 | 122.70 |
| 1 | A | 634 | ASN | O-C-N | 6.37 | 132.89 | 122.70 |
| 2 | B | 271 | GLU | N-CA-C | 6.37 | 128.19 | 111.00 |
| 2 | B | 615 | SER | O-C-N | 6.37 | 132.89 | 122.70 |
| 2 | B | 123 | LEU | CA-C-O | -6.37 | 106.73 | 120.10 |
| 2 | B | 610 | ARG | O-C-N | 6.37 | 132.88 | 122.70 |
| 4 | M | 86 | PRO | O-C-N | 6.37 | 132.89 | 122.70 |
| 1 | A | 211 | ASP | O-C-N | 6.36 | 132.88 | 122.70 |
| 1 | A | 454 | ILE | O-C-N | 6.36 | 132.87 | 122.70 |
| 2 | B | 614 | ILE | O-C-N | 6.36 | 132.87 | 122.70 |
| 1 | A | 202 | LYS | O-C-N | 6.36 | 132.87 | 122.70 |
| 1 | A | 128 | LEU | O-C-N | 6.35 | 132.86 | 122.70 |
| 2 | B | 388 | PRO | C-N-CA | 6.35 | 137.57 | 121.70 |
| 2 | B | 592 | TYR | O-C-N | 6.34 | 132.85 | 122.70 |
| 2 | B | 341 | GLU | O-C-N | 6.34 | 132.84 | 122.70 |
| 1 | A | 278 | ILE | C-N-CA | 6.34 | 137.54 | 121.70 |
| 4 | M | 16 | PHE | CA-C-O | 6.34 | 133.41 | 120.10 |
| 1 | A | 332 | TYR | O-C-N | 6.33 | 132.83 | 122.70 |
| 4 | M | 90 | PHE | O-C-N | 6.33 | 132.84 | 122.70 |
| 1 | A | 331 | ARG | O-C-N | 6.33 | 132.83 | 122.70 |
| 3 | S | 1 | MET | O-C-N | -6.33 | 112.57 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 4 | M | 51 | LEU | O-C-N | -6.33 | 112.57 | 122.70 |
| 4 | M | 3 | LEU | CA-C-O | 6.33 | 133.38 | 120.10 |
| 1 | A | 186 | PHE | O-C-N | 6.32 | 132.81 | 122.70 |
| 2 | B | 209 | SER | O-C-N | 6.32 | 132.81 | 122.70 |
| 4 | M | 402 | SER | CA-C-N | 6.32 | 131.10 | 117.20 |
| 3 | S | 165 | SER | C-N-CA | -6.32 | 105.91 | 121.70 |
| 1 | A | 421 | PRO | O-C-N | 6.31 | 132.80 | 122.70 |
| 1 | A | 603 | VAL | CA-C-O | -6.31 | 106.84 | 120.10 |
| 4 | M | 232 | HIS | O-C-N | -6.31 | 112.60 | 122.70 |
| 1 | A | 185 | LEU | O-C-N | 6.31 | 132.80 | 122.70 |
| 2 | B | 67 | ILE | O-C-N | 6.31 | 132.80 | 122.70 |
| 2 | B | 177 | ILE | O-C-N | 6.31 | 132.79 | 122.70 |
| 2 | B | 435 | SER | O-C-N | 6.31 | 132.79 | 122.70 |
| 1 | A | 492 | ILE | O-C-N | 6.31 | 132.79 | 122.70 |
| 1 | A | 428 | MET | O-C-N | 6.30 | 132.78 | 122.70 |
| 1 | A | 316 | LEU | O-C-N | 6.30 | 132.78 | 122.70 |
| 2 | B | 302 | PHE | CA-C-O | -6.30 | 106.87 | 120.10 |
| 1 | A | 110 | ALA | O-C-N | -6.30 | 112.62 | 122.70 |
| 2 | B | 409 | LYS | O-C-N | 6.29 | 132.77 | 122.70 |
| 1 | A | 155 | THR | CA-C-O | -6.29 | 106.88 | 120.10 |
| 2 | B | 595 | VAL | O-C-N | 6.29 | 132.77 | 122.70 |
| 1 | A | 395 | PHE | C-N-CA | -6.29 | 105.99 | 121.70 |
| 2 | B | 101 | ILE | O-C-N | 6.29 | 132.76 | 122.70 |
| 2 | B | 262 | LYS | C-N-CA | -6.29 | 95.60 | 122.00 |
| 3 | S | 130 | SER | O-C-N | 6.29 | 132.76 | 122.70 |
| 2 | B | 490 | ILE | O-C-N | 6.28 | 132.75 | 122.70 |
| 2 | B | 550 | VAL | O-C-N | 6.28 | 132.75 | 122.70 |
| 1 | A | 139 | ASP | O-C-N | 6.28 | 132.74 | 122.70 |
| 1 | A | 620 | GLY | CA-C-O | -6.28 | 109.30 | 120.60 |
| 1 | A | 337 | LEU | O-C-N | 6.28 | 132.74 | 122.70 |
| 1 | A | 552 | ILE | O-C-N | 6.28 | 132.74 | 122.70 |
| 3 | S | 80 | TYR | O-C-N | -6.28 | 112.66 | 122.70 |
| 1 | A | 252 | ILE | O-C-N | 6.27 | 132.73 | 122.70 |
| 1 | A | 298 | ILE | C-N-CA | -6.27 | 106.03 | 121.70 |
| 1 | A | 473 | ILE | O-C-N | 6.27 | 133.86 | 123.20 |
| 2 | B | 193 | LEU | O-C-N | 6.27 | 132.73 | 122.70 |
| 4 | M | 126 | ASN | CA-C-O | -6.27 | 106.94 | 120.10 |
| 1 | A | 117 | ASP | O-C-N | 6.27 | 132.72 | 122.70 |
| 1 | A | 625 | LEU | O-C-N | -6.27 | 112.67 | 122.70 |
| 2 | B | 394 | TRP | O-C-N | 6.26 | 132.72 | 122.70 |
| 2 | B | 587 | ARG | O-C-N | 6.26 | 132.72 | 122.70 |
| 1 | A | 569 | ASP | CA-C-O | -6.26 | 106.95 | 120.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | B | 346 | THR | O-C-N | 6.26 | 132.71 | 122.70 |
| 2 | B | 64 | LYS | O-C-N | 6.25 | 132.70 | 122.70 |
| 2 | B | 549 | LEU | O-C-N | 6.25 | 132.71 | 122.70 |
| 1 | A | 387 | ILE | O-C-N | 6.25 | 132.70 | 122.70 |
| 1 | A | 574 | ILE | O-C-N | 6.25 | 132.70 | 122.70 |
| 2 | B | 432 | ALA | O-C-N | 6.25 | 132.70 | 122.70 |
| 4 | M | 55 | MET | C-N-CA | -6.25 | 106.08 | 121.70 |
| 3 | S | 120 | ASP | O-C-N | 6.25 | 132.69 | 122.70 |
| 1 | A | 333 | ILE | O-C-N | 6.24 | 132.69 | 122.70 |
| 1 | A | 68 | THR | O-C-N | 6.24 | 132.69 | 122.70 |
| 1 | A | 439 | ASP | N-CA-CB | 6.24 | 121.83 | 110.60 |
| 2 | B | 374 | PHE | O-C-N | 6.24 | 132.68 | 122.70 |
| 1 | A | 576 | MET | O-C-N | 6.23 | 132.67 | 122.70 |
| 4 | M | 368 | ASP | CA-C-O | -6.23 | 107.01 | 120.10 |
| 2 | B | 249 | ILE | O-C-N | 6.23 | 132.67 | 122.70 |
| 1 | A | 335 | CYS | O-C-N | 6.23 | 132.66 | 122.70 |
| 1 | A | 421 | PRO | CA-C-O | -6.23 | 105.26 | 120.20 |
| 3 | S | 85 | PHE | CA-C-O | 6.23 | 133.18 | 120.10 |
| 4 | M | 394 | GLN | O-C-N | -6.23 | 112.61 | 123.20 |
| 1 | A | 632 | PHE | O-C-N | 6.22 | 132.66 | 122.70 |
| 2 | B | 426 | GLU | O-C-N | 6.22 | 132.66 | 122.70 |
| 2 | B | 111 | ASN | N-CA-C | 6.22 | 127.79 | 111.00 |
| 2 | B | 272 | GLY | N-CA-C | -6.22 | 97.55 | 113.10 |
| 2 | B | 522 | GLU | O-C-N | 6.22 | 132.65 | 122.70 |
| 1 | A | 492 | ILE | CA-C-O | -6.22 | 107.04 | 120.10 |
| 1 | A | 353 | ASP | O-C-N | 6.22 | 132.65 | 122.70 |
| 4 | M | 77 | LEU | CA-C-O | 6.22 | 133.15 | 120.10 |
| 2 | B | 59 | VAL | O-C-N | 6.21 | 132.64 | 122.70 |
| 2 | B | 363 | ILE | CA-C-O | -6.21 | 107.05 | 120.10 |
| 1 | A | 98 | ASN | O-C-N | -6.21 | 112.76 | 122.70 |
| 1 | A | 372 | ILE | O-C-N | 6.21 | 132.63 | 122.70 |
| 1 | A | 274 | LEU | C-N-CA | -6.20 | 106.19 | 121.70 |
| 2 | B | 455 | ILE | O-C-N | 6.20 | 132.62 | 122.70 |
| 3 | S | 149 | ILE | O-C-N | 6.20 | 132.62 | 122.70 |
| 4 | M | 272 | LEU | C-N-CA | 6.19 | 137.18 | 121.70 |
| 2 | B | 155 | LEU | O-C-N | 6.19 | 132.60 | 122.70 |
| 1 | A | 140 | VAL | C-N-CA | -6.19 | 106.23 | 121.70 |
| 2 | B | 605 | PHE | O-C-N | 6.19 | 132.60 | 122.70 |
| 1 | A | 108 | LEU | CA-C-O | -6.18 | 107.11 | 120.10 |
| 1 | A | 429 | VAL | O-C-N | 6.18 | 132.60 | 122.70 |
| 2 | B | 119 | SER | O-C-N | 6.18 | 132.60 | 122.70 |
| 2 | B | 430 | ILE | O-C-N | 6.18 | 132.59 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | A | 628 | VAL | O-C-N | 6.18 | 132.59 | 122.70 |
| 2 | B | 543 | GLU | O-C-N | 6.18 | 132.59 | 122.70 |
| 2 | B | 593 | ASN | O-C-N | 6.18 | 132.59 | 122.70 |
| 2 | B | 410 | GLU | O-C-N | 6.18 | 132.59 | 122.70 |
| 1 | A | 458 | ALA | O-C-N | 6.18 | 132.58 | 122.70 |
| 2 | B | 251 | LEU | O-C-N | 6.18 | 132.58 | 122.70 |
| 4 | M | 65 | TYR | O-C-N | 6.17 | 132.58 | 122.70 |
| 1 | A | 138 | ASN | O-C-N | 6.17 | 132.57 | 122.70 |
| 2 | B | 495 | ASP | O-C-N | 6.16 | 132.56 | 122.70 |
| 2 | B | 58 | GLU | O-C-N | 6.16 | 132.56 | 122.70 |
| 2 | B | 511 | ILE | CA-C-O | 6.16 | 133.03 | 120.10 |
| 4 | M | 111 | ILE | O-C-N | 6.16 | 132.55 | 122.70 |
| 4 | M | 421 | GLY | CA-C-O | 6.16 | 131.68 | 120.60 |
| 1 | A | 241 | TYR | O-C-N | 6.16 | 132.55 | 122.70 |
| 2 | B | 532 | ARG | O-C-N | 6.16 | 132.55 | 122.70 |
| 2 | B | 248 | LEU | O-C-N | 6.15 | 132.55 | 122.70 |
| 2 | B | 429 | VAL | O-C-N | 6.15 | 132.55 | 122.70 |
| 2 | B | 136 | CYS | O-C-N | 6.15 | 132.54 | 122.70 |
| 2 | B | 145 | MET | CA-C-N | 6.15 | 130.73 | 117.20 |
| 3 | S | 43 | ASN | C-N-CA | -6.15 | 106.33 | 121.70 |
| 1 | A | 295 | VAL | CA-C-O | -6.15 | 107.19 | 120.10 |
| 1 | A | 339 | TYR | O-C-N | 6.15 | 132.53 | 122.70 |
| 1 | A | 142 | LYS | O-C-N | 6.14 | 132.53 | 122.70 |
| 2 | B | 233 | TYR | O-C-N | 6.14 | 132.53 | 122.70 |
| 4 | M | 429 | ASP | C-N-CA | -6.14 | 106.34 | 121.70 |
| 2 | B | 196 | LEU | O-C-N | 6.14 | 132.53 | 122.70 |
| 1 | A | 312 | ALA | O-C-N | 6.14 | 132.52 | 122.70 |
| 3 | S | 83 | LEU | O-C-N | -6.14 | 112.88 | 122.70 |
| 2 | B | 337 | THR | O-C-N | 6.14 | 132.52 | 122.70 |
| 4 | M | 107 | ASP | CA-C-O | -6.14 | 107.22 | 120.10 |
| 2 | B | 551 | LEU | O-C-N | 6.13 | 132.51 | 122.70 |
| 3 | S | 70 | ASN | CA-C-O | 6.13 | 132.98 | 120.10 |
| 2 | B | 82 | TYR | O-C-N | -6.13 | 112.89 | 122.70 |
| 2 | B | 324 | ALA | O-C-N | 6.13 | 132.50 | 122.70 |
| 3 | S | 145 | ASN | O-C-N | 6.13 | 132.50 | 122.70 |
| 1 | A | 143 | VAL | O-C-N | 6.13 | 133.62 | 123.20 |
| 2 | B | 464 | SER | O-C-N | 6.13 | 132.50 | 122.70 |
| 3 | S | 21 | THR | C-N-CA | -6.13 | 96.27 | 122.00 |
| 2 | B | 195 | ILE | O-C-N | 6.12 | 132.49 | 122.70 |
| 2 | B | 512 | VAL | O-C-N | 6.12 | 132.49 | 122.70 |
| 3 | S | 81 | ALA | N-CA-C | -6.12 | 94.48 | 111.00 |
| 1 | A | 491 | THR | O-C-N | 6.11 | 132.48 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3 | S | 64 | ASN | C-N-CA | -6.11 | 106.42 | 121.70 |
| 4 | M | 290 | PHE | N-CA-C | -6.11 | 94.51 | 111.00 |
| 1 | A | 598 | GLU | O-C-N | 6.11 | 132.47 | 122.70 |
| 2 | B | 510 | GLY | O-C-N | 6.11 | 132.47 | 122.70 |
| 1 | A | 313 | MET | O-C-N | 6.11 | 132.47 | 122.70 |
| 1 | A | 237 | SER | CA-C-O | -6.10 | 107.29 | 120.10 |
| 1 | A | 584 | PHE | O-C-N | 6.10 | 132.46 | 122.70 |
| 4 | M | 135 | ASN | N-CA-CB | 6.10 | 121.57 | 110.60 |
| 3 | S | 38 | LEU | O-C-N | 6.10 | 132.45 | 122.70 |
| 2 | B | 178 | ILE | O-C-N | 6.09 | 132.45 | 122.70 |
| 2 | B | 553 | ALA | O-C-N | 6.09 | 132.44 | 122.70 |
| 4 | M | 398 | ILE | O-C-N | -6.09 | 112.95 | 122.70 |
| 2 | B | 244 | SER | CA-C-O | -6.09 | 107.32 | 120.10 |
| 2 | B | 582 | ASP | O-C-N | -6.08 | 112.97 | 122.70 |
| 1 | A | 390 | THR | O-C-N | 6.08 | 132.42 | 122.70 |
| 2 | B | 74 | ASP | C-N-CA | 6.07 | 136.88 | 121.70 |
| 2 | B | 44 | PRO | O-C-N | 6.07 | 132.41 | 122.70 |
| 2 | B | 355 | ASN | CA-C-O | -6.07 | 107.36 | 120.10 |
| 3 | S | 139 | GLY | N-CA-C | -6.07 | 97.93 | 113.10 |
| 2 | B | 166 | SER | O-C-N | 6.06 | 132.40 | 122.70 |
| 1 | A | 158 | LEU | CA-C-O | -6.06 | 107.38 | 120.10 |
| 1 | A | 578 | LEU | O-C-N | 6.06 | 132.39 | 122.70 |
| 1 | A | 81 | GLY | C-N-CA | 6.06 | 136.84 | 121.70 |
| 1 | A | 533 | ILE | CA-C-O | -6.05 | 107.39 | 120.10 |
| 1 | A | 557 | LYS | O-C-N | 6.05 | 132.39 | 122.70 |
| 3 | S | 85 | PHE | O-C-N | -6.05 | 113.01 | 122.70 |
| 4 | M | 381 | ASN | N-CA-C | -6.05 | 94.65 | 111.00 |
| 1 | A | 631 | SER | CA-C-O | -6.05 | 107.39 | 120.10 |
| 4 | M | 91 | THR | O-C-N | 6.05 | 132.38 | 122.70 |
| 2 | B | 131 | ASN | O-C-N | 6.05 | 132.38 | 122.70 |
| 2 | B | 469 | ASP | CA-C-O | -6.05 | 107.40 | 120.10 |
| 2 | B | 568 | VAL | O-C-N | 6.05 | 132.37 | 122.70 |
| 3 | S | 16 | LEU | CA-C-O | 6.04 | 132.79 | 120.10 |
| 2 | B | 189 | HIS | O-C-N | 6.04 | 132.37 | 122.70 |
| 4 | M | 131 | ALA | C-N-CA | 6.04 | 134.98 | 122.30 |
| 1 | A | 104 | ARG | O-C-N | 6.04 | 132.36 | 122.70 |
| 4 | M | 237 | THR | O-C-N | -6.04 | 112.93 | 123.20 |
| 1 | A | 122 | MET | O-C-N | 6.04 | 132.36 | 122.70 |
| 2 | B | 207 | VAL | O-C-N | 6.04 | 132.36 | 122.70 |
| 2 | B | 585 | GLY | CA-C-O | -6.04 | 109.73 | 120.60 |
| 1 | A | 125 | THR | O-C-N | 6.03 | 132.35 | 122.70 |
| 2 | B | 358 | MET | O-C-N | 6.03 | 132.35 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3 | S | 32 | LEU | CA-C-O | -6.03 | 107.43 | 120.10 |
| 2 | B | 525 | ILE | O-C-N | 6.03 | 132.35 | 122.70 |
| 1 | A | 494 | ASN | O-C-N | 6.03 | 132.35 | 122.70 |
| 2 | B | 155 | LEU | CA-C-O | -6.03 | 107.44 | 120.10 |
| 1 | A | 296 | ASN | CA-C-O | -6.03 | 107.45 | 120.10 |
| 1 | A | 633 | PHE | CA-C-O | -6.03 | 107.45 | 120.10 |
| 2 | B | 150 | LEU | CA-C-O | -6.03 | 107.45 | 120.10 |
| 1 | A | 229 | ASN | C-N-CD | 6.02 | 141.05 | 128.40 |
| 3 | S | 96 | LEU | CA-C-O | -6.02 | 107.45 | 120.10 |
| 2 | B | 255 | TYR | O-C-N | 6.02 | 132.33 | 122.70 |
| 2 | B | 184 | GLY | CA-C-O | 6.01 | 131.42 | 120.60 |
| 2 | B | 190 | GLU | O-C-N | 6.01 | 132.32 | 122.70 |
| 1 | A | 71 | VAL | CA-C-O | -6.01 | 107.48 | 120.10 |
| 4 | M | 426 | LYS | N-CA-C | -6.01 | 94.78 | 111.00 |
| 2 | B | 103 | LEU | O-C-N | 6.01 | 132.31 | 122.70 |
| 2 | B | 462 | ASN | C-N-CA | -6.01 | 106.68 | 121.70 |
| 1 | A | 545 | HIS | CA-C-O | 6.00 | 132.70 | 120.10 |
| 2 | B | 209 | SER | CA-C-O | -6.00 | 107.50 | 120.10 |
| 2 | B | 413 | LYS | O-C-N | 6.00 | 132.30 | 122.70 |
| 1 | A | 336 | ILE | O-C-N | 6.00 | 132.30 | 122.70 |
| 1 | A | 538 | GLU | C-N-CA | -6.00 | 106.71 | 121.70 |
| 2 | B | 433 | VAL | O-C-N | 6.00 | 132.29 | 122.70 |
| 2 | B | 303 | LEU | O-C-N | 5.99 | 132.29 | 122.70 |
| 1 | A | 154 | ILE | C-N-CA | -5.99 | 106.72 | 121.70 |
| 1 | A | 108 | LEU | O-C-N | 5.99 | 132.28 | 122.70 |
| 2 | B | 437 | SER | O-C-N | 5.99 | 132.28 | 122.70 |
| 1 | A | 121 | LEU | O-C-N | 5.98 | 132.27 | 122.70 |
| 2 | B | 314 | ASN | O-C-N | 5.98 | 132.47 | 121.10 |
| 4 | M | 6 | TYR | CA-C-O | 5.98 | 132.66 | 120.10 |
| 4 | M | 283 | PHE | N-CA-C | -5.98 | 94.84 | 111.00 |
| 1 | A | 625 | LEU | C-N-CA | -5.98 | 106.75 | 121.70 |
| 1 | A | 249 | ASN | O-C-N | 5.98 | 132.27 | 122.70 |
| 4 | M | 117 | ASN | CA-C-O | -5.98 | 107.55 | 120.10 |
| 4 | M | 131 | ALA | N-CA-C | 5.98 | 127.14 | 111.00 |
| 2 | B | 523 | PHE | C-N-CA | -5.98 | 106.76 | 121.70 |
| 1 | A | 162 | ILE | CA-C-O | -5.97 | 107.56 | 120.10 |
| 1 | A | 230 | PRO | CA-C-O | -5.97 | 105.88 | 120.20 |
| 1 | A | 600 | SER | CA-C-O | -5.97 | 107.56 | 120.10 |
| 1 | A | 325 | SER | CA-C-N | -5.97 | 104.07 | 117.20 |
| 2 | B | 98 | LYS | O-C-N | 5.97 | 132.25 | 122.70 |
| 1 | A | 454 | ILE | CA-C-O | -5.96 | 107.58 | 120.10 |
| 2 | B | 47 | LEU | O-C-N | 5.96 | 132.24 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | A | 217 | ALA | CA-C-O | -5.95 | 107.60 | 120.10 |
| 1 | A | 448 | GLU | C-N-CA | 5.95 | 136.58 | 121.70 |
| 1 | A | 130 | LYS | O-C-N | 5.95 | 132.22 | 122.70 |
| 1 | A | 323 | CYS | CA-C-N | 5.95 | 130.29 | 117.20 |
| 1 | A | 491 | THR | CA-C-O | -5.95 | 107.60 | 120.10 |
| 2 | B | 204 | ASP | O-C-N | 5.95 | 132.41 | 121.10 |
| 1 | A | 155 | THR | O-C-N | 5.95 | 132.40 | 121.10 |
| 1 | A | 499 | ILE | C-N-CA | -5.95 | 106.83 | 121.70 |
| 2 | B | 333 | GLN | N-CA-C | -5.95 | 94.94 | 111.00 |
| 1 | A | 309 | PHE | O-C-N | 5.95 | 132.21 | 122.70 |
| 2 | B | 238 | LYS | C-N-CA | 5.95 | 136.56 | 121.70 |
| 1 | A | 271 | ARG | CA-C-O | -5.94 | 107.62 | 120.10 |
| 1 | A | 513 | ARG | CA-C-O | -5.94 | 107.62 | 120.10 |
| 4 | M | 120 | ARG | O-C-N | 5.94 | 132.20 | 122.70 |
| 4 | M | 74 | TYR | O-C-N | -5.94 | 113.20 | 122.70 |
| 1 | A | 566 | PHE | C-N-CA | 5.93 | 136.53 | 121.70 |
| 1 | A | 369 | SER | O-C-N | 5.93 | 132.19 | 122.70 |
| 3 | S | 107 | GLU | O-C-N | 5.93 | 132.19 | 122.70 |
| 1 | A | 325 | SER | C-N-CA | 5.92 | 136.51 | 121.70 |
| 2 | B | 407 | ASN | O-C-N | 5.92 | 132.18 | 122.70 |
| 4 | M | 367 | ALA | N-CA-C | -5.92 | 95.00 | 111.00 |
| 1 | A | 371 | ALA | O-C-N | 5.92 | 132.18 | 122.70 |
| 1 | A | 518 | CYS | CA-C-O | -5.92 | 107.66 | 120.10 |
| 1 | A | 278 | ILE | O-C-N | -5.92 | 113.22 | 122.70 |
| 2 | B | 402 | LEU | N-CA-C | 5.92 | 126.98 | 111.00 |
| 1 | A | 452 | ALA | O-C-N | 5.92 | 132.16 | 122.70 |
| 2 | B | 586 | SER | O-C-N | 5.91 | 132.16 | 122.70 |
| 2 | B | 247 | TYR | O-C-N | 5.91 | 132.16 | 122.70 |
| 3 | S | 154 | ASP | O-C-N | 5.91 | 132.15 | 122.70 |
| 1 | A | 400 | VAL | O-C-N | 5.91 | 132.15 | 122.70 |
| 3 | S | 152 | SER | O-C-N | 5.91 | 132.15 | 122.70 |
| 2 | B | 174 | ALA | CA-C-O | 5.90 | 132.50 | 120.10 |
| 2 | B | 446 | TRP | O-C-N | 5.90 | 132.15 | 122.70 |
| 1 | A | 287 | ALA | N-CA-C | 5.90 | 126.94 | 111.00 |
| 1 | A | 268 | PRO | O-C-N | 5.90 | 132.14 | 122.70 |
| 1 | A | 500 | SER | O-C-N | -5.90 | 113.26 | 122.70 |
| 2 | B | 250 | GLU | O-C-N | 5.90 | 132.14 | 122.70 |
| 2 | B | 444 | THR | CA-C-O | 5.90 | 132.49 | 120.10 |
| 2 | B | 239 | GLN | C-N-CA | 5.90 | 136.44 | 121.70 |
| 2 | B | 579 | PRO | N-CA-C | 5.90 | 127.43 | 112.10 |
| 1 | A | 490 | VAL | O-C-N | 5.90 | 132.13 | 122.70 |
| 3 | S | 61 | ASN | C-N-CA | -5.89 | 106.97 | 121.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | B | 469 | ASP | O-C-N | 5.89 | 132.13 | 122.70 |
| 2 | B | 590 | GLN | O-C-N | 5.89 | 132.13 | 122.70 |
| 2 | B | 396 | ILE | O-C-N | 5.89 | 132.12 | 122.70 |
| 2 | B | 496 | LEU | O-C-N | 5.89 | 132.12 | 122.70 |
| 4 | M | 280 | ASP | CA-C-N | -5.89 | 104.42 | 116.20 |
| 4 | M | 306 | LEU | CA-C-O | 5.89 | 132.46 | 120.10 |
| 1 | A | 553 | LEU | O-C-N | 5.88 | 132.11 | 122.70 |
| 2 | B | 214 | ALA | O-C-N | 5.88 | 132.12 | 122.70 |
| 2 | B | 546 | CYS | O-C-N | 5.88 | 132.12 | 122.70 |
| 3 | S | 159 | ALA | O-C-N | 5.88 | 132.11 | 122.70 |
| 2 | B | 530 | LEU | O-C-N | 5.88 | 132.11 | 122.70 |
| 1 | A | 419 | ILE | N-CA-C | 5.88 | 126.88 | 111.00 |
| 1 | A | 257 | LEU | CA-C-O | -5.88 | 107.76 | 120.10 |
| 1 | A | 106 | GLY | CA-C-O | -5.88 | 110.02 | 120.60 |
| 4 | M | 121 | ILE | O-C-N | 5.87 | 132.10 | 122.70 |
| 1 | A | 276 | PRO | O-C-N | -5.87 | 113.31 | 122.70 |
| 2 | B | 393 | ILE | O-C-N | 5.87 | 132.09 | 122.70 |
| 2 | B | 526 | CYS | CA-C-O | -5.86 | 107.79 | 120.10 |
| 1 | A | 436 | CYS | C-N-CA | -5.86 | 107.05 | 121.70 |
| 4 | M | 46 | SER | O-C-N | -5.86 | 113.32 | 122.70 |
| 1 | A | 251 | TRP | O-C-N | 5.86 | 132.07 | 122.70 |
| 2 | B | 412 | PHE | CA-C-O | -5.86 | 107.80 | 120.10 |
| 2 | B | 471 | TYR | O-C-N | 5.86 | 132.07 | 122.70 |
| 2 | B | 36 | THR | O-C-N | 5.86 | 132.07 | 122.70 |
| 2 | B | 490 | ILE | CA-C-O | -5.86 | 107.80 | 120.10 |
| 3 | S | 117 | ASN | O-C-N | 5.85 | 132.07 | 122.70 |
| 1 | A | 535 | ILE | O-C-N | -5.85 | 113.34 | 122.70 |
| 2 | B | 211 | ALA | CA-C-O | -5.85 | 107.81 | 120.10 |
| 2 | B | 293 | VAL | O-C-N | -5.85 | 113.33 | 122.70 |
| 2 | B | 96 | LYS | O-C-N | 5.85 | 132.06 | 122.70 |
| 2 | B | 212 | VAL | C-N-CA | -5.85 | 107.07 | 121.70 |
| 2 | B | 449 | HIS | O-C-N | 5.85 | 132.06 | 122.70 |
| 2 | B | 232 | ARG | O-C-N | 5.85 | 132.05 | 122.70 |
| 2 | B | 476 | ARG | O-C-N | 5.84 | 132.05 | 122.70 |
| 2 | B | 569 | THR | CA-C-N | -5.84 | 104.51 | 116.20 |
| 2 | B | 189 | HIS | CA-C-O | -5.84 | 107.83 | 120.10 |
| 2 | B | 545 | ARG | O-C-N | 5.84 | 132.05 | 122.70 |
| 1 | A | 404 | GLN | C-N-CA | 5.84 | 136.30 | 121.70 |
| 1 | A | 417 | PRO | N-CA-C | -5.84 | 96.92 | 112.10 |
| 2 | B | 79 | VAL | O-C-N | 5.84 | 132.04 | 122.70 |
| 1 | A | 442 | SER | N-CA-CB | 5.84 | 119.26 | 110.50 |
| 4 | M | 60 | LEU | N-CA-C | -5.84 | 95.24 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4 | M | 278 | ILE | CA-C-N | -5.84 | 104.36 | 117.20 |
| 4 | M | 367 | ALA | N-CA-CB | -5.83 | 101.93 | 110.10 |
| 1 | A | 214 | VAL | O-C-N | 5.83 | 132.03 | 122.70 |
| 1 | A | 333 | ILE | CA-C-O | -5.83 | 107.86 | 120.10 |
| 2 | B | 547 | GLN | O-C-N | 5.83 | 132.02 | 122.70 |
| 4 | M | 59 | ASP | O-C-N | -5.83 | 113.38 | 122.70 |
| 1 | A | 217 | ALA | O-C-N | 5.82 | 132.01 | 122.70 |
| 1 | A | 474 | GLY | CA-C-O | -5.82 | 110.12 | 120.60 |
| 4 | M | 133 | GLU | C-N-CA | -5.82 | 97.56 | 122.00 |
| 2 | B | 245 | GLN | O-C-N | 5.82 | 132.01 | 122.70 |
| 2 | B | 60 | ARG | O-C-N | 5.82 | 132.00 | 122.70 |
| 3 | S | 58 | LEU | N-CA-CB | 5.82 | 122.03 | 110.40 |
| 2 | B | 519 | ALA | N-CA-CB | -5.81 | 101.97 | 110.10 |
| 1 | A | 265 | GLN | C-N-CA | 5.81 | 136.22 | 121.70 |
| 1 | A | 413 | SER | C-N-CA | -5.81 | 107.18 | 121.70 |
| 3 | S | 155 | GLU | O-C-N | 5.81 | 132.00 | 122.70 |
| 4 | M | 223 | HIS | O-C-N | -5.80 | 113.41 | 122.70 |
| 2 | B | 112 | ASP | N-CA-C | 5.80 | 126.67 | 111.00 |
| 2 | B | 418 | TYR | O-C-N | -5.80 | 113.42 | 122.70 |
| 1 | A | 75 | THR | O-C-N | 5.80 | 131.98 | 122.70 |
| 1 | A | 430 | ASN | O-C-N | 5.80 | 131.97 | 122.70 |
| 2 | B | 448 | SER | O-C-N | 5.80 | 131.97 | 122.70 |
| 1 | A | 317 | GLU | O-C-N | 5.79 | 131.97 | 122.70 |
| 1 | A | 316 | LEU | CA-C-O | -5.79 | 107.94 | 120.10 |
| 2 | B | 567 | GLN | C-N-CA | -5.79 | 107.22 | 121.70 |
| 3 | S | 76 | ILE | O-C-N | -5.79 | 113.44 | 122.70 |
| 4 | M | 401 | LYS | C-N-CA | -5.79 | 107.23 | 121.70 |
| 1 | A | 105 | VAL | C-N-CA | 5.79 | 134.45 | 122.30 |
| 1 | A | 572 | PHE | O-C-N | 5.79 | 131.96 | 122.70 |
| 1 | A | 599 | ARG | CA-C-O | -5.78 | 107.95 | 120.10 |
| 1 | A | 422 | GLU | CA-C-O | -5.78 | 107.96 | 120.10 |
| 2 | B | 468 | LEU | O-C-N | 5.78 | 131.95 | 122.70 |
| 2 | B | 436 | LEU | O-C-N | 5.78 | 131.94 | 122.70 |
| 3 | S | 48 | SER | C-N-CA | -5.78 | 107.26 | 121.70 |
| 2 | B | 466 | SER | O-C-N | 5.78 | 131.94 | 122.70 |
| 2 | B | 303 | LEU | CA-C-O | -5.77 | 107.98 | 120.10 |
| 3 | S | 150 | VAL | CA-C-O | -5.77 | 107.98 | 120.10 |
| 4 | M | 265 | ASN | CA-C-O | -5.77 | 107.98 | 120.10 |
| 1 | A | 315 | CYS | O-C-N | 5.77 | 131.93 | 122.70 |
| 3 | S | 84 | TYR | CA-C-O | 5.77 | 132.21 | 120.10 |
| 1 | A | 528 | ASN | O-C-N | -5.76 | 113.40 | 123.20 |
| 2 | B | 457 | HIS | O-C-N | -5.76 | 113.48 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | B | 33 | SER | O-C-N | 5.76 | 131.92 | 122.70 |
| 2 | B | 67 | ILE | CA-C-O | -5.76 | 108.00 | 120.10 |
| 1 | A | 426 | ILE | O-C-N | 5.76 | 131.91 | 122.70 |
| 2 | B | 55 | ASN | O-C-N | 5.76 | 131.91 | 122.70 |
| 3 | S | 86 | THR | O-C-N | -5.76 | 113.49 | 122.70 |
| 1 | A | 106 | GLY | O-C-N | 5.75 | 131.91 | 122.70 |
| 2 | B | 423 | HIS | N-CA-C | -5.75 | 95.46 | 111.00 |
| 1 | A | 145 | ILE | CA-C-O | -5.75 | 108.02 | 120.10 |
| 1 | A | 216 | SER | O-C-N | 5.75 | 131.91 | 122.70 |
| 2 | B | 36 | THR | CA-C-O | -5.75 | 108.02 | 120.10 |
| 4 | M | 130 | GLU | CB-CA-C | 5.75 | 121.89 | 110.40 |
| 2 | B | 322 | CYS | CA-C-O | -5.74 | 108.04 | 120.10 |
| 2 | B | 604 | GLU | CA-C-N | -5.74 | 104.56 | 117.20 |
| 3 | S | 137 | GLN | CA-C-O | 5.74 | 132.16 | 120.10 |
| 4 | M | 447 | ILE | CA-C-O | 5.74 | 132.16 | 120.10 |
| 2 | B | 529 | VAL | O-C-N | 5.74 | 131.89 | 122.70 |
| 2 | B | 395 | LYS | CA-C-O | -5.74 | 108.05 | 120.10 |
| 1 | A | 493 | ALA | O-C-N | 5.73 | 131.87 | 122.70 |
| 1 | A | 582 | ILE | CA-C-O | -5.73 | 108.06 | 120.10 |
| 2 | B | 341 | GLU | CA-C-O | -5.73 | 108.06 | 120.10 |
| 3 | S | 87 | PHE | CA-C-O | 5.73 | 132.13 | 120.10 |
| 4 | M | 354 | ASP | N-CA-CB | 5.73 | 120.91 | 110.60 |
| 3 | S | 117 | ASN | CA-C-O | -5.73 | 108.07 | 120.10 |
| 2 | B | 371 | GLN | O-C-N | 5.73 | 131.86 | 122.70 |
| 3 | S | 35 | VAL | O-C-N | 5.72 | 131.86 | 122.70 |
| 1 | A | 152 | THR | C-N-CA | -5.72 | 107.39 | 121.70 |
| 1 | A | 630 | PRO | O-C-N | 5.72 | 131.86 | 122.70 |
| 4 | M | 135 | ASN | O-C-N | 5.72 | 131.86 | 122.70 |
| 1 | A | 543 | TYR | N-CA-C | 5.72 | 126.44 | 111.00 |
| 2 | B | 216 | LYS | O-C-N | -5.72 | 113.55 | 122.70 |
| 2 | B | 318 | ILE | CA-C-O | -5.72 | 108.09 | 120.10 |
| 1 | A | 572 | PHE | C-N-CA | 5.71 | 135.98 | 121.70 |
| 2 | B | 275 | ARG | N-CA-CB | 5.71 | 120.89 | 110.60 |
| 4 | M | 384 | GLY | O-C-N | 5.71 | 131.84 | 122.70 |
| 2 | B | 391 | ALA | O-C-N | 5.71 | 131.84 | 122.70 |
| 2 | B | 388 | PRO | O-C-N | 5.71 | 131.84 | 122.70 |
| 1 | A | 64 | LEU | C-N-CA | -5.71 | 107.43 | 121.70 |
| 1 | A | 135 | ASP | CA-C-N | 5.70 | 127.61 | 116.20 |
| 1 | A | 163 | ALA | O-C-N | -5.70 | 113.57 | 122.70 |
| 1 | A | 237 | SER | O-C-N | 5.70 | 131.93 | 121.10 |
| 2 | B | 176 | ALA | O-C-N | 5.70 | 131.82 | 122.70 |
| 2 | B | 265 | VAL | CA-C-N | -5.70 | 104.67 | 117.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | A | 427 | LYS | O-C-N | 5.70 | 131.81 | 122.70 |
| 3 | S | 131 | VAL | O-C-N | 5.70 | 131.81 | 122.70 |
| 1 | A | 501 | ASN | C-N-CA | 5.69 | 135.93 | 121.70 |
| 2 | B | 366 | LEU | CA-C-O | 5.69 | 132.05 | 120.10 |
| 1 | A | 350 | SER | C-N-CA | -5.69 | 107.47 | 121.70 |
| 2 | B | 324 | ALA | CA-C-O | -5.69 | 108.16 | 120.10 |
| 2 | B | 300 | ASP | O-C-N | 5.68 | 131.79 | 122.70 |
| 1 | A | 397 | ASP | O-C-N | -5.68 | 113.61 | 122.70 |
| 2 | B | 241 | ASP | O-C-N | 5.68 | 131.79 | 122.70 |
| 4 | M | 306 | LEU | C-N-CA | -5.68 | 107.51 | 121.70 |
| 1 | A | 123 | LEU | O-C-N | 5.67 | 131.78 | 122.70 |
| 4 | M | 321 | GLY | C-N-CA | -5.67 | 107.51 | 121.70 |
| 1 | A | 575 | LYS | O-C-N | 5.67 | 131.78 | 122.70 |
| 2 | B | 596 | LEU | O-C-N | 5.67 | 131.78 | 122.70 |
| 1 | A | 275 | LEU | O-C-N | -5.67 | 110.33 | 121.10 |
| 4 | M | 136 | VAL | CA-C-O | 5.67 | 132.00 | 120.10 |
| 1 | A | 230 | PRO | CA-N-CD | 5.66 | 119.63 | 111.70 |
| 1 | A | 253 | ILE | O-C-N | 5.66 | 131.76 | 122.70 |
| 1 | A | 575 | LYS | CA-C-O | -5.66 | 108.20 | 120.10 |
| 2 | B | 99 | ARG | CA-C-O | -5.66 | 108.22 | 120.10 |
| 2 | B | 188 | TYR | O-C-N | 5.66 | 131.75 | 122.70 |
| 1 | A | 173 | THR | C-N-CA | 5.65 | 135.83 | 121.70 |
| 1 | A | 580 | GLU | O-C-N | 5.65 | 131.73 | 122.70 |
| 2 | B | 48 | VAL | O-C-N | 5.65 | 131.74 | 122.70 |
| 2 | B | 522 | GLU | N-CA-C | 5.65 | 126.25 | 111.00 |
| 2 | B | 428 | VAL | CA-C-O | -5.64 | 108.25 | 120.10 |
| 4 | M | 267 | ILE | C-N-CA | -5.64 | 110.45 | 122.30 |
| 2 | B | 477 | MET | O-C-N | 5.64 | 131.73 | 122.70 |
| 1 | A | 305 | GLU | CA-C-N | 5.64 | 129.61 | 117.20 |
| 2 | B | 431 | MET | O-C-N | 5.64 | 131.72 | 122.70 |
| 1 | A | 368 | ARG | O-C-N | 5.64 | 131.72 | 122.70 |
| 1 | A | 233 | PHE | CA-C-O | 5.63 | 131.93 | 120.10 |
| 4 | M | 261 | ASN | C-N-CA | -5.63 | 107.63 | 121.70 |
| 2 | B | 173 | VAL | O-C-N | 5.63 | 131.71 | 122.70 |
| 2 | B | 593 | ASN | CA-C-O | -5.63 | 108.28 | 120.10 |
| 1 | A | 188 | VAL | CA-C-O | -5.63 | 108.28 | 120.10 |
| 1 | A | 577 | VAL | O-C-N | 5.63 | 131.70 | 122.70 |
| 2 | B | 569 | THR | C-N-CA | 5.63 | 134.12 | 122.30 |
| 1 | A | 330 | LEU | CA-C-O | -5.62 | 108.29 | 120.10 |
| 3 | S | 87 | PHE | O-C-N | -5.62 | 113.70 | 122.70 |
| 1 | A | 109 | ALA | O-C-N | 5.62 | 131.69 | 122.70 |
| 1 | A | 184 | ALA | O-C-N | 5.62 | 131.69 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 3 | S | 60 | SER | C-N-CA | 5.62 | 135.75 | 121.70 |
| 4 | M | 61 | GLU | CA-C-N | -5.62 | 104.84 | 117.20 |
| 1 | A | 88 | ASN | O-C-N | -5.62 | 113.71 | 122.70 |
| 3 | S | 1 | MET | CA-C-O | 5.62 | 131.89 | 120.10 |
| 2 | B | 156 | HIS | O-C-N | 5.61 | 131.68 | 122.70 |
| 2 | B | 438 | ARG | O-C-N | 5.61 | 131.68 | 122.70 |
| 4 | M | 18 | TYR | CA-C-O | 5.61 | 131.88 | 120.10 |
| 1 | A | 293 | GLU | O-C-N | 5.61 | 131.67 | 122.70 |
| 1 | A | 467 | LYS | C-N-CA | -5.61 | 107.68 | 121.70 |
| 1 | A | 341 | ILE | O-C-N | 5.60 | 132.72 | 123.20 |
| 2 | B | 122 | SER | O-C-N | 5.60 | 131.66 | 122.70 |
| 1 | A | 551 | LEU | CA-C-O | -5.60 | 108.35 | 120.10 |
| 2 | B | 179 | LYS | O-C-N | 5.60 | 131.65 | 122.70 |
| 1 | A | 105 | VAL | CA-C-O | -5.59 | 108.35 | 120.10 |
| 2 | B | 365 | PHE | CA-C-O | -5.59 | 108.35 | 120.10 |
| 1 | A | 199 | ASN | O-C-N | 5.59 | 131.65 | 122.70 |
| 3 | S | 49 | SER | CA-C-N | 5.59 | 129.50 | 117.20 |
| 1 | A | 124 | ALA | O-C-N | 5.59 | 131.64 | 122.70 |
| 1 | A | 624 | LEU | CA-C-O | -5.59 | 108.37 | 120.10 |
| 2 | B | 434 | LYS | O-C-N | 5.59 | 131.64 | 122.70 |
| 1 | A | 277 | LYS | CA-C-N | 5.58 | 129.49 | 117.20 |
| 2 | B | 138 | ALA | CA-C-O | -5.58 | 108.37 | 120.10 |
| 2 | B | 223 | LEU | CA-C-O | 5.58 | 131.83 | 120.10 |
| 2 | B | 554 | LYS | CA-C-O | -5.58 | 108.37 | 120.10 |
| 2 | B | 169 | VAL | CA-C-O | -5.58 | 108.38 | 120.10 |
| 2 | B | 172 | GLU | C-N-CA | -5.58 | 107.75 | 121.70 |
| 2 | B | 319 | LEU | O-C-N | 5.58 | 131.63 | 122.70 |
| 4 | M | 421 | GLY | C-N-CD | 5.58 | 140.12 | 128.40 |
| 1 | A | 160 | ARG | O-C-N | 5.58 | 131.62 | 122.70 |
| 1 | A | 507 | GLN | C-N-CA | -5.58 | 107.75 | 121.70 |
| 4 | M | 387 | GLU | O-C-N | -5.58 | 113.78 | 122.70 |
| 2 | B | 458 | MET | C-N-CA | -5.58 | 107.76 | 121.70 |
| 4 | M | 292 | PRO | C-N-CD | -5.58 | 108.33 | 120.60 |
| 1 | A | 191 | GLN | C-N-CA | 5.57 | 135.63 | 121.70 |
| 2 | B | 290 | SER | N-CA-C | 5.57 | 126.05 | 111.00 |
| 2 | B | 86 | VAL | O-C-N | 5.57 | 131.62 | 122.70 |
| 1 | A | 583 | GLU | O-C-N | 5.57 | 131.61 | 122.70 |
| 2 | B | 117 | LEU | O-C-N | 5.57 | 131.60 | 122.70 |
| 4 | M | 368 | ASP | O-C-N | 5.57 | 131.68 | 121.10 |
| 4 | M | 225 | VAL | O-C-N | 5.56 | 131.60 | 122.70 |
| 1 | A | 636 | TYR | CB-CG-CD2 | -5.56 | 117.66 | 121.00 |
| 1 | A | 588 | LEU | CA-C-O | 5.56 | 131.78 | 120.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2 | B | 120 | ILE | O-C-N | 5.56 | 131.60 | 122.70 |
| 4 | M | 103 | TYR | N-CA-CB | 5.56 | 120.61 | 110.60 |
| 2 | B | 283 | TYR | CB-CG-CD2 | -5.55 | 117.67 | 121.00 |
| 1 | A | 265 | GLN | CB-CA-C | 5.55 | 121.50 | 110.40 |
| 4 | M | 284 | SER | C-N-CD | 5.55 | 140.06 | 128.40 |
| 2 | B | 551 | LEU | CA-C-O | -5.55 | 108.44 | 120.10 |
| 2 | B | 605 | PHE | CA-C-O | -5.55 | 108.45 | 120.10 |
| 2 | B | 194 | ASP | O-C-N | 5.55 | 131.58 | 122.70 |
| 2 | B | 492 | LYS | O-C-N | 5.54 | 131.57 | 122.70 |
| 1 | A | 229 | ASN | C-N-CA | -5.54 | 98.71 | 122.00 |
| 1 | A | 242 | GLU | CA-C-O | -5.54 | 108.46 | 120.10 |
| 2 | B | 340 | ILE | O-C-N | 5.54 | 131.57 | 122.70 |
| 2 | B | 365 | PHE | O-C-N | 5.54 | 131.57 | 122.70 |
| 4 | M | 385 | ARG | CA-C-O | 5.54 | 131.74 | 120.10 |
| 2 | B | 430 | ILE | CA-C-O | -5.54 | 108.46 | 120.10 |
| 2 | B | 215 | TYR | CA-C-O | -5.54 | 108.47 | 120.10 |
| 3 | S | 164 | ASP | O-C-N | -5.54 | 113.84 | 122.70 |
| 1 | A | 294 | SER | O-C-N | 5.53 | 131.55 | 122.70 |
| 4 | M | 25 | PRO | N-CA-C | -5.53 | 97.72 | 112.10 |
| 4 | M | 256 | VAL | O-C-N | 5.53 | 131.54 | 122.70 |
| 2 | B | 457 | HIS | C-N-CA | -5.53 | 107.89 | 121.70 |
| 2 | B | 456 | ASP | O-C-N | 5.52 | 131.54 | 122.70 |
| 1 | A | 126 | ASN | O-C-N | 5.52 | 131.53 | 122.70 |
| 1 | A | 103 | LYS | C-N-CA | -5.51 | 107.91 | 121.70 |
| 1 | A | 356 | ILE | O-C-N | 5.51 | 131.52 | 122.70 |
| 2 | B | 318 | ILE | O-C-N | 5.51 | 131.52 | 122.70 |
| 3 | S | 151 | ALA | O-C-N | 5.51 | 131.52 | 122.70 |
| 1 | A | 156 | PRO | CA-C-O | 5.51 | 133.43 | 120.20 |
| 3 | S | 109 | LEU | C-N-CA | -5.51 | 107.93 | 121.70 |
| 2 | B | 204 | ASP | CA-C-O | -5.51 | 108.54 | 120.10 |
| 1 | A | 165 | ASP | O-C-N | 5.50 | 131.50 | 122.70 |
| 1 | A | 278 | ILE | CA-C-O | -5.50 | 108.55 | 120.10 |
| 2 | B | 120 | ILE | CA-C-O | -5.50 | 108.55 | 120.10 |
| 1 | A | 456 | ASP | O-C-N | 5.50 | 131.50 | 122.70 |
| 2 | B | 334 | MET | N-CA-C | 5.50 | 125.84 | 111.00 |
| 1 | A | 558 | VAL | CA-C-O | -5.50 | 108.56 | 120.10 |
| 1 | A | 125 | THR | CA-C-O | -5.49 | 108.57 | 120.10 |
| 1 | A | 181 | ALA | O-C-N | 5.49 | 131.48 | 122.70 |
| 1 | A | 341 | ILE | CA-C-O | -5.49 | 108.58 | 120.10 |
| 1 | A | 416 | ILE | C-N-CA | -5.49 | 98.94 | 122.00 |
| 1 | A | 501 | ASN | N-CA-CB | 5.49 | 120.48 | 110.60 |
| 4 | M | 230 | LYS | O-C-N | -5.49 | 113.92 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | B | 275 | ARG | CA-C-N | -5.49 | 105.13 | 117.20 |
| 1 | A | 129 | LYS | O-C-N | 5.49 | 131.48 | 122.70 |
| 4 | M | 441 | GLY | CA-C-N | -5.49 | 105.13 | 117.20 |
| 2 | B | 451 | MET | O-C-N | 5.48 | 131.47 | 122.70 |
| 2 | B | 540 | GLU | N-CA-C | 5.48 | 125.80 | 111.00 |
| 2 | B | 586 | SER | CA-C-O | -5.48 | 108.59 | 120.10 |
| 1 | A | 528 | ASN | C-N-CA | -5.48 | 110.79 | 122.30 |
| 2 | B | 287 | GLU | O-C-N | 5.48 | 131.47 | 122.70 |
| 2 | B | 415 | LEU | CA-C-O | -5.48 | 108.59 | 120.10 |
| 1 | A | 496 | ILE | CA-C-O | -5.48 | 108.59 | 120.10 |
| 1 | A | 175 | PRO | O-C-N | 5.47 | 131.46 | 122.70 |
| 1 | A | 604 | LEU | CA-C-O | -5.47 | 108.61 | 120.10 |
| 1 | A | 433 | ILE | CA-C-O | -5.47 | 108.61 | 120.10 |
| 1 | A | 593 | THR | O-C-N | 5.47 | 131.46 | 122.70 |
| 2 | B | 178 | ILE | CA-C-O | -5.47 | 108.61 | 120.10 |
| 4 | M | 90 | PHE | CA-C-O | -5.47 | 108.61 | 120.10 |
| 2 | B | 225 | LEU | CA-C-N | -5.47 | 105.17 | 117.20 |
| 4 | M | 343 | ASN | C-N-CA | -5.47 | 108.04 | 121.70 |
| 2 | B | 321 | CYS | O-C-N | 5.46 | 131.44 | 122.70 |
| 2 | B | 354 | GLY | N-CA-C | -5.46 | 99.44 | 113.10 |
| 2 | B | 436 | LEU | CA-C-O | -5.46 | 108.62 | 120.10 |
| 3 | S | 74 | GLN | CA-C-O | 5.46 | 131.57 | 120.10 |
| 1 | A | 505 | ASN | O-C-N | -5.46 | 113.97 | 122.70 |
| 3 | S | 124 | ASN | O-C-N | 5.46 | 131.44 | 122.70 |
| 4 | M | 85 | GLY | CA-C-O | -5.46 | 110.78 | 120.60 |
| 4 | M | 103 | TYR | CB-CA-C | 5.46 | 121.31 | 110.40 |
| 1 | A | 319 | LEU | CA-C-O | 5.45 | 131.55 | 120.10 |
| 4 | M | 51 | LEU | N-CA-CB | -5.45 | 99.50 | 110.40 |
| 3 | S | 98 | ILE | CA-C-O | -5.45 | 108.67 | 120.10 |
| 4 | M | 88 | ASP | O-C-N | 5.45 | 131.41 | 122.70 |
| 1 | A | 308 | ASP | N-CA-C | 5.44 | 125.70 | 111.00 |
| 1 | A | 470 | GLY | O-C-N | 5.44 | 131.41 | 122.70 |
| 2 | B | 73 | ASP | C-N-CA | -5.44 | 108.09 | 121.70 |
| 1 | A | 578 | LEU | CA-C-O | -5.44 | 108.68 | 120.10 |
| 4 | M | 58 | ARG | C-N-CA | -5.44 | 108.11 | 121.70 |
| 2 | B | 133 | GLU | O-C-N | 5.44 | 131.40 | 122.70 |
| 2 | B | 531 | ARG | CA-C-O | -5.44 | 108.68 | 120.10 |
| 1 | A | 63 | ASP | N-CA-C | 5.43 | 125.67 | 111.00 |
| 2 | B | 323 | ASN | CA-C-O | -5.43 | 108.69 | 120.10 |
| 3 | S | 158 | LYS | CA-C-O | -5.43 | 108.69 | 120.10 |
| 4 | M | 377 | LYS | N-CA-C | 5.43 | 125.67 | 111.00 |
| 1 | A | 370 | LYS | CA-C-O | -5.43 | 108.70 | 120.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | B | 245 | GLN | CA-C-O | -5.43 | 108.70 | 120.10 |
| 2 | B | 475 | ILE | CA-C-O | -5.43 | 108.70 | 120.10 |
| 4 | M | 354 | ASP | CB-CA-C | 5.42 | 121.24 | 110.40 |
| 1 | A | 137 | ASN | C-N-CA | -5.42 | 108.15 | 121.70 |
| 1 | A | 335 | CYS | CA-C-O | -5.41 | 108.73 | 120.10 |
| 2 | B | 387 | ASP | N-CA-C | 5.41 | 125.62 | 111.00 |
| 1 | A | 244 | LEU | CA-C-O | 5.41 | 131.46 | 120.10 |
| 1 | A | 375 | VAL | O-C-N | -5.41 | 114.04 | 122.70 |
| 1 | A | 419 | ILE | CA-C-N | -5.41 | 105.30 | 117.20 |
| 4 | M | 57 | GLY | O-C-N | -5.41 | 114.05 | 122.70 |
| 1 | A | 334 | SER | O-C-N | 5.41 | 131.35 | 122.70 |
| 3 | S | 37 | GLU | CA-C-O | -5.41 | 108.75 | 120.10 |
| 1 | A | 255 | ARG | O-C-N | 5.41 | 131.35 | 122.70 |
| 1 | A | 466 | ASP | N-CA-C | -5.41 | 96.40 | 111.00 |
| 4 | M | 87 | LEU | O-C-N | 5.41 | 131.35 | 122.70 |
| 4 | M | 279 | ASN | CA-C-O | -5.40 | 108.76 | 120.10 |
| 2 | B | 109 | ALA | CB-CA-C | -5.40 | 102.00 | 110.10 |
| 3 | S | 49 | SER | CA-C-O | -5.40 | 108.76 | 120.10 |
| 1 | A | 611 | LEU | CA-C-O | -5.40 | 108.77 | 120.10 |
| 1 | A | 139 | ASP | CA-C-O | -5.40 | 108.77 | 120.10 |
| 1 | A | 391 | LEU | CA-C-O | 5.39 | 131.43 | 120.10 |
| 4 | M | 130 | GLU | O-C-N | 5.39 | 131.33 | 122.70 |
| 1 | A | 514 | GLU | CA-C-O | -5.39 | 108.78 | 120.10 |
| 2 | B | 192 | LEU | CA-C-O | -5.39 | 108.78 | 120.10 |
| 1 | A | 73 | LYS | O-C-N | 5.39 | 131.32 | 122.70 |
| 1 | A | 614 | LEU | C-N-CA | -5.38 | 108.24 | 121.70 |
| 4 | M | 307 | SER | O-C-N | 5.38 | 131.31 | 122.70 |
| 2 | B | 127 | LEU | C-N-CA | -5.38 | 108.25 | 121.70 |
| 1 | A | 94 | VAL | CA-C-O | 5.38 | 131.39 | 120.10 |
| 1 | A | 501 | ASN | N-CA-C | -5.38 | 96.48 | 111.00 |
| 4 | M | 396 | GLN | O-C-N | -5.38 | 114.10 | 122.70 |
| 1 | A | 80 | TYR | CB-CA-C | 5.38 | 121.15 | 110.40 |
| 1 | A | 312 | ALA | CA-C-O | -5.38 | 108.81 | 120.10 |
| 2 | B | 420 | ALA | N-CA-CB | -5.37 | 102.58 | 110.10 |
| 1 | A | 85 | ALA | O-C-N | 5.37 | 131.29 | 122.70 |
| 2 | B | 491 | PHE | O-C-N | 5.37 | 131.29 | 122.70 |
| 1 | A | 313 | MET | CA-C-O | -5.37 | 108.83 | 120.10 |
| 2 | B | 493 | LEU | CA-C-O | -5.37 | 108.83 | 120.10 |
| 4 | M | 450 | GLU | O-C-N | -5.37 | 114.12 | 122.70 |
| 1 | A | 289 | SER | C-N-CA | -5.36 | 108.29 | 121.70 |
| 1 | A | 346 | THR | CA-C-O | 5.36 | 131.36 | 120.10 |
| 2 | B | 357 | GLU | O-C-N | 5.36 | 131.28 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | A | 90 | HIS | O-C-N | 5.36 | 131.27 | 122.70 |
| 2 | B | 392 | SER | O-C-N | 5.36 | 131.27 | 122.70 |
| 4 | M | 444 | ALA | N-CA-CB | -5.36 | 102.60 | 110.10 |
| 4 | M | 104 | PHE | CA-C-O | 5.35 | 131.34 | 120.10 |
| 1 | A | 597 | GLN | O-C-N | 5.35 | 131.26 | 122.70 |
| 3 | S | 103 | GLN | CA-C-O | -5.35 | 108.86 | 120.10 |
| 2 | B | 562 | ASN | O-C-N | 5.35 | 131.26 | 122.70 |
| 2 | B | 273 | SER | C-N-CA | 5.35 | 144.46 | 122.00 |
| 4 | M | 447 | ILE | O-C-N | -5.35 | 114.15 | 122.70 |
| 1 | A | 518 | CYS | O-C-N | 5.34 | 131.25 | 122.70 |
| 2 | B | 196 | LEU | CA-C-O | -5.34 | 108.88 | 120.10 |
| 1 | A | 455 | MET | O-C-N | 5.34 | 131.24 | 122.70 |
| 1 | A | 99 | LYS | O-C-N | 5.33 | 131.24 | 122.70 |
| 2 | B | 222 | HIS | O-C-N | 5.33 | 131.23 | 122.70 |
| 4 | M | 405 | THR | N-CA-CB | -5.33 | 100.17 | 110.30 |
| 1 | A | 352 | PHE | O-C-N | 5.33 | 131.22 | 122.70 |
| 1 | A | 370 | LYS | O-C-N | 5.33 | 131.22 | 122.70 |
| 2 | B | 482 | ASN | O-C-N | 5.33 | 131.22 | 121.10 |
| 1 | A | 134 | TYR | C-N-CA | -5.33 | 108.38 | 121.70 |
| 1 | A | 380 | ASP | O-C-N | 5.33 | 131.22 | 122.70 |
| 2 | B | 126 | SER | CA-C-O | 5.32 | 131.28 | 120.10 |
| 1 | A | 439 | ASP | C-N-CA | 5.32 | 135.00 | 121.70 |
| 4 | M | 61 | GLU | N-CA-CB | 5.32 | 120.17 | 110.60 |
| 1 | A | 85 | ALA | N-CA-CB | -5.32 | 102.65 | 110.10 |
| 2 | B | 467 | VAL | CA-C-O | -5.31 | 108.94 | 120.10 |
| 2 | B | 595 | VAL | CA-C-O | -5.31 | 108.94 | 120.10 |
| 1 | A | 636 | TYR | CD1-CG-CD2 | 5.31 | 123.74 | 117.90 |
| 1 | A | 295 | VAL | O-C-N | 5.31 | 131.20 | 122.70 |
| 2 | B | 472 | VAL | C-N-CA | -5.31 | 108.43 | 121.70 |
| 1 | A | 216 | SER | CA-C-O | -5.31 | 108.95 | 120.10 |
| 1 | A | 398 | GLU | N-CA-C | 5.31 | 125.33 | 111.00 |
| 2 | B | 219 | TYR | N-CA-C | 5.31 | 125.33 | 111.00 |
| 2 | B | 34 | SER | O-C-N | 5.30 | 131.19 | 122.70 |
| 4 | M | 296 | LYS | C-N-CA | -5.30 | 108.44 | 121.70 |
| 1 | A | 193 | PRO | CA-C-O | -5.30 | 107.49 | 120.20 |
| 2 | B | 383 | VAL | CA-C-N | -5.30 | 105.55 | 117.20 |
| 2 | B | 489 | ILE | CA-C-O | -5.30 | 108.98 | 120.10 |
| 2 | B | 283 | TYR | CD1-CG-CD2 | 5.29 | 123.72 | 117.90 |
| 3 | S | 34 | GLN | O-C-N | 5.29 | 131.17 | 122.70 |
| 1 | A | 613 | ALA | CA-C-O | -5.29 | 108.99 | 120.10 |
| 2 | B | 213 | LEU | CA-C-O | -5.29 | 108.99 | 120.10 |
| 2 | B | 83 | PHE | CA-C-N | -5.29 | 105.56 | 117.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | B | 616 | SER | O-C-N | 5.29 | 131.16 | 122.70 |
| 1 | A | 177 | ILE | CA-C-O | -5.28 | 109.00 | 120.10 |
| 1 | A | 390 | THR | CA-C-O | -5.28 | 109.00 | 120.10 |
| 1 | A | 633 | PHE | O-C-N | 5.28 | 131.15 | 122.70 |
| 2 | B | 364 | HIS | O-C-N | 5.28 | 131.15 | 122.70 |
| 2 | B | 54 | ARG | N-CA-C | 5.28 | 125.26 | 111.00 |
| 1 | A | 512 | LEU | O-C-N | 5.28 | 131.15 | 122.70 |
| 2 | B | 351 | GLU | CA-C-O | 5.28 | 131.19 | 120.10 |
| 1 | A | 72 | LEU | O-C-N | 5.28 | 131.15 | 122.70 |
| 1 | A | 222 | ILE | O-C-N | 5.28 | 131.15 | 122.70 |
| 1 | A | 292 | TYR | O-C-N | 5.28 | 131.15 | 122.70 |
| 2 | B | 592 | TYR | CA-C-O | -5.28 | 109.01 | 120.10 |
| 2 | B | 398 | ILE | O-C-N | 5.28 | 131.15 | 122.70 |
| 1 | A | 110 | ALA | CA-C-O | 5.28 | 131.18 | 120.10 |
| 1 | A | 280 | GLU | O-C-N | 5.28 | 131.14 | 122.70 |
| 1 | A | 221 | VAL | CA-C-O | -5.27 | 109.03 | 120.10 |
| 2 | B | 609 | ASP | O-C-N | 5.27 | 131.14 | 122.70 |
| 2 | B | 494 | ALA | CA-C-O | -5.27 | 109.04 | 120.10 |
| 2 | B | 566 | ALA | N-CA-CB | -5.27 | 102.72 | 110.10 |
| 4 | M | 39 | PRO | O-C-N | 5.27 | 131.13 | 122.70 |
| 1 | A | 163 | ALA | CA-C-O | 5.27 | 131.16 | 120.10 |
| 1 | A | 429 | VAL | CA-C-O | -5.27 | 109.04 | 120.10 |
| 3 | S | 18 | LYS | CA-C-O | 5.27 | 131.16 | 120.10 |
| 4 | M | 1 | MET | C-N-CA | -5.27 | 108.53 | 121.70 |
| 4 | M | 59 | ASP | N-CA-C | -5.27 | 96.78 | 111.00 |
| 2 | B | 608 | ARG | O-C-N | 5.26 | 131.12 | 122.70 |
| 2 | B | 555 | LEU | CA-C-O | -5.26 | 109.05 | 120.10 |
| 4 | M | 7 | ILE | CA-C-O | -5.26 | 109.05 | 120.10 |
| 2 | B | 399 | LEU | O-C-N | -5.25 | 114.30 | 122.70 |
| 3 | S | 68 | VAL | N-CA-CB | -5.25 | 99.95 | 111.50 |
| 1 | A | 254 | ILE | O-C-N | 5.25 | 131.10 | 122.70 |
| 2 | B | 470 | ALA | O-C-N | 5.25 | 131.09 | 122.70 |
| 1 | A | 305 | GLU | CA-C-O | -5.25 | 109.08 | 120.10 |
| 2 | B | 68 | SER | O-C-N | 5.25 | 131.09 | 122.70 |
| 2 | B | 166 | SER | C-N-CA | 5.25 | 134.81 | 121.70 |
| 2 | B | 222 | HIS | N-CA-C | 5.24 | 125.15 | 111.00 |
| 1 | A | 146 | ALA | CA-C-O | -5.24 | 109.09 | 120.10 |
| 2 | B | 482 | ASN | CA-C-O | -5.24 | 109.09 | 120.10 |
| 3 | S | 153 | VAL | CA-C-O | -5.24 | 109.09 | 120.10 |
| 1 | A | 383 | ASN | CA-C-O | -5.24 | 109.10 | 120.10 |
| 2 | B | 280 | PRO | N-CA-C | -5.24 | 98.48 | 112.10 |
| 4 | M | 16 | PHE | O-C-N | -5.24 | 114.32 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | A | 516 | ILE | CA-C-O | -5.24 | 109.11 | 120.10 |
| 2 | B | 297 | PRO | CA-C-O | -5.24 | 107.64 | 120.20 |
| 2 | B | 319 | LEU | CA-C-O | -5.24 | 109.11 | 120.10 |
| 2 | B | 577 | ASN | C-N-CA | -5.24 | 100.01 | 122.00 |
| 4 | M | 284 | SER | CA-C-O | 5.24 | 131.09 | 120.10 |
| 1 | A | 327 | ASP | O-C-N | 5.23 | 131.04 | 121.10 |
| 3 | S | 89 | VAL | C-N-CA | -5.23 | 108.63 | 121.70 |
| 1 | A | 91 | ILE | CA-C-O | -5.23 | 109.12 | 120.10 |
| 1 | A | 559 | PHE | CA-C-O | -5.23 | 109.13 | 120.10 |
| 1 | A | 304 | LEU | CA-C-N | 5.22 | 128.69 | 117.20 |
| 4 | M | 234 | ARG | O-C-N | -5.22 | 114.34 | 122.70 |
| 1 | A | 226 | SER | C-N-CA | -5.22 | 108.64 | 121.70 |
| 1 | A | 337 | LEU | CA-C-O | -5.22 | 109.13 | 120.10 |
| 3 | S | 78 | LYS | CA-C-O | 5.22 | 131.07 | 120.10 |
| 2 | B | 500 | GLN | N-CA-C | 5.22 | 125.10 | 111.00 |
| 3 | S | 138 | GLY | C-N-CA | 5.22 | 133.26 | 122.30 |
| 2 | B | 286 | ILE | CA-C-N | -5.22 | 105.72 | 117.20 |
| 4 | M | 21 | GLY | CA-C-N | -5.22 | 105.72 | 117.20 |
| 1 | A | 172 | SER | C-N-CA | -5.22 | 108.66 | 121.70 |
| 1 | A | 634 | ASN | CA-C-O | -5.21 | 109.15 | 120.10 |
| 2 | B | 63 | MET | CA-C-O | -5.21 | 109.16 | 120.10 |
| 1 | A | 144 | GLY | O-C-N | 5.21 | 131.03 | 122.70 |
| 1 | A | 620 | GLY | O-C-N | 5.21 | 131.03 | 122.70 |
| 2 | B | 248 | LEU | CA-C-O | -5.20 | 109.17 | 120.10 |
| 2 | B | 350 | THR | N-CA-C | 5.20 | 125.05 | 111.00 |
| 4 | M | 55 | MET | O-C-N | -5.20 | 114.37 | 122.70 |
| 2 | B | 451 | MET | CA-C-O | -5.20 | 109.18 | 120.10 |
| 2 | B | 216 | LYS | CA-C-O | 5.20 | 131.02 | 120.10 |
| 3 | S | 154 | ASP | CA-C-O | -5.20 | 109.18 | 120.10 |
| 2 | B | 118 | LEU | O-C-N | 5.20 | 131.01 | 122.70 |
| 2 | B | 544 | THR | CA-C-O | -5.20 | 109.19 | 120.10 |
| 4 | M | 60 | LEU | CA-C-N | -5.20 | 105.77 | 117.20 |
| 1 | A | 562 | TRP | CA-C-O | -5.19 | 109.19 | 120.10 |
| 2 | B | 48 | VAL | CA-C-O | -5.19 | 109.19 | 120.10 |
| 2 | B | 533 | LEU | O-C-N | 5.19 | 131.01 | 122.70 |
| 4 | M | 122 | SER | CA-C-O | -5.19 | 109.19 | 120.10 |
| 2 | B | 112 | ASP | CA-C-O | -5.19 | 109.20 | 120.10 |
| 4 | M | 77 | LEU | O-C-N | -5.19 | 114.39 | 122.70 |
| 4 | M | 331 | LEU | CA-C-N | -5.19 | 105.82 | 116.20 |
| 1 | A | 121 | LEU | CA-C-O | -5.19 | 109.20 | 120.10 |
| 1 | A | 526 | VAL | C-N-CA | 5.19 | 134.67 | 121.70 |
| 1 | A | 422 | GLU | O-C-N | 5.19 | 131.00 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | A | 314 | ALA | O-C-N | 5.19 | 131.00 | 122.70 |
| 1 | A | 502 | ASP | O-C-N | 5.19 | 131.00 | 122.70 |
| 2 | B | 606 | ASP | O-C-N | 5.18 | 130.99 | 122.70 |
| 2 | B | 360 | LEU | CA-C-O | -5.18 | 109.22 | 120.10 |
| 4 | M | 379 | LEU | CA-C-O | 5.18 | 130.97 | 120.10 |
| 2 | B | 584 | SER | CB-CA-C | -5.18 | 100.26 | 110.10 |
| 1 | A | 239 | LEU | O-C-N | 5.17 | 130.98 | 122.70 |
| 1 | A | 437 | SER | N-CA-C | 5.17 | 124.96 | 111.00 |
| 1 | A | 115 | TYR | C-N-CA | 5.17 | 134.62 | 121.70 |
| 2 | B | 411 | ILE | CA-C-O | -5.17 | 109.25 | 120.10 |
| 4 | M | 59 | ASP | CA-C-O | -5.17 | 109.25 | 120.10 |
| 1 | A | 440 | ASN | N-CA-C | -5.16 | 97.06 | 111.00 |
| 2 | B | 391 | ALA | CA-C-O | -5.16 | 109.26 | 120.10 |
| 1 | A | 323 | CYS | O-C-N | -5.16 | 114.44 | 122.70 |
| 1 | A | 635 | ALA | CA-C-O | -5.16 | 109.27 | 120.10 |
| 1 | A | 493 | ALA | CA-C-O | -5.16 | 109.27 | 120.10 |
| 3 | S | 164 | ASP | CA-C-N | 5.16 | 128.55 | 117.20 |
| 3 | S | 54 | PRO | CA-C-N | 5.16 | 131.53 | 117.10 |
| 1 | A | 566 | PHE | O-C-N | 5.15 | 130.94 | 122.70 |
| 1 | A | 230 | PRO | O-C-N | 5.15 | 130.94 | 122.70 |
| 2 | B | 242 | SER | N-CA-C | 5.15 | 124.90 | 111.00 |
| 2 | B | 116 | THR | CA-C-O | -5.14 | 109.30 | 120.10 |
| 4 | M | 46 | SER | CA-C-N | 5.14 | 128.51 | 117.20 |
| 2 | B | 552 | SER | CA-C-O | -5.14 | 109.31 | 120.10 |
| 2 | B | 615 | SER | CA-C-O | -5.14 | 109.31 | 120.10 |
| 2 | B | 60 | ARG | CA-C-O | -5.14 | 109.31 | 120.10 |
| 2 | B | 84 | ALA | O-C-N | 5.14 | 130.92 | 122.70 |
| 2 | B | 518 | ILE | O-C-N | 5.14 | 130.92 | 122.70 |
| 3 | S | 141 | VAL | N-CA-C | -5.14 | 97.13 | 111.00 |
| 4 | M | 309 | GLN | O-C-N | 5.13 | 130.91 | 122.70 |
| 1 | A | 71 | VAL | O-C-N | 5.13 | 130.91 | 122.70 |
| 2 | B | 548 | ILE | CA-C-O | -5.13 | 109.32 | 120.10 |
| 2 | B | 614 | ILE | CA-C-O | -5.13 | 109.32 | 120.10 |
| 1 | A | 434 | SER | CA-C-O | -5.13 | 109.33 | 120.10 |
| 2 | B | 345 | ARG | O-C-N | 5.13 | 130.91 | 122.70 |
| 3 | S | 78 | LYS | O-C-N | -5.13 | 114.50 | 122.70 |
| 2 | B | 530 | LEU | CA-C-O | -5.13 | 109.34 | 120.10 |
| 1 | A | 389 | GLN | O-C-N | 5.12 | 130.90 | 122.70 |
| 2 | B | 439 | CYS | CA-C-O | -5.12 | 109.34 | 120.10 |
| 1 | A | 302 | ASN | N-CA-CB | 5.12 | 119.82 | 110.60 |
| 1 | A | 219 | VAL | O-C-N | 5.12 | 130.89 | 122.70 |
| 2 | B | 210 | CYS | CA-C-O | -5.12 | 109.34 | 120.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4 | M | 278 | ILE | C-N-CA | -5.12 | 108.90 | 121.70 |
| 1 | A | 602 | GLU | CA-C-O | -5.12 | 109.35 | 120.10 |
| 2 | B | 61 | ASP | O-C-N | 5.12 | 130.89 | 122.70 |
| 1 | A | 178 | ARG | O-C-N | 5.12 | 130.89 | 122.70 |
| 2 | B | 176 | ALA | CA-C-O | -5.12 | 109.36 | 120.10 |
| 4 | M | 117 | ASN | C-N-CA | 5.12 | 134.49 | 121.70 |
| 1 | A | 193 | PRO | O-C-N | 5.12 | 130.88 | 122.70 |
| 2 | B | 94 | ASP | O-C-N | 5.12 | 130.88 | 122.70 |
| 2 | B | 340 | ILE | CA-C-O | -5.11 | 109.36 | 120.10 |
| 2 | B | 532 | ARG | CA-C-O | -5.11 | 109.36 | 120.10 |
| 1 | A | 387 | ILE | CA-C-O | -5.11 | 109.37 | 120.10 |
| 1 | A | 555 | LEU | CA-C-O | -5.11 | 109.37 | 120.10 |
| 2 | B | 589 | SER | CA-C-O | -5.11 | 109.37 | 120.10 |
| 1 | A | 479 | ASN | CA-C-O | -5.11 | 109.38 | 120.10 |
| 2 | B | 474 | VAL | CA-C-O | -5.11 | 109.38 | 120.10 |
| 2 | B | 588 | ILE | CA-C-O | -5.11 | 109.38 | 120.10 |
| 3 | S | 36 | TYR | CA-C-O | -5.11 | 109.38 | 120.10 |
| 3 | S | 146 | VAL | CA-C-O | -5.11 | 109.38 | 120.10 |
| 4 | M | 110 | SER | CA-C-O | -5.11 | 109.38 | 120.10 |
| 2 | B | 274 | PRO | CA-N-CD | -5.10 | 104.36 | 111.50 |
| 2 | B | 401 | THR | C-N-CA | 5.10 | 134.46 | 121.70 |
| 2 | B | 292 | GLU | CA-C-N | -5.10 | 105.98 | 117.20 |
| 2 | B | 577 | ASN | N-CA-CB | -5.10 | 101.42 | 110.60 |
| 1 | A | 560 | SER | O-C-N | 5.10 | 130.85 | 122.70 |
| 1 | A | 445 | ASN | N-CA-C | -5.09 | 97.25 | 111.00 |
| 2 | B | 317 | VAL | CA-C-O | -5.09 | 109.40 | 120.10 |
| 2 | B | 443 | SER | CA-C-N | -5.09 | 105.99 | 117.20 |
| 1 | A | 85 | ALA | CA-C-N | -5.09 | 106.00 | 117.20 |
| 2 | B | 55 | ASN | C-N-CA | 5.09 | 134.43 | 121.70 |
| 2 | B | 336 | ASN | O-C-N | 5.09 | 130.85 | 122.70 |
| 1 | A | 174 | ARG | C-N-CD | -5.09 | 109.41 | 120.60 |
| 3 | S | 12 | CYS | C-N-CA | -5.09 | 108.98 | 121.70 |
| 2 | B | 450 | VAL | CA-C-O | -5.08 | 109.44 | 120.10 |
| 4 | M | 63 | TYR | CG-CD1-CE1 | -5.08 | 117.24 | 121.30 |
| 1 | A | 441 | TYR | N-CA-C | -5.07 | 97.31 | 111.00 |
| 4 | M | 24 | ALA | C-N-CD | 5.07 | 139.04 | 128.40 |
| 2 | B | 132 | SER | CA-C-O | 5.07 | 130.74 | 120.10 |
| 2 | B | 69 | ILE | C-N-CA | -5.06 | 109.04 | 121.70 |
| 4 | M | 282 | VAL | C-N-CA | -5.06 | 109.05 | 121.70 |
| 2 | B | 502 | SER | C-N-CA | -5.06 | 109.06 | 121.70 |
| 1 | A | 174 | ARG | O-C-N | 5.06 | 130.71 | 121.10 |
| 2 | B | 426 | GLU | CA-C-O | -5.05 | 109.49 | 120.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3 | S | 132 | LEU | CA-C-O | -5.05 | 109.49 | 120.10 |
| 2 | B | 138 | ALA | O-C-N | 5.05 | 130.78 | 122.70 |
| 4 | M | 323 | MET | C-N-CA | -5.05 | 109.08 | 121.70 |
| 1 | A | 253 | ILE | CA-C-O | -5.05 | 109.50 | 120.10 |
| 2 | B | 596 | LEU | CA-C-O | -5.04 | 109.51 | 120.10 |
| 3 | S | 63 | ASN | N-CA-CB | 5.04 | 119.68 | 110.60 |
| 3 | S | 89 | VAL | CA-C-O | 5.04 | 130.69 | 120.10 |
| 2 | B | 350 | THR | C-N-CA | 5.04 | 134.30 | 121.70 |
| 1 | A | 375 | VAL | CA-C-O | 5.04 | 130.68 | 120.10 |
| 2 | B | 134 | LEU | CA-C-O | -5.04 | 109.52 | 120.10 |
| 1 | A | 239 | LEU | C-N-CA | -5.04 | 109.10 | 121.70 |
| 1 | A | 469 | LEU | CA-C-N | -5.04 | 106.13 | 116.20 |
| 2 | B | 229 | HIS | O-C-N | 5.03 | 130.75 | 122.70 |
| 2 | B | 435 | SER | CA-C-O | -5.03 | 109.53 | 120.10 |
| 2 | B | 465 | ALA | O-C-N | 5.03 | 130.75 | 122.70 |
| 4 | M | 405 | THR | CA-C-O | 5.03 | 130.66 | 120.10 |
| 1 | A | 425 | LYS | CA-C-O | -5.03 | 109.55 | 120.10 |
| 3 | S | 29 | LYS | CA-C-O | -5.03 | 109.55 | 120.10 |
| 4 | M | 266 | ASP | C-N-CA | 5.02 | 134.24 | 121.70 |
| 2 | B | 444 | THR | C-N-CA | -5.02 | 109.16 | 121.70 |
| 2 | B | 492 | LYS | CA-C-O | -5.02 | 109.57 | 120.10 |
| 2 | B | 503 | LEU | CA-C-N | -5.01 | 106.17 | 117.20 |
| 4 | M | 136 | VAL | O-C-N | 5.01 | 130.71 | 122.70 |
| 1 | A | 535 | ILE | CA-C-N | -5.00 | 106.19 | 117.20 |
| 4 | M | 103 | TYR | CA-C-O | 5.00 | 130.61 | 120.10 |

All (2) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 3 | S | 69 | ASN | CA |
| 4 | M | 22 | ALA | CA |

All (127) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | A | 117 | ASP | Mainchain |
| 1 | A | 174 | ARG | Mainchain |
| 1 | A | 192 | TYR | Mainchain |
| 1 | A | 199 | ASN | Mainchain |
| 1 | A | 204 | VAL | Mainchain |
| 1 | A | 219 | VAL | Mainchain |
| 1 | A | 233 | PHE | Mainchain |

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| Mol | Chain | Res | Type | Group |
|------------|--------------|------------|-------------|--------------|
| 1 | A | 240 | LEU | Mainchain |
| 1 | A | 244 | LEU | Mainchain |
| 1 | A | 260 | PHE | Mainchain |
| 1 | A | 275 | LEU | Mainchain |
| 1 | A | 277 | LYS | Mainchain |
| 1 | A | 278 | ILE | Mainchain |
| 1 | A | 282 | MET | Mainchain |
| 1 | A | 288 | THR | Mainchain |
| 1 | A | 289 | SER | Mainchain |
| 1 | A | 290 | VAL | Mainchain |
| 1 | A | 298 | ILE | Mainchain |
| 1 | A | 302 | ASN | Mainchain |
| 1 | A | 306 | GLU | Mainchain |
| 1 | A | 319 | LEU | Mainchain |
| 1 | A | 320 | HIS | Mainchain |
| 1 | A | 323 | CYS | Mainchain |
| 1 | A | 325 | SER | Mainchain |
| 1 | A | 328 | PRO | Mainchain |
| 1 | A | 350 | SER | Mainchain |
| 1 | A | 381 | GLU | Mainchain |
| 1 | A | 399 | ASP | Peptide |
| 1 | A | 400 | VAL | Peptide |
| 1 | A | 436 | CYS | Mainchain |
| 1 | A | 441 | TYR | Mainchain |
| 1 | A | 462 | GLN | Mainchain |
| 1 | A | 487 | MET | Mainchain |
| 1 | A | 500 | SER | Mainchain |
| 1 | A | 501 | ASN | Mainchain |
| 1 | A | 505 | ASN | Mainchain |
| 1 | A | 506 | LYS | Mainchain |
| 1 | A | 527 | GLU | Mainchain |
| 1 | A | 528 | ASN | Mainchain |
| 1 | A | 529 | GLY | Mainchain |
| 1 | A | 531 | ASP | Mainchain |
| 1 | A | 535 | ILE | Mainchain |
| 1 | A | 536 | MET | Mainchain |
| 1 | A | 538 | GLU | Mainchain |
| 1 | A | 539 | ASN | Mainchain |
| 1 | A | 565 | ASN | Mainchain |
| 1 | A | 569 | ASP | Mainchain |
| 1 | A | 571 | ARG | Mainchain |
| 1 | A | 586 | GLU | Mainchain |

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| Mol | Chain | Res | Type | Group |
|------------|--------------|------------|-------------|--------------|
| 1 | A | 588 | LEU | Mainchain |
| 1 | A | 64 | LEU | Mainchain |
| 1 | A | 80 | TYR | Mainchain |
| 1 | A | 84 | MET | Mainchain |
| 1 | A | 94 | VAL | Mainchain |
| 2 | B | 126 | SER | Mainchain |
| 2 | B | 142 | LEU | Mainchain |
| 2 | B | 147 | MET | Mainchain |
| 2 | B | 181 | TYR | Mainchain |
| 2 | B | 186 | ASN | Mainchain |
| 2 | B | 237 | ILE | Mainchain |
| 2 | B | 267 | ASP | Mainchain |
| 2 | B | 278 | PRO | Peptide |
| 2 | B | 293 | VAL | Mainchain |
| 2 | B | 310 | ILE | Mainchain |
| 2 | B | 326 | TYR | Mainchain |
| 2 | B | 375 | LEU | Mainchain |
| 2 | B | 377 | TYR | Mainchain |
| 2 | B | 384 | PHE | Mainchain |
| 2 | B | 404 | ASN | Mainchain |
| 2 | B | 444 | THR | Mainchain |
| 2 | B | 459 | GLU | Mainchain |
| 2 | B | 485 | LYS | Mainchain |
| 2 | B | 497 | LEU | Mainchain |
| 2 | B | 523 | PHE | Mainchain |
| 2 | B | 536 | ASN | Mainchain |
| 2 | B | 557 | SER | Mainchain |
| 2 | B | 56 | SER | Mainchain |
| 2 | B | 565 | GLN | Mainchain |
| 2 | B | 569 | THR | Mainchain |
| 2 | B | 573 | GLU | Mainchain |
| 2 | B | 581 | TYR | Mainchain |
| 2 | B | 584 | SER | Mainchain |
| 2 | B | 78 | ASP | Mainchain |
| 2 | B | 82 | TYR | Mainchain |
| 2 | B | 88 | LYS | Mainchain |
| 4 | M | 102 | GLU | Mainchain |
| 4 | M | 103 | TYR | Mainchain |
| 4 | M | 104 | PHE | Mainchain |
| 4 | M | 105 | ASP | Peptide |
| 4 | M | 131 | ALA | Mainchain |
| 4 | M | 132 | GLY | Mainchain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 4 | M | 134 | PRO | Mainchain |
| 4 | M | 265 | ASN | Mainchain |
| 4 | M | 284 | SER | Mainchain |
| 4 | M | 292 | PRO | Peptide |
| 4 | M | 40 | GLN | Mainchain |
| 4 | M | 405 | THR | Mainchain |
| 4 | M | 421 | GLY | Mainchain |
| 4 | M | 426 | LYS | Peptide |
| 4 | M | 445 | SER | Peptide |
| 4 | M | 45 | SER | Peptide |
| 4 | M | 456 | SER | Mainchain |
| 4 | M | 462 | LYS | Peptide |
| 4 | M | 477 | GLY | Peptide |
| 4 | M | 51 | LEU | Peptide |
| 4 | M | 57 | GLY | Mainchain |
| 4 | M | 79 | SER | Mainchain |
| 4 | M | 8 | THR | Mainchain |
| 4 | M | 85 | GLY | Mainchain |
| 3 | S | 101 | LEU | Mainchain |
| 3 | S | 102 | ILE | Mainchain |
| 3 | S | 135 | ILE | Mainchain |
| 3 | S | 161 | GLU | Mainchain |
| 3 | S | 163 | THR | Peptide |
| 3 | S | 167 | ILE | Peptide |
| 3 | S | 22 | PRO | Mainchain |
| 3 | S | 43 | ASN | Mainchain |
| 3 | S | 46 | PHE | Mainchain |
| 3 | S | 50 | PHE | Mainchain |
| 3 | S | 53 | THR | Mainchain |
| 3 | S | 56 | SER | Mainchain |
| 3 | S | 57 | LEU | Mainchain |
| 3 | S | 58 | LEU | Peptide |
| 3 | S | 64 | ASN | Mainchain |
| 3 | S | 66 | ASP | Mainchain |
| 3 | S | 69 | ASN | Mainchain |
| 3 | S | 99 | LEU | Mainchain |

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 | 4625 | 0 | 4703 | 1294 | 0 |
| 2 | B | 4963 | 0 | 4983 | 2778 | 0 |
| 3 | S | 1358 | 0 | 1335 | 469 | 0 |
| 4 | M | 3158 | 0 | 3098 | 1734 | 0 |
| All | All | 14104 | 0 | 14119 | 5611 | 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 199.

All (5611) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:17:VAL:HG21 | 2:B:35:TYR:CD2 | 1.29 | 1.68 |
| 2:B:243:TRP:CH2 | 4:M:98:ARG:HD3 | 1.17 | 1.63 |
| 2:B:106:LEU:CD1 | 2:B:144:ASP:HB3 | 1.23 | 1.62 |
| 1:A:606:PHE:CZ | 1:A:633:PHE:HB2 | 1.23 | 1.62 |
| 2:B:578:PRO:HD2 | 2:B:581:TYR:CE2 | 1.21 | 1.61 |
| 2:B:106:LEU:CD2 | 4:M:130:GLU:HB3 | 1.26 | 1.61 |
| 2:B:2:VAL:HG11 | 4:M:54:SER:CB | 1.24 | 1.60 |
| 2:B:106:LEU:HD13 | 2:B:144:ASP:CB | 1.32 | 1.60 |
| 2:B:479:VAL:CG1 | 2:B:486:HIS:CE1 | 1.80 | 1.60 |
| 4:M:131:ALA:CA | 4:M:131:ALA:CB | 1.80 | 1.59 |
| 4:M:344:ILE:CG2 | 4:M:347:PHE:HB3 | 1.24 | 1.58 |
| 2:B:523:PHE:HZ | 2:B:580:TYR:CE2 | 1.17 | 1.58 |
| 2:B:73:ASP:HA | 4:M:19:LEU:CD2 | 1.29 | 1.58 |
| 2:B:403:ILE:HD13 | 2:B:439:CYS:CA | 1.34 | 1.57 |
| 2:B:216:LYS:CB | 2:B:251:LEU:HD13 | 1.12 | 1.57 |
| 2:B:226:LEU:HD23 | 2:B:255:TYR:CD1 | 1.38 | 1.55 |
| 2:B:17:VAL:CG2 | 2:B:35:TYR:HD2 | 1.20 | 1.54 |
| 4:M:282:VAL:N | 4:M:282:VAL:CA | 1.69 | 1.54 |
| 1:A:594:PHE:HE2 | 2:B:477:MET:SD | 1.28 | 1.53 |
| 4:M:244:VAL:HA | 4:M:472:TYR:CD2 | 1.37 | 1.52 |
| 2:B:106:LEU:HD23 | 4:M:130:GLU:CB | 1.05 | 1.51 |
| 2:B:107:ARG:CZ | 4:M:20:LEU:HD23 | 1.37 | 1.51 |
| 4:M:281:GLY:CA | 4:M:281:GLY:C | 1.78 | 1.51 |
| 2:B:73:ASP:CA | 4:M:19:LEU:HD22 | 1.11 | 1.51 |
| 2:B:1:MET:SD | 4:M:39:PRO:HD2 | 1.48 | 1.50 |
| 3:S:64:ASN:CA | 3:S:64:ASN:C | 1.80 | 1.49 |
| 2:B:72:SER:CA | 4:M:17:GLN:HE22 | 1.25 | 1.49 |
| 2:B:512:VAL:HG13 | 2:B:533:LEU:CD1 | 1.40 | 1.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:72:SER:HA | 4:M:17:GLN:NE2 | 1.28 | 1.47 |
| 1:A:329:ASN:CA | 3:S:50:PHE:CZ | 1.82 | 1.47 |
| 2:B:219:TYR:CE2 | 2:B:226:LEU:HD13 | 1.45 | 1.47 |
| 2:B:486:HIS:CE1 | 2:B:518:ILE:HD13 | 1.45 | 1.46 |
| 1:A:405:THR:HA | 2:B:7:ARG:NH2 | 1.24 | 1.46 |
| 1:A:406:GLY:C | 3:S:64:ASN:HD21 | 1.14 | 1.45 |
| 4:M:432:THR:OG1 | 4:M:480:GLN:CG | 1.63 | 1.45 |
| 2:B:230:PHE:CZ | 2:B:252:LEU:HD22 | 1.49 | 1.45 |
| 2:B:211:ALA:CB | 2:B:233:TYR:OH | 1.64 | 1.45 |
| 3:S:163:THR:CA | 3:S:163:THR:C | 1.83 | 1.45 |
| 2:B:73:ASP:CA | 4:M:19:LEU:CD2 | 1.87 | 1.45 |
| 4:M:245:ASP:O | 4:M:472:TYR:CE1 | 1.68 | 1.44 |
| 2:B:12:LEU:HD13 | 4:M:13:LYS:CG | 1.47 | 1.44 |
| 2:B:14:THR:HG22 | 2:B:36:THR:CG2 | 1.47 | 1.44 |
| 2:B:106:LEU:HD23 | 4:M:130:GLU:CA | 1.46 | 1.43 |
| 2:B:224:GLU:CB | 2:B:259:TYR:OH | 1.64 | 1.43 |
| 2:B:374:PHE:CE2 | 2:B:402:LEU:CD1 | 1.77 | 1.43 |
| 1:A:328:PRO:C | 3:S:50:PHE:HZ | 1.20 | 1.43 |
| 1:A:251:TRP:CE3 | 3:S:97:ALA:CA | 1.92 | 1.43 |
| 1:A:506:LYS:NZ | 4:M:82:LYS:HD2 | 1.28 | 1.43 |
| 2:B:215:TYR:CD2 | 2:B:233:TYR:HE2 | 1.37 | 1.43 |
| 2:B:423:HIS:NE2 | 4:M:365:GLU:HB3 | 1.28 | 1.43 |
| 2:B:523:PHE:CZ | 2:B:580:TYR:CE2 | 2.06 | 1.43 |
| 2:B:256:CYS:SG | 2:B:328:LEU:HD22 | 1.57 | 1.43 |
| 2:B:223:LEU:HD11 | 2:B:258:GLN:CB | 1.46 | 1.42 |
| 2:B:107:ARG:HH22 | 4:M:20:LEU:CD2 | 1.31 | 1.42 |
| 2:B:293:VAL:O | 2:B:299:LEU:CG | 1.65 | 1.42 |
| 2:B:337:THR:CA | 2:B:373:LEU:HD11 | 0.97 | 1.42 |
| 4:M:347:PHE:CE1 | 4:M:350:VAL:CG1 | 2.02 | 1.42 |
| 2:B:12:LEU:HD13 | 4:M:13:LYS:CB | 1.48 | 1.41 |
| 2:B:337:THR:HA | 2:B:373:LEU:CD1 | 0.93 | 1.41 |
| 2:B:564:LYS:CD | 2:B:621:GLY:O | 1.67 | 1.41 |
| 2:B:437:SER:CB | 2:B:474:VAL:HG13 | 1.49 | 1.41 |
| 2:B:20:ARG:NH1 | 4:M:118:TYR:HB3 | 1.09 | 1.41 |
| 2:B:158:VAL:HG11 | 2:B:177:ILE:CG1 | 1.45 | 1.41 |
| 2:B:223:LEU:HD13 | 2:B:259:TYR:N | 1.15 | 1.41 |
| 2:B:106:LEU:CG | 4:M:130:GLU:HB3 | 1.49 | 1.40 |
| 2:B:178:ILE:CG2 | 2:B:217:GLU:HB2 | 1.48 | 1.40 |
| 1:A:595:GLU:OE1 | 2:B:513:TRP:CZ3 | 1.73 | 1.40 |
| 2:B:243:TRP:CH2 | 4:M:98:ARG:CD | 2.02 | 1.40 |
| 2:B:20:ARG:HH12 | 4:M:118:TYR:CB | 1.31 | 1.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:11:ALA:HA | 2:B:40:GLN:NE2 | 1.18 | 1.40 |
| 2:B:403:ILE:CD1 | 2:B:439:CYS:CA | 2.00 | 1.40 |
| 2:B:374:PHE:HZ | 2:B:381:PHE:CD2 | 1.40 | 1.40 |
| 2:B:578:PRO:CD | 2:B:581:TYR:CE2 | 2.02 | 1.40 |
| 2:B:259:TYR:O | 2:B:261:PRO:CD | 1.66 | 1.39 |
| 1:A:595:GLU:CD | 2:B:513:TRP:CZ3 | 1.95 | 1.39 |
| 2:B:178:ILE:HG13 | 2:B:214:ALA:C | 1.41 | 1.39 |
| 2:B:25:VAL:HG22 | 2:B:30:LEU:C | 1.13 | 1.39 |
| 2:B:107:ARG:NH1 | 4:M:20:LEU:HD23 | 1.32 | 1.39 |
| 2:B:479:VAL:HG11 | 2:B:486:HIS:NE2 | 1.34 | 1.39 |
| 2:B:278:PRO:HD2 | 2:B:292:GLU:CB | 1.54 | 1.38 |
| 1:A:329:ASN:N | 3:S:50:PHE:CZ | 1.87 | 1.38 |
| 2:B:28:SER:CB | 2:B:30:LEU:O | 1.69 | 1.38 |
| 2:B:107:ARG:NH2 | 4:M:20:LEU:HD23 | 1.36 | 1.37 |
| 2:B:252:LEU:HD13 | 2:B:302:PHE:CD1 | 1.59 | 1.37 |
| 2:B:290:SER:O | 2:B:292:GLU:N | 1.56 | 1.37 |
| 2:B:293:VAL:O | 2:B:299:LEU:CD1 | 1.69 | 1.37 |
| 2:B:403:ILE:CD1 | 2:B:439:CYS:O | 1.69 | 1.37 |
| 2:B:337:THR:CB | 2:B:373:LEU:HD11 | 1.55 | 1.37 |
| 2:B:396:ILE:CG2 | 2:B:432:ALA:HA | 1.54 | 1.37 |
| 1:A:595:GLU:OE2 | 2:B:513:TRP:CZ3 | 1.77 | 1.37 |
| 2:B:12:LEU:CD1 | 4:M:13:LYS:HA | 1.54 | 1.37 |
| 2:B:193:LEU:CD2 | 2:B:225:LEU:CB | 2.00 | 1.37 |
| 4:M:219:LEU:CB | 4:M:472:TYR:O | 1.71 | 1.36 |
| 1:A:407:SER:C | 3:S:64:ASN:HD22 | 1.24 | 1.36 |
| 2:B:12:LEU:CD1 | 4:M:13:LYS:HG3 | 1.53 | 1.36 |
| 2:B:38:TYR:CE2 | 2:B:43:ASN:O | 1.78 | 1.36 |
| 4:M:222:PHE:O | 4:M:479:PHE:CE1 | 1.79 | 1.35 |
| 2:B:403:ILE:HD13 | 2:B:439:CYS:CB | 1.56 | 1.35 |
| 4:M:245:ASP:N | 4:M:472:TYR:CD1 | 1.93 | 1.35 |
| 2:B:28:SER:OG | 2:B:30:LEU:C | 1.64 | 1.35 |
| 2:B:252:LEU:HB2 | 2:B:302:PHE:CZ | 1.60 | 1.35 |
| 1:A:179:LYS:CE | 3:S:137:GLN:O | 1.74 | 1.34 |
| 2:B:479:VAL:HG13 | 2:B:486:HIS:ND1 | 1.41 | 1.34 |
| 1:A:595:GLU:OE2 | 2:B:513:TRP:CE3 | 1.78 | 1.34 |
| 1:A:503:ASN:HA | 4:M:59:ASP:O | 1.24 | 1.34 |
| 1:A:504:ILE:HA | 4:M:59:ASP:OD2 | 1.23 | 1.34 |
| 1:A:594:PHE:CE2 | 2:B:477:MET:SD | 2.18 | 1.34 |
| 2:B:25:VAL:CG2 | 2:B:30:LEU:C | 1.94 | 1.34 |
| 2:B:512:VAL:CG1 | 2:B:533:LEU:HD13 | 1.55 | 1.34 |
| 3:S:29:LYS:NZ | 3:S:33:GLU:OE2 | 1.59 | 1.34 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:606:PHE:HZ | 1:A:633:PHE:CB | 1.38 | 1.33 |
| 2:B:216:LYS:CB | 2:B:251:LEU:CD1 | 2.03 | 1.33 |
| 2:B:213:LEU:CD1 | 4:M:135:ASN:OD1 | 1.74 | 1.33 |
| 2:B:501:THR:O | 2:B:508:ARG:NH2 | 1.59 | 1.33 |
| 1:A:638:LEU:HD21 | 2:B:561:ASP:N | 1.43 | 1.33 |
| 2:B:374:PHE:CE2 | 2:B:402:LEU:HD11 | 1.15 | 1.33 |
| 2:B:403:ILE:HD11 | 2:B:439:CYS:O | 1.16 | 1.33 |
| 2:B:162:VAL:HG21 | 2:B:195:ILE:CG2 | 1.56 | 1.32 |
| 2:B:437:SER:HB2 | 2:B:474:VAL:CG1 | 1.59 | 1.32 |
| 1:A:504:ILE:HD13 | 4:M:59:ASP:OD2 | 1.20 | 1.32 |
| 1:A:606:PHE:CZ | 1:A:633:PHE:CB | 2.12 | 1.32 |
| 2:B:73:ASP:N | 4:M:19:LEU:CD2 | 1.89 | 1.32 |
| 2:B:226:LEU:CD2 | 2:B:255:TYR:CD1 | 2.10 | 1.32 |
| 2:B:295:ASN:O | 2:B:300:ASP:CB | 1.75 | 1.32 |
| 2:B:230:PHE:CE2 | 2:B:252:LEU:HD23 | 1.63 | 1.32 |
| 2:B:259:TYR:O | 2:B:261:PRO:N | 1.60 | 1.32 |
| 2:B:276:SER:O | 2:B:295:ASN:HB2 | 1.19 | 1.32 |
| 2:B:9:ALA:CB | 4:M:14:LEU:HB2 | 1.57 | 1.32 |
| 2:B:193:LEU:HD22 | 2:B:225:LEU:CB | 1.26 | 1.32 |
| 4:M:435:LEU:O | 4:M:479:PHE:CD1 | 1.82 | 1.32 |
| 2:B:106:LEU:CD1 | 2:B:144:ASP:CB | 1.93 | 1.31 |
| 2:B:224:GLU:HA | 2:B:259:TYR:CZ | 1.10 | 1.31 |
| 2:B:375:LEU:CD1 | 2:B:404:ASN:HD22 | 1.40 | 1.31 |
| 2:B:433:VAL:HG11 | 2:B:471:TYR:CA | 1.58 | 1.31 |
| 4:M:41:LEU:CD1 | 4:M:52:ASP:H | 1.39 | 1.31 |
| 2:B:9:ALA:O | 4:M:14:LEU:HB3 | 1.27 | 1.31 |
| 2:B:375:LEU:CD1 | 2:B:404:ASN:ND2 | 1.93 | 1.31 |
| 2:B:17:VAL:CG2 | 2:B:35:TYR:CD2 | 1.97 | 1.31 |
| 2:B:479:VAL:HG13 | 2:B:486:HIS:CE1 | 1.43 | 1.31 |
| 4:M:223:HIS:HA | 4:M:479:PHE:CD1 | 1.62 | 1.31 |
| 1:A:251:TRP:CE3 | 3:S:97:ALA:HA | 1.02 | 1.31 |
| 2:B:38:TYR:OH | 2:B:46:GLN:CG | 1.78 | 1.31 |
| 2:B:400:SER:HB3 | 2:B:435:SER:CB | 1.60 | 1.31 |
| 4:M:243:ILE:O | 4:M:472:TYR:CB | 1.77 | 1.31 |
| 2:B:278:PRO:CD | 2:B:292:GLU:HB2 | 1.60 | 1.31 |
| 2:B:396:ILE:HG21 | 2:B:432:ALA:CA | 1.61 | 1.31 |
| 2:B:243:TRP:CZ3 | 4:M:98:ARG:CD | 2.13 | 1.30 |
| 1:A:407:SER:O | 3:S:64:ASN:ND2 | 1.63 | 1.30 |
| 2:B:5:ILE:CG2 | 4:M:42:LEU:HD11 | 1.61 | 1.30 |
| 2:B:12:LEU:CG | 4:M:13:LYS:HG3 | 1.59 | 1.30 |
| 2:B:274:PRO:HG2 | 2:B:295:ASN:CB | 1.61 | 1.30 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:506:LYS:NZ | 4:M:82:LYS:CD | 1.94 | 1.30 |
| 4:M:344:ILE:CG2 | 4:M:347:PHE:CB | 2.09 | 1.30 |
| 1:A:503:ASN:OD1 | 4:M:60:LEU:CA | 1.79 | 1.30 |
| 2:B:234:CYS:O | 2:B:237:ILE:HG22 | 1.18 | 1.30 |
| 2:B:274:PRO:CB | 2:B:295:ASN:OD1 | 1.80 | 1.30 |
| 1:A:503:ASN:OD1 | 4:M:60:LEU:HD23 | 1.31 | 1.30 |
| 2:B:200:MET:SD | 2:B:229:HIS:O | 0.91 | 1.30 |
| 2:B:337:THR:HA | 2:B:373:LEU:CG | 1.60 | 1.30 |
| 2:B:75:ASP:OD1 | 4:M:24:ALA:HB3 | 1.16 | 1.29 |
| 4:M:355:ASP:OD2 | 4:M:357:LYS:NZ | 1.61 | 1.29 |
| 1:A:402:ILE:CD1 | 3:S:62:GLU:O | 1.79 | 1.29 |
| 2:B:73:ASP:HB3 | 4:M:25:PRO:O | 1.32 | 1.29 |
| 2:B:230:PHE:CE2 | 2:B:252:LEU:CD2 | 2.16 | 1.29 |
| 1:A:506:LYS:HE2 | 4:M:82:LYS:CB | 1.62 | 1.28 |
| 4:M:219:LEU:CD1 | 4:M:472:TYR:O | 1.81 | 1.28 |
| 1:A:556:VAL:HG21 | 1:A:603:VAL:CG2 | 1.63 | 1.28 |
| 2:B:181:TYR:CE1 | 2:B:222:HIS:CD2 | 2.20 | 1.28 |
| 2:B:216:LYS:HE3 | 4:M:133:GLU:OE2 | 1.32 | 1.28 |
| 2:B:256:CYS:SG | 2:B:328:LEU:CD2 | 2.21 | 1.28 |
| 2:B:274:PRO:CG | 2:B:295:ASN:OD1 | 1.80 | 1.28 |
| 2:B:433:VAL:CG1 | 2:B:471:TYR:HA | 1.63 | 1.28 |
| 4:M:218:LEU:HA | 4:M:472:TYR:CE2 | 1.67 | 1.28 |
| 2:B:230:PHE:CE1 | 2:B:234:CYS:SG | 2.26 | 1.28 |
| 2:B:296:ASP:OD1 | 2:B:297:PRO:HD2 | 1.22 | 1.28 |
| 1:A:462:GLN:O | 4:M:58:ARG:HA | 1.24 | 1.28 |
| 2:B:25:VAL:CG2 | 2:B:32:GLU:H | 1.47 | 1.28 |
| 2:B:73:ASP:OD1 | 4:M:19:LEU:HD13 | 1.26 | 1.28 |
| 2:B:219:TYR:CE2 | 2:B:226:LEU:CD1 | 2.14 | 1.27 |
| 1:A:402:ILE:CG2 | 3:S:62:GLU:O | 1.81 | 1.27 |
| 1:A:402:ILE:HG21 | 3:S:62:GLU:O | 1.16 | 1.27 |
| 2:B:155:LEU:HD23 | 2:B:192:LEU:CD1 | 1.62 | 1.27 |
| 2:B:274:PRO:HG2 | 2:B:295:ASN:CG | 1.52 | 1.27 |
| 2:B:17:VAL:HG21 | 2:B:35:TYR:CE2 | 1.69 | 1.27 |
| 2:B:28:SER:O | 2:B:58:GLU:HG2 | 1.12 | 1.27 |
| 2:B:38:TYR:CE2 | 2:B:43:ASN:N | 2.01 | 1.27 |
| 1:A:186:PHE:CE2 | 1:A:224:GLU:CB | 2.17 | 1.27 |
| 2:B:347:VAL:HG22 | 2:B:359:LEU:CB | 1.64 | 1.27 |
| 1:A:405:THR:CA | 2:B:7:ARG:HH21 | 1.46 | 1.26 |
| 2:B:374:PHE:CZ | 2:B:381:PHE:CD2 | 2.21 | 1.26 |
| 4:M:218:LEU:O | 4:M:441:GLY:N | 1.64 | 1.26 |
| 2:B:278:PRO:HD2 | 2:B:292:GLU:CG | 1.66 | 1.26 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:M:96:ILE:HG21 | 4:M:125:PHE:CZ | 1.68 | 1.26 |
| 4:M:223:HIS:HA | 4:M:479:PHE:CE1 | 1.70 | 1.26 |
| 2:B:231:ARG:NH2 | 2:B:279:LEU:HD21 | 1.47 | 1.26 |
| 1:A:333:ILE:CD1 | 3:S:95:GLU:OE1 | 1.83 | 1.26 |
| 2:B:403:ILE:CD1 | 2:B:439:CYS:C | 2.02 | 1.26 |
| 2:B:567:GLN:O | 2:B:569:THR:N | 1.68 | 1.26 |
| 2:B:73:ASP:OD1 | 4:M:24:ALA:HB1 | 1.12 | 1.26 |
| 2:B:200:MET:CE | 2:B:229:HIS:O | 1.81 | 1.26 |
| 2:B:479:VAL:CG1 | 2:B:486:HIS:NE2 | 1.92 | 1.26 |
| 2:B:309:LEU:HB3 | 2:B:317:VAL:CG1 | 1.66 | 1.25 |
| 2:B:418:TYR:OH | 2:B:432:ALA:HB2 | 1.34 | 1.25 |
| 2:B:74:ASP:O | 2:B:77:ILE:HG12 | 1.15 | 1.25 |
| 2:B:22:ALA:HB2 | 2:B:33:SER:OG | 1.37 | 1.25 |
| 2:B:178:ILE:HG13 | 2:B:214:ALA:CA | 1.66 | 1.25 |
| 2:B:73:ASP:OD1 | 4:M:19:LEU:CD1 | 1.83 | 1.25 |
| 2:B:219:TYR:CZ | 2:B:226:LEU:HB2 | 1.71 | 1.25 |
| 2:B:25:VAL:HG23 | 2:B:32:GLU:N | 1.53 | 1.24 |
| 2:B:144:ASP:CG | 4:M:131:ALA:HA | 1.57 | 1.24 |
| 2:B:219:TYR:CD2 | 2:B:226:LEU:HD22 | 1.71 | 1.24 |
| 2:B:243:TRP:CZ3 | 4:M:98:ARG:HD3 | 1.72 | 1.24 |
| 2:B:556:LEU:CA | 2:B:588:ILE:HD11 | 1.65 | 1.24 |
| 4:M:65:TYR:CZ | 4:M:86:PRO:HB3 | 1.69 | 1.24 |
| 2:B:230:PHE:CZ | 2:B:252:LEU:CD2 | 2.17 | 1.24 |
| 2:B:337:THR:CB | 2:B:373:LEU:CD1 | 2.13 | 1.24 |
| 2:B:216:LYS:HA | 2:B:251:LEU:CD1 | 1.67 | 1.24 |
| 3:S:32:LEU:O | 3:S:35:VAL:HG22 | 1.33 | 1.24 |
| 2:B:197:LYS:HB2 | 2:B:229:HIS:NE2 | 1.51 | 1.24 |
| 2:B:216:LYS:CA | 2:B:251:LEU:CD1 | 2.15 | 1.23 |
| 2:B:347:VAL:CG2 | 2:B:359:LEU:HB3 | 1.66 | 1.23 |
| 1:A:329:ASN:HA | 3:S:50:PHE:CZ | 1.39 | 1.23 |
| 2:B:200:MET:SD | 2:B:229:HIS:C | 2.14 | 1.23 |
| 2:B:341:GLU:HG3 | 2:B:377:TYR:CE1 | 1.50 | 1.23 |
| 2:B:107:ARG:HH12 | 4:M:20:LEU:CD2 | 1.49 | 1.23 |
| 2:B:215:TYR:CD2 | 2:B:233:TYR:CE2 | 2.27 | 1.23 |
| 4:M:218:LEU:HA | 4:M:472:TYR:CD2 | 1.71 | 1.23 |
| 4:M:222:PHE:CD1 | 4:M:240:ILE:HG23 | 1.72 | 1.23 |
| 1:A:422:GLU:OE1 | 3:S:62:GLU:HG2 | 1.37 | 1.23 |
| 1:A:450:TYR:OH | 1:A:476:GLN:CG | 1.87 | 1.23 |
| 2:B:13:ASP:OD1 | 4:M:14:LEU:C | 1.75 | 1.23 |
| 2:B:216:LYS:HB2 | 2:B:251:LEU:CD1 | 1.66 | 1.23 |
| 2:B:219:TYR:CE2 | 2:B:226:LEU:HB2 | 1.71 | 1.23 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:258:LYS:NZ | 3:S:93:GLU:CA | 2.02 | 1.22 |
| 2:B:2:VAL:CG1 | 4:M:54:SER:CB | 2.17 | 1.22 |
| 2:B:73:ASP:OD1 | 4:M:24:ALA:CB | 1.85 | 1.22 |
| 2:B:375:LEU:HD13 | 2:B:404:ASN:CB | 1.67 | 1.22 |
| 3:S:135:ILE:O | 3:S:141:VAL:HA | 1.33 | 1.22 |
| 1:A:506:LYS:HZ1 | 4:M:82:LYS:CD | 1.50 | 1.22 |
| 2:B:293:VAL:O | 2:B:299:LEU:HG | 1.21 | 1.22 |
| 2:B:104:TYR:O | 2:B:107:ARG:HB2 | 1.40 | 1.22 |
| 2:B:259:TYR:CD1 | 2:B:261:PRO:HG3 | 1.75 | 1.22 |
| 4:M:363:ASN:ND2 | 4:M:431:GLN:OE1 | 1.72 | 1.22 |
| 2:B:103:LEU:CD1 | 4:M:123:LEU:HD11 | 1.68 | 1.21 |
| 2:B:277:CYS:O | 2:B:288:TYR:HB3 | 1.38 | 1.21 |
| 2:B:563:PHE:O | 2:B:566:ALA:HB3 | 1.32 | 1.21 |
| 4:M:245:ASP:N | 4:M:472:TYR:CE1 | 2.08 | 1.21 |
| 2:B:567:GLN:O | 2:B:569:THR:OG1 | 1.53 | 1.21 |
| 2:B:584:SER:O | 2:B:588:ILE:HG22 | 1.35 | 1.21 |
| 4:M:44:ASP:CB | 4:M:50:TYR:CD2 | 2.23 | 1.21 |
| 2:B:107:ARG:NH2 | 4:M:20:LEU:CD2 | 1.96 | 1.21 |
| 2:B:143:SER:OG | 2:B:179:LYS:HD2 | 1.36 | 1.21 |
| 2:B:178:ILE:CG1 | 2:B:214:ALA:HB1 | 1.69 | 1.21 |
| 2:B:196:LEU:O | 2:B:215:TYR:OH | 1.58 | 1.21 |
| 2:B:237:ILE:O | 2:B:238:LYS:C | 1.69 | 1.21 |
| 2:B:336:ASN:C | 2:B:373:LEU:HD21 | 1.60 | 1.21 |
| 2:B:567:GLN:O | 2:B:569:THR:CB | 1.89 | 1.21 |
| 2:B:14:THR:CG2 | 2:B:36:THR:CG2 | 2.19 | 1.21 |
| 2:B:318:ILE:HD13 | 2:B:346:THR:OG1 | 1.08 | 1.21 |
| 1:A:406:GLY:C | 3:S:64:ASN:ND2 | 1.93 | 1.20 |
| 2:B:1:MET:SD | 4:M:39:PRO:CD | 2.28 | 1.20 |
| 1:A:329:ASN:N | 3:S:50:PHE:CE2 | 2.09 | 1.20 |
| 4:M:350:VAL:HG13 | 4:M:442:GLN:CB | 1.71 | 1.20 |
| 2:B:5:ILE:HG21 | 4:M:42:LEU:CD1 | 1.70 | 1.20 |
| 2:B:106:LEU:HD22 | 2:B:144:ASP:OD2 | 1.42 | 1.20 |
| 2:B:479:VAL:CG2 | 2:B:486:HIS:CD2 | 2.25 | 1.20 |
| 1:A:328:PRO:C | 3:S:50:PHE:CZ | 2.09 | 1.20 |
| 2:B:72:SER:CB | 4:M:17:GLN:OE1 | 1.89 | 1.20 |
| 2:B:106:LEU:CD2 | 4:M:130:GLU:CB | 1.91 | 1.20 |
| 2:B:139:LEU:CD2 | 2:B:173:VAL:HA | 1.72 | 1.20 |
| 2:B:279:LEU:N | 2:B:288:TYR:HB2 | 1.54 | 1.20 |
| 1:A:606:PHE:CE1 | 1:A:633:PHE:HB2 | 1.75 | 1.20 |
| 2:B:12:LEU:HB3 | 4:M:13:LYS:CG | 1.70 | 1.20 |
| 2:B:28:SER:C | 2:B:58:GLU:HG2 | 1.62 | 1.20 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:313:SER:OG | 4:M:269:ILE:O | 1.60 | 1.19 |
| 4:M:221:THR:N | 4:M:474:THR:OG1 | 1.73 | 1.19 |
| 1:A:329:ASN:HA | 3:S:50:PHE:CE1 | 1.75 | 1.19 |
| 1:A:563:CYS:HB3 | 1:A:621:LEU:HD11 | 1.24 | 1.19 |
| 2:B:523:PHE:CE2 | 2:B:580:TYR:CD2 | 2.30 | 1.19 |
| 1:A:410:TYR:CD1 | 3:S:43:ASN:ND2 | 2.10 | 1.19 |
| 2:B:375:LEU:HD13 | 2:B:404:ASN:HB2 | 1.21 | 1.19 |
| 4:M:121:ILE:O | 4:M:125:PHE:CD1 | 1.95 | 1.19 |
| 2:B:226:LEU:HD23 | 2:B:255:TYR:CE1 | 1.77 | 1.19 |
| 2:B:256:CYS:CB | 2:B:328:LEU:CD2 | 2.19 | 1.19 |
| 2:B:268:LYS:O | 2:B:273:SER:OG | 1.55 | 1.19 |
| 2:B:375:LEU:HD13 | 2:B:404:ASN:ND2 | 1.52 | 1.19 |
| 2:B:403:ILE:CD1 | 2:B:439:CYS:HA | 1.62 | 1.19 |
| 2:B:523:PHE:CZ | 2:B:580:TYR:CD2 | 2.30 | 1.19 |
| 1:A:407:SER:C | 3:S:64:ASN:ND2 | 1.95 | 1.18 |
| 2:B:2:VAL:CG1 | 4:M:54:SER:OG | 1.89 | 1.18 |
| 2:B:106:LEU:CD2 | 4:M:130:GLU:CA | 2.14 | 1.18 |
| 2:B:136:CYS:SG | 2:B:169:VAL:HA | 1.83 | 1.18 |
| 1:A:215:VAL:CG1 | 1:A:243:ILE:HG21 | 1.74 | 1.18 |
| 1:A:186:PHE:CE2 | 1:A:224:GLU:HB2 | 1.77 | 1.18 |
| 2:B:11:ALA:CA | 2:B:40:GLN:NE2 | 2.06 | 1.18 |
| 2:B:261:PRO:CD | 2:B:293:VAL:HG23 | 1.74 | 1.18 |
| 2:B:274:PRO:HG2 | 2:B:295:ASN:OD1 | 1.37 | 1.18 |
| 2:B:351:GLU:HB3 | 4:M:476:THR:CB | 1.74 | 1.18 |
| 2:B:223:LEU:CD1 | 2:B:259:TYR:N | 2.05 | 1.18 |
| 2:B:252:LEU:CD1 | 2:B:302:PHE:CD1 | 2.27 | 1.18 |
| 2:B:278:PRO:HA | 2:B:288:TYR:CB | 1.73 | 1.18 |
| 1:A:503:ASN:HB3 | 4:M:59:ASP:C | 1.63 | 1.17 |
| 2:B:144:ASP:OD1 | 4:M:131:ALA:HA | 1.40 | 1.17 |
| 2:B:219:TYR:CZ | 2:B:226:LEU:CA | 2.27 | 1.17 |
| 2:B:335:LYS:HA | 2:B:370:ASP:OD2 | 1.43 | 1.17 |
| 2:B:155:LEU:CD2 | 2:B:192:LEU:HD11 | 1.75 | 1.17 |
| 2:B:433:VAL:HG12 | 2:B:474:VAL:CG2 | 1.73 | 1.17 |
| 2:B:158:VAL:CG1 | 2:B:177:ILE:CG1 | 2.22 | 1.17 |
| 2:B:383:VAL:O | 2:B:385:PRO:HD3 | 1.45 | 1.17 |
| 2:B:374:PHE:CE2 | 2:B:402:LEU:HD13 | 1.75 | 1.17 |
| 4:M:275:CYS:SG | 4:M:293:PRO:HB3 | 1.85 | 1.17 |
| 4:M:432:THR:OG1 | 4:M:480:GLN:HG3 | 1.00 | 1.17 |
| 2:B:28:SER:O | 2:B:58:GLU:CG | 1.90 | 1.16 |
| 2:B:155:LEU:CD2 | 2:B:192:LEU:CD1 | 2.23 | 1.16 |
| 2:B:564:LYS:HD2 | 2:B:621:GLY:O | 1.02 | 1.16 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:252:LEU:HB2 | 2:B:302:PHE:CE1 | 1.79 | 1.16 |
| 2:B:322:CYS:SG | 2:B:366:LEU:HD11 | 1.83 | 1.16 |
| 2:B:400:SER:HB3 | 2:B:435:SER:HB3 | 1.18 | 1.16 |
| 3:S:8:PHE:HB3 | 3:S:36:TYR:OH | 1.42 | 1.16 |
| 2:B:16:LYS:HD3 | 4:M:115:VAL:HG21 | 1.21 | 1.16 |
| 2:B:296:ASP:OD1 | 2:B:297:PRO:CD | 1.93 | 1.16 |
| 2:B:479:VAL:HG22 | 2:B:486:HIS:CD2 | 1.79 | 1.16 |
| 4:M:219:LEU:HD22 | 4:M:473:LYS:HA | 1.16 | 1.16 |
| 2:B:38:TYR:OH | 2:B:46:GLN:CB | 1.92 | 1.16 |
| 2:B:73:ASP:N | 4:M:19:LEU:HD22 | 1.51 | 1.16 |
| 2:B:106:LEU:CD1 | 2:B:144:ASP:O | 1.92 | 1.16 |
| 2:B:216:LYS:CA | 2:B:251:LEU:HD13 | 1.76 | 1.16 |
| 2:B:245:GLN:CD | 2:B:309:LEU:HD11 | 1.66 | 1.16 |
| 2:B:568:VAL:HG12 | 2:B:571:SER:OG | 1.44 | 1.16 |
| 1:A:258:LYS:NZ | 3:S:93:GLU:HA | 1.57 | 1.15 |
| 1:A:410:TYR:CE1 | 3:S:43:ASN:ND2 | 2.13 | 1.15 |
| 2:B:2:VAL:CG1 | 4:M:54:SER:HB3 | 1.74 | 1.15 |
| 2:B:178:ILE:HG12 | 2:B:214:ALA:HB1 | 1.19 | 1.15 |
| 2:B:476:ARG:HA | 2:B:514:LEU:HD13 | 1.16 | 1.15 |
| 2:B:158:VAL:HG11 | 2:B:177:ILE:HG13 | 1.27 | 1.15 |
| 4:M:302:TYR:CD1 | 4:M:445:SER:HB3 | 1.80 | 1.15 |
| 1:A:179:LYS:HE3 | 3:S:140:MET:CB | 1.75 | 1.15 |
| 1:A:411:GLU:OE2 | 3:S:46:PHE:CE1 | 1.99 | 1.15 |
| 2:B:64:LYS:NZ | 4:M:120:ARG:NH1 | 1.94 | 1.15 |
| 2:B:219:TYR:CE1 | 2:B:226:LEU:HB2 | 1.81 | 1.15 |
| 1:A:186:PHE:CE2 | 1:A:224:GLU:CG | 2.30 | 1.15 |
| 1:A:260:PHE:O | 1:A:261:THR:C | 1.69 | 1.15 |
| 2:B:219:TYR:CE2 | 2:B:226:LEU:CB | 2.28 | 1.15 |
| 2:B:313:SER:CB | 4:M:269:ILE:HB | 1.64 | 1.15 |
| 1:A:254:ILE:HG21 | 3:S:94:SER:OG | 1.44 | 1.15 |
| 2:B:16:LYS:CD | 4:M:115:VAL:HG21 | 1.76 | 1.15 |
| 2:B:236:ILE:CG2 | 2:B:240:LEU:HD11 | 1.77 | 1.15 |
| 2:B:259:TYR:O | 2:B:261:PRO:HD3 | 1.31 | 1.15 |
| 4:M:241:HIS:O | 4:M:474:THR:CB | 1.94 | 1.15 |
| 4:M:344:ILE:HG23 | 4:M:347:PHE:CB | 1.71 | 1.15 |
| 2:B:212:VAL:HG21 | 2:B:248:LEU:HD21 | 1.29 | 1.14 |
| 4:M:41:LEU:HD12 | 4:M:52:ASP:H | 1.02 | 1.14 |
| 1:A:504:ILE:HA | 4:M:59:ASP:CG | 1.68 | 1.14 |
| 2:B:13:ASP:O | 2:B:17:VAL:HG22 | 1.46 | 1.14 |
| 2:B:236:ILE:HG22 | 2:B:240:LEU:CD1 | 1.77 | 1.14 |
| 2:B:252:LEU:HB3 | 2:B:302:PHE:CD2 | 1.81 | 1.14 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:343:LEU:HD23 | 2:B:363:ILE:HD13 | 1.15 | 1.14 |
| 4:M:244:VAL:HA | 4:M:472:TYR:CE2 | 1.81 | 1.14 |
| 4:M:347:PHE:CE1 | 4:M:350:VAL:HG11 | 1.69 | 1.14 |
| 2:B:245:GLN:CD | 2:B:309:LEU:CD1 | 2.16 | 1.14 |
| 2:B:375:LEU:O | 2:B:377:TYR:N | 1.78 | 1.14 |
| 2:B:556:LEU:HD22 | 2:B:588:ILE:HG12 | 1.26 | 1.14 |
| 2:B:25:VAL:HG22 | 2:B:30:LEU:O | 1.45 | 1.14 |
| 1:A:186:PHE:CE2 | 1:A:224:GLU:HG2 | 1.83 | 1.14 |
| 1:A:638:LEU:HD23 | 2:B:561:ASP:CG | 1.65 | 1.14 |
| 2:B:2:VAL:HG11 | 4:M:54:SER:OG | 1.39 | 1.14 |
| 3:S:17:VAL:HG21 | 3:S:19:PHE:CZ | 1.83 | 1.14 |
| 4:M:95:THR:OG1 | 4:M:137:SER:O | 1.64 | 1.14 |
| 4:M:343:ASN:HA | 4:M:408:VAL:HG13 | 1.15 | 1.14 |
| 1:A:275:LEU:O | 1:A:276:PRO:C | 1.73 | 1.13 |
| 1:A:406:GLY:O | 3:S:64:ASN:ND2 | 1.76 | 1.13 |
| 1:A:408:ILE:HG21 | 3:S:41:GLN:HB3 | 1.14 | 1.13 |
| 2:B:14:THR:CG2 | 2:B:36:THR:HG22 | 1.77 | 1.13 |
| 2:B:20:ARG:NH1 | 4:M:118:TYR:CB | 1.99 | 1.13 |
| 2:B:70:MET:HE1 | 2:B:107:ARG:HG3 | 1.29 | 1.13 |
| 2:B:216:LYS:HA | 2:B:251:LEU:HD11 | 1.14 | 1.13 |
| 4:M:262:THR:CG2 | 4:M:265:ASN:H | 1.61 | 1.13 |
| 2:B:219:TYR:CD2 | 2:B:226:LEU:HB2 | 1.84 | 1.13 |
| 2:B:341:GLU:CG | 2:B:377:TYR:CE1 | 2.25 | 1.13 |
| 2:B:344:VAL:HG13 | 2:B:381:PHE:CE2 | 1.82 | 1.13 |
| 4:M:222:PHE:O | 4:M:479:PHE:CZ | 2.00 | 1.13 |
| 1:A:503:ASN:CB | 4:M:59:ASP:C | 2.16 | 1.13 |
| 2:B:127:LEU:HD13 | 2:B:157:THR:HG21 | 1.30 | 1.13 |
| 2:B:325:LEU:HD13 | 2:B:339:PHE:HB3 | 1.18 | 1.13 |
| 4:M:71:LYS:HB3 | 4:M:74:TYR:CZ | 1.83 | 1.13 |
| 1:A:638:LEU:CD1 | 2:B:557:SER:C | 2.17 | 1.13 |
| 1:A:114:PHE:CZ | 1:A:153:ILE:HA | 1.83 | 1.12 |
| 1:A:530:ASN:ND2 | 1:A:573:GLU:OE1 | 1.80 | 1.13 |
| 2:B:103:LEU:HB3 | 4:M:126:ASN:HD22 | 1.00 | 1.12 |
| 2:B:469:ASP:OD2 | 2:B:506:ASN:HB2 | 1.47 | 1.12 |
| 1:A:333:ILE:HD13 | 3:S:95:GLU:OE1 | 1.47 | 1.12 |
| 2:B:143:SER:HB2 | 2:B:179:LYS:CB | 1.79 | 1.12 |
| 4:M:222:PHE:C | 4:M:479:PHE:CZ | 2.23 | 1.12 |
| 2:B:18:ILE:CD1 | 2:B:36:THR:HG21 | 1.76 | 1.12 |
| 2:B:72:SER:HB3 | 4:M:17:GLN:OE1 | 1.42 | 1.12 |
| 2:B:486:HIS:CE1 | 2:B:518:ILE:CD1 | 2.33 | 1.12 |
| 4:M:302:TYR:CE1 | 4:M:445:SER:HB3 | 1.84 | 1.12 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:M:350:VAL:HG13 | 4:M:442:GLN:HB3 | 1.16 | 1.12 |
| 1:A:503:ASN:CA | 4:M:59:ASP:O | 1.98 | 1.12 |
| 2:B:73:ASP:CG | 4:M:24:ALA:HB1 | 1.68 | 1.12 |
| 2:B:106:LEU:HG | 4:M:130:GLU:OE1 | 1.47 | 1.12 |
| 2:B:219:TYR:CZ | 2:B:226:LEU:CB | 2.31 | 1.12 |
| 4:M:219:LEU:HB2 | 4:M:472:TYR:O | 1.43 | 1.12 |
| 1:A:606:PHE:HZ | 1:A:633:PHE:CG | 1.68 | 1.12 |
| 2:B:12:LEU:CD1 | 4:M:13:LYS:CA | 2.27 | 1.12 |
| 2:B:12:LEU:CB | 4:M:13:LYS:HG3 | 1.80 | 1.12 |
| 2:B:38:TYR:HE2 | 2:B:43:ASN:O | 1.12 | 1.12 |
| 2:B:82:TYR:HB2 | 2:B:104:TYR:OH | 1.50 | 1.12 |
| 2:B:230:PHE:O | 2:B:231:ARG:O | 1.66 | 1.12 |
| 2:B:261:PRO:HD3 | 2:B:293:VAL:HG23 | 1.26 | 1.12 |
| 2:B:422:ALA:HB3 | 2:B:424:PHE:CE2 | 1.85 | 1.12 |
| 2:B:181:TYR:CE1 | 2:B:185:LYS:HG3 | 1.85 | 1.11 |
| 4:M:219:LEU:HD13 | 4:M:472:TYR:O | 1.40 | 1.11 |
| 2:B:9:ALA:HB1 | 4:M:14:LEU:CB | 1.80 | 1.11 |
| 2:B:293:VAL:C | 2:B:299:LEU:HG | 1.71 | 1.11 |
| 2:B:223:LEU:CD1 | 2:B:258:GLN:C | 2.19 | 1.11 |
| 1:A:233:PHE:O | 1:A:234:ILE:C | 1.71 | 1.11 |
| 2:B:12:LEU:HD12 | 4:M:13:LYS:HA | 1.11 | 1.11 |
| 2:B:25:VAL:HG22 | 2:B:31:GLY:N | 1.64 | 1.11 |
| 1:A:556:VAL:HG21 | 1:A:603:VAL:HG21 | 1.15 | 1.11 |
| 2:B:16:LYS:HB3 | 4:M:115:VAL:HG11 | 1.19 | 1.11 |
| 2:B:29:LYS:N | 2:B:30:LEU:HA | 1.56 | 1.11 |
| 2:B:107:ARG:NH1 | 4:M:20:LEU:CD2 | 2.09 | 1.11 |
| 4:M:244:VAL:CA | 4:M:472:TYR:CD2 | 2.33 | 1.11 |
| 4:M:268:GLY:N | 4:M:302:TYR:OH | 1.83 | 1.11 |
| 1:A:215:VAL:CG1 | 1:A:243:ILE:CG2 | 2.28 | 1.10 |
| 1:A:503:ASN:CG | 4:M:60:LEU:HD23 | 1.71 | 1.10 |
| 2:B:252:LEU:CB | 2:B:302:PHE:CZ | 2.35 | 1.10 |
| 4:M:2:TYR:OH | 4:M:64:LYS:NZ | 1.82 | 1.10 |
| 4:M:347:PHE:CE1 | 4:M:350:VAL:HG12 | 1.84 | 1.10 |
| 1:A:429:VAL:CB | 1:A:469:LEU:HD11 | 1.81 | 1.10 |
| 1:A:503:ASN:OD1 | 4:M:60:LEU:HA | 0.93 | 1.10 |
| 2:B:211:ALA:C | 2:B:233:TYR:OH | 1.90 | 1.10 |
| 2:B:303:LEU:HD22 | 2:B:339:PHE:CZ | 1.85 | 1.10 |
| 2:B:348:THR:HG21 | 2:B:380:LYS:HB3 | 1.18 | 1.10 |
| 2:B:107:ARG:HH22 | 4:M:20:LEU:HD21 | 1.00 | 1.10 |
| 2:B:344:VAL:HG11 | 2:B:377:TYR:HB3 | 1.18 | 1.10 |
| 2:B:219:TYR:CD2 | 2:B:226:LEU:HD13 | 1.85 | 1.10 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:280:PRO:HG2 | 2:B:283:TYR:CD2 | 1.86 | 1.10 |
| 2:B:318:ILE:CD1 | 2:B:346:THR:OG1 | 2.00 | 1.10 |
| 2:B:337:THR:N | 2:B:373:LEU:HD21 | 1.66 | 1.10 |
| 2:B:451:MET:HG3 | 2:B:489:ILE:HG12 | 1.32 | 1.10 |
| 4:M:341:SER:OG | 4:M:343:ASN:ND2 | 1.84 | 1.10 |
| 1:A:125:THR:OG1 | 1:A:158:LEU:HD13 | 1.48 | 1.09 |
| 1:A:638:LEU:HD12 | 2:B:557:SER:C | 1.71 | 1.09 |
| 2:B:211:ALA:HB3 | 2:B:233:TYR:OH | 1.48 | 1.09 |
| 2:B:310:ILE:CG2 | 2:B:342:ALA:HB1 | 1.82 | 1.09 |
| 3:S:16:LEU:HB2 | 3:S:125:TRP:NE1 | 1.66 | 1.09 |
| 4:M:44:ASP:HB3 | 4:M:50:TYR:CD2 | 1.86 | 1.09 |
| 4:M:51:LEU:HB3 | 4:M:68:VAL:HG21 | 1.31 | 1.09 |
| 2:B:11:ALA:CA | 2:B:40:GLN:HE22 | 1.60 | 1.09 |
| 2:B:70:MET:CE | 2:B:107:ARG:HG3 | 1.80 | 1.09 |
| 2:B:106:LEU:HD13 | 2:B:144:ASP:HB2 | 1.18 | 1.09 |
| 2:B:158:VAL:HG11 | 2:B:177:ILE:HG12 | 1.10 | 1.09 |
| 2:B:274:PRO:CA | 2:B:295:ASN:OD1 | 2.00 | 1.09 |
| 2:B:479:VAL:HG11 | 2:B:486:HIS:CE1 | 1.60 | 1.09 |
| 4:M:350:VAL:CG2 | 4:M:442:GLN:HG2 | 1.82 | 1.09 |
| 2:B:310:ILE:HD11 | 2:B:321:CYS:HB2 | 1.29 | 1.09 |
| 2:B:479:VAL:HG13 | 2:B:486:HIS:CG | 1.87 | 1.09 |
| 2:B:224:GLU:CA | 2:B:259:TYR:OH | 0.79 | 1.09 |
| 3:S:35:VAL:HG12 | 3:S:77:TYR:OH | 1.53 | 1.09 |
| 4:M:76:CYS:SG | 4:M:97:ASP:OD1 | 2.10 | 1.09 |
| 4:M:262:THR:O | 4:M:264:GLY:N | 1.85 | 1.09 |
| 1:A:68:THR:HB | 3:S:166:LYS:CB | 1.83 | 1.09 |
| 1:A:114:PHE:CD1 | 1:A:153:ILE:HG23 | 1.88 | 1.09 |
| 2:B:20:ARG:CZ | 4:M:118:TYR:HB3 | 1.82 | 1.09 |
| 2:B:276:SER:O | 2:B:295:ASN:CB | 1.99 | 1.09 |
| 1:A:179:LYS:HE3 | 3:S:140:MET:HB3 | 1.12 | 1.08 |
| 2:B:24:ALA:HB3 | 2:B:32:GLU:HG2 | 1.12 | 1.08 |
| 2:B:280:PRO:CG | 2:B:283:TYR:CD2 | 2.36 | 1.08 |
| 4:M:20:LEU:HD22 | 4:M:129:VAL:HG21 | 1.29 | 1.08 |
| 4:M:106:LYS:CE | 4:M:296:LYS:HE3 | 1.82 | 1.08 |
| 4:M:350:VAL:HG22 | 4:M:442:GLN:HG2 | 1.09 | 1.08 |
| 1:A:429:VAL:HB | 1:A:469:LEU:HD11 | 1.33 | 1.08 |
| 1:A:506:LYS:CE | 4:M:82:LYS:CB | 2.31 | 1.08 |
| 2:B:340:ILE:HG12 | 2:B:373:LEU:HD23 | 1.36 | 1.08 |
| 4:M:44:ASP:HB2 | 4:M:50:TYR:CD2 | 1.88 | 1.08 |
| 4:M:106:LYS:HE2 | 4:M:296:LYS:CE | 1.83 | 1.08 |
| 4:M:219:LEU:CG | 4:M:472:TYR:O | 2.02 | 1.08 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:18:ILE:HD13 | 2:B:36:THR:HG21 | 1.33 | 1.08 |
| 2:B:23:ALA:C | 2:B:32:GLU:OE1 | 1.90 | 1.08 |
| 2:B:375:LEU:HD12 | 2:B:404:ASN:HD22 | 1.19 | 1.08 |
| 4:M:69:ILE:O | 4:M:75:TRP:HA | 1.53 | 1.08 |
| 1:A:595:GLU:OE1 | 2:B:513:TRP:HZ3 | 1.14 | 1.08 |
| 2:B:158:VAL:CG1 | 2:B:177:ILE:HG13 | 1.82 | 1.08 |
| 2:B:237:ILE:O | 2:B:239:GLN:N | 1.85 | 1.08 |
| 4:M:106:LYS:HE2 | 4:M:296:LYS:HE3 | 1.18 | 1.08 |
| 4:M:306:LEU:CD2 | 4:M:317:MET:CE | 2.32 | 1.08 |
| 2:B:1:MET:HG2 | 4:M:39:PRO:HD3 | 1.30 | 1.08 |
| 2:B:104:TYR:O | 2:B:107:ARG:CB | 2.01 | 1.08 |
| 2:B:140:SER:HB2 | 2:B:172:GLU:OE1 | 1.51 | 1.08 |
| 2:B:236:ILE:O | 2:B:240:LEU:HG | 1.54 | 1.08 |
| 2:B:418:TYR:OH | 2:B:432:ALA:CB | 2.02 | 1.08 |
| 1:A:111:SER:HB2 | 1:A:152:THR:OG1 | 1.54 | 1.07 |
| 1:A:536:MET:CG | 1:A:551:LEU:HD11 | 1.83 | 1.07 |
| 1:A:559:PHE:CE2 | 1:A:581:LEU:HD22 | 1.88 | 1.07 |
| 1:A:585:PHE:CE2 | 1:A:603:VAL:CG1 | 2.37 | 1.07 |
| 2:B:18:ILE:HD13 | 2:B:36:THR:CG2 | 1.81 | 1.07 |
| 2:B:103:LEU:HB3 | 4:M:126:ASN:ND2 | 1.68 | 1.07 |
| 2:B:433:VAL:HG21 | 2:B:471:TYR:CD2 | 1.88 | 1.07 |
| 2:B:556:LEU:CB | 2:B:588:ILE:HD11 | 1.82 | 1.07 |
| 3:S:8:PHE:CD2 | 3:S:84:TYR:HB2 | 1.89 | 1.07 |
| 2:B:197:LYS:HB2 | 2:B:229:HIS:HE2 | 1.02 | 1.07 |
| 2:B:231:ARG:HG3 | 2:B:298:ASP:OD1 | 1.52 | 1.07 |
| 2:B:256:CYS:HB2 | 2:B:328:LEU:HD23 | 1.32 | 1.07 |
| 4:M:9:ASP:HB2 | 4:M:111:ILE:CG2 | 1.83 | 1.07 |
| 2:B:106:LEU:CB | 4:M:130:GLU:HB3 | 1.85 | 1.07 |
| 2:B:247:TYR:CD1 | 4:M:136:VAL:HG12 | 1.89 | 1.07 |
| 2:B:386:LYS:NZ | 4:M:478:ASN:OD1 | 1.86 | 1.07 |
| 2:B:433:VAL:HG11 | 2:B:471:TYR:N | 1.69 | 1.07 |
| 2:B:556:LEU:HA | 2:B:588:ILE:HD11 | 1.31 | 1.07 |
| 4:M:347:PHE:CD1 | 4:M:350:VAL:HB | 1.89 | 1.07 |
| 2:B:223:LEU:CD1 | 2:B:258:GLN:CB | 2.33 | 1.07 |
| 2:B:348:THR:CG2 | 2:B:380:LYS:HB3 | 1.84 | 1.07 |
| 2:B:38:TYR:OH | 2:B:46:GLN:HB2 | 1.52 | 1.07 |
| 2:B:278:PRO:HG2 | 2:B:292:GLU:OE1 | 1.54 | 1.07 |
| 2:B:293:VAL:O | 2:B:299:LEU:HD12 | 1.52 | 1.07 |
| 2:B:325:LEU:HD13 | 2:B:339:PHE:CB | 1.84 | 1.07 |
| 2:B:461:HIS:O | 2:B:462:ASN:HB3 | 1.43 | 1.07 |
| 4:M:223:HIS:ND1 | 4:M:476:THR:OG1 | 1.81 | 1.07 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:137:ASN:O | 1:A:139:ASP:N | 1.88 | 1.06 |
| 2:B:74:ASP:O | 2:B:77:ILE:CG1 | 2.03 | 1.06 |
| 2:B:341:GLU:CG | 2:B:377:TYR:HE1 | 1.61 | 1.06 |
| 2:B:375:LEU:HD13 | 2:B:404:ASN:CG | 1.74 | 1.06 |
| 2:B:400:SER:HB3 | 2:B:435:SER:CA | 1.85 | 1.06 |
| 4:M:375:LYS:HE2 | 4:M:418:GLU:OE1 | 1.55 | 1.06 |
| 1:A:225:LEU:HB3 | 1:A:233:PHE:CE2 | 1.89 | 1.06 |
| 4:M:261:ASN:HB2 | 4:M:450:GLU:CG | 1.85 | 1.06 |
| 1:A:504:ILE:CA | 4:M:59:ASP:OD2 | 2.01 | 1.06 |
| 2:B:178:ILE:HG23 | 2:B:217:GLU:HB2 | 1.16 | 1.06 |
| 2:B:564:LYS:CE | 2:B:621:GLY:O | 2.02 | 1.06 |
| 4:M:106:LYS:O | 4:M:107:ASP:C | 1.89 | 1.06 |
| 4:M:443:SER:HB3 | 4:M:447:ILE:CG1 | 1.85 | 1.06 |
| 1:A:186:PHE:HE2 | 1:A:224:GLU:HB2 | 0.94 | 1.06 |
| 2:B:1:MET:CG | 4:M:39:PRO:CD | 2.34 | 1.06 |
| 2:B:139:LEU:HG | 2:B:176:ALA:HB2 | 1.37 | 1.06 |
| 2:B:309:LEU:HB3 | 2:B:317:VAL:HG12 | 1.35 | 1.06 |
| 2:B:374:PHE:CE1 | 2:B:381:PHE:CE2 | 2.44 | 1.06 |
| 2:B:433:VAL:HG12 | 2:B:474:VAL:HG21 | 1.36 | 1.06 |
| 2:B:556:LEU:HA | 2:B:588:ILE:CD1 | 1.84 | 1.06 |
| 2:B:569:THR:HG22 | 2:B:569:THR:O | 1.47 | 1.06 |
| 4:M:96:ILE:HG23 | 4:M:125:PHE:CE1 | 1.90 | 1.06 |
| 4:M:96:ILE:CG2 | 4:M:125:PHE:CE1 | 2.39 | 1.06 |
| 1:A:504:ILE:CD1 | 4:M:59:ASP:OD2 | 2.04 | 1.06 |
| 2:B:25:VAL:CG2 | 2:B:32:GLU:N | 2.12 | 1.06 |
| 2:B:199:LEU:O | 2:B:201:ALA:N | 1.87 | 1.06 |
| 2:B:403:ILE:HG21 | 2:B:439:CYS:SG | 1.95 | 1.06 |
| 4:M:243:ILE:O | 4:M:472:TYR:CD2 | 2.09 | 1.06 |
| 4:M:273:HIS:HB2 | 4:M:298:ARG:O | 1.55 | 1.06 |
| 1:A:200:PHE:CZ | 1:A:236:LEU:HD21 | 1.90 | 1.05 |
| 2:B:73:ASP:H | 4:M:19:LEU:HD23 | 1.20 | 1.05 |
| 2:B:219:TYR:HB3 | 2:B:223:LEU:HD23 | 1.33 | 1.05 |
| 4:M:243:ILE:O | 4:M:472:TYR:CG | 2.08 | 1.05 |
| 4:M:379:LEU:HD23 | 4:M:411:LEU:HG | 1.33 | 1.05 |
| 2:B:70:MET:HE1 | 2:B:107:ARG:CG | 1.85 | 1.05 |
| 2:B:196:LEU:HB3 | 2:B:215:TYR:CZ | 1.91 | 1.05 |
| 2:B:476:ARG:HA | 2:B:514:LEU:CD1 | 1.84 | 1.05 |
| 2:B:73:ASP:CB | 4:M:19:LEU:HD22 | 1.87 | 1.05 |
| 2:B:100:LEU:HD21 | 4:M:123:LEU:HD22 | 1.38 | 1.05 |
| 4:M:48:ASP:O | 4:M:70:ASN:HB3 | 1.56 | 1.05 |
| 4:M:323:MET:SD | 4:M:342:LEU:HA | 1.96 | 1.05 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:186:PHE:CZ | 1:A:224:GLU:HG2 | 1.92 | 1.05 |
| 1:A:582:ILE:HG23 | 1:A:604:LEU:HG | 1.33 | 1.05 |
| 2:B:70:MET:CE | 2:B:107:ARG:CG | 2.34 | 1.05 |
| 2:B:396:ILE:HD13 | 2:B:432:ALA:HB2 | 1.36 | 1.05 |
| 1:A:585:PHE:CE2 | 1:A:603:VAL:HG11 | 1.91 | 1.05 |
| 2:B:12:LEU:CD1 | 4:M:13:LYS:CG | 2.23 | 1.05 |
| 2:B:64:LYS:NZ | 4:M:120:ARG:HH12 | 1.50 | 1.05 |
| 2:B:73:ASP:H | 4:M:19:LEU:CD2 | 1.60 | 1.05 |
| 2:B:106:LEU:HD11 | 2:B:144:ASP:HB3 | 1.07 | 1.05 |
| 2:B:162:VAL:HG21 | 2:B:195:ILE:HG22 | 1.31 | 1.05 |
| 2:B:310:ILE:HG12 | 2:B:318:ILE:HA | 1.39 | 1.05 |
| 1:A:186:PHE:HE2 | 1:A:224:GLU:CB | 1.62 | 1.04 |
| 2:B:12:LEU:HD13 | 4:M:13:LYS:CA | 1.88 | 1.04 |
| 2:B:69:ILE:O | 2:B:71:ALA:N | 1.90 | 1.04 |
| 2:B:313:SER:HB3 | 4:M:269:ILE:HB | 1.09 | 1.04 |
| 2:B:461:HIS:O | 2:B:462:ASN:CB | 1.98 | 1.04 |
| 3:S:32:LEU:O | 3:S:35:VAL:CG2 | 2.04 | 1.04 |
| 1:A:506:LYS:HE2 | 4:M:82:LYS:HB3 | 1.04 | 1.04 |
| 2:B:38:TYR:OH | 2:B:46:GLN:HG3 | 1.56 | 1.04 |
| 2:B:143:SER:CB | 2:B:179:LYS:HB2 | 1.86 | 1.04 |
| 2:B:223:LEU:HD13 | 2:B:258:GLN:C | 1.76 | 1.04 |
| 2:B:223:LEU:CD1 | 2:B:258:GLN:HB3 | 1.88 | 1.04 |
| 2:B:295:ASN:O | 2:B:300:ASP:HB2 | 0.89 | 1.04 |
| 1:A:225:LEU:HD13 | 1:A:233:PHE:HZ | 1.14 | 1.04 |
| 4:M:41:LEU:CD1 | 4:M:52:ASP:N | 2.20 | 1.04 |
| 4:M:344:ILE:HG22 | 4:M:347:PHE:HB3 | 1.09 | 1.04 |
| 1:A:333:ILE:HD11 | 3:S:95:GLU:OE1 | 1.52 | 1.04 |
| 1:A:638:LEU:CD2 | 2:B:561:ASP:H | 1.70 | 1.04 |
| 2:B:103:LEU:HD12 | 4:M:123:LEU:HD11 | 1.06 | 1.04 |
| 2:B:143:SER:CB | 2:B:179:LYS:HD2 | 1.88 | 1.04 |
| 2:B:178:ILE:HD12 | 2:B:218:CYS:H | 1.23 | 1.04 |
| 2:B:216:LYS:CA | 2:B:251:LEU:HD11 | 1.85 | 1.04 |
| 2:B:299:LEU:O | 2:B:302:PHE:HB3 | 1.58 | 1.04 |
| 2:B:379:LYS:HE2 | 2:B:410:GLU:HG3 | 1.06 | 1.04 |
| 2:B:556:LEU:HD22 | 2:B:588:ILE:CG1 | 1.88 | 1.04 |
| 4:M:220:GLU:HG2 | 4:M:439:TYR:HB2 | 1.38 | 1.04 |
| 1:A:179:LYS:HE2 | 3:S:137:GLN:O | 0.86 | 1.03 |
| 2:B:106:LEU:HD22 | 2:B:144:ASP:CG | 1.77 | 1.03 |
| 2:B:196:LEU:HB3 | 2:B:215:TYR:CE1 | 1.92 | 1.03 |
| 2:B:552:SER:O | 2:B:556:LEU:HG | 1.58 | 1.03 |
| 2:B:9:ALA:CA | 4:M:14:LEU:HB2 | 1.89 | 1.03 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:512:VAL:C | 2:B:551:LEU:HD13 | 1.78 | 1.03 |
| 1:A:503:ASN:CG | 4:M:60:LEU:CA | 2.26 | 1.03 |
| 2:B:17:VAL:CB | 2:B:35:TYR:CD2 | 2.40 | 1.03 |
| 2:B:212:VAL:O | 2:B:213:LEU:C | 1.94 | 1.03 |
| 3:S:53:THR:HG21 | 3:S:68:VAL:HA | 1.36 | 1.03 |
| 3:S:73:ILE:CG2 | 3:S:88:ILE:HG23 | 1.87 | 1.03 |
| 1:A:638:LEU:HD13 | 2:B:557:SER:OG | 1.58 | 1.03 |
| 2:B:17:VAL:CB | 2:B:35:TYR:HD2 | 1.71 | 1.03 |
| 2:B:178:ILE:CG1 | 2:B:214:ALA:C | 2.27 | 1.03 |
| 2:B:212:VAL:HG23 | 2:B:233:TYR:CE1 | 1.94 | 1.03 |
| 2:B:344:VAL:CG1 | 2:B:377:TYR:HB3 | 1.90 | 1.02 |
| 2:B:347:VAL:HG11 | 2:B:381:PHE:CE1 | 1.94 | 1.02 |
| 4:M:105:ASP:O | 4:M:106:LYS:CB | 2.02 | 1.02 |
| 4:M:350:VAL:HA | 4:M:442:GLN:HB2 | 1.38 | 1.02 |
| 4:M:383:HIS:CG | 4:M:403:THR:HG1 | 1.76 | 1.02 |
| 2:B:224:GLU:CA | 2:B:259:TYR:CZ | 1.87 | 1.02 |
| 2:B:309:LEU:HB3 | 2:B:317:VAL:HG11 | 1.38 | 1.02 |
| 1:A:215:VAL:HG11 | 1:A:243:ILE:HG23 | 1.40 | 1.02 |
| 1:A:422:GLU:OE1 | 3:S:62:GLU:CG | 2.07 | 1.02 |
| 1:A:462:GLN:OE1 | 4:M:58:ARG:CB | 2.02 | 1.02 |
| 2:B:75:ASP:OD1 | 4:M:24:ALA:CB | 2.07 | 1.02 |
| 2:B:103:LEU:CD1 | 4:M:123:LEU:CD1 | 2.37 | 1.02 |
| 2:B:174:ALA:HB1 | 2:B:211:ALA:HA | 1.40 | 1.02 |
| 2:B:245:GLN:OE1 | 2:B:309:LEU:HD12 | 1.59 | 1.02 |
| 2:B:337:THR:OG1 | 2:B:373:LEU:HD13 | 1.58 | 1.02 |
| 4:M:243:ILE:O | 4:M:472:TYR:HB3 | 1.54 | 1.02 |
| 4:M:245:ASP:O | 4:M:472:TYR:HE1 | 1.11 | 1.02 |
| 1:A:289:SER:O | 1:A:290:VAL:C | 1.83 | 1.02 |
| 1:A:503:ASN:CG | 4:M:60:LEU:HA | 1.79 | 1.02 |
| 2:B:313:SER:HB3 | 4:M:269:ILE:CB | 1.89 | 1.02 |
| 4:M:54:SER:H | 4:M:66:PHE:HD2 | 1.05 | 1.02 |
| 4:M:224:VAL:H | 4:M:479:PHE:CB | 1.73 | 1.02 |
| 1:A:503:ASN:OD1 | 4:M:60:LEU:CD2 | 2.08 | 1.02 |
| 2:B:79:VAL:HG23 | 2:B:108:PHE:CE2 | 1.94 | 1.02 |
| 2:B:256:CYS:HB2 | 2:B:328:LEU:CD2 | 1.84 | 1.02 |
| 2:B:351:GLU:HB3 | 4:M:476:THR:HB | 1.02 | 1.02 |
| 4:M:65:TYR:O | 4:M:79:SER:HA | 1.58 | 1.02 |
| 1:A:68:THR:HB | 3:S:166:LYS:HB3 | 1.03 | 1.01 |
| 2:B:219:TYR:CD1 | 2:B:226:LEU:HB2 | 1.95 | 1.01 |
| 2:B:328:LEU:HB3 | 2:B:333:GLN:HE22 | 1.22 | 1.01 |
| 2:B:343:LEU:CD2 | 2:B:363:ILE:HD13 | 1.90 | 1.01 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:389:ILE:CG1 | 2:B:425:PRO:HG2 | 1.88 | 1.01 |
| 2:B:397:GLN:HE21 | 2:B:431:MET:HE3 | 1.21 | 1.01 |
| 4:M:15:ILE:HG23 | 4:M:115:VAL:CG2 | 1.90 | 1.01 |
| 4:M:306:LEU:HD22 | 4:M:317:MET:CE | 1.89 | 1.01 |
| 2:B:12:LEU:CD1 | 4:M:13:LYS:CB | 2.39 | 1.01 |
| 2:B:252:LEU:CB | 2:B:302:PHE:CE2 | 2.44 | 1.01 |
| 2:B:567:GLN:C | 2:B:569:THR:N | 2.11 | 1.01 |
| 1:A:585:PHE:HE2 | 1:A:603:VAL:CG1 | 1.73 | 1.01 |
| 1:A:585:PHE:O | 1:A:600:SER:OG | 1.79 | 1.01 |
| 2:B:14:THR:HA | 2:B:36:THR:HA | 1.41 | 1.01 |
| 2:B:38:TYR:CD2 | 2:B:43:ASN:N | 2.09 | 1.01 |
| 2:B:193:LEU:CD2 | 2:B:225:LEU:HB3 | 1.75 | 1.01 |
| 2:B:433:VAL:HG11 | 2:B:471:TYR:HA | 1.06 | 1.01 |
| 3:S:127:THR:CG2 | 3:S:153:VAL:HG13 | 1.90 | 1.01 |
| 1:A:411:GLU:HG3 | 3:S:46:PHE:CZ | 1.95 | 1.01 |
| 1:A:462:GLN:C | 4:M:58:ARG:HA | 1.81 | 1.01 |
| 1:A:573:GLU:O | 1:A:574:ILE:C | 1.77 | 1.01 |
| 2:B:12:LEU:HB3 | 4:M:13:LYS:HG2 | 1.40 | 1.01 |
| 2:B:73:ASP:CB | 4:M:25:PRO:O | 2.07 | 1.01 |
| 2:B:167:ALA:O | 2:B:207:VAL:CG2 | 2.07 | 1.01 |
| 2:B:418:TYR:CD1 | 2:B:418:TYR:C | 2.34 | 1.01 |
| 2:B:423:HIS:NE2 | 4:M:365:GLU:CB | 2.23 | 1.01 |
| 4:M:261:ASN:HB2 | 4:M:450:GLU:HG3 | 1.42 | 1.01 |
| 4:M:443:SER:CB | 4:M:447:ILE:HG13 | 1.91 | 1.01 |
| 1:A:556:VAL:CG2 | 1:A:603:VAL:HG21 | 1.90 | 1.01 |
| 2:B:219:TYR:CD2 | 2:B:226:LEU:CD2 | 2.43 | 1.01 |
| 2:B:259:TYR:HD1 | 2:B:261:PRO:HG3 | 1.15 | 1.01 |
| 2:B:375:LEU:CD1 | 2:B:404:ASN:HB2 | 1.91 | 1.01 |
| 2:B:447:GLU:OE1 | 2:B:485:LYS:HG3 | 1.61 | 1.01 |
| 4:M:218:LEU:O | 4:M:441:GLY:CA | 2.09 | 1.01 |
| 4:M:302:TYR:CE1 | 4:M:445:SER:CB | 2.44 | 1.01 |
| 2:B:5:ILE:CG2 | 4:M:42:LEU:CD1 | 2.32 | 1.00 |
| 2:B:44:PRO:HB3 | 2:B:82:TYR:OH | 1.59 | 1.00 |
| 2:B:278:PRO:CD | 2:B:292:GLU:CB | 2.28 | 1.00 |
| 2:B:563:PHE:HD1 | 2:B:584:SER:CB | 1.73 | 1.00 |
| 4:M:68:VAL:HA | 4:M:76:CYS:O | 1.59 | 1.00 |
| 2:B:224:GLU:N | 2:B:259:TYR:OH | 1.74 | 1.00 |
| 2:B:398:ILE:CG2 | 2:B:402:LEU:HD11 | 1.91 | 1.00 |
| 1:A:409:VAL:CG1 | 3:S:42:ARG:HH12 | 1.74 | 1.00 |
| 1:A:506:LYS:CE | 4:M:82:LYS:HB2 | 1.92 | 1.00 |
| 1:A:556:VAL:HG22 | 1:A:603:VAL:HG11 | 1.40 | 1.00 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:267:ASP:H | 2:B:289:PRO:HG3 | 1.23 | 1.00 |
| 2:B:174:ALA:CB | 2:B:211:ALA:HA | 1.90 | 1.00 |
| 2:B:213:LEU:HD13 | 4:M:135:ASN:CG | 1.81 | 1.00 |
| 2:B:245:GLN:NE2 | 2:B:309:LEU:HD11 | 1.74 | 1.00 |
| 2:B:279:LEU:HG | 2:B:288:TYR:HD2 | 1.25 | 1.00 |
| 2:B:578:PRO:HD2 | 2:B:581:TYR:CD2 | 1.97 | 1.00 |
| 4:M:214:LEU:HD23 | 4:M:214:LEU:O | 1.62 | 1.00 |
| 4:M:245:ASP:CA | 4:M:472:TYR:CE1 | 2.45 | 1.00 |
| 4:M:347:PHE:CZ | 4:M:350:VAL:HG12 | 1.95 | 1.00 |
| 2:B:155:LEU:HD21 | 2:B:192:LEU:HD12 | 1.44 | 1.00 |
| 2:B:212:VAL:HG21 | 2:B:248:LEU:CD2 | 1.92 | 1.00 |
| 2:B:193:LEU:CD2 | 2:B:225:LEU:HB2 | 1.88 | 1.00 |
| 2:B:437:SER:CA | 2:B:474:VAL:HG13 | 1.91 | 1.00 |
| 3:S:8:PHE:CE2 | 3:S:84:TYR:CB | 2.45 | 1.00 |
| 1:A:589:SER:CA | 1:A:597:GLN:HG3 | 1.92 | 1.00 |
| 2:B:136:CYS:HB3 | 2:B:172:GLU:HG3 | 1.38 | 0.99 |
| 2:B:243:TRP:CZ3 | 4:M:98:ARG:HD2 | 1.96 | 0.99 |
| 2:B:252:LEU:O | 2:B:302:PHE:CE2 | 2.14 | 0.99 |
| 2:B:336:ASN:C | 2:B:373:LEU:CD2 | 2.29 | 0.99 |
| 2:B:344:VAL:HG21 | 2:B:377:TYR:CB | 1.92 | 0.99 |
| 1:A:323:CYS:SG | 1:A:334:SER:HB3 | 2.02 | 0.99 |
| 2:B:219:TYR:CG | 2:B:226:LEU:HB2 | 1.96 | 0.99 |
| 2:B:403:ILE:HD13 | 2:B:439:CYS:HA | 1.19 | 0.99 |
| 2:B:337:THR:CA | 2:B:373:LEU:CD1 | 1.76 | 0.99 |
| 1:A:450:TYR:OH | 1:A:476:GLN:HG3 | 1.57 | 0.99 |
| 2:B:17:VAL:HG11 | 2:B:35:TYR:CE2 | 1.98 | 0.99 |
| 2:B:261:PRO:HD3 | 2:B:293:VAL:CG2 | 1.91 | 0.99 |
| 4:M:20:LEU:HD22 | 4:M:129:VAL:CG2 | 1.91 | 0.99 |
| 2:B:73:ASP:CG | 4:M:19:LEU:HD13 | 1.82 | 0.99 |
| 2:B:252:LEU:HB3 | 2:B:302:PHE:CE2 | 1.97 | 0.99 |
| 4:M:74:TYR:CB | 4:M:114:ILE:HD11 | 1.93 | 0.99 |
| 4:M:220:GLU:HG3 | 4:M:439:TYR:CD2 | 1.96 | 0.99 |
| 2:B:211:ALA:HB1 | 2:B:233:TYR:OH | 1.58 | 0.99 |
| 2:B:274:PRO:C | 2:B:295:ASN:OD1 | 1.69 | 0.99 |
| 2:B:38:TYR:CE2 | 2:B:43:ASN:C | 2.35 | 0.99 |
| 2:B:106:LEU:CD2 | 4:M:130:GLU:HA | 1.92 | 0.99 |
| 2:B:256:CYS:SG | 2:B:299:LEU:HD23 | 2.03 | 0.99 |
| 3:S:35:VAL:CG1 | 3:S:77:TYR:OH | 2.10 | 0.99 |
| 4:M:245:ASP:CB | 4:M:472:TYR:CD1 | 2.46 | 0.99 |
| 4:M:245:ASP:C | 4:M:472:TYR:CE1 | 2.35 | 0.99 |
| 1:A:402:ILE:CG1 | 3:S:62:GLU:O | 2.09 | 0.99 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:25:VAL:CG2 | 2:B:31:GLY:N | 2.20 | 0.99 |
| 2:B:211:ALA:CA | 2:B:233:TYR:OH | 2.09 | 0.99 |
| 4:M:344:ILE:HG23 | 4:M:347:PHE:HB3 | 1.29 | 0.99 |
| 2:B:519:ALA:O | 2:B:523:PHE:HB3 | 1.61 | 0.99 |
| 2:B:584:SER:O | 2:B:588:ILE:CG2 | 2.10 | 0.99 |
| 4:M:95:THR:CG2 | 4:M:137:SER:O | 2.09 | 0.99 |
| 4:M:244:VAL:O | 4:M:299:LEU:N | 1.95 | 0.99 |
| 1:A:288:THR:HG23 | 3:S:96:LEU:HD21 | 1.40 | 0.99 |
| 2:B:34:SER:O | 2:B:37:TYR:HB3 | 1.63 | 0.99 |
| 2:B:193:LEU:HB3 | 2:B:225:LEU:HD12 | 1.44 | 0.99 |
| 2:B:396:ILE:HG22 | 2:B:435:SER:OG | 1.61 | 0.99 |
| 2:B:14:THR:HG22 | 2:B:36:THR:HG22 | 0.99 | 0.98 |
| 2:B:70:MET:HE1 | 2:B:107:ARG:CB | 1.93 | 0.98 |
| 2:B:216:LYS:CE | 4:M:133:GLU:OE2 | 2.10 | 0.98 |
| 2:B:219:TYR:OH | 2:B:226:LEU:HA | 1.63 | 0.98 |
| 4:M:443:SER:HB3 | 4:M:447:ILE:HG13 | 1.41 | 0.98 |
| 2:B:469:ASP:OD1 | 2:B:507:ALA:N | 1.97 | 0.98 |
| 1:A:225:LEU:CD1 | 1:A:233:PHE:CZ | 2.44 | 0.98 |
| 2:B:475:ILE:HG23 | 2:B:489:ILE:HG21 | 1.45 | 0.98 |
| 4:M:96:ILE:CG2 | 4:M:125:PHE:CZ | 2.45 | 0.98 |
| 1:A:136:GLY:O | 1:A:139:ASP:HB3 | 1.64 | 0.98 |
| 2:B:143:SER:HB2 | 2:B:179:LYS:HB2 | 0.99 | 0.98 |
| 2:B:215:TYR:HD2 | 2:B:233:TYR:CE2 | 1.70 | 0.98 |
| 2:B:389:ILE:HG12 | 2:B:425:PRO:CG | 1.92 | 0.98 |
| 2:B:403:ILE:HD13 | 2:B:439:CYS:HB3 | 1.44 | 0.98 |
| 1:A:213:SER:HB3 | 3:S:142:ILE:O | 1.62 | 0.98 |
| 2:B:469:ASP:CG | 2:B:506:ASN:HB2 | 1.84 | 0.98 |
| 4:M:375:LYS:CE | 4:M:418:GLU:OE1 | 2.10 | 0.98 |
| 4:M:354:ASP:HB2 | 4:M:440:ILE:CD1 | 1.94 | 0.98 |
| 4:M:375:LYS:N | 4:M:416:GLU:O | 1.96 | 0.98 |
| 2:B:178:ILE:HG13 | 2:B:214:ALA:CB | 1.94 | 0.97 |
| 2:B:178:ILE:CG1 | 2:B:214:ALA:CB | 2.42 | 0.97 |
| 2:B:322:CYS:SG | 2:B:366:LEU:CD1 | 2.51 | 0.97 |
| 2:B:213:LEU:HD13 | 4:M:135:ASN:OD1 | 0.80 | 0.97 |
| 2:B:230:PHE:HE2 | 2:B:252:LEU:HD23 | 1.17 | 0.97 |
| 4:M:271:SER:O | 4:M:300:LEU:HA | 1.64 | 0.97 |
| 4:M:354:ASP:HB2 | 4:M:440:ILE:HD12 | 1.44 | 0.97 |
| 1:A:508:LEU:HD12 | 4:M:59:ASP:OD2 | 1.62 | 0.97 |
| 2:B:5:ILE:HD13 | 4:M:42:LEU:HD12 | 1.41 | 0.97 |
| 2:B:24:ALA:CB | 2:B:32:GLU:HG2 | 1.88 | 0.97 |
| 2:B:167:ALA:O | 2:B:207:VAL:HG22 | 1.63 | 0.97 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:13:ASP:OD1 | 4:M:14:LEU:O | 1.81 | 0.97 |
| 2:B:374:PHE:CZ | 2:B:381:PHE:CE2 | 2.51 | 0.97 |
| 3:S:8:PHE:HB3 | 3:S:36:TYR:CZ | 1.98 | 0.97 |
| 2:B:344:VAL:HG22 | 2:B:374:PHE:CE1 | 1.98 | 0.97 |
| 2:B:542:PRO:O | 2:B:607:ILE:HD11 | 1.64 | 0.97 |
| 4:M:96:ILE:HD12 | 4:M:125:PHE:CD1 | 1.99 | 0.97 |
| 2:B:162:VAL:CG2 | 2:B:195:ILE:CG2 | 2.41 | 0.97 |
| 2:B:400:SER:CB | 2:B:435:SER:HA | 1.94 | 0.97 |
| 2:B:588:ILE:HG23 | 2:B:618:PHE:CZ | 1.99 | 0.97 |
| 2:B:25:VAL:HG23 | 2:B:32:GLU:H | 1.11 | 0.97 |
| 2:B:341:GLU:HA | 2:B:377:TYR:CE1 | 1.65 | 0.97 |
| 2:B:73:ASP:N | 4:M:19:LEU:CB | 2.28 | 0.97 |
| 2:B:106:LEU:HD23 | 4:M:130:GLU:HB2 | 1.47 | 0.97 |
| 2:B:523:PHE:HE2 | 2:B:580:TYR:CD2 | 1.80 | 0.97 |
| 1:A:556:VAL:HG22 | 1:A:603:VAL:CG1 | 1.94 | 0.97 |
| 4:M:353:VAL:O | 4:M:401:LYS:HA | 1.65 | 0.97 |
| 2:B:9:ALA:O | 4:M:14:LEU:CB | 2.13 | 0.96 |
| 2:B:106:LEU:CD2 | 2:B:144:ASP:CB | 2.43 | 0.96 |
| 2:B:261:PRO:HB2 | 2:B:290:SER:HB3 | 1.46 | 0.96 |
| 2:B:328:LEU:CB | 2:B:333:GLN:HE22 | 1.78 | 0.96 |
| 2:B:422:ALA:HB3 | 2:B:424:PHE:CD2 | 2.00 | 0.96 |
| 1:A:225:LEU:CB | 1:A:233:PHE:CZ | 2.47 | 0.96 |
| 2:B:109:ALA:HB2 | 2:B:145:MET:SD | 2.05 | 0.96 |
| 1:A:309:PHE:CZ | 1:A:348:PHE:CZ | 2.53 | 0.96 |
| 2:B:227:HIS:O | 2:B:298:ASP:OD2 | 1.82 | 0.96 |
| 2:B:318:ILE:HD13 | 2:B:346:THR:CB | 1.93 | 0.96 |
| 2:B:347:VAL:HG11 | 2:B:381:PHE:HE1 | 1.30 | 0.96 |
| 4:M:244:VAL:HG13 | 4:M:472:TYR:CE2 | 2.00 | 0.96 |
| 4:M:323:MET:HB3 | 4:M:340:LEU:HD11 | 1.46 | 0.96 |
| 2:B:143:SER:C | 2:B:179:LYS:HD3 | 1.85 | 0.96 |
| 2:B:475:ILE:HG23 | 2:B:489:ILE:CG2 | 1.96 | 0.96 |
| 1:A:263:LEU:O | 1:A:266:VAL:N | 1.98 | 0.96 |
| 2:B:34:SER:HB3 | 2:B:65:ARG:NH1 | 1.80 | 0.96 |
| 2:B:396:ILE:CD1 | 2:B:432:ALA:HB2 | 1.94 | 0.96 |
| 4:M:243:ILE:H | 4:M:474:THR:CG2 | 1.77 | 0.96 |
| 2:B:497:LEU:O | 2:B:499:VAL:N | 1.98 | 0.96 |
| 4:M:405:THR:C | 4:M:407:THR:N | 2.09 | 0.96 |
| 1:A:528:ASN:O | 1:A:529:GLY:C | 1.98 | 0.96 |
| 2:B:396:ILE:HD13 | 2:B:432:ALA:CB | 1.95 | 0.96 |
| 2:B:523:PHE:CE2 | 2:B:580:TYR:CG | 2.53 | 0.96 |
| 2:B:69:ILE:O | 2:B:70:MET:C | 2.00 | 0.96 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:139:LEU:HD21 | 2:B:173:VAL:HA | 1.45 | 0.96 |
| 2:B:161:LEU:HB3 | 2:B:173:VAL:HG22 | 1.46 | 0.96 |
| 2:B:556:LEU:HB3 | 2:B:588:ILE:HD11 | 1.45 | 0.96 |
| 4:M:41:LEU:HD12 | 4:M:52:ASP:N | 1.80 | 0.96 |
| 4:M:220:GLU:OE2 | 4:M:439:TYR:CD2 | 2.17 | 0.96 |
| 2:B:260:LEU:HA | 2:B:293:VAL:HG21 | 1.48 | 0.96 |
| 2:B:278:PRO:HD3 | 2:B:289:PRO:O | 1.64 | 0.96 |
| 4:M:379:LEU:HA | 4:M:412:ARG:O | 1.66 | 0.96 |
| 2:B:139:LEU:HD23 | 2:B:173:VAL:HA | 1.44 | 0.96 |
| 2:B:144:ASP:OD2 | 4:M:131:ALA:HA | 1.66 | 0.96 |
| 2:B:556:LEU:CD2 | 2:B:588:ILE:CG1 | 2.44 | 0.96 |
| 1:A:215:VAL:HG11 | 1:A:243:ILE:CG2 | 1.93 | 0.95 |
| 2:B:16:LYS:NZ | 4:M:111:ILE:HD12 | 1.81 | 0.95 |
| 2:B:223:LEU:HD13 | 2:B:259:TYR:H | 1.14 | 0.95 |
| 3:S:35:VAL:HB | 3:S:77:TYR:CE2 | 2.00 | 0.95 |
| 4:M:265:ASN:HB3 | 4:M:309:GLN:HG3 | 1.46 | 0.95 |
| 1:A:68:THR:CB | 3:S:166:LYS:HB3 | 1.96 | 0.95 |
| 2:B:155:LEU:CD2 | 2:B:192:LEU:HD12 | 1.95 | 0.95 |
| 2:B:278:PRO:C | 2:B:288:TYR:HB2 | 1.85 | 0.95 |
| 2:B:297:PRO:O | 2:B:301:LEU:CG | 2.13 | 0.95 |
| 2:B:389:ILE:HG12 | 2:B:425:PRO:HG2 | 0.97 | 0.95 |
| 2:B:497:LEU:O | 2:B:498:THR:C | 1.92 | 0.95 |
| 4:M:350:VAL:HG22 | 4:M:442:GLN:CG | 1.96 | 0.95 |
| 2:B:236:ILE:HG22 | 2:B:240:LEU:HD11 | 0.97 | 0.95 |
| 2:B:256:CYS:CB | 2:B:328:LEU:HD22 | 1.88 | 0.95 |
| 2:B:523:PHE:CZ | 2:B:580:TYR:CZ | 2.55 | 0.95 |
| 1:A:323:CYS:SG | 1:A:334:SER:CB | 2.55 | 0.95 |
| 1:A:424:TYR:CD1 | 3:S:63:ASN:ND2 | 2.34 | 0.95 |
| 1:A:563:CYS:HB3 | 1:A:621:LEU:CD1 | 1.95 | 0.95 |
| 1:A:638:LEU:HD21 | 2:B:561:ASP:H | 0.82 | 0.95 |
| 3:S:8:PHE:CE2 | 3:S:84:TYR:HB2 | 1.99 | 0.95 |
| 4:M:290:PHE:CE2 | 4:M:297:PHE:CZ | 2.53 | 0.95 |
| 4:M:374:TYR:O | 4:M:390:ILE:HD12 | 1.66 | 0.95 |
| 1:A:213:SER:HB2 | 3:S:142:ILE:CA | 1.96 | 0.95 |
| 1:A:605:GLU:OE1 | 1:A:636:TYR:OH | 1.83 | 0.95 |
| 2:B:208:ILE:HD13 | 2:B:236:ILE:HG21 | 1.47 | 0.95 |
| 2:B:560:ILE:HG23 | 2:B:564:LYS:HB2 | 1.47 | 0.95 |
| 4:M:41:LEU:HD13 | 4:M:52:ASP:H | 1.27 | 0.95 |
| 2:B:371:GLN:HB3 | 2:B:401:THR:O | 1.67 | 0.95 |
| 2:B:397:GLN:NE2 | 2:B:431:MET:CE | 2.30 | 0.95 |
| 1:A:114:PHE:O | 1:A:115:TYR:C | 2.03 | 0.95 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:215:VAL:HG13 | 1:A:243:ILE:HG21 | 1.44 | 0.95 |
| 1:A:239:LEU:O | 1:A:242:GLU:O | 1.84 | 0.95 |
| 1:A:258:LYS:HZ1 | 3:S:93:GLU:HA | 1.17 | 0.95 |
| 1:A:450:TYR:OH | 1:A:476:GLN:HG2 | 1.65 | 0.95 |
| 3:S:130:SER:OG | 3:S:156:LEU:HD12 | 1.66 | 0.95 |
| 4:M:432:THR:OG1 | 4:M:480:GLN:HG2 | 1.63 | 0.95 |
| 1:A:581:LEU:HD23 | 1:A:607:LEU:HD11 | 1.46 | 0.95 |
| 4:M:220:GLU:CD | 4:M:439:TYR:HD2 | 1.71 | 0.95 |
| 1:A:137:ASN:C | 1:A:139:ASP:N | 2.12 | 0.95 |
| 1:A:558:VAL:CG1 | 1:A:562:TRP:CE2 | 2.49 | 0.95 |
| 2:B:162:VAL:HG21 | 2:B:195:ILE:HG23 | 1.48 | 0.95 |
| 2:B:184:GLY:O | 2:B:188:TYR:HD2 | 1.47 | 0.95 |
| 2:B:556:LEU:HD23 | 2:B:588:ILE:HG13 | 1.46 | 0.95 |
| 4:M:219:LEU:HD22 | 4:M:473:LYS:CA | 1.97 | 0.95 |
| 2:B:213:LEU:HD21 | 4:M:136:VAL:HB | 1.49 | 0.94 |
| 2:B:216:LYS:CG | 2:B:251:LEU:HD13 | 1.97 | 0.94 |
| 2:B:227:HIS:C | 2:B:298:ASP:OD2 | 2.06 | 0.94 |
| 2:B:234:CYS:O | 2:B:237:ILE:CG2 | 2.14 | 0.94 |
| 2:B:387:ASP:CB | 2:B:388:PRO:HD2 | 1.97 | 0.94 |
| 2:B:566:ALA:HA | 2:B:574:ASN:HB3 | 1.48 | 0.94 |
| 4:M:51:LEU:CB | 4:M:68:VAL:HG21 | 1.97 | 0.94 |
| 4:M:347:PHE:CG | 4:M:350:VAL:HB | 2.01 | 0.94 |
| 4:M:436:GLU:HA | 4:M:479:PHE:CE1 | 2.00 | 0.94 |
| 1:A:295:VAL:HG22 | 1:A:315:CYS:HB3 | 1.49 | 0.94 |
| 2:B:513:TRP:HA | 2:B:551:LEU:CD2 | 1.97 | 0.94 |
| 2:B:519:ALA:O | 2:B:523:PHE:CB | 2.15 | 0.94 |
| 1:A:225:LEU:CB | 1:A:233:PHE:CE2 | 2.50 | 0.94 |
| 1:A:319:LEU:O | 1:A:320:HIS:C | 2.02 | 0.94 |
| 2:B:9:ALA:HB1 | 4:M:14:LEU:HB2 | 0.94 | 0.94 |
| 2:B:144:ASP:OD2 | 4:M:131:ALA:CA | 2.14 | 0.94 |
| 2:B:310:ILE:O | 2:B:311:TYR:C | 1.95 | 0.94 |
| 2:B:337:THR:N | 2:B:373:LEU:CD2 | 2.30 | 0.94 |
| 2:B:348:THR:OG1 | 4:M:305:ASP:OD2 | 1.84 | 0.94 |
| 3:S:17:VAL:CG2 | 3:S:19:PHE:CZ | 2.49 | 0.94 |
| 2:B:312:SER:C | 4:M:269:ILE:HD13 | 1.73 | 0.94 |
| 4:M:20:LEU:CD2 | 4:M:129:VAL:HG21 | 1.97 | 0.94 |
| 4:M:44:ASP:O | 4:M:47:SER:N | 2.00 | 0.94 |
| 4:M:222:PHE:O | 4:M:479:PHE:HE1 | 1.48 | 0.94 |
| 4:M:245:ASP:CA | 4:M:472:TYR:CD1 | 2.50 | 0.94 |
| 2:B:86:VAL:HG12 | 2:B:101:ILE:HG23 | 1.48 | 0.94 |
| 2:B:278:PRO:HA | 2:B:288:TYR:C | 1.87 | 0.94 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:476:ARG:CA | 2:B:514:LEU:HD13 | 1.95 | 0.94 |
| 2:B:563:PHE:C | 2:B:566:ALA:HB3 | 1.87 | 0.94 |
| 2:B:25:VAL:HG21 | 2:B:32:GLU:H | 1.31 | 0.94 |
| 2:B:335:LYS:CA | 2:B:370:ASP:OD2 | 2.16 | 0.94 |
| 2:B:405:GLU:O | 2:B:446:TRP:NE1 | 2.01 | 0.94 |
| 3:S:46:PHE:O | 3:S:48:SER:N | 2.00 | 0.94 |
| 1:A:405:THR:CA | 2:B:7:ARG:NH2 | 2.13 | 0.94 |
| 1:A:179:LYS:NZ | 3:S:142:ILE:N | 2.16 | 0.94 |
| 1:A:225:LEU:HD13 | 1:A:233:PHE:CZ | 2.01 | 0.94 |
| 1:A:257:LEU:HD22 | 1:A:278:ILE:CG2 | 1.97 | 0.94 |
| 1:A:462:GLN:O | 4:M:58:ARG:CA | 2.15 | 0.94 |
| 2:B:70:MET:CE | 2:B:107:ARG:CB | 2.46 | 0.94 |
| 2:B:325:LEU:CD1 | 2:B:339:PHE:HB3 | 1.96 | 0.94 |
| 4:M:224:VAL:N | 4:M:479:PHE:CG | 2.35 | 0.94 |
| 4:M:276:VAL:HG22 | 4:M:290:PHE:HD1 | 1.30 | 0.94 |
| 1:A:121:LEU:HD21 | 1:A:158:LEU:HB2 | 1.49 | 0.94 |
| 2:B:136:CYS:HB3 | 2:B:172:GLU:CG | 1.97 | 0.94 |
| 2:B:200:MET:HG2 | 2:B:232:ARG:HB3 | 1.49 | 0.94 |
| 2:B:231:ARG:NH2 | 2:B:279:LEU:CD2 | 2.30 | 0.94 |
| 4:M:258:VAL:HG13 | 4:M:449:VAL:HG13 | 1.49 | 0.94 |
| 1:A:77:LEU:O | 1:A:80:TYR:O | 1.86 | 0.94 |
| 2:B:479:VAL:CG1 | 2:B:486:HIS:CD2 | 2.50 | 0.94 |
| 2:B:563:PHE:O | 2:B:566:ALA:CB | 2.15 | 0.94 |
| 1:A:581:LEU:HD11 | 1:A:585:PHE:CZ | 2.03 | 0.93 |
| 2:B:16:LYS:HZ3 | 4:M:111:ILE:CG1 | 1.82 | 0.93 |
| 2:B:178:ILE:CG2 | 2:B:217:GLU:CB | 2.44 | 0.93 |
| 2:B:181:TYR:CE1 | 2:B:222:HIS:HD2 | 1.75 | 0.93 |
| 2:B:226:LEU:HD23 | 2:B:255:TYR:HD1 | 1.17 | 0.93 |
| 2:B:256:CYS:SG | 2:B:299:LEU:CD2 | 2.57 | 0.93 |
| 4:M:435:LEU:O | 4:M:479:PHE:CG | 2.20 | 0.93 |
| 2:B:106:LEU:HD22 | 2:B:144:ASP:CB | 1.98 | 0.93 |
| 2:B:237:ILE:HG23 | 2:B:238:LYS:N | 1.80 | 0.93 |
| 2:B:325:LEU:HB3 | 2:B:334:MET:SD | 2.08 | 0.93 |
| 3:S:8:PHE:CB | 3:S:36:TYR:HE1 | 1.81 | 0.93 |
| 4:M:95:THR:HG21 | 4:M:137:SER:O | 1.68 | 0.93 |
| 4:M:262:THR:HG22 | 4:M:265:ASN:H | 1.32 | 0.93 |
| 4:M:309:GLN:NE2 | 4:M:445:SER:O | 2.00 | 0.93 |
| 2:B:337:THR:CG2 | 2:B:373:LEU:CD1 | 2.45 | 0.93 |
| 2:B:341:GLU:CA | 2:B:377:TYR:CE1 | 2.36 | 0.93 |
| 2:B:400:SER:CB | 2:B:435:SER:CA | 2.47 | 0.93 |
| 3:S:8:PHE:CB | 3:S:36:TYR:CE1 | 2.52 | 0.93 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:M:220:GLU:CG | 4:M:439:TYR:HD2 | 1.78 | 0.93 |
| 4:M:245:ASP:O | 4:M:472:TYR:CZ | 2.22 | 0.93 |
| 2:B:313:SER:CB | 4:M:269:ILE:O | 2.16 | 0.93 |
| 2:B:568:VAL:O | 2:B:571:SER:HB2 | 1.66 | 0.93 |
| 1:A:220:SER:O | 1:A:223:CYS:HB3 | 1.69 | 0.93 |
| 2:B:179:LYS:NZ | 4:M:131:ALA:HA | 1.82 | 0.93 |
| 2:B:259:TYR:HD1 | 2:B:261:PRO:CG | 1.82 | 0.93 |
| 2:B:337:THR:HG23 | 2:B:373:LEU:HD12 | 1.49 | 0.93 |
| 2:B:374:PHE:O | 2:B:402:LEU:HD22 | 1.68 | 0.93 |
| 1:A:179:LYS:CE | 3:S:140:MET:HB3 | 1.98 | 0.93 |
| 1:A:225:LEU:CD1 | 1:A:233:PHE:HZ | 1.80 | 0.93 |
| 2:B:152:PRO:HA | 2:B:188:TYR:CE1 | 2.03 | 0.93 |
| 2:B:196:LEU:C | 2:B:215:TYR:OH | 2.06 | 0.93 |
| 2:B:310:ILE:HG22 | 2:B:342:ALA:HB1 | 1.50 | 0.93 |
| 4:M:405:THR:O | 4:M:407:THR:HG23 | 1.68 | 0.93 |
| 2:B:106:LEU:CD2 | 2:B:144:ASP:CG | 2.37 | 0.93 |
| 2:B:231:ARG:HH22 | 2:B:279:LEU:HD21 | 1.10 | 0.93 |
| 4:M:241:HIS:O | 4:M:474:THR:HB | 1.68 | 0.93 |
| 1:A:391:LEU:O | 1:A:392:MET:C | 1.88 | 0.93 |
| 2:B:340:ILE:HG12 | 2:B:373:LEU:CD2 | 1.98 | 0.93 |
| 1:A:429:VAL:HB | 1:A:469:LEU:CD1 | 1.98 | 0.93 |
| 2:B:161:LEU:HB3 | 2:B:173:VAL:CG2 | 1.98 | 0.93 |
| 2:B:181:TYR:CD2 | 2:B:218:CYS:O | 2.22 | 0.93 |
| 2:B:219:TYR:CZ | 2:B:226:LEU:HA | 1.98 | 0.93 |
| 2:B:243:TRP:HH2 | 4:M:98:ARG:CD | 1.59 | 0.93 |
| 2:B:325:LEU:HD13 | 2:B:339:PHE:CG | 2.04 | 0.93 |
| 2:B:5:ILE:HD11 | 4:M:39:PRO:CG | 1.98 | 0.93 |
| 2:B:310:ILE:HG23 | 2:B:318:ILE:HG23 | 1.48 | 0.93 |
| 2:B:415:LEU:HD12 | 2:B:436:LEU:HD21 | 1.49 | 0.93 |
| 4:M:104:PHE:CZ | 4:M:117:ASN:HB3 | 2.04 | 0.93 |
| 2:B:1:MET:HG2 | 4:M:39:PRO:CD | 1.98 | 0.92 |
| 2:B:73:ASP:HA | 4:M:19:LEU:HD21 | 1.52 | 0.92 |
| 1:A:213:SER:HB2 | 3:S:142:ILE:HA | 1.48 | 0.92 |
| 1:A:462:GLN:OE1 | 4:M:58:ARG:HB3 | 1.69 | 0.92 |
| 1:A:506:LYS:HZ3 | 4:M:82:LYS:CD | 1.79 | 0.92 |
| 2:B:513:TRP:HA | 2:B:551:LEU:HD22 | 1.49 | 0.92 |
| 2:B:518:ILE:O | 2:B:518:ILE:HD12 | 1.69 | 0.92 |
| 4:M:74:TYR:HB3 | 4:M:114:ILE:HD11 | 1.51 | 0.92 |
| 4:M:218:LEU:CA | 4:M:472:TYR:CE2 | 2.52 | 0.92 |
| 1:A:601:VAL:O | 1:A:602:GLU:C | 1.91 | 0.92 |
| 2:B:220:ALA:HA | 2:B:258:GLN:HG3 | 1.50 | 0.92 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:570:LYS:HD3 | 1:A:618:THR:HG22 | 1.51 | 0.92 |
| 2:B:1:MET:CG | 4:M:39:PRO:HD3 | 1.98 | 0.92 |
| 2:B:252:LEU:CB | 2:B:302:PHE:CE1 | 2.51 | 0.92 |
| 2:B:336:ASN:O | 2:B:373:LEU:HD21 | 1.69 | 0.92 |
| 2:B:433:VAL:HG12 | 2:B:474:VAL:HG23 | 1.48 | 0.92 |
| 2:B:472:VAL:CG1 | 2:B:510:GLY:HA3 | 1.99 | 0.92 |
| 1:A:381:GLU:O | 1:A:382:ASP:C | 1.91 | 0.92 |
| 2:B:16:LYS:HZ3 | 4:M:111:ILE:HG13 | 1.35 | 0.92 |
| 2:B:181:TYR:CE2 | 2:B:218:CYS:O | 2.22 | 0.92 |
| 4:M:222:PHE:CD1 | 4:M:240:ILE:CG2 | 2.53 | 0.92 |
| 2:B:136:CYS:SG | 2:B:169:VAL:CA | 2.58 | 0.92 |
| 2:B:224:GLU:C | 2:B:259:TYR:OH | 2.07 | 0.92 |
| 2:B:374:PHE:CE2 | 2:B:398:ILE:CG2 | 2.52 | 0.92 |
| 4:M:9:ASP:CB | 4:M:111:ILE:CG2 | 2.47 | 0.92 |
| 2:B:178:ILE:HG21 | 2:B:217:GLU:HB2 | 1.49 | 0.92 |
| 2:B:565:GLN:OE1 | 2:B:581:TYR:OH | 1.87 | 0.92 |
| 1:A:103:LYS:HB3 | 1:A:107:TYR:CE2 | 2.03 | 0.92 |
| 1:A:254:ILE:CG2 | 3:S:94:SER:OG | 2.18 | 0.92 |
| 2:B:219:TYR:CD2 | 2:B:226:LEU:CG | 2.53 | 0.92 |
| 2:B:230:PHE:O | 2:B:231:ARG:C | 1.96 | 0.92 |
| 2:B:119:SER:O | 2:B:123:LEU:HG | 1.70 | 0.92 |
| 2:B:336:ASN:HB3 | 2:B:339:PHE:CE2 | 2.04 | 0.92 |
| 4:M:362:PHE:O | 4:M:363:ASN:C | 2.06 | 0.92 |
| 1:A:556:VAL:CG2 | 1:A:603:VAL:CG2 | 2.44 | 0.92 |
| 2:B:337:THR:HG23 | 2:B:373:LEU:CD1 | 2.00 | 0.92 |
| 4:M:344:ILE:HG23 | 4:M:347:PHE:HB2 | 1.50 | 0.92 |
| 2:B:107:ARG:HH12 | 4:M:20:LEU:HB3 | 1.35 | 0.91 |
| 4:M:351:SER:HB2 | 4:M:440:ILE:O | 1.68 | 0.91 |
| 2:B:5:ILE:HG21 | 4:M:42:LEU:HD11 | 0.94 | 0.91 |
| 2:B:237:ILE:CG2 | 2:B:238:LYS:N | 2.34 | 0.91 |
| 2:B:297:PRO:O | 2:B:301:LEU:HD12 | 1.70 | 0.91 |
| 3:S:130:SER:OG | 3:S:156:LEU:CD1 | 2.16 | 0.91 |
| 1:A:309:PHE:CE1 | 1:A:348:PHE:CE2 | 2.58 | 0.91 |
| 2:B:72:SER:OG | 4:M:17:GLN:OE1 | 1.87 | 0.91 |
| 2:B:578:PRO:CD | 2:B:581:TYR:HE2 | 1.57 | 0.91 |
| 2:B:124:GLN:HA | 2:B:127:LEU:HD12 | 1.51 | 0.91 |
| 2:B:178:ILE:HD13 | 2:B:218:CYS:HB2 | 1.50 | 0.91 |
| 2:B:256:CYS:CB | 2:B:328:LEU:HD23 | 1.94 | 0.91 |
| 4:M:9:ASP:HB2 | 4:M:111:ILE:HG21 | 1.50 | 0.91 |
| 2:B:297:PRO:O | 2:B:301:LEU:HG | 1.71 | 0.91 |
| 2:B:329:ALA:HB2 | 2:B:334:MET:HG2 | 1.51 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:M:344:ILE:HG21 | 4:M:347:PHE:HB3 | 1.50 | 0.91 |
| 1:A:114:PHE:CE1 | 1:A:153:ILE:HA | 2.05 | 0.91 |
| 2:B:12:LEU:HD12 | 4:M:13:LYS:CA | 1.96 | 0.91 |
| 2:B:80:GLN:N | 2:B:108:PHE:HE2 | 1.68 | 0.91 |
| 2:B:219:TYR:CG | 2:B:226:LEU:HD22 | 2.05 | 0.91 |
| 2:B:523:PHE:HZ | 2:B:580:TYR:CZ | 1.88 | 0.91 |
| 2:B:578:PRO:HD3 | 2:B:581:TYR:HE2 | 1.33 | 0.91 |
| 4:M:479:PHE:H | 4:M:479:PHE:HD1 | 1.18 | 0.91 |
| 3:S:4:ALA:HA | 3:S:18:LYS:O | 1.69 | 0.91 |
| 4:M:44:ASP:HB2 | 4:M:50:TYR:HD2 | 1.29 | 0.91 |
| 4:M:113:LYS:O | 4:M:116:ASN:HB2 | 1.70 | 0.91 |
| 1:A:575:LYS:NZ | 1:A:615:GLU:OE1 | 2.04 | 0.91 |
| 2:B:16:LYS:HB3 | 4:M:115:VAL:CG1 | 2.01 | 0.91 |
| 2:B:151:ALA:CB | 2:B:188:TYR:CE2 | 2.54 | 0.91 |
| 3:S:73:ILE:CG2 | 3:S:88:ILE:CG2 | 2.49 | 0.91 |
| 1:A:556:VAL:HG21 | 1:A:603:VAL:HG22 | 1.53 | 0.91 |
| 2:B:533:LEU:O | 2:B:536:ASN:N | 2.04 | 0.91 |
| 4:M:306:LEU:CD1 | 4:M:317:MET:CE | 2.49 | 0.91 |
| 2:B:223:LEU:HD11 | 2:B:258:GLN:HB3 | 0.91 | 0.91 |
| 2:B:560:ILE:HA | 2:B:563:PHE:HB2 | 1.53 | 0.91 |
| 2:B:578:PRO:HD2 | 2:B:581:TYR:CZ | 2.05 | 0.91 |
| 3:S:135:ILE:O | 3:S:141:VAL:CA | 2.18 | 0.91 |
| 1:A:257:LEU:HD22 | 1:A:278:ILE:HG22 | 1.53 | 0.90 |
| 2:B:12:LEU:CB | 4:M:13:LYS:CG | 2.40 | 0.90 |
| 2:B:437:SER:HB2 | 2:B:474:VAL:CB | 2.00 | 0.90 |
| 2:B:513:TRP:N | 2:B:551:LEU:HD13 | 1.86 | 0.90 |
| 4:M:243:ILE:O | 4:M:472:TYR:HB2 | 1.70 | 0.90 |
| 1:A:578:LEU:HD23 | 1:A:607:LEU:HD22 | 1.54 | 0.90 |
| 2:B:25:VAL:HG23 | 2:B:32:GLU:HG3 | 1.52 | 0.90 |
| 2:B:106:LEU:CD2 | 2:B:144:ASP:OD2 | 2.19 | 0.90 |
| 3:S:53:THR:OG1 | 3:S:68:VAL:CA | 2.18 | 0.90 |
| 1:A:283:GLU:OE1 | 1:A:318:ARG:NH2 | 2.03 | 0.90 |
| 1:A:503:ASN:HD21 | 4:M:60:LEU:CD2 | 1.85 | 0.90 |
| 2:B:387:ASP:HB3 | 2:B:388:PRO:HD2 | 1.52 | 0.90 |
| 2:B:398:ILE:O | 2:B:401:THR:N | 2.03 | 0.90 |
| 2:B:556:LEU:CD2 | 2:B:588:ILE:HG13 | 1.99 | 0.90 |
| 4:M:95:THR:CB | 4:M:137:SER:O | 2.19 | 0.90 |
| 4:M:293:PRO:HD2 | 4:M:293:PRO:O | 1.68 | 0.90 |
| 4:M:347:PHE:CD1 | 4:M:350:VAL:CB | 2.53 | 0.90 |
| 2:B:139:LEU:CG | 2:B:176:ALA:HB2 | 1.99 | 0.90 |
| 2:B:396:ILE:HD13 | 2:B:432:ALA:CA | 2.00 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:M:100:LEU:CD2 | 4:M:121:ILE:HG12 | 2.00 | 0.90 |
| 2:B:109:ALA:O | 2:B:110:GLU:C | 1.99 | 0.90 |
| 1:A:121:LEU:HD12 | 1:A:153:ILE:CG2 | 2.01 | 0.90 |
| 2:B:38:TYR:CZ | 2:B:43:ASN:O | 2.25 | 0.90 |
| 2:B:436:LEU:HD12 | 2:B:454:LEU:CD2 | 2.01 | 0.90 |
| 1:A:316:LEU:CD1 | 1:A:348:PHE:CD2 | 2.54 | 0.90 |
| 1:A:424:TYR:CE1 | 3:S:63:ASN:ND2 | 2.40 | 0.90 |
| 2:B:155:LEU:HD23 | 2:B:192:LEU:HD11 | 0.91 | 0.90 |
| 2:B:297:PRO:O | 2:B:301:LEU:CD1 | 2.19 | 0.90 |
| 2:B:562:ASN:O | 2:B:581:TYR:HA | 1.72 | 0.90 |
| 4:M:317:MET:HB2 | 4:M:322:LEU:H | 1.33 | 0.90 |
| 4:M:347:PHE:O | 4:M:348:LYS:C | 2.09 | 0.90 |
| 1:A:179:LYS:HE2 | 3:S:137:GLN:C | 1.92 | 0.90 |
| 1:A:213:SER:HB2 | 3:S:142:ILE:CB | 2.02 | 0.90 |
| 2:B:29:LYS:N | 2:B:30:LEU:CA | 2.34 | 0.90 |
| 4:M:16:PHE:HE2 | 4:M:125:PHE:CE2 | 1.90 | 0.90 |
| 4:M:244:VAL:CA | 4:M:472:TYR:CE2 | 2.53 | 0.90 |
| 2:B:80:GLN:CG | 2:B:108:PHE:HZ | 1.85 | 0.90 |
| 2:B:278:PRO:HD3 | 2:B:292:GLU:HB2 | 1.52 | 0.90 |
| 2:B:279:LEU:H | 2:B:288:TYR:HB2 | 1.12 | 0.90 |
| 4:M:56:VAL:H | 4:M:64:LYS:HG3 | 1.36 | 0.90 |
| 4:M:242:GLY:HA2 | 4:M:474:THR:HG21 | 1.52 | 0.90 |
| 1:A:276:PRO:O | 1:A:278:ILE:O | 1.88 | 0.90 |
| 2:B:11:ALA:HA | 2:B:40:GLN:HE21 | 1.32 | 0.90 |
| 2:B:231:ARG:CG | 2:B:298:ASP:OD1 | 2.19 | 0.90 |
| 2:B:278:PRO:HD2 | 2:B:292:GLU:HG3 | 1.52 | 0.90 |
| 2:B:348:THR:HG21 | 2:B:380:LYS:CB | 2.01 | 0.90 |
| 2:B:567:GLN:O | 2:B:569:THR:CA | 2.18 | 0.90 |
| 1:A:349:ILE:HG21 | 1:A:378:ILE:HG22 | 1.54 | 0.89 |
| 2:B:23:ALA:C | 2:B:32:GLU:CD | 2.10 | 0.89 |
| 2:B:25:VAL:HG22 | 2:B:28:SER:OG | 1.70 | 0.89 |
| 2:B:215:TYR:HD2 | 2:B:233:TYR:HE2 | 0.91 | 0.89 |
| 2:B:436:LEU:CD1 | 2:B:454:LEU:HD21 | 2.02 | 0.89 |
| 2:B:20:ARG:HH12 | 4:M:118:TYR:CA | 1.84 | 0.89 |
| 2:B:56:SER:O | 2:B:57:ARG:C | 2.00 | 0.89 |
| 2:B:300:ASP:OD2 | 2:B:304:GLN:NE2 | 2.06 | 0.89 |
| 4:M:222:PHE:CE1 | 4:M:240:ILE:CG2 | 2.54 | 0.89 |
| 2:B:403:ILE:HD12 | 2:B:439:CYS:O | 1.68 | 0.89 |
| 2:B:522:GLU:O | 2:B:522:GLU:HG2 | 1.70 | 0.89 |
| 2:B:597:TYR:O | 2:B:601:TYR:CD2 | 2.25 | 0.89 |
| 3:S:131:VAL:CG2 | 3:S:153:VAL:HG22 | 2.02 | 0.89 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:609:LEU:HG | 1:A:628:VAL:CG1 | 2.02 | 0.89 |
| 2:B:347:VAL:HG21 | 2:B:381:PHE:CE1 | 2.08 | 0.89 |
| 3:S:16:LEU:HD13 | 3:S:125:TRP:HE1 | 1.36 | 0.89 |
| 4:M:241:HIS:O | 4:M:474:THR:OG1 | 1.90 | 0.89 |
| 4:M:253:ASN:HA | 4:M:292:PRO:HG2 | 1.54 | 0.89 |
| 1:A:585:PHE:C | 1:A:600:SER:HG | 1.74 | 0.89 |
| 2:B:243:TRP:HZ3 | 4:M:98:ARG:CD | 1.80 | 0.89 |
| 4:M:240:ILE:HG21 | 4:M:444:ALA:HA | 1.54 | 0.89 |
| 2:B:216:LYS:CG | 2:B:251:LEU:CD1 | 2.51 | 0.89 |
| 2:B:340:ILE:HG21 | 2:B:374:PHE:HA | 1.55 | 0.89 |
| 2:B:397:GLN:HE21 | 2:B:431:MET:CE | 1.83 | 0.89 |
| 4:M:48:ASP:HA | 4:M:70:ASN:HD22 | 1.37 | 0.89 |
| 2:B:16:LYS:HZ1 | 4:M:111:ILE:HD12 | 1.34 | 0.89 |
| 2:B:38:TYR:CE2 | 2:B:43:ASN:CA | 2.55 | 0.89 |
| 2:B:193:LEU:HD21 | 2:B:225:LEU:HB2 | 1.53 | 0.89 |
| 2:B:345:ARG:O | 2:B:349:MET:HG3 | 1.72 | 0.89 |
| 2:B:396:ILE:HG21 | 2:B:432:ALA:HA | 0.90 | 0.89 |
| 2:B:400:SER:HA | 2:B:439:CYS:SG | 2.13 | 0.89 |
| 4:M:247:ARG:H | 4:M:470:ALA:HB2 | 1.35 | 0.89 |
| 1:A:464:ILE:O | 1:A:465:SER:C | 1.92 | 0.89 |
| 2:B:2:VAL:HG11 | 4:M:54:SER:HB3 | 0.91 | 0.89 |
| 2:B:17:VAL:O | 2:B:21:GLU:HG2 | 1.73 | 0.89 |
| 2:B:174:ALA:O | 2:B:175:LEU:C | 2.02 | 0.89 |
| 1:A:638:LEU:CD1 | 2:B:557:SER:OG | 2.21 | 0.89 |
| 2:B:72:SER:C | 4:M:19:LEU:HB2 | 1.92 | 0.89 |
| 2:B:232:ARG:HG3 | 2:B:236:ILE:HD11 | 1.55 | 0.89 |
| 2:B:252:LEU:HB3 | 2:B:302:PHE:CG | 2.06 | 0.89 |
| 2:B:378:THR:O | 2:B:381:PHE:N | 2.05 | 0.89 |
| 3:S:16:LEU:HB2 | 3:S:125:TRP:HE1 | 1.32 | 0.89 |
| 4:M:9:ASP:CB | 4:M:111:ILE:HG22 | 2.03 | 0.89 |
| 4:M:121:ILE:O | 4:M:125:PHE:CE1 | 2.26 | 0.89 |
| 1:A:410:TYR:HD1 | 3:S:43:ASN:ND2 | 1.63 | 0.89 |
| 1:A:503:ASN:CG | 4:M:60:LEU:N | 2.25 | 0.89 |
| 2:B:11:ALA:N | 2:B:40:GLN:HE22 | 1.71 | 0.89 |
| 2:B:278:PRO:CA | 2:B:288:TYR:CB | 2.51 | 0.89 |
| 2:B:294:VAL:HG23 | 2:B:333:GLN:HG2 | 1.54 | 0.89 |
| 2:B:397:GLN:NE2 | 2:B:431:MET:HE3 | 1.87 | 0.89 |
| 3:S:5:VAL:O | 3:S:17:VAL:HA | 1.73 | 0.89 |
| 4:M:9:ASP:HB2 | 4:M:111:ILE:HG22 | 1.53 | 0.89 |
| 4:M:44:ASP:HB3 | 4:M:50:TYR:CE2 | 2.07 | 0.89 |
| 4:M:240:ILE:CG2 | 4:M:444:ALA:HA | 2.02 | 0.89 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:M:260:LEU:CD2 | 4:M:449:VAL:HG22 | 2.02 | 0.89 |
| 4:M:437:TYR:CD1 | 4:M:479:PHE:CZ | 2.61 | 0.89 |
| 2:B:13:ASP:O | 2:B:17:VAL:CG2 | 2.20 | 0.88 |
| 2:B:151:ALA:HA | 2:B:180:LEU:HD11 | 1.55 | 0.88 |
| 2:B:276:SER:O | 2:B:295:ASN:ND2 | 2.06 | 0.88 |
| 4:M:350:VAL:HG13 | 4:M:442:GLN:CG | 2.03 | 0.88 |
| 2:B:310:ILE:HD11 | 2:B:321:CYS:CB | 2.03 | 0.88 |
| 2:B:437:SER:HB2 | 2:B:474:VAL:HG13 | 0.90 | 0.88 |
| 2:B:486:HIS:ND1 | 2:B:518:ILE:HD13 | 1.88 | 0.88 |
| 4:M:350:VAL:CG1 | 4:M:442:GLN:HB3 | 2.02 | 0.88 |
| 1:A:503:ASN:HD21 | 4:M:60:LEU:HG | 1.39 | 0.88 |
| 2:B:2:VAL:HG13 | 4:M:54:SER:OG | 1.73 | 0.88 |
| 2:B:11:ALA:HA | 2:B:40:GLN:HE22 | 1.07 | 0.88 |
| 2:B:162:VAL:HG22 | 2:B:199:LEU:HD11 | 1.54 | 0.88 |
| 2:B:375:LEU:HD13 | 2:B:404:ASN:HD22 | 1.14 | 0.88 |
| 2:B:568:VAL:CG1 | 2:B:571:SER:OG | 2.21 | 0.88 |
| 4:M:356:LEU:CD2 | 4:M:358:ILE:HG13 | 2.04 | 0.88 |
| 1:A:84:MET:O | 1:A:85:ALA:C | 2.05 | 0.88 |
| 2:B:70:MET:CE | 2:B:107:ARG:HB3 | 2.03 | 0.88 |
| 2:B:158:VAL:HG13 | 2:B:173:VAL:HG12 | 1.53 | 0.88 |
| 2:B:274:PRO:CG | 2:B:295:ASN:CB | 2.52 | 0.88 |
| 4:M:219:LEU:HB3 | 4:M:472:TYR:O | 1.71 | 0.88 |
| 1:A:88:ASN:O | 1:A:89:PHE:C | 2.04 | 0.88 |
| 1:A:100:LEU:O | 1:A:101:GLN:C | 1.98 | 0.88 |
| 1:A:266:VAL:O | 1:A:267:GLU:CB | 2.22 | 0.88 |
| 1:A:585:PHE:CA | 1:A:600:SER:OG | 2.22 | 0.88 |
| 2:B:14:THR:HG21 | 2:B:40:GLN:HG2 | 1.53 | 0.88 |
| 2:B:151:ALA:HB1 | 2:B:188:TYR:CE2 | 2.08 | 0.88 |
| 2:B:351:GLU:CB | 4:M:476:THR:HB | 1.99 | 0.88 |
| 4:M:219:LEU:CD2 | 4:M:473:LYS:HA | 2.01 | 0.88 |
| 2:B:37:TYR:HD2 | 2:B:38:TYR:CD1 | 1.92 | 0.88 |
| 2:B:144:ASP:HA | 2:B:179:LYS:HD3 | 1.54 | 0.88 |
| 2:B:367:SER:HB2 | 2:B:401:THR:HB | 1.53 | 0.88 |
| 2:B:433:VAL:CG1 | 2:B:474:VAL:HG21 | 2.04 | 0.88 |
| 2:B:457:HIS:HA | 2:B:461:HIS:HD2 | 1.37 | 0.88 |
| 4:M:15:ILE:HG23 | 4:M:115:VAL:HG23 | 1.54 | 0.88 |
| 1:A:88:ASN:HB3 | 1:A:120:ILE:HG23 | 1.56 | 0.88 |
| 1:A:216:SER:HB3 | 3:S:140:MET:SD | 2.13 | 0.88 |
| 1:A:495:ILE:HG23 | 1:A:515:CYS:SG | 2.13 | 0.88 |
| 2:B:337:THR:CG2 | 2:B:373:LEU:HD11 | 2.02 | 0.88 |
| 3:S:8:PHE:HB3 | 3:S:36:TYR:CE1 | 2.08 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:M:245:ASP:HB3 | 4:M:472:TYR:CD1 | 2.09 | 0.88 |
| 2:B:219:TYR:CE2 | 2:B:226:LEU:CG | 2.56 | 0.88 |
| 2:B:280:PRO:HG3 | 2:B:283:TYR:CD2 | 2.09 | 0.88 |
| 2:B:367:SER:HB2 | 2:B:401:THR:CB | 2.03 | 0.88 |
| 4:M:272:LEU:HD21 | 4:M:278:ILE:HB | 1.56 | 0.88 |
| 4:M:288:ILE:CD1 | 4:M:300:LEU:HD22 | 2.03 | 0.88 |
| 1:A:621:LEU:O | 1:A:622:PRO:C | 1.96 | 0.88 |
| 2:B:38:TYR:CZ | 2:B:43:ASN:N | 2.31 | 0.88 |
| 1:A:381:GLU:HA | 1:A:384:LEU:HD23 | 1.53 | 0.87 |
| 2:B:143:SER:HB3 | 2:B:176:ALA:HA | 1.54 | 0.87 |
| 2:B:178:ILE:HG23 | 2:B:217:GLU:CB | 2.03 | 0.87 |
| 2:B:568:VAL:HG12 | 2:B:571:SER:CB | 2.03 | 0.87 |
| 4:M:221:THR:H | 4:M:474:THR:HG1 | 0.93 | 0.87 |
| 1:A:411:GLU:HG3 | 3:S:46:PHE:HZ | 1.34 | 0.87 |
| 1:A:536:MET:O | 1:A:537:THR:C | 1.89 | 0.87 |
| 2:B:230:PHE:CD1 | 2:B:298:ASP:HB3 | 2.08 | 0.87 |
| 2:B:341:GLU:HG3 | 2:B:377:TYR:HE1 | 0.77 | 0.87 |
| 2:B:374:PHE:HE1 | 2:B:381:PHE:CE2 | 1.90 | 0.87 |
| 4:M:306:LEU:HD22 | 4:M:317:MET:HE3 | 1.52 | 0.87 |
| 2:B:136:CYS:CB | 2:B:172:GLU:HG3 | 2.04 | 0.87 |
| 4:M:347:PHE:HE1 | 4:M:350:VAL:HG11 | 1.32 | 0.87 |
| 4:M:383:HIS:CG | 4:M:403:THR:OG1 | 2.26 | 0.87 |
| 1:A:503:ASN:CB | 4:M:59:ASP:O | 2.20 | 0.87 |
| 1:A:595:GLU:OE2 | 2:B:513:TRP:CH2 | 2.27 | 0.87 |
| 2:B:279:LEU:HG | 2:B:288:TYR:CD2 | 2.09 | 0.87 |
| 4:M:219:LEU:HB3 | 4:M:472:TYR:C | 1.94 | 0.87 |
| 4:M:240:ILE:HG22 | 4:M:444:ALA:CB | 2.04 | 0.87 |
| 1:A:68:THR:H | 3:S:166:LYS:HD3 | 1.40 | 0.87 |
| 2:B:106:LEU:CG | 2:B:144:ASP:HB3 | 2.04 | 0.87 |
| 2:B:214:ALA:O | 2:B:217:GLU:N | 2.07 | 0.87 |
| 2:B:563:PHE:HD1 | 2:B:584:SER:HB3 | 1.39 | 0.87 |
| 3:S:131:VAL:HG22 | 3:S:153:VAL:HG22 | 1.57 | 0.87 |
| 1:A:462:GLN:C | 4:M:58:ARG:CA | 2.43 | 0.87 |
| 2:B:197:LYS:CB | 2:B:229:HIS:NE2 | 2.36 | 0.87 |
| 2:B:237:ILE:CG2 | 2:B:238:LYS:H | 1.86 | 0.87 |
| 2:B:367:SER:CB | 2:B:401:THR:OG1 | 2.22 | 0.87 |
| 4:M:220:GLU:CG | 4:M:439:TYR:HB2 | 2.04 | 0.87 |
| 1:A:488:ARG:O | 1:A:491:THR:OG1 | 1.93 | 0.87 |
| 2:B:181:TYR:HE1 | 2:B:222:HIS:CD2 | 1.90 | 0.87 |
| 2:B:253:ILE:HG12 | 2:B:324:ALA:HA | 1.55 | 0.87 |
| 4:M:92:PHE:HE2 | 4:M:128:CYS:O | 1.58 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:M:219:LEU:CB | 4:M:472:TYR:C | 2.41 | 0.87 |
| 1:A:103:LYS:O | 1:A:107:TYR:CD2 | 2.28 | 0.87 |
| 1:A:251:TRP:HE3 | 3:S:97:ALA:HA | 1.16 | 0.87 |
| 2:B:553:ALA:HB2 | 2:B:614:ILE:HD13 | 1.55 | 0.87 |
| 2:B:569:THR:O | 2:B:569:THR:CG2 | 2.22 | 0.87 |
| 4:M:74:TYR:HB3 | 4:M:114:ILE:CD1 | 2.05 | 0.87 |
| 4:M:223:HIS:CA | 4:M:479:PHE:CE1 | 2.57 | 0.87 |
| 4:M:306:LEU:O | 4:M:307:SER:C | 2.03 | 0.87 |
| 1:A:433:ILE:HG23 | 1:A:476:GLN:HB2 | 1.57 | 0.87 |
| 4:M:4:SER:O | 4:M:78:ALA:HA | 1.72 | 0.87 |
| 2:B:34:SER:OG | 2:B:65:ARG:CZ | 2.23 | 0.86 |
| 2:B:69:ILE:HG23 | 2:B:74:ASP:HB3 | 1.57 | 0.86 |
| 2:B:386:LYS:HE3 | 4:M:480:GLN:HB2 | 1.55 | 0.86 |
| 2:B:224:GLU:CG | 2:B:259:TYR:OH | 2.23 | 0.86 |
| 2:B:366:LEU:O | 2:B:367:SER:C | 2.02 | 0.86 |
| 2:B:479:VAL:HG21 | 2:B:486:HIS:CD2 | 2.09 | 0.86 |
| 2:B:523:PHE:HE2 | 2:B:580:TYR:CG | 1.91 | 0.86 |
| 2:B:556:LEU:CA | 2:B:588:ILE:CD1 | 2.48 | 0.86 |
| 3:S:8:PHE:CE2 | 3:S:84:TYR:HB3 | 2.08 | 0.86 |
| 1:A:506:LYS:NZ | 4:M:82:LYS:HD3 | 1.88 | 0.86 |
| 2:B:158:VAL:CG1 | 2:B:177:ILE:HG12 | 1.99 | 0.86 |
| 2:B:278:PRO:HA | 2:B:288:TYR:HB3 | 1.55 | 0.86 |
| 1:A:66:SER:N | 3:S:166:LYS:HE2 | 1.89 | 0.86 |
| 2:B:72:SER:O | 2:B:73:ASP:HB2 | 1.75 | 0.86 |
| 2:B:107:ARG:HH12 | 4:M:20:LEU:CB | 1.88 | 0.86 |
| 2:B:344:VAL:HG11 | 2:B:377:TYR:CB | 2.05 | 0.86 |
| 2:B:436:LEU:HD12 | 2:B:454:LEU:HD21 | 1.57 | 0.86 |
| 4:M:222:PHE:CE1 | 4:M:240:ILE:HG23 | 2.10 | 0.86 |
| 1:A:288:THR:HG23 | 3:S:96:LEU:CD2 | 2.05 | 0.86 |
| 2:B:261:PRO:HD2 | 2:B:293:VAL:HG23 | 1.55 | 0.86 |
| 4:M:41:LEU:HD13 | 4:M:52:ASP:N | 1.85 | 0.86 |
| 4:M:74:TYR:CB | 4:M:114:ILE:CD1 | 2.52 | 0.86 |
| 4:M:105:ASP:O | 4:M:106:LYS:HB3 | 1.74 | 0.86 |
| 4:M:306:LEU:HD13 | 4:M:317:MET:HE3 | 1.54 | 0.86 |
| 1:A:114:PHE:CD2 | 1:A:153:ILE:HG12 | 2.10 | 0.86 |
| 1:A:408:ILE:HG22 | 3:S:64:ASN:HB3 | 1.56 | 0.86 |
| 1:A:629:LEU:O | 1:A:630:PRO:C | 2.01 | 0.86 |
| 2:B:28:SER:C | 2:B:58:GLU:CG | 2.34 | 0.86 |
| 2:B:260:LEU:HD22 | 2:B:291:TYR:OH | 1.75 | 0.86 |
| 2:B:274:PRO:CG | 2:B:295:ASN:HA | 2.05 | 0.86 |
| 1:A:462:GLN:C | 4:M:58:ARG:CB | 2.41 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:M:215:TYR:CG | 4:M:468:LYS:HA | 2.11 | 0.86 |
| 4:M:223:HIS:CA | 4:M:479:PHE:CD1 | 2.55 | 0.86 |
| 1:A:182:ILE:HG22 | 1:A:221:VAL:HG21 | 1.58 | 0.86 |
| 2:B:189:HIS:NE2 | 2:B:222:HIS:HB3 | 1.91 | 0.86 |
| 2:B:239:GLN:O | 4:M:279:ASN:HA | 1.75 | 0.86 |
| 2:B:310:ILE:CD1 | 2:B:321:CYS:HB2 | 2.05 | 0.86 |
| 2:B:418:TYR:CD1 | 2:B:424:PHE:CE2 | 2.64 | 0.86 |
| 2:B:424:PHE:CD1 | 2:B:428:VAL:HG11 | 2.10 | 0.86 |
| 1:A:373:GLU:HG3 | 1:A:427:LYS:HE2 | 1.58 | 0.86 |
| 2:B:143:SER:C | 2:B:179:LYS:CD | 2.44 | 0.86 |
| 2:B:360:LEU:HB3 | 2:B:394:TRP:HB3 | 1.58 | 0.86 |
| 2:B:472:VAL:HG11 | 2:B:510:GLY:HA3 | 1.55 | 0.86 |
| 2:B:537:PHE:CE2 | 2:B:545:ARG:HB3 | 2.11 | 0.86 |
| 2:B:599:ALA:O | 2:B:601:TYR:N | 2.09 | 0.86 |
| 4:M:96:ILE:HG21 | 4:M:125:PHE:CE1 | 2.09 | 0.86 |
| 4:M:215:TYR:CD1 | 4:M:467:TYR:O | 2.28 | 0.86 |
| 2:B:162:VAL:CG2 | 2:B:199:LEU:HD11 | 2.05 | 0.86 |
| 2:B:172:GLU:O | 2:B:173:VAL:C | 2.06 | 0.86 |
| 4:M:290:PHE:CZ | 4:M:293:PRO:HD3 | 2.10 | 0.86 |
| 2:B:559:ASP:O | 2:B:563:PHE:N | 2.09 | 0.85 |
| 4:M:15:ILE:HG23 | 4:M:115:VAL:HG22 | 1.57 | 0.85 |
| 4:M:245:ASP:N | 4:M:472:TYR:CG | 2.29 | 0.85 |
| 1:A:595:GLU:OE2 | 2:B:513:TRP:CD2 | 2.29 | 0.85 |
| 2:B:219:TYR:CD2 | 2:B:226:LEU:CB | 2.53 | 0.85 |
| 2:B:344:VAL:HG13 | 2:B:381:PHE:HE2 | 1.32 | 0.85 |
| 2:B:596:LEU:HD12 | 2:B:611:ALA:HB1 | 1.58 | 0.85 |
| 2:B:212:VAL:CG2 | 2:B:248:LEU:HD21 | 2.05 | 0.85 |
| 4:M:443:SER:HG | 4:M:447:ILE:C | 1.79 | 0.85 |
| 1:A:225:LEU:HB3 | 1:A:233:PHE:CZ | 2.11 | 0.85 |
| 1:A:411:GLU:CG | 3:S:46:PHE:CZ | 2.58 | 0.85 |
| 1:A:506:LYS:HZ3 | 4:M:82:LYS:HD3 | 1.38 | 0.85 |
| 2:B:227:HIS:CA | 2:B:298:ASP:OD2 | 2.24 | 0.85 |
| 2:B:256:CYS:SG | 2:B:328:LEU:HD21 | 2.15 | 0.85 |
| 2:B:337:THR:CA | 2:B:373:LEU:CD2 | 2.55 | 0.85 |
| 2:B:517:GLU:OE2 | 2:B:554:LYS:NZ | 2.09 | 0.85 |
| 4:M:290:PHE:HB2 | 4:M:299:LEU:CD1 | 2.05 | 0.85 |
| 2:B:343:LEU:CD2 | 2:B:366:LEU:HD12 | 2.06 | 0.85 |
| 4:M:347:PHE:CE1 | 4:M:350:VAL:CB | 2.60 | 0.85 |
| 2:B:5:ILE:HD11 | 4:M:39:PRO:CD | 2.07 | 0.85 |
| 2:B:5:ILE:HD11 | 4:M:39:PRO:N | 1.90 | 0.85 |
| 2:B:14:THR:CG2 | 2:B:36:THR:HG23 | 1.94 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:70:MET:SD | 2:B:107:ARG:HB3 | 2.17 | 0.85 |
| 2:B:75:ASP:CG | 4:M:24:ALA:HB3 | 1.95 | 0.85 |
| 2:B:293:VAL:CA | 2:B:299:LEU:HG | 2.06 | 0.85 |
| 2:B:433:VAL:CG2 | 2:B:471:TYR:CD2 | 2.58 | 0.85 |
| 2:B:479:VAL:HG13 | 2:B:486:HIS:CD2 | 2.10 | 0.85 |
| 3:S:53:THR:CB | 3:S:68:VAL:C | 2.44 | 0.85 |
| 3:S:135:ILE:HG23 | 3:S:141:VAL:HG13 | 1.58 | 0.85 |
| 4:M:215:TYR:CD1 | 4:M:468:LYS:HA | 2.11 | 0.85 |
| 2:B:80:GLN:HG3 | 2:B:108:PHE:HZ | 1.41 | 0.85 |
| 2:B:337:THR:CA | 2:B:373:LEU:HD21 | 2.07 | 0.85 |
| 4:M:212:ASN:HA | 4:M:249:TYR:O | 1.75 | 0.85 |
| 2:B:50:LEU:HD23 | 2:B:62:ALA:HA | 1.56 | 0.85 |
| 2:B:181:TYR:HE1 | 2:B:185:LYS:HG3 | 1.37 | 0.85 |
| 2:B:216:LYS:HG3 | 2:B:251:LEU:HD12 | 1.58 | 0.85 |
| 2:B:322:CYS:SG | 2:B:362:ALA:HB1 | 2.16 | 0.85 |
| 1:A:102:GLN:NE2 | 3:S:166:LYS:NZ | 2.25 | 0.85 |
| 1:A:309:PHE:CE1 | 1:A:348:PHE:CZ | 2.64 | 0.85 |
| 1:A:585:PHE:CE2 | 1:A:603:VAL:HG12 | 2.11 | 0.85 |
| 2:B:9:ALA:C | 4:M:14:LEU:CB | 2.44 | 0.85 |
| 2:B:73:ASP:CA | 4:M:19:LEU:HD23 | 2.00 | 0.85 |
| 2:B:261:PRO:CD | 2:B:293:VAL:CG2 | 2.53 | 0.85 |
| 2:B:278:PRO:HA | 2:B:288:TYR:CA | 2.06 | 0.85 |
| 2:B:351:GLU:CB | 4:M:476:THR:CG2 | 2.55 | 0.85 |
| 4:M:215:TYR:HD1 | 4:M:467:TYR:O | 1.59 | 0.85 |
| 4:M:222:PHE:CD2 | 4:M:439:TYR:HE2 | 1.95 | 0.85 |
| 4:M:262:THR:C | 4:M:264:GLY:H | 1.80 | 0.85 |
| 1:A:411:GLU:CG | 3:S:46:PHE:HZ | 1.89 | 0.85 |
| 1:A:601:VAL:O | 1:A:602:GLU:O | 1.94 | 0.85 |
| 2:B:34:SER:CB | 2:B:65:ARG:NH1 | 2.40 | 0.85 |
| 2:B:215:TYR:HD1 | 2:B:219:TYR:CE2 | 1.93 | 0.85 |
| 1:A:183:THR:O | 1:A:186:PHE:HB3 | 1.77 | 0.84 |
| 1:A:244:LEU:HD11 | 1:A:281:LEU:CD1 | 2.07 | 0.84 |
| 1:A:410:TYR:HE1 | 3:S:43:ASN:ND2 | 1.71 | 0.84 |
| 1:A:503:ASN:HD21 | 4:M:60:LEU:CG | 1.90 | 0.84 |
| 2:B:106:LEU:HD13 | 2:B:144:ASP:CA | 2.06 | 0.84 |
| 2:B:219:TYR:CD2 | 2:B:226:LEU:CD1 | 2.53 | 0.84 |
| 2:B:429:VAL:HG12 | 2:B:467:VAL:HG13 | 1.57 | 0.84 |
| 1:A:536:MET:HG2 | 1:A:551:LEU:HD11 | 1.58 | 0.84 |
| 1:A:581:LEU:HD23 | 1:A:607:LEU:HD21 | 1.58 | 0.84 |
| 4:M:240:ILE:HG22 | 4:M:444:ALA:HB1 | 1.57 | 0.84 |
| 4:M:306:LEU:HD11 | 4:M:317:MET:HE1 | 1.58 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:M:376:ILE:CG2 | 4:M:379:LEU:CD1 | 2.54 | 0.84 |
| 2:B:274:PRO:HB2 | 2:B:295:ASN:OD1 | 1.75 | 0.84 |
| 4:M:215:TYR:HB2 | 4:M:467:TYR:C | 1.95 | 0.84 |
| 1:A:114:PHE:O | 1:A:115:TYR:O | 1.95 | 0.84 |
| 1:A:261:THR:OG1 | 1:A:297:CYS:SG | 2.33 | 0.84 |
| 1:A:402:ILE:CB | 3:S:62:GLU:O | 2.23 | 0.84 |
| 1:A:511:VAL:O | 1:A:515:CYS:SG | 2.36 | 0.84 |
| 2:B:104:TYR:O | 2:B:107:ARG:N | 2.09 | 0.84 |
| 2:B:107:ARG:NH1 | 4:M:20:LEU:HB3 | 1.92 | 0.84 |
| 2:B:596:LEU:HD22 | 2:B:615:SER:OG | 1.76 | 0.84 |
| 4:M:306:LEU:CD1 | 4:M:317:MET:HE1 | 2.06 | 0.84 |
| 4:M:362:PHE:O | 4:M:363:ASN:O | 1.95 | 0.84 |
| 4:M:443:SER:HB3 | 4:M:447:ILE:N | 1.93 | 0.84 |
| 1:A:204:VAL:O | 1:A:205:SER:C | 2.09 | 0.84 |
| 1:A:395:PHE:CE1 | 1:A:428:MET:HG3 | 2.12 | 0.84 |
| 1:A:409:VAL:HG12 | 3:S:42:ARG:NH1 | 1.92 | 0.84 |
| 1:A:409:VAL:HG12 | 3:S:42:ARG:HH12 | 1.42 | 0.84 |
| 1:A:581:LEU:HD23 | 1:A:607:LEU:CD1 | 2.07 | 0.84 |
| 2:B:103:LEU:HD11 | 4:M:127:CYS:SG | 2.17 | 0.84 |
| 3:S:109:LEU:HD12 | 3:S:113:PHE:CD1 | 2.12 | 0.84 |
| 4:M:92:PHE:CZ | 4:M:128:CYS:HB2 | 2.12 | 0.84 |
| 4:M:258:VAL:HG13 | 4:M:449:VAL:CG1 | 2.07 | 0.84 |
| 1:A:328:PRO:O | 1:A:329:ASN:C | 2.11 | 0.84 |
| 1:A:589:SER:HA | 1:A:597:GLN:HG3 | 1.59 | 0.84 |
| 2:B:70:MET:HE3 | 2:B:107:ARG:CG | 2.05 | 0.84 |
| 2:B:433:VAL:CG2 | 2:B:471:TYR:CE2 | 2.61 | 0.84 |
| 3:S:53:THR:OG1 | 3:S:68:VAL:N | 2.11 | 0.84 |
| 4:M:6:TYR:HA | 4:M:16:PHE:O | 1.77 | 0.84 |
| 1:A:190:LEU:HD11 | 1:A:228:LYS:HE3 | 1.60 | 0.84 |
| 1:A:495:ILE:HG21 | 1:A:515:CYS:HB3 | 1.59 | 0.84 |
| 1:A:503:ASN:ND2 | 4:M:60:LEU:CD2 | 2.40 | 0.84 |
| 1:A:581:LEU:CD2 | 1:A:607:LEU:HD11 | 2.07 | 0.84 |
| 2:B:127:LEU:HB3 | 2:B:157:THR:HG23 | 1.59 | 0.84 |
| 2:B:418:TYR:C | 2:B:418:TYR:HD1 | 1.77 | 0.84 |
| 2:B:430:ILE:HD11 | 2:B:466:SER:HB2 | 1.58 | 0.84 |
| 4:M:432:THR:HA | 4:M:481:VAL:O | 1.77 | 0.84 |
| 2:B:106:LEU:HD12 | 2:B:144:ASP:O | 1.74 | 0.84 |
| 2:B:226:LEU:HD21 | 2:B:255:TYR:CD1 | 2.11 | 0.84 |
| 2:B:398:ILE:HG22 | 2:B:402:LEU:CD1 | 2.08 | 0.84 |
| 2:B:549:LEU:HD13 | 2:B:595:VAL:HG12 | 1.59 | 0.84 |
| 4:M:271:SER:HB3 | 4:M:301:GLU:HG3 | 1.60 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:M:339:GLU:HG3 | 4:M:412:ARG:HG2 | 1.58 | 0.84 |
| 1:A:581:LEU:HG | 1:A:585:PHE:CE2 | 2.13 | 0.84 |
| 2:B:219:TYR:CZ | 2:B:226:LEU:N | 2.46 | 0.84 |
| 2:B:403:ILE:CG2 | 2:B:439:CYS:SG | 2.66 | 0.84 |
| 4:M:336:ASP:OD1 | 4:M:415:ILE:O | 1.96 | 0.84 |
| 1:A:274:LEU:O | 1:A:275:LEU:C | 2.13 | 0.83 |
| 1:A:450:TYR:HH | 1:A:476:GLN:HG2 | 1.38 | 0.83 |
| 2:B:512:VAL:HG22 | 2:B:533:LEU:HD22 | 1.59 | 0.83 |
| 4:M:212:ASN:ND2 | 4:M:249:TYR:O | 2.11 | 0.83 |
| 4:M:243:ILE:N | 4:M:474:THR:HG22 | 1.93 | 0.83 |
| 4:M:364:VAL:O | 4:M:367:ALA:O | 1.95 | 0.83 |
| 4:M:378:ILE:O | 4:M:413:GLY:HA3 | 1.77 | 0.83 |
| 1:A:189:PHE:CB | 1:A:225:LEU:HD21 | 2.08 | 0.83 |
| 2:B:9:ALA:C | 4:M:14:LEU:HB3 | 1.97 | 0.83 |
| 2:B:103:LEU:HD12 | 4:M:123:LEU:CD1 | 1.97 | 0.83 |
| 2:B:274:PRO:HG2 | 2:B:295:ASN:CA | 2.08 | 0.83 |
| 2:B:403:ILE:CD1 | 2:B:439:CYS:CB | 2.49 | 0.83 |
| 2:B:515:PHE:CD2 | 2:B:529:VAL:HG21 | 2.13 | 0.83 |
| 3:S:31:LEU:O | 3:S:35:VAL:HG13 | 1.79 | 0.83 |
| 4:M:47:SER:HB2 | 4:M:50:TYR:CD1 | 2.12 | 0.83 |
| 4:M:65:TYR:CE1 | 4:M:86:PRO:HB3 | 2.13 | 0.83 |
| 4:M:442:GLN:HG3 | 4:M:443:SER:H | 1.43 | 0.83 |
| 1:A:107:TYR:CD1 | 1:A:128:LEU:HD21 | 2.13 | 0.83 |
| 2:B:230:PHE:HZ | 2:B:252:LEU:HD22 | 1.10 | 0.83 |
| 2:B:252:LEU:HD13 | 2:B:302:PHE:HD1 | 1.35 | 0.83 |
| 3:S:25:LEU:O | 3:S:26:PRO:C | 2.16 | 0.83 |
| 4:M:478:ASN:O | 4:M:479:PHE:O | 1.96 | 0.83 |
| 1:A:88:ASN:CB | 1:A:120:ILE:HD12 | 2.09 | 0.83 |
| 2:B:162:VAL:HG23 | 2:B:173:VAL:HG11 | 1.58 | 0.83 |
| 2:B:217:GLU:OE2 | 4:M:133:GLU:OE1 | 1.97 | 0.83 |
| 2:B:340:ILE:CG1 | 2:B:373:LEU:HD23 | 2.08 | 0.83 |
| 2:B:347:VAL:O | 2:B:350:THR:N | 2.10 | 0.83 |
| 3:S:16:LEU:HD13 | 3:S:125:TRP:NE1 | 1.92 | 0.83 |
| 4:M:261:ASN:HB2 | 4:M:450:GLU:HG2 | 1.59 | 0.83 |
| 1:A:240:LEU:O | 1:A:241:TYR:C | 2.09 | 0.83 |
| 1:A:504:ILE:O | 1:A:505:ASN:C | 2.10 | 0.83 |
| 2:B:27:THR:HB | 2:B:57:ARG:HD2 | 1.60 | 0.83 |
| 2:B:423:HIS:CD2 | 4:M:365:GLU:HB3 | 2.12 | 0.83 |
| 4:M:244:VAL:HB | 4:M:300:LEU:HG | 1.60 | 0.83 |
| 4:M:443:SER:OG | 4:M:447:ILE:C | 2.17 | 0.83 |
| 1:A:568:GLU:OE1 | 1:A:571:ARG:NH1 | 2.10 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:351:GLU:HB3 | 4:M:476:THR:CG2 | 2.09 | 0.83 |
| 3:S:130:SER:CB | 3:S:156:LEU:CD1 | 2.57 | 0.83 |
| 4:M:380:ARG:O | 4:M:411:LEU:HA | 1.76 | 0.83 |
| 2:B:29:LYS:H | 2:B:30:LEU:HA | 1.44 | 0.83 |
| 2:B:378:THR:HG23 | 2:B:379:LYS:N | 1.94 | 0.83 |
| 2:B:127:LEU:HD11 | 2:B:142:LEU:CD1 | 2.09 | 0.83 |
| 2:B:436:LEU:CD1 | 2:B:454:LEU:CD2 | 2.56 | 0.83 |
| 2:B:519:ALA:O | 2:B:523:PHE:CD1 | 2.31 | 0.83 |
| 3:S:35:VAL:CB | 3:S:77:TYR:OH | 2.26 | 0.83 |
| 2:B:34:SER:O | 2:B:37:TYR:CB | 2.25 | 0.83 |
| 2:B:83:PHE:CD1 | 2:B:115:LEU:HD12 | 2.14 | 0.83 |
| 1:A:99:LYS:HG2 | 1:A:101:GLN:H | 1.44 | 0.83 |
| 1:A:495:ILE:CG2 | 1:A:515:CYS:HB3 | 2.07 | 0.83 |
| 2:B:152:PRO:HA | 2:B:188:TYR:HE1 | 1.44 | 0.83 |
| 2:B:181:TYR:HE1 | 2:B:222:HIS:NE2 | 1.76 | 0.83 |
| 2:B:252:LEU:CD1 | 2:B:302:PHE:CE1 | 2.62 | 0.83 |
| 2:B:340:ILE:HB | 2:B:373:LEU:HG | 1.61 | 0.83 |
| 2:B:403:ILE:HD12 | 2:B:439:CYS:C | 1.99 | 0.83 |
| 2:B:408:VAL:HB | 2:B:446:TRP:CD1 | 2.14 | 0.83 |
| 4:M:223:HIS:CG | 4:M:476:THR:HG1 | 1.95 | 0.83 |
| 4:M:276:VAL:HG22 | 4:M:290:PHE:CD1 | 2.13 | 0.83 |
| 2:B:374:PHE:HE2 | 2:B:402:LEU:CD1 | 1.42 | 0.82 |
| 2:B:398:ILE:HG22 | 2:B:402:LEU:HD11 | 1.58 | 0.82 |
| 4:M:235:LEU:HD13 | 4:M:310:VAL:HG21 | 1.59 | 0.82 |
| 4:M:374:TYR:OH | 4:M:394:GLN:C | 2.17 | 0.82 |
| 2:B:90:ILE:N | 2:B:101:ILE:HD13 | 1.94 | 0.82 |
| 2:B:318:ILE:HD13 | 2:B:346:THR:HG1 | 1.41 | 0.82 |
| 2:B:429:VAL:HG12 | 2:B:467:VAL:CG1 | 2.09 | 0.82 |
| 4:M:220:GLU:CG | 4:M:439:TYR:CD2 | 2.59 | 0.82 |
| 2:B:100:LEU:HD21 | 4:M:123:LEU:CD2 | 2.09 | 0.82 |
| 2:B:106:LEU:CG | 4:M:130:GLU:CB | 2.40 | 0.82 |
| 2:B:337:THR:CB | 2:B:373:LEU:HD13 | 2.05 | 0.82 |
| 2:B:415:LEU:HD12 | 2:B:436:LEU:CD2 | 2.09 | 0.82 |
| 4:M:245:ASP:HB3 | 4:M:472:TYR:HD1 | 1.41 | 0.82 |
| 4:M:327:PHE:CE1 | 4:M:336:ASP:HB2 | 2.14 | 0.82 |
| 2:B:72:SER:C | 4:M:17:GLN:HE22 | 1.82 | 0.82 |
| 2:B:301:LEU:O | 2:B:305:SER:OG | 1.97 | 0.82 |
| 3:S:16:LEU:CD1 | 3:S:125:TRP:HE1 | 1.92 | 0.82 |
| 1:A:222:ILE:HG21 | 1:A:240:LEU:HD11 | 1.61 | 0.82 |
| 1:A:536:MET:SD | 1:A:551:LEU:CD1 | 2.68 | 0.82 |
| 3:S:16:LEU:CB | 3:S:125:TRP:HE1 | 1.91 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:409:VAL:CG1 | 3:S:42:ARG:NH1 | 2.42 | 0.82 |
| 2:B:5:ILE:HD11 | 4:M:39:PRO:HG3 | 1.60 | 0.82 |
| 2:B:302:PHE:CE2 | 2:B:328:LEU:HD11 | 2.13 | 0.82 |
| 2:B:458:MET:SD | 2:B:471:TYR:HB3 | 2.19 | 0.82 |
| 2:B:580:TYR:HB3 | 2:B:582:ASP:CG | 1.99 | 0.82 |
| 3:S:54:PRO:HD2 | 3:S:57:LEU:HB2 | 1.59 | 0.82 |
| 4:M:97:ASP:O | 4:M:100:LEU:HB2 | 1.77 | 0.82 |
| 2:B:212:VAL:CG2 | 2:B:233:TYR:CE1 | 2.62 | 0.82 |
| 4:M:100:LEU:HD22 | 4:M:121:ILE:HG12 | 1.60 | 0.82 |
| 1:A:384:LEU:HD22 | 1:A:441:TYR:CD2 | 2.15 | 0.82 |
| 1:A:411:GLU:OE2 | 3:S:46:PHE:HE1 | 1.62 | 0.82 |
| 2:B:127:LEU:CD1 | 2:B:157:THR:HG21 | 2.10 | 0.82 |
| 2:B:139:LEU:HD11 | 2:B:176:ALA:CB | 2.09 | 0.82 |
| 2:B:219:TYR:HE2 | 2:B:226:LEU:HD13 | 1.03 | 0.82 |
| 2:B:343:LEU:HD22 | 2:B:366:LEU:HD12 | 1.61 | 0.82 |
| 2:B:563:PHE:CD1 | 2:B:584:SER:CA | 2.62 | 0.82 |
| 4:M:47:SER:O | 4:M:75:TRP:HH2 | 1.61 | 0.82 |
| 4:M:243:ILE:N | 4:M:474:THR:CG2 | 2.42 | 0.82 |
| 1:A:503:ASN:ND2 | 4:M:60:LEU:HG | 1.95 | 0.82 |
| 2:B:259:TYR:C | 2:B:261:PRO:N | 2.23 | 0.82 |
| 2:B:267:ASP:H | 2:B:289:PRO:CG | 1.92 | 0.82 |
| 2:B:337:THR:C | 2:B:373:LEU:HD11 | 1.95 | 0.82 |
| 1:A:606:PHE:CZ | 1:A:633:PHE:CD1 | 2.68 | 0.82 |
| 2:B:136:CYS:C | 2:B:172:GLU:HG3 | 2.00 | 0.82 |
| 2:B:216:LYS:NZ | 4:M:136:VAL:HG21 | 1.95 | 0.82 |
| 3:S:6:LEU:HD22 | 3:S:32:LEU:HD22 | 1.62 | 0.82 |
| 4:M:271:SER:HB3 | 4:M:301:GLU:CG | 2.08 | 0.82 |
| 1:A:213:SER:CB | 3:S:142:ILE:HB | 2.10 | 0.81 |
| 2:B:107:ARG:NH2 | 4:M:18:TYR:OH | 2.12 | 0.81 |
| 2:B:109:ALA:CB | 2:B:145:MET:SD | 2.69 | 0.81 |
| 2:B:219:TYR:HB3 | 2:B:223:LEU:CD2 | 2.10 | 0.81 |
| 2:B:253:ILE:HG12 | 2:B:324:ALA:CA | 2.10 | 0.81 |
| 2:B:379:LYS:HE2 | 2:B:410:GLU:CG | 2.02 | 0.81 |
| 2:B:438:ARG:HA | 2:B:441:GLN:HE21 | 1.45 | 0.81 |
| 2:B:513:TRP:O | 2:B:516:GLY:N | 2.12 | 0.81 |
| 1:A:100:LEU:O | 1:A:101:GLN:O | 1.96 | 0.81 |
| 1:A:216:SER:O | 1:A:219:VAL:HB | 1.80 | 0.81 |
| 2:B:347:VAL:CG1 | 2:B:381:PHE:CE1 | 2.63 | 0.81 |
| 4:M:304:VAL:HG11 | 4:M:445:SER:HA | 1.62 | 0.81 |
| 1:A:504:ILE:CA | 4:M:59:ASP:CG | 2.46 | 0.81 |
| 1:A:581:LEU:HB3 | 1:A:607:LEU:HD13 | 1.61 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:17:VAL:HB | 2:B:35:TYR:CD2 | 2.14 | 0.81 |
| 2:B:252:LEU:C | 2:B:302:PHE:CE2 | 2.53 | 0.81 |
| 2:B:278:PRO:CA | 2:B:288:TYR:HB2 | 2.10 | 0.81 |
| 4:M:212:ASN:HB3 | 4:M:250:LEU:HA | 1.62 | 0.81 |
| 4:M:223:HIS:HA | 4:M:479:PHE:CG | 2.14 | 0.81 |
| 4:M:272:LEU:CD2 | 4:M:278:ILE:HB | 2.08 | 0.81 |
| 1:A:204:VAL:HG13 | 1:A:239:LEU:CD1 | 2.09 | 0.81 |
| 1:A:346:THR:O | 1:A:347:ASP:C | 2.15 | 0.81 |
| 1:A:638:LEU:CD2 | 2:B:561:ASP:CG | 2.47 | 0.81 |
| 2:B:67:ILE:O | 4:M:18:TYR:HE1 | 1.62 | 0.81 |
| 2:B:230:PHE:HE1 | 2:B:234:CYS:SG | 1.96 | 0.81 |
| 2:B:486:HIS:HE1 | 2:B:518:ILE:HD13 | 1.39 | 0.81 |
| 3:S:89:VAL:HG11 | 3:S:98:ILE:CG1 | 2.10 | 0.81 |
| 4:M:288:ILE:HD12 | 4:M:300:LEU:HD22 | 1.61 | 0.81 |
| 1:A:92:LEU:HD23 | 1:A:95:MET:HE3 | 1.63 | 0.81 |
| 1:A:121:LEU:HD13 | 1:A:155:THR:HG23 | 1.60 | 0.81 |
| 1:A:492:ILE:HG21 | 1:A:526:VAL:HG21 | 1.62 | 0.81 |
| 2:B:14:THR:CG2 | 2:B:40:GLN:HG2 | 2.09 | 0.81 |
| 2:B:38:TYR:CZ | 2:B:46:GLN:HB2 | 2.16 | 0.81 |
| 2:B:70:MET:HE3 | 2:B:107:ARG:CD | 2.10 | 0.81 |
| 2:B:348:THR:CB | 4:M:305:ASP:OD2 | 2.28 | 0.81 |
| 4:M:67:SER:OG | 4:M:90:PHE:HD1 | 1.62 | 0.81 |
| 4:M:293:PRO:HB2 | 4:M:294:ASP:O | 1.79 | 0.81 |
| 1:A:503:ASN:ND2 | 4:M:60:LEU:HD23 | 1.94 | 0.81 |
| 1:A:585:PHE:HE2 | 1:A:603:VAL:HG11 | 1.33 | 0.81 |
| 2:B:13:ASP:O | 2:B:17:VAL:HG13 | 1.80 | 0.81 |
| 2:B:106:LEU:HB3 | 4:M:130:GLU:CB | 2.11 | 0.81 |
| 2:B:344:VAL:HG21 | 2:B:377:TYR:CG | 2.15 | 0.81 |
| 4:M:350:VAL:CG1 | 4:M:442:GLN:CB | 2.57 | 0.81 |
| 1:A:506:LYS:HE3 | 4:M:82:LYS:HB2 | 1.59 | 0.81 |
| 2:B:268:LYS:HA | 2:B:276:SER:HB2 | 1.60 | 0.81 |
| 2:B:399:LEU:HD12 | 2:B:415:LEU:HD21 | 1.62 | 0.81 |
| 2:B:563:PHE:CD1 | 2:B:584:SER:CB | 2.62 | 0.81 |
| 2:B:588:ILE:HG23 | 2:B:618:PHE:HZ | 1.46 | 0.81 |
| 3:S:80:TYR:O | 3:S:82:THR:N | 2.14 | 0.81 |
| 3:S:89:VAL:HG11 | 3:S:98:ILE:CG2 | 2.11 | 0.81 |
| 4:M:218:LEU:O | 4:M:441:GLY:HA2 | 1.81 | 0.81 |
| 2:B:72:SER:HA | 4:M:17:GLN:HE22 | 0.64 | 0.81 |
| 2:B:261:PRO:HB2 | 2:B:290:SER:CB | 2.10 | 0.81 |
| 4:M:306:LEU:HD13 | 4:M:317:MET:CE | 2.10 | 0.81 |
| 4:M:327:PHE:CE1 | 4:M:336:ASP:OD2 | 2.33 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:M:354:ASP:O | 4:M:438:SER:O | 1.99 | 0.81 |
| 4:M:435:LEU:O | 4:M:479:PHE:CE1 | 2.32 | 0.81 |
| 1:A:429:VAL:HG11 | 1:A:473:ILE:CG1 | 2.11 | 0.81 |
| 1:A:506:LYS:O | 1:A:507:GLN:HB2 | 1.79 | 0.81 |
| 2:B:106:LEU:HB3 | 4:M:130:GLU:HB3 | 1.62 | 0.81 |
| 2:B:290:SER:O | 2:B:291:TYR:C | 1.88 | 0.81 |
| 2:B:377:TYR:O | 2:B:380:LYS:HB2 | 1.80 | 0.81 |
| 3:S:3:HIS:NE2 | 3:S:90:ASP:OD2 | 2.13 | 0.81 |
| 2:B:70:MET:HE3 | 2:B:107:ARG:HD2 | 1.62 | 0.81 |
| 2:B:197:LYS:HB2 | 2:B:229:HIS:CD2 | 2.16 | 0.81 |
| 2:B:227:HIS:HA | 2:B:298:ASP:OD2 | 1.81 | 0.81 |
| 2:B:383:VAL:O | 2:B:385:PRO:CD | 2.29 | 0.81 |
| 2:B:566:ALA:HB2 | 2:B:581:TYR:CD1 | 2.16 | 0.81 |
| 3:S:6:LEU:HD11 | 3:S:14:PRO:HB3 | 1.63 | 0.81 |
| 1:A:128:LEU:HD13 | 1:A:150:LEU:HG | 1.62 | 0.80 |
| 2:B:44:PRO:CB | 2:B:82:TYR:OH | 2.28 | 0.80 |
| 2:B:106:LEU:HD21 | 4:M:130:GLU:CA | 2.10 | 0.80 |
| 2:B:435:SER:O | 2:B:438:ARG:N | 2.13 | 0.80 |
| 4:M:223:HIS:CD2 | 4:M:478:ASN:HA | 2.16 | 0.80 |
| 4:M:428:VAL:O | 4:M:429:ASP:C | 2.17 | 0.80 |
| 2:B:252:LEU:O | 2:B:302:PHE:HE2 | 1.62 | 0.80 |
| 2:B:278:PRO:CG | 2:B:292:GLU:OE1 | 2.28 | 0.80 |
| 2:B:308:CYS:O | 2:B:312:SER:N | 2.10 | 0.80 |
| 2:B:337:THR:HA | 2:B:373:LEU:CD2 | 2.11 | 0.80 |
| 2:B:349:MET:HG2 | 4:M:305:ASP:HB2 | 1.63 | 0.80 |
| 1:A:189:PHE:HB2 | 1:A:225:LEU:HD21 | 1.61 | 0.80 |
| 2:B:16:LYS:NZ | 4:M:111:ILE:CD1 | 2.44 | 0.80 |
| 2:B:193:LEU:HD22 | 2:B:225:LEU:HB3 | 0.81 | 0.80 |
| 2:B:232:ARG:O | 2:B:236:ILE:HG13 | 1.81 | 0.80 |
| 2:B:243:TRP:HZ3 | 4:M:98:ARG:HD2 | 1.37 | 0.80 |
| 2:B:430:ILE:HG12 | 2:B:467:VAL:HA | 1.64 | 0.80 |
| 2:B:599:ALA:C | 2:B:601:TYR:N | 2.31 | 0.80 |
| 3:S:80:TYR:O | 3:S:81:ALA:C | 2.14 | 0.80 |
| 4:M:120:ARG:O | 4:M:124:ILE:HD12 | 1.81 | 0.80 |
| 2:B:219:TYR:CE1 | 2:B:226:LEU:N | 2.48 | 0.80 |
| 2:B:267:ASP:N | 2:B:289:PRO:HG3 | 1.96 | 0.80 |
| 4:M:51:LEU:HB3 | 4:M:68:VAL:CG2 | 2.09 | 0.80 |
| 4:M:288:ILE:HD12 | 4:M:300:LEU:CD2 | 2.11 | 0.80 |
| 2:B:278:PRO:HA | 2:B:288:TYR:HB2 | 1.62 | 0.80 |
| 2:B:418:TYR:O | 2:B:419:VAL:C | 2.08 | 0.80 |
| 2:B:430:ILE:HD11 | 2:B:466:SER:CB | 2.12 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:M:66:PHE:HD1 | 4:M:78:ALA:O | 1.64 | 0.80 |
| 1:A:121:LEU:HD12 | 1:A:153:ILE:HG22 | 1.63 | 0.80 |
| 1:A:533:ILE:HG12 | 1:A:562:TRP:CH2 | 2.16 | 0.80 |
| 2:B:22:ALA:CB | 2:B:33:SER:OG | 2.27 | 0.80 |
| 2:B:193:LEU:HB3 | 2:B:225:LEU:CD1 | 2.11 | 0.80 |
| 2:B:213:LEU:CD2 | 4:M:136:VAL:HB | 2.11 | 0.80 |
| 2:B:274:PRO:HG2 | 2:B:295:ASN:HB3 | 1.64 | 0.80 |
| 2:B:310:ILE:HA | 2:B:318:ILE:HG12 | 1.62 | 0.80 |
| 2:B:343:LEU:HD22 | 2:B:366:LEU:CD1 | 2.12 | 0.80 |
| 3:S:55:PRO:HA | 3:S:69:ASN:HB3 | 1.63 | 0.80 |
| 4:M:449:VAL:CG1 | 4:M:452:ILE:HG13 | 2.11 | 0.80 |
| 1:A:136:GLY:O | 1:A:139:ASP:CB | 2.30 | 0.80 |
| 1:A:411:GLU:OE2 | 3:S:46:PHE:CZ | 2.35 | 0.80 |
| 1:A:536:MET:O | 1:A:537:THR:O | 2.00 | 0.80 |
| 2:B:73:ASP:N | 4:M:19:LEU:HD23 | 1.76 | 0.80 |
| 2:B:396:ILE:HG21 | 2:B:432:ALA:N | 1.96 | 0.80 |
| 4:M:347:PHE:CD1 | 4:M:350:VAL:CG1 | 2.65 | 0.80 |
| 4:M:353:VAL:HG23 | 4:M:438:SER:O | 1.81 | 0.80 |
| 1:A:536:MET:SD | 1:A:551:LEU:HD11 | 2.21 | 0.80 |
| 1:A:606:PHE:CZ | 1:A:633:PHE:CG | 2.59 | 0.80 |
| 2:B:243:TRP:HH2 | 4:M:98:ARG:HH11 | 1.30 | 0.80 |
| 2:B:389:ILE:O | 2:B:390:VAL:C | 2.12 | 0.80 |
| 2:B:69:ILE:C | 2:B:71:ALA:N | 2.34 | 0.80 |
| 2:B:243:TRP:HH2 | 4:M:98:ARG:NH1 | 1.78 | 0.80 |
| 3:S:53:THR:CG2 | 3:S:68:VAL:HA | 2.11 | 0.80 |
| 4:M:122:SER:O | 4:M:125:PHE:HB2 | 1.81 | 0.80 |
| 1:A:298:ILE:O | 1:A:299:VAL:C | 2.18 | 0.80 |
| 2:B:14:THR:CB | 2:B:40:GLN:HG2 | 2.12 | 0.80 |
| 2:B:103:LEU:HD21 | 4:M:127:CYS:SG | 2.22 | 0.80 |
| 2:B:144:ASP:OD1 | 4:M:131:ALA:CA | 2.28 | 0.79 |
| 2:B:162:VAL:HG22 | 2:B:199:LEU:CG | 2.12 | 0.79 |
| 2:B:278:PRO:HB3 | 2:B:288:TYR:O | 1.82 | 0.79 |
| 2:B:318:ILE:HG21 | 2:B:346:THR:CB | 2.12 | 0.79 |
| 2:B:344:VAL:HG22 | 2:B:374:PHE:HE1 | 1.43 | 0.79 |
| 2:B:347:VAL:CB | 2:B:381:PHE:CE1 | 2.65 | 0.79 |
| 3:S:43:ASN:O | 3:S:44:SER:C | 2.15 | 0.79 |
| 4:M:16:PHE:CE2 | 4:M:125:PHE:CE2 | 2.69 | 0.79 |
| 4:M:222:PHE:CE2 | 4:M:439:TYR:HE2 | 1.99 | 0.79 |
| 1:A:536:MET:HG2 | 1:A:551:LEU:CD1 | 2.11 | 0.79 |
| 1:A:225:LEU:HB2 | 1:A:233:PHE:CZ | 2.16 | 0.79 |
| 1:A:399:ASP:H | 1:A:418:ILE:HD11 | 1.46 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:162:VAL:HG22 | 2:B:199:LEU:CD1 | 2.12 | 0.79 |
| 2:B:405:GLU:C | 2:B:446:TRP:HE1 | 1.84 | 0.79 |
| 1:A:506:LYS:CE | 4:M:82:LYS:HB3 | 1.98 | 0.79 |
| 1:A:609:LEU:HG | 1:A:628:VAL:HG11 | 1.65 | 0.79 |
| 3:S:53:THR:HB | 3:S:69:ASN:CB | 2.13 | 0.79 |
| 4:M:290:PHE:HB2 | 4:M:299:LEU:HD11 | 1.63 | 0.79 |
| 1:A:599:ARG:NE | 2:B:610:ARG:HH22 | 1.79 | 0.79 |
| 2:B:16:LYS:HZ3 | 4:M:111:ILE:CD1 | 1.95 | 0.79 |
| 2:B:69:ILE:HG22 | 2:B:77:ILE:HG13 | 1.62 | 0.79 |
| 2:B:378:THR:O | 2:B:380:LYS:N | 2.15 | 0.79 |
| 2:B:474:VAL:O | 2:B:477:MET:N | 2.14 | 0.79 |
| 2:B:580:TYR:HB3 | 2:B:582:ASP:OD1 | 1.83 | 0.79 |
| 4:M:343:ASN:HA | 4:M:408:VAL:CG1 | 2.08 | 0.79 |
| 1:A:182:ILE:HG22 | 1:A:221:VAL:CG2 | 2.12 | 0.79 |
| 1:A:558:VAL:HG13 | 1:A:562:TRP:NE1 | 1.97 | 0.79 |
| 2:B:18:ILE:CD1 | 2:B:36:THR:CG2 | 2.49 | 0.79 |
| 2:B:53:SER:OG | 2:B:58:GLU:OE1 | 2.00 | 0.79 |
| 2:B:108:PHE:O | 2:B:111:ASN:N | 2.15 | 0.79 |
| 2:B:199:LEU:C | 2:B:201:ALA:H | 1.86 | 0.79 |
| 2:B:215:TYR:HD1 | 2:B:219:TYR:HE2 | 1.25 | 0.79 |
| 2:B:277:CYS:SG | 2:B:292:GLU:HG3 | 2.22 | 0.79 |
| 3:S:8:PHE:CG | 3:S:36:TYR:CE1 | 2.71 | 0.79 |
| 1:A:251:TRP:CZ3 | 3:S:97:ALA:C | 2.31 | 0.79 |
| 1:A:328:PRO:O | 3:S:50:PHE:HZ | 1.65 | 0.79 |
| 2:B:179:LYS:NZ | 4:M:131:ALA:CA | 2.46 | 0.79 |
| 2:B:589:SER:HA | 2:B:592:TYR:HD2 | 1.47 | 0.79 |
| 4:M:65:TYR:CZ | 4:M:86:PRO:CB | 2.61 | 0.79 |
| 4:M:104:PHE:CZ | 4:M:117:ASN:CB | 2.65 | 0.79 |
| 4:M:334:ASP:O | 4:M:417:TYR:N | 2.15 | 0.79 |
| 2:B:106:LEU:CG | 2:B:144:ASP:CB | 2.61 | 0.79 |
| 2:B:107:ARG:HH12 | 4:M:20:LEU:CG | 1.95 | 0.79 |
| 2:B:167:ALA:O | 2:B:207:VAL:HG21 | 1.82 | 0.79 |
| 4:M:120:ARG:O | 4:M:124:ILE:CD1 | 2.31 | 0.79 |
| 4:M:235:LEU:CD1 | 4:M:306:LEU:HB3 | 2.12 | 0.79 |
| 4:M:240:ILE:CG2 | 4:M:444:ALA:CA | 2.61 | 0.79 |
| 2:B:12:LEU:CD2 | 4:M:13:LYS:HG3 | 2.13 | 0.79 |
| 2:B:82:TYR:HB2 | 2:B:104:TYR:CZ | 2.17 | 0.79 |
| 4:M:44:ASP:CB | 4:M:50:TYR:CE2 | 2.64 | 0.79 |
| 4:M:218:LEU:HG | 4:M:244:VAL:HG22 | 1.64 | 0.79 |
| 1:A:558:VAL:HG12 | 1:A:562:TRP:CE2 | 2.17 | 0.79 |
| 2:B:158:VAL:HG13 | 2:B:173:VAL:CG1 | 2.12 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:M:217:ASP:CB | 4:M:470:ALA:O | 2.30 | 0.79 |
| 1:A:394:GLN:O | 1:A:398:GLU:N | 2.14 | 0.78 |
| 2:B:103:LEU:HD13 | 4:M:123:LEU:CD1 | 2.12 | 0.78 |
| 2:B:243:TRP:CH2 | 4:M:98:ARG:NH1 | 2.51 | 0.78 |
| 1:A:244:LEU:HG | 1:A:281:LEU:HD11 | 1.64 | 0.78 |
| 1:A:638:LEU:HD11 | 2:B:557:SER:C | 2.01 | 0.78 |
| 2:B:12:LEU:HB3 | 4:M:13:LYS:HG3 | 1.46 | 0.78 |
| 2:B:223:LEU:HD11 | 2:B:258:GLN:HB2 | 1.60 | 0.78 |
| 2:B:310:ILE:CG2 | 2:B:342:ALA:CB | 2.60 | 0.78 |
| 3:S:53:THR:OG1 | 3:S:68:VAL:C | 2.21 | 0.78 |
| 4:M:383:HIS:CB | 4:M:403:THR:OG1 | 2.32 | 0.78 |
| 1:A:395:PHE:CE2 | 1:A:420:ILE:HD13 | 2.18 | 0.78 |
| 2:B:16:LYS:HD3 | 4:M:115:VAL:CG2 | 2.09 | 0.78 |
| 2:B:80:GLN:CG | 2:B:108:PHE:CZ | 2.66 | 0.78 |
| 2:B:252:LEU:HD12 | 2:B:302:PHE:CE1 | 2.18 | 0.78 |
| 2:B:274:PRO:HG2 | 2:B:275:ARG:O | 1.69 | 0.78 |
| 1:A:179:LYS:HZ3 | 3:S:141:VAL:C | 1.87 | 0.78 |
| 1:A:182:ILE:CG2 | 1:A:221:VAL:HG21 | 2.12 | 0.78 |
| 1:A:320:HIS:O | 1:A:321:THR:C | 2.19 | 0.78 |
| 4:M:7:ILE:CD1 | 4:M:121:ILE:HG21 | 2.12 | 0.78 |
| 4:M:214:LEU:O | 4:M:467:TYR:N | 2.16 | 0.78 |
| 4:M:356:LEU:CD2 | 4:M:358:ILE:CG1 | 2.62 | 0.78 |
| 1:A:405:THR:HA | 2:B:7:ARG:HH21 | 0.64 | 0.78 |
| 4:M:317:MET:HB3 | 4:M:320:ILE:O | 1.84 | 0.78 |
| 1:A:95:MET:SD | 1:A:107:TYR:CD1 | 2.75 | 0.78 |
| 1:A:223:CYS:O | 1:A:226:SER:OG | 2.00 | 0.78 |
| 1:A:536:MET:CG | 1:A:551:LEU:CD1 | 2.61 | 0.78 |
| 1:A:605:GLU:OE2 | 1:A:608:ARG:NH2 | 2.16 | 0.78 |
| 2:B:232:ARG:HG3 | 2:B:236:ILE:CD1 | 2.13 | 0.78 |
| 3:S:4:ALA:HB2 | 3:S:19:PHE:HD1 | 1.49 | 0.78 |
| 3:S:15:ARG:O | 3:S:125:TRP:CZ2 | 2.36 | 0.78 |
| 1:A:332:TYR:CZ | 1:A:336:ILE:HD11 | 2.18 | 0.78 |
| 1:A:384:LEU:HG | 1:A:385:LYS:H | 1.49 | 0.78 |
| 2:B:106:LEU:C | 4:M:130:GLU:OE1 | 2.22 | 0.78 |
| 2:B:178:ILE:HG13 | 2:B:214:ALA:O | 1.84 | 0.78 |
| 2:B:212:VAL:CG2 | 2:B:248:LEU:CD2 | 2.60 | 0.78 |
| 2:B:272:GLY:O | 2:B:274:PRO:HD3 | 1.84 | 0.78 |
| 2:B:309:LEU:CB | 2:B:317:VAL:CG1 | 2.57 | 0.78 |
| 4:M:306:LEU:CD1 | 4:M:317:MET:HE3 | 2.14 | 0.78 |
| 2:B:309:LEU:CB | 2:B:317:VAL:HG11 | 2.13 | 0.78 |
| 2:B:310:ILE:O | 2:B:311:TYR:O | 2.01 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:313:SER:CB | 4:M:269:ILE:CB | 2.42 | 0.78 |
| 2:B:340:ILE:HG13 | 2:B:373:LEU:HB3 | 1.66 | 0.78 |
| 2:B:444:THR:HG22 | 2:B:482:ASN:OD1 | 1.84 | 0.78 |
| 3:S:35:VAL:HB | 3:S:77:TYR:CZ | 2.18 | 0.78 |
| 4:M:240:ILE:HG22 | 4:M:444:ALA:CA | 2.14 | 0.78 |
| 1:A:104:ARG:HA | 1:A:145:ILE:HG21 | 1.66 | 0.78 |
| 1:A:200:PHE:CZ | 1:A:236:LEU:CD2 | 2.66 | 0.78 |
| 1:A:558:VAL:CG1 | 1:A:562:TRP:NE1 | 2.47 | 0.78 |
| 2:B:12:LEU:HD13 | 4:M:13:LYS:HG3 | 1.14 | 0.78 |
| 2:B:72:SER:C | 4:M:19:LEU:CB | 2.52 | 0.78 |
| 2:B:347:VAL:CG1 | 2:B:381:PHE:HE1 | 1.95 | 0.78 |
| 4:M:9:ASP:CB | 4:M:111:ILE:HG21 | 2.11 | 0.78 |
| 4:M:78:ALA:CB | 4:M:89:CYS:SG | 2.72 | 0.78 |
| 4:M:293:PRO:O | 4:M:293:PRO:CD | 2.32 | 0.78 |
| 4:M:319:SER:HB3 | 4:M:343:ASN:O | 1.84 | 0.78 |
| 2:B:16:LYS:NZ | 4:M:111:ILE:CG1 | 2.46 | 0.78 |
| 2:B:162:VAL:CG2 | 2:B:195:ILE:HG23 | 2.09 | 0.78 |
| 2:B:178:ILE:CG1 | 2:B:214:ALA:CA | 2.57 | 0.78 |
| 2:B:189:HIS:NE2 | 2:B:193:LEU:HD11 | 1.99 | 0.78 |
| 2:B:245:GLN:NE2 | 2:B:309:LEU:CD1 | 2.40 | 0.78 |
| 2:B:274:PRO:CG | 2:B:295:ASN:CA | 2.61 | 0.78 |
| 4:M:121:ILE:O | 4:M:125:PHE:HD1 | 1.67 | 0.78 |
| 4:M:284:SER:O | 4:M:285:PRO:C | 2.11 | 0.78 |
| 1:A:397:ASP:O | 1:A:418:ILE:HG13 | 1.84 | 0.77 |
| 2:B:140:SER:HB2 | 2:B:172:GLU:CD | 2.05 | 0.77 |
| 2:B:188:TYR:O | 2:B:192:LEU:HD13 | 1.82 | 0.77 |
| 2:B:199:LEU:C | 2:B:201:ALA:N | 2.33 | 0.77 |
| 2:B:215:TYR:CD1 | 2:B:219:TYR:HE2 | 2.01 | 0.77 |
| 2:B:534:ILE:HD13 | 2:B:591:MET:O | 1.84 | 0.77 |
| 2:B:534:ILE:CD1 | 2:B:591:MET:O | 2.32 | 0.77 |
| 4:M:7:ILE:HA | 4:M:76:CYS:HA | 1.66 | 0.77 |
| 4:M:131:ALA:CB | 4:M:131:ALA:N | 2.44 | 0.77 |
| 4:M:243:ILE:HD13 | 4:M:301:GLU:HB3 | 1.66 | 0.77 |
| 4:M:343:ASN:H | 4:M:343:ASN:HD22 | 1.28 | 0.77 |
| 1:A:103:LYS:HB3 | 1:A:107:TYR:HE2 | 1.49 | 0.77 |
| 2:B:274:PRO:HG3 | 2:B:295:ASN:HA | 1.65 | 0.77 |
| 2:B:340:ILE:HG21 | 2:B:374:PHE:CA | 2.14 | 0.77 |
| 1:A:213:SER:CB | 3:S:142:ILE:CA | 2.62 | 0.77 |
| 2:B:38:TYR:OH | 2:B:46:GLN:CD | 2.17 | 0.77 |
| 2:B:102:HIS:ND1 | 2:B:137:PHE:HB3 | 1.99 | 0.77 |
| 4:M:350:VAL:HA | 4:M:442:GLN:CB | 2.13 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:72:SER:CA | 4:M:17:GLN:NE2 | 2.05 | 0.77 |
| 2:B:565:GLN:HB2 | 2:B:581:TYR:CE1 | 2.19 | 0.77 |
| 4:M:265:ASN:HA | 4:M:313:SER:OG | 1.85 | 0.77 |
| 4:M:282:VAL:N | 4:M:282:VAL:C | 2.35 | 0.77 |
| 2:B:278:PRO:CD | 2:B:289:PRO:O | 2.32 | 0.77 |
| 2:B:294:VAL:C | 2:B:299:LEU:HD12 | 2.05 | 0.77 |
| 2:B:437:SER:OG | 2:B:477:MET:HB2 | 1.84 | 0.77 |
| 4:M:215:TYR:N | 4:M:467:TYR:HB3 | 1.98 | 0.77 |
| 4:M:222:PHE:CE1 | 4:M:240:ILE:HG21 | 2.18 | 0.77 |
| 4:M:224:VAL:N | 4:M:479:PHE:CD2 | 2.52 | 0.77 |
| 2:B:63:MET:HG2 | 2:B:100:LEU:HB3 | 1.65 | 0.77 |
| 2:B:219:TYR:CE1 | 2:B:226:LEU:CB | 2.57 | 0.77 |
| 2:B:328:LEU:HB3 | 2:B:333:GLN:NE2 | 2.00 | 0.77 |
| 4:M:45:SER:HB2 | 4:M:75:TRP:CZ2 | 2.19 | 0.77 |
| 4:M:43:GLU:O | 4:M:45:SER:N | 2.17 | 0.77 |
| 4:M:51:LEU:HB2 | 4:M:68:VAL:CB | 2.15 | 0.77 |
| 4:M:59:ASP:O | 4:M:61:GLU:N | 2.17 | 0.77 |
| 4:M:323:MET:SD | 4:M:342:LEU:CA | 2.73 | 0.77 |
| 2:B:126:SER:O | 2:B:135:ARG:HG2 | 1.83 | 0.77 |
| 2:B:574:ASN:O | 2:B:576:GLN:O | 2.02 | 0.77 |
| 3:S:53:THR:HB | 3:S:68:VAL:C | 2.05 | 0.77 |
| 4:M:224:VAL:HG22 | 4:M:306:LEU:HD12 | 1.65 | 0.77 |
| 4:M:253:ASN:OD1 | 4:M:292:PRO:HD2 | 1.84 | 0.77 |
| 4:M:283:PHE:CE2 | 4:M:289:THR:CB | 2.68 | 0.77 |
| 4:M:306:LEU:HD21 | 4:M:317:MET:CE | 2.14 | 0.77 |
| 4:M:343:ASN:CA | 4:M:408:VAL:HG13 | 2.06 | 0.77 |
| 1:A:151:SER:HB2 | 1:A:187:LYS:HB2 | 1.65 | 0.77 |
| 2:B:14:THR:HA | 2:B:17:VAL:HG22 | 1.66 | 0.77 |
| 3:S:53:THR:HB | 3:S:69:ASN:N | 2.00 | 0.77 |
| 4:M:96:ILE:HD11 | 4:M:125:PHE:HA | 1.67 | 0.77 |
| 4:M:224:VAL:O | 4:M:479:PHE:HB3 | 1.84 | 0.77 |
| 4:M:262:THR:HG22 | 4:M:264:GLY:N | 2.00 | 0.77 |
| 2:B:102:HIS:O | 2:B:103:LEU:C | 2.18 | 0.77 |
| 2:B:403:ILE:HG21 | 2:B:439:CYS:CB | 2.15 | 0.77 |
| 2:B:433:VAL:CG1 | 2:B:474:VAL:CG2 | 2.60 | 0.77 |
| 2:B:438:ARG:HA | 2:B:441:GLN:NE2 | 1.99 | 0.77 |
| 2:B:564:LYS:HG3 | 2:B:568:VAL:HG23 | 1.67 | 0.77 |
| 4:M:5:PHE:CE2 | 4:M:20:LEU:CD1 | 2.68 | 0.77 |
| 4:M:69:ILE:CG2 | 4:M:97:ASP:OD2 | 2.33 | 0.77 |
| 4:M:131:ALA:CB | 4:M:131:ALA:C | 2.47 | 0.77 |
| 1:A:300:LYS:C | 1:A:302:ASN:N | 2.34 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:348:PHE:O | 1:A:352:PHE:CD2 | 2.38 | 0.76 |
| 2:B:14:THR:OG1 | 2:B:40:GLN:HG2 | 1.85 | 0.76 |
| 2:B:415:LEU:CD1 | 2:B:436:LEU:HD21 | 2.15 | 0.76 |
| 2:B:444:THR:O | 2:B:445:SER:C | 2.19 | 0.76 |
| 2:B:477:MET:O | 2:B:480:GLN:HB2 | 1.85 | 0.76 |
| 2:B:16:LYS:HD2 | 4:M:115:VAL:HG21 | 1.64 | 0.76 |
| 3:S:35:VAL:HB | 3:S:77:TYR:HE2 | 1.47 | 0.76 |
| 4:M:262:THR:CG2 | 4:M:265:ASN:N | 2.43 | 0.76 |
| 1:A:349:ILE:CG2 | 1:A:378:ILE:HG22 | 2.15 | 0.76 |
| 1:A:426:ILE:HD13 | 1:A:466:ASP:OD2 | 1.85 | 0.76 |
| 1:A:462:GLN:C | 4:M:58:ARG:HB3 | 2.04 | 0.76 |
| 2:B:13:ASP:C | 2:B:17:VAL:HG22 | 2.04 | 0.76 |
| 2:B:38:TYR:HE2 | 2:B:43:ASN:C | 1.81 | 0.76 |
| 2:B:186:ASN:C | 2:B:188:TYR:N | 2.37 | 0.76 |
| 2:B:568:VAL:O | 2:B:571:SER:CB | 2.32 | 0.76 |
| 4:M:131:ALA:C | 4:M:133:GLU:H | 1.85 | 0.76 |
| 4:M:220:GLU:N | 4:M:439:TYR:O | 2.13 | 0.76 |
| 2:B:151:ALA:CA | 2:B:180:LEU:HD11 | 2.14 | 0.76 |
| 2:B:243:TRP:CH2 | 4:M:98:ARG:NE | 2.52 | 0.76 |
| 2:B:433:VAL:HG13 | 2:B:471:TYR:HA | 1.66 | 0.76 |
| 4:M:45:SER:HB2 | 4:M:75:TRP:CH2 | 2.21 | 0.76 |
| 4:M:71:LYS:HB3 | 4:M:74:TYR:CE1 | 2.20 | 0.76 |
| 4:M:222:PHE:C | 4:M:479:PHE:CE1 | 2.53 | 0.76 |
| 1:A:121:LEU:CD1 | 1:A:153:ILE:HG22 | 2.16 | 0.76 |
| 1:A:281:LEU:O | 1:A:282:MET:C | 2.12 | 0.76 |
| 1:A:316:LEU:HD11 | 1:A:348:PHE:CD2 | 2.20 | 0.76 |
| 1:A:402:ILE:HD13 | 3:S:62:GLU:O | 1.11 | 0.76 |
| 2:B:519:ALA:O | 2:B:523:PHE:HD1 | 1.66 | 0.76 |
| 4:M:6:TYR:CD2 | 4:M:17:GLN:HG2 | 2.21 | 0.76 |
| 4:M:47:SER:O | 4:M:49:ASP:N | 2.19 | 0.76 |
| 4:M:105:ASP:O | 4:M:106:LYS:HB2 | 1.83 | 0.76 |
| 4:M:317:MET:O | 4:M:322:LEU:HB3 | 1.86 | 0.76 |
| 1:A:83:ASP:OD2 | 1:A:85:ALA:N | 2.18 | 0.76 |
| 1:A:581:LEU:HD23 | 1:A:607:LEU:CD2 | 2.16 | 0.76 |
| 2:B:106:LEU:CG | 4:M:130:GLU:OE1 | 2.32 | 0.76 |
| 2:B:162:VAL:CB | 2:B:195:ILE:HG23 | 2.15 | 0.76 |
| 3:S:73:ILE:HG23 | 3:S:88:ILE:CG2 | 2.13 | 0.76 |
| 3:S:109:LEU:O | 3:S:110:ASP:C | 2.10 | 0.76 |
| 4:M:437:TYR:HD1 | 4:M:479:PHE:CZ | 2.01 | 0.76 |
| 1:A:407:SER:N | 3:S:64:ASN:HD21 | 1.84 | 0.76 |
| 2:B:9:ALA:CA | 4:M:14:LEU:CB | 2.64 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:23:ALA:O | 2:B:32:GLU:OE2 | 2.01 | 0.76 |
| 2:B:189:HIS:CE1 | 2:B:193:LEU:HD11 | 2.20 | 0.76 |
| 4:M:20:LEU:HD22 | 4:M:129:VAL:CB | 2.14 | 0.76 |
| 4:M:104:PHE:CE2 | 4:M:117:ASN:HB2 | 2.20 | 0.76 |
| 1:A:295:VAL:HG11 | 1:A:319:LEU:HD11 | 1.67 | 0.76 |
| 2:B:219:TYR:HD2 | 2:B:226:LEU:HD22 | 1.49 | 0.76 |
| 2:B:559:ASP:CB | 2:B:563:PHE:CD2 | 2.69 | 0.76 |
| 3:S:71:GLU:O | 3:S:73:ILE:N | 2.19 | 0.76 |
| 2:B:268:LYS:O | 2:B:273:SER:CB | 2.33 | 0.76 |
| 2:B:347:VAL:HG22 | 2:B:359:LEU:HB3 | 0.82 | 0.76 |
| 3:S:8:PHE:N | 3:S:8:PHE:CD1 | 2.51 | 0.76 |
| 3:S:48:SER:OG | 3:S:50:PHE:N | 2.18 | 0.76 |
| 3:S:53:THR:HB | 3:S:69:ASN:CA | 2.15 | 0.76 |
| 4:M:67:SER:HG | 4:M:90:PHE:HD1 | 1.33 | 0.76 |
| 4:M:242:GLY:O | 4:M:301:GLU:HA | 1.86 | 0.76 |
| 4:M:354:ASP:HA | 4:M:401:LYS:HB3 | 1.67 | 0.76 |
| 4:M:445:SER:OG | 4:M:447:ILE:HG23 | 1.84 | 0.76 |
| 1:A:309:PHE:CZ | 1:A:348:PHE:CE1 | 2.74 | 0.76 |
| 1:A:519:LEU:O | 1:A:520:GLY:C | 2.16 | 0.76 |
| 2:B:80:GLN:HG2 | 2:B:108:PHE:CZ | 2.21 | 0.76 |
| 2:B:101:ILE:O | 2:B:105:LEU:HD13 | 1.85 | 0.76 |
| 2:B:178:ILE:HD13 | 2:B:218:CYS:CB | 2.16 | 0.76 |
| 3:S:53:THR:HB | 3:S:69:ASN:HB2 | 1.66 | 0.76 |
| 4:M:243:ILE:H | 4:M:474:THR:HG22 | 1.49 | 0.76 |
| 1:A:88:ASN:CG | 1:A:120:ILE:HG21 | 2.07 | 0.75 |
| 1:A:570:LYS:O | 1:A:571:ARG:HB2 | 1.84 | 0.75 |
| 2:B:223:LEU:O | 2:B:224:GLU:C | 2.16 | 0.75 |
| 2:B:261:PRO:HG2 | 2:B:292:GLU:HB3 | 1.67 | 0.75 |
| 4:M:6:TYR:O | 4:M:77:LEU:N | 2.16 | 0.75 |
| 4:M:217:ASP:HB2 | 4:M:470:ALA:O | 1.86 | 0.75 |
| 1:A:203:PHE:CZ | 1:A:221:VAL:HG11 | 2.22 | 0.75 |
| 2:B:18:ILE:HD13 | 2:B:36:THR:HG22 | 1.65 | 0.75 |
| 2:B:83:PHE:CE1 | 2:B:87:VAL:CG2 | 2.68 | 0.75 |
| 2:B:468:LEU:HD13 | 2:B:503:LEU:CD2 | 2.15 | 0.75 |
| 4:M:66:PHE:CD1 | 4:M:78:ALA:O | 2.39 | 0.75 |
| 1:A:147:LEU:HD22 | 1:A:166:LEU:HD23 | 1.66 | 0.75 |
| 2:B:278:PRO:CB | 2:B:288:TYR:O | 2.35 | 0.75 |
| 2:B:344:VAL:HG21 | 2:B:377:TYR:HB3 | 1.66 | 0.75 |
| 2:B:418:TYR:CZ | 2:B:432:ALA:HB2 | 2.21 | 0.75 |
| 2:B:513:TRP:N | 2:B:551:LEU:CD1 | 2.49 | 0.75 |
| 2:B:5:ILE:CD1 | 4:M:39:PRO:N | 2.49 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:106:LEU:CB | 4:M:130:GLU:CB | 2.65 | 0.75 |
| 2:B:127:LEU:HD11 | 2:B:142:LEU:HD12 | 1.69 | 0.75 |
| 2:B:197:LYS:HA | 2:B:229:HIS:CD2 | 2.21 | 0.75 |
| 2:B:248:LEU:O | 2:B:252:LEU:HG | 1.86 | 0.75 |
| 2:B:278:PRO:CA | 2:B:288:TYR:C | 2.55 | 0.75 |
| 4:M:54:SER:HB2 | 4:M:66:PHE:CE2 | 2.21 | 0.75 |
| 4:M:323:MET:CE | 4:M:342:LEU:HB3 | 2.16 | 0.75 |
| 1:A:101:GLN:O | 1:A:104:ARG:N | 2.19 | 0.75 |
| 2:B:82:TYR:HB2 | 2:B:104:TYR:HH | 1.52 | 0.75 |
| 2:B:250:GLU:O | 2:B:253:ILE:HB | 1.86 | 0.75 |
| 2:B:280:PRO:HG3 | 2:B:283:TYR:CE2 | 2.21 | 0.75 |
| 2:B:515:PHE:O | 2:B:516:GLY:C | 2.17 | 0.75 |
| 4:M:15:ILE:CG2 | 4:M:114:ILE:HG22 | 2.17 | 0.75 |
| 4:M:41:LEU:HB3 | 4:M:51:LEU:HA | 1.67 | 0.75 |
| 1:A:492:ILE:HD11 | 1:A:522:PHE:HB2 | 1.68 | 0.75 |
| 2:B:79:VAL:C | 2:B:108:PHE:HE2 | 1.89 | 0.75 |
| 2:B:185:LYS:NZ | 2:B:221:ASP:OD2 | 2.19 | 0.75 |
| 2:B:277:CYS:HA | 2:B:292:GLU:HA | 1.69 | 0.75 |
| 2:B:473:ASN:O | 2:B:476:ARG:HB3 | 1.86 | 0.75 |
| 4:M:379:LEU:HD23 | 4:M:411:LEU:CG | 2.16 | 0.75 |
| 1:A:369:SER:HB2 | 1:A:424:TYR:CE2 | 2.21 | 0.75 |
| 1:A:395:PHE:CZ | 1:A:428:MET:HG3 | 2.22 | 0.75 |
| 2:B:483:PRO:HA | 2:B:486:HIS:HB2 | 1.69 | 0.75 |
| 4:M:70:ASN:HA | 4:M:74:TYR:O | 1.85 | 0.75 |
| 4:M:220:GLU:HG3 | 4:M:439:TYR:HD2 | 1.36 | 0.75 |
| 4:M:245:ASP:CB | 4:M:472:TYR:HD1 | 1.92 | 0.75 |
| 2:B:178:ILE:HD12 | 2:B:218:CYS:N | 1.98 | 0.75 |
| 2:B:307:ASN:O | 2:B:311:TYR:N | 2.20 | 0.75 |
| 2:B:427:ASN:HA | 2:B:430:ILE:HD12 | 1.67 | 0.75 |
| 2:B:470:ALA:O | 2:B:473:ASN:N | 2.20 | 0.75 |
| 2:B:512:VAL:HG13 | 2:B:533:LEU:HD11 | 1.62 | 0.75 |
| 1:A:88:ASN:HB2 | 1:A:120:ILE:HD12 | 1.69 | 0.75 |
| 1:A:372:ILE:CG2 | 1:A:431:VAL:HG21 | 2.17 | 0.75 |
| 1:A:469:LEU:O | 1:A:470:GLY:C | 2.21 | 0.75 |
| 2:B:37:TYR:HD2 | 2:B:38:TYR:HD1 | 1.31 | 0.75 |
| 2:B:144:ASP:CA | 2:B:179:LYS:HD3 | 2.16 | 0.75 |
| 2:B:219:TYR:O | 2:B:223:LEU:CD2 | 2.34 | 0.75 |
| 2:B:526:CYS:N | 2:B:527:PRO:CD | 2.48 | 0.75 |
| 4:M:65:TYR:CE2 | 4:M:86:PRO:HA | 2.22 | 0.75 |
| 4:M:320:ILE:HG23 | 4:M:439:TYR:OH | 1.86 | 0.75 |
| 1:A:503:ASN:ND2 | 4:M:60:LEU:CG | 2.50 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:181:TYR:CE1 | 2:B:222:HIS:NE2 | 2.54 | 0.74 |
| 2:B:212:VAL:O | 2:B:214:ALA:N | 2.19 | 0.74 |
| 2:B:219:TYR:O | 2:B:220:ALA:C | 2.23 | 0.74 |
| 2:B:567:GLN:C | 2:B:569:THR:OG1 | 2.24 | 0.74 |
| 3:S:1:MET:N | 3:S:93:GLU:OE1 | 2.19 | 0.74 |
| 4:M:282:VAL:N | 4:M:283:PHE:N | 2.34 | 0.74 |
| 4:M:362:PHE:CE1 | 4:M:374:TYR:CZ | 2.74 | 0.74 |
| 1:A:254:ILE:HG13 | 1:A:290:VAL:HG22 | 1.69 | 0.74 |
| 1:A:282:MET:O | 1:A:283:GLU:C | 2.22 | 0.74 |
| 2:B:231:ARG:O | 2:B:233:TYR:N | 2.20 | 0.74 |
| 2:B:231:ARG:HG2 | 2:B:297:PRO:HB2 | 1.69 | 0.74 |
| 3:S:73:ILE:HG23 | 3:S:88:ILE:HG23 | 1.69 | 0.74 |
| 4:M:268:GLY:H | 4:M:302:TYR:HH | 1.34 | 0.74 |
| 4:M:377:LYS:NZ | 4:M:416:GLU:OE1 | 2.20 | 0.74 |
| 1:A:196:LEU:O | 1:A:196:LEU:HD22 | 1.87 | 0.74 |
| 1:A:379:VAL:HG11 | 1:A:441:TYR:OH | 1.86 | 0.74 |
| 1:A:429:VAL:CG2 | 1:A:469:LEU:HD11 | 2.17 | 0.74 |
| 2:B:549:LEU:CD2 | 2:B:607:ILE:O | 2.34 | 0.74 |
| 4:M:6:TYR:CD2 | 4:M:17:GLN:CG | 2.70 | 0.74 |
| 4:M:15:ILE:HG21 | 4:M:114:ILE:CG2 | 2.17 | 0.74 |
| 4:M:283:PHE:CE2 | 4:M:289:THR:OG1 | 2.40 | 0.74 |
| 4:M:327:PHE:HE1 | 4:M:336:ASP:HB2 | 1.52 | 0.74 |
| 4:M:380:ARG:O | 4:M:410:VAL:O | 2.05 | 0.74 |
| 1:A:258:LYS:NZ | 3:S:93:GLU:C | 2.40 | 0.74 |
| 2:B:17:VAL:HG23 | 2:B:35:TYR:HD2 | 1.43 | 0.74 |
| 2:B:120:ILE:CD1 | 2:B:150:LEU:HD13 | 2.17 | 0.74 |
| 2:B:216:LYS:HG3 | 2:B:251:LEU:CD1 | 2.16 | 0.74 |
| 2:B:374:PHE:CE2 | 2:B:398:ILE:HG21 | 2.20 | 0.74 |
| 2:B:559:ASP:HB2 | 2:B:563:PHE:CD2 | 2.22 | 0.74 |
| 4:M:71:LYS:HG2 | 4:M:74:TYR:OH | 1.87 | 0.74 |
| 4:M:478:ASN:O | 4:M:479:PHE:C | 2.25 | 0.74 |
| 1:A:492:ILE:HG23 | 1:A:519:LEU:CD2 | 2.18 | 0.74 |
| 1:A:545:HIS:O | 1:A:546:SER:C | 2.17 | 0.74 |
| 2:B:5:ILE:HD11 | 4:M:39:PRO:CA | 2.17 | 0.74 |
| 2:B:69:ILE:C | 2:B:71:ALA:H | 1.91 | 0.74 |
| 1:A:68:THR:CB | 3:S:166:LYS:HD3 | 2.17 | 0.74 |
| 2:B:34:SER:O | 2:B:37:TYR:N | 2.20 | 0.74 |
| 2:B:347:VAL:HA | 2:B:359:LEU:HG | 1.68 | 0.74 |
| 4:M:54:SER:N | 4:M:66:PHE:HD2 | 1.84 | 0.74 |
| 4:M:245:ASP:N | 4:M:472:TYR:CZ | 2.55 | 0.74 |
| 1:A:136:GLY:O | 1:A:139:ASP:CA | 2.35 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:25:VAL:HG21 | 2:B:31:GLY:N | 2.01 | 0.74 |
| 2:B:216:LYS:HB2 | 2:B:251:LEU:HD13 | 0.74 | 0.74 |
| 2:B:422:ALA:CB | 2:B:424:PHE:CE2 | 2.67 | 0.74 |
| 4:M:71:LYS:O | 4:M:74:TYR:CD2 | 2.41 | 0.74 |
| 4:M:235:LEU:HD11 | 4:M:306:LEU:HB3 | 1.67 | 0.74 |
| 4:M:267:ILE:HD12 | 4:M:445:SER:OG | 1.88 | 0.74 |
| 1:A:260:PHE:CG | 1:A:274:LEU:HG | 2.22 | 0.74 |
| 2:B:312:SER:C | 4:M:269:ILE:CD1 | 2.50 | 0.74 |
| 4:M:12:ASN:CG | 4:M:42:LEU:HB3 | 2.08 | 0.74 |
| 4:M:262:THR:HG22 | 4:M:264:GLY:CA | 2.18 | 0.74 |
| 2:B:123:LEU:HD13 | 2:B:142:LEU:HG | 1.68 | 0.74 |
| 2:B:151:ALA:HB3 | 2:B:188:TYR:CE2 | 2.23 | 0.74 |
| 2:B:400:SER:CB | 2:B:435:SER:HB3 | 2.09 | 0.74 |
| 2:B:478:LEU:O | 2:B:479:VAL:C | 2.19 | 0.74 |
| 2:B:560:ILE:CG2 | 2:B:564:LYS:HB2 | 2.18 | 0.74 |
| 4:M:226:PHE:HB2 | 4:M:481:VAL:HG22 | 1.69 | 0.74 |
| 1:A:566:PHE:CD1 | 1:A:570:LYS:HA | 2.23 | 0.74 |
| 2:B:120:ILE:HA | 2:B:142:LEU:HD21 | 1.70 | 0.74 |
| 2:B:223:LEU:HD11 | 2:B:258:GLN:CA | 2.15 | 0.74 |
| 3:S:75:ILE:HG22 | 3:S:77:TYR:CE1 | 2.23 | 0.74 |
| 4:M:70:ASN:HB2 | 4:M:75:TRP:CE3 | 2.23 | 0.74 |
| 1:A:186:PHE:CD2 | 1:A:224:GLU:CB | 2.71 | 0.73 |
| 2:B:17:VAL:HG11 | 2:B:35:TYR:HE2 | 1.53 | 0.73 |
| 2:B:124:GLN:CD | 2:B:153:ILE:HG23 | 2.09 | 0.73 |
| 2:B:197:LYS:CB | 2:B:229:HIS:CD2 | 2.71 | 0.73 |
| 2:B:276:SER:C | 2:B:295:ASN:HB2 | 2.06 | 0.73 |
| 2:B:472:VAL:HG11 | 2:B:510:GLY:CA | 2.17 | 0.73 |
| 3:S:130:SER:CB | 3:S:156:LEU:HD13 | 2.18 | 0.73 |
| 1:A:158:LEU:HG | 1:A:162:ILE:CD1 | 2.18 | 0.73 |
| 1:A:213:SER:CB | 3:S:142:ILE:HA | 2.18 | 0.73 |
| 1:A:421:PRO:HB3 | 3:S:63:ASN:N | 2.02 | 0.73 |
| 2:B:136:CYS:CA | 2:B:172:GLU:HG3 | 2.17 | 0.73 |
| 2:B:139:LEU:CD1 | 2:B:176:ALA:HB2 | 2.18 | 0.73 |
| 2:B:140:SER:CB | 2:B:172:GLU:OE1 | 2.36 | 0.73 |
| 2:B:179:LYS:CE | 4:M:131:ALA:O | 2.36 | 0.73 |
| 2:B:472:VAL:HG11 | 2:B:511:ILE:N | 2.03 | 0.73 |
| 4:M:283:PHE:CE2 | 4:M:289:THR:HB | 2.23 | 0.73 |
| 4:M:374:TYR:HA | 4:M:417:TYR:HA | 1.70 | 0.73 |
| 1:A:71:VAL:CG1 | 1:A:105:VAL:HG12 | 2.17 | 0.73 |
| 2:B:12:LEU:HD22 | 4:M:13:LYS:HE3 | 1.70 | 0.73 |
| 3:S:35:VAL:HB | 3:S:77:TYR:OH | 1.87 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:M:250:LEU:CD1 | 4:M:254:PRO:HG2 | 2.18 | 0.73 |
| 1:A:579:LYS:O | 1:A:582:ILE:HB | 1.89 | 0.73 |
| 2:B:253:ILE:CG1 | 2:B:324:ALA:CB | 2.66 | 0.73 |
| 2:B:374:PHE:C | 2:B:402:LEU:HD22 | 2.08 | 0.73 |
| 3:S:49:SER:O | 3:S:77:TYR:HB2 | 1.89 | 0.73 |
| 4:M:214:LEU:C | 4:M:467:TYR:H | 1.91 | 0.73 |
| 1:A:163:ALA:O | 1:A:164:ASP:C | 2.24 | 0.73 |
| 2:B:279:LEU:HD12 | 2:B:285:GLU:HG2 | 1.69 | 0.73 |
| 2:B:367:SER:CB | 2:B:401:THR:HG1 | 2.02 | 0.73 |
| 2:B:375:LEU:CD1 | 2:B:404:ASN:CB | 2.56 | 0.73 |
| 2:B:554:LYS:O | 2:B:557:SER:N | 2.21 | 0.73 |
| 2:B:559:ASP:HA | 2:B:562:ASN:HB2 | 1.69 | 0.73 |
| 3:S:135:ILE:HG23 | 3:S:141:VAL:CG1 | 2.18 | 0.73 |
| 4:M:42:LEU:HD23 | 4:M:51:LEU:HD21 | 1.69 | 0.73 |
| 1:A:215:VAL:O | 1:A:216:SER:C | 2.19 | 0.73 |
| 2:B:12:LEU:HD13 | 4:M:13:LYS:HB2 | 1.63 | 0.73 |
| 2:B:28:SER:CA | 2:B:58:GLU:HG2 | 2.19 | 0.73 |
| 2:B:69:ILE:CG2 | 2:B:77:ILE:HG13 | 2.19 | 0.73 |
| 2:B:204:ASP:O | 2:B:207:VAL:HB | 1.89 | 0.73 |
| 2:B:223:LEU:HD13 | 2:B:259:TYR:CA | 2.15 | 0.73 |
| 2:B:596:LEU:HD12 | 2:B:611:ALA:CB | 2.18 | 0.73 |
| 4:M:19:LEU:HD21 | 4:M:24:ALA:CB | 2.19 | 0.73 |
| 4:M:224:VAL:HG11 | 4:M:226:PHE:CZ | 2.23 | 0.73 |
| 4:M:225:VAL:HB | 4:M:237:THR:OG1 | 1.88 | 0.73 |
| 4:M:375:LYS:HE3 | 4:M:418:GLU:OE1 | 1.88 | 0.73 |
| 4:M:449:VAL:HG11 | 4:M:452:ILE:CG1 | 2.19 | 0.73 |
| 1:A:114:PHE:CG | 1:A:153:ILE:HG12 | 2.22 | 0.73 |
| 2:B:1:MET:HG3 | 4:M:39:PRO:HG2 | 1.71 | 0.73 |
| 2:B:5:ILE:HG23 | 4:M:42:LEU:CD1 | 2.18 | 0.73 |
| 2:B:318:ILE:HD13 | 2:B:346:THR:CG2 | 2.18 | 0.73 |
| 2:B:318:ILE:HG21 | 2:B:346:THR:OG1 | 1.87 | 0.73 |
| 2:B:63:MET:CG | 2:B:100:LEU:HB3 | 2.18 | 0.73 |
| 2:B:73:ASP:HA | 4:M:19:LEU:HD22 | 0.88 | 0.73 |
| 2:B:249:ILE:HG12 | 2:B:306:LEU:CD2 | 2.19 | 0.73 |
| 2:B:375:LEU:HD12 | 2:B:404:ASN:ND2 | 1.82 | 0.73 |
| 3:S:89:VAL:HG11 | 3:S:98:ILE:HG13 | 1.68 | 0.73 |
| 1:A:536:MET:CB | 1:A:551:LEU:HD11 | 2.18 | 0.73 |
| 2:B:215:TYR:CE2 | 2:B:233:TYR:CE2 | 2.76 | 0.73 |
| 2:B:259:TYR:CD1 | 2:B:261:PRO:CG | 2.61 | 0.73 |
| 2:B:347:VAL:HG21 | 2:B:381:PHE:HE1 | 1.54 | 0.73 |
| 2:B:375:LEU:HD22 | 2:B:404:ASN:HB2 | 1.70 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:403:ILE:CD1 | 2:B:439:CYS:HB3 | 2.16 | 0.73 |
| 3:S:53:THR:O | 3:S:69:ASN:CG | 2.27 | 0.73 |
| 3:S:73:ILE:HG21 | 3:S:88:ILE:CG2 | 2.17 | 0.73 |
| 4:M:224:VAL:O | 4:M:480:GLN:N | 2.20 | 0.73 |
| 4:M:246:VAL:O | 4:M:297:PHE:CE1 | 2.42 | 0.73 |
| 4:M:362:PHE:CE1 | 4:M:374:TYR:CE2 | 2.77 | 0.73 |
| 4:M:373:ALA:HB3 | 4:M:418:GLU:O | 1.88 | 0.73 |
| 4:M:405:THR:C | 4:M:407:THR:H | 1.90 | 0.73 |
| 1:A:88:ASN:HB3 | 1:A:120:ILE:HD12 | 1.71 | 0.73 |
| 1:A:92:LEU:O | 1:A:95:MET:N | 2.22 | 0.73 |
| 1:A:420:ILE:HG23 | 1:A:424:TYR:HB2 | 1.71 | 0.73 |
| 1:A:595:GLU:CD | 2:B:513:TRP:CH2 | 2.63 | 0.73 |
| 1:A:606:PHE:HZ | 1:A:633:PHE:CD1 | 2.05 | 0.73 |
| 2:B:109:ALA:O | 2:B:111:ASN:N | 2.22 | 0.73 |
| 2:B:178:ILE:HD11 | 2:B:215:TYR:HA | 1.71 | 0.73 |
| 2:B:253:ILE:HG12 | 2:B:324:ALA:CB | 2.19 | 0.73 |
| 2:B:373:LEU:C | 2:B:375:LEU:H | 1.92 | 0.73 |
| 2:B:501:THR:C | 2:B:508:ARG:NH2 | 2.41 | 0.73 |
| 3:S:16:LEU:CG | 3:S:125:TRP:HE1 | 2.02 | 0.73 |
| 4:M:106:LYS:NZ | 4:M:296:LYS:HE3 | 2.03 | 0.73 |
| 1:A:186:PHE:HB2 | 1:A:221:VAL:HG13 | 1.72 | 0.72 |
| 1:A:219:VAL:HG21 | 1:A:256:LEU:HD21 | 1.70 | 0.72 |
| 1:A:409:VAL:HG11 | 3:S:42:ARG:HH12 | 1.50 | 0.72 |
| 2:B:25:VAL:HG23 | 2:B:32:GLU:CG | 2.19 | 0.72 |
| 2:B:35:TYR:CE1 | 4:M:118:TYR:OH | 2.42 | 0.72 |
| 2:B:404:ASN:O | 2:B:405:GLU:C | 2.08 | 0.72 |
| 4:M:215:TYR:O | 4:M:246:VAL:HG13 | 1.89 | 0.72 |
| 4:M:262:THR:HG22 | 4:M:265:ASN:N | 2.04 | 0.72 |
| 2:B:72:SER:CB | 4:M:17:GLN:CD | 2.56 | 0.72 |
| 2:B:129:ASP:O | 2:B:135:ARG:HD3 | 1.88 | 0.72 |
| 2:B:328:LEU:CB | 2:B:333:GLN:NE2 | 2.49 | 0.72 |
| 1:A:488:ARG:HD2 | 1:A:522:PHE:CE2 | 2.24 | 0.72 |
| 2:B:208:ILE:HD13 | 2:B:236:ILE:CG2 | 2.18 | 0.72 |
| 2:B:249:ILE:CD1 | 2:B:321:CYS:SG | 2.77 | 0.72 |
| 4:M:214:LEU:HD23 | 4:M:214:LEU:C | 2.09 | 0.72 |
| 4:M:344:ILE:HG22 | 4:M:347:PHE:CB | 1.97 | 0.72 |
| 4:M:347:PHE:CE1 | 4:M:350:VAL:HB | 2.23 | 0.72 |
| 4:M:347:PHE:CD1 | 4:M:350:VAL:HG11 | 2.22 | 0.72 |
| 4:M:19:LEU:HD21 | 4:M:24:ALA:HB3 | 1.70 | 0.72 |
| 1:A:405:THR:O | 2:B:7:ARG:CZ | 2.38 | 0.72 |
| 2:B:196:LEU:HB3 | 2:B:215:TYR:OH | 1.88 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:363:ILE:HG22 | 2:B:398:ILE:HG12 | 1.70 | 0.72 |
| 2:B:494:ALA:HB2 | 2:B:515:PHE:CZ | 2.24 | 0.72 |
| 2:B:549:LEU:CD1 | 2:B:595:VAL:HG12 | 2.20 | 0.72 |
| 4:M:53:HIS:HA | 4:M:66:PHE:HB2 | 1.70 | 0.72 |
| 1:A:136:GLY:O | 1:A:137:ASN:C | 2.18 | 0.72 |
| 1:A:186:PHE:CD2 | 1:A:224:GLU:HB3 | 2.23 | 0.72 |
| 2:B:158:VAL:HG13 | 2:B:177:ILE:HG13 | 1.71 | 0.72 |
| 2:B:512:VAL:HG22 | 2:B:533:LEU:CD2 | 2.19 | 0.72 |
| 2:B:540:GLU:OE1 | 2:B:548:ILE:CD1 | 2.37 | 0.72 |
| 4:M:220:GLU:OE2 | 4:M:439:TYR:HD2 | 1.65 | 0.72 |
| 4:M:235:LEU:HD11 | 4:M:306:LEU:CB | 2.19 | 0.72 |
| 4:M:242:GLY:CA | 4:M:474:THR:HG21 | 2.20 | 0.72 |
| 4:M:352:GLN:HG3 | 4:M:440:ILE:HB | 1.70 | 0.72 |
| 1:A:316:LEU:HD13 | 1:A:348:PHE:CG | 2.24 | 0.72 |
| 1:A:407:SER:N | 3:S:64:ASN:ND2 | 2.38 | 0.72 |
| 2:B:13:ASP:OD1 | 4:M:15:ILE:N | 2.22 | 0.72 |
| 2:B:25:VAL:HA | 2:B:28:SER:H | 1.55 | 0.72 |
| 2:B:260:LEU:CA | 2:B:293:VAL:HG21 | 2.18 | 0.72 |
| 2:B:347:VAL:HG21 | 2:B:381:PHE:CZ | 2.25 | 0.72 |
| 2:B:397:GLN:HG2 | 2:B:431:MET:SD | 2.29 | 0.72 |
| 4:M:281:GLY:C | 4:M:281:GLY:N | 2.41 | 0.72 |
| 1:A:503:ASN:HB3 | 4:M:60:LEU:N | 2.04 | 0.72 |
| 1:A:513:ARG:HG3 | 1:A:547:VAL:HG22 | 1.69 | 0.72 |
| 2:B:294:VAL:O | 2:B:299:LEU:HD12 | 1.90 | 0.72 |
| 4:M:218:LEU:CA | 4:M:472:TYR:CD2 | 2.64 | 0.72 |
| 4:M:302:TYR:CE1 | 4:M:445:SER:HB2 | 2.24 | 0.72 |
| 4:M:437:TYR:CD1 | 4:M:437:TYR:N | 2.54 | 0.72 |
| 2:B:247:TYR:HD1 | 4:M:136:VAL:HG12 | 1.51 | 0.72 |
| 2:B:360:LEU:CD2 | 2:B:395:LYS:HD3 | 2.20 | 0.72 |
| 2:B:549:LEU:HD21 | 2:B:611:ALA:N | 2.04 | 0.72 |
| 4:M:244:VAL:HG13 | 4:M:472:TYR:CZ | 2.25 | 0.72 |
| 4:M:343:ASN:HD22 | 4:M:343:ASN:N | 1.87 | 0.72 |
| 4:M:433:VAL:HG12 | 4:M:481:VAL:HB | 1.70 | 0.72 |
| 1:A:114:PHE:C | 1:A:115:TYR:O | 2.27 | 0.72 |
| 1:A:322:PHE:CD1 | 1:A:330:LEU:HD21 | 2.24 | 0.72 |
| 1:A:535:ILE:O | 1:A:535:ILE:HG22 | 1.89 | 0.72 |
| 1:A:566:PHE:C | 1:A:568:GLU:H | 1.90 | 0.72 |
| 2:B:231:ARG:O | 2:B:234:CYS:N | 2.23 | 0.72 |
| 2:B:259:TYR:O | 2:B:293:VAL:CG2 | 2.37 | 0.72 |
| 2:B:360:LEU:HD21 | 2:B:395:LYS:HD3 | 1.71 | 0.72 |
| 2:B:367:SER:OG | 2:B:401:THR:HG21 | 1.89 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:415:LEU:CD1 | 2:B:436:LEU:CD2 | 2.68 | 0.72 |
| 1:A:212:ILE:O | 1:A:213:SER:C | 2.16 | 0.71 |
| 1:A:585:PHE:HB3 | 1:A:600:SER:OG | 1.89 | 0.71 |
| 2:B:472:VAL:O | 2:B:473:ASN:C | 2.18 | 0.71 |
| 2:B:512:VAL:CG1 | 2:B:533:LEU:CD1 | 2.36 | 0.71 |
| 4:M:223:HIS:CG | 4:M:476:THR:OG1 | 2.43 | 0.71 |
| 1:A:213:SER:CB | 3:S:142:ILE:CB | 2.67 | 0.71 |
| 3:S:1:MET:H2 | 3:S:93:GLU:HB2 | 1.54 | 0.71 |
| 3:S:112:CYS:HB2 | 3:S:113:PHE:CD1 | 2.25 | 0.71 |
| 4:M:67:SER:O | 4:M:77:LEU:HA | 1.91 | 0.71 |
| 4:M:99:ILE:O | 4:M:99:ILE:CG2 | 2.38 | 0.71 |
| 4:M:443:SER:OG | 4:M:448:TYR:N | 2.23 | 0.71 |
| 2:B:143:SER:CB | 2:B:179:LYS:CD | 2.67 | 0.71 |
| 2:B:219:TYR:O | 2:B:223:LEU:HD21 | 1.91 | 0.71 |
| 4:M:279:ASN:HB2 | 4:M:283:PHE:CD2 | 2.24 | 0.71 |
| 4:M:449:VAL:HG11 | 4:M:452:ILE:HG13 | 1.69 | 0.71 |
| 1:A:405:THR:HB | 2:B:7:ARG:HE | 1.54 | 0.71 |
| 1:A:503:ASN:CB | 4:M:60:LEU:N | 2.52 | 0.71 |
| 1:A:539:ASN:O | 1:A:540:ILE:C | 2.18 | 0.71 |
| 2:B:73:ASP:H | 4:M:19:LEU:CB | 1.98 | 0.71 |
| 4:M:437:TYR:CD1 | 4:M:479:PHE:CE2 | 2.78 | 0.71 |
| 2:B:80:GLN:HA | 2:B:108:PHE:CE2 | 2.26 | 0.71 |
| 2:B:106:LEU:HD21 | 4:M:130:GLU:HA | 1.72 | 0.71 |
| 2:B:347:VAL:CG2 | 2:B:381:PHE:CE1 | 2.73 | 0.71 |
| 3:S:57:LEU:O | 3:S:59:LEU:HA | 1.90 | 0.71 |
| 4:M:6:TYR:CD1 | 4:M:77:LEU:HD23 | 2.26 | 0.71 |
| 4:M:435:LEU:HB2 | 4:M:437:TYR:CE1 | 2.25 | 0.71 |
| 1:A:225:LEU:HD12 | 1:A:233:PHE:CZ | 2.26 | 0.71 |
| 1:A:266:VAL:O | 1:A:267:GLU:HB3 | 1.91 | 0.71 |
| 1:A:292:TYR:CD1 | 1:A:292:TYR:O | 2.44 | 0.71 |
| 1:A:562:TRP:O | 1:A:565:ASN:N | 2.23 | 0.71 |
| 1:A:573:GLU:O | 1:A:575:LYS:N | 2.23 | 0.71 |
| 2:B:24:ALA:HB3 | 2:B:32:GLU:CG | 2.07 | 0.71 |
| 2:B:28:SER:O | 2:B:58:GLU:CD | 2.28 | 0.71 |
| 2:B:367:SER:CB | 2:B:401:THR:CB | 2.68 | 0.71 |
| 2:B:379:LYS:CE | 2:B:410:GLU:HG3 | 2.02 | 0.71 |
| 3:S:4:ALA:CB | 3:S:19:PHE:CD1 | 2.74 | 0.71 |
| 3:S:55:PRO:O | 3:S:58:LEU:CB | 2.39 | 0.71 |
| 4:M:244:VAL:HA | 4:M:472:TYR:CG | 2.18 | 0.71 |
| 1:A:350:SER:O | 1:A:351:ARG:C | 2.23 | 0.71 |
| 1:A:366:SER:HB3 | 3:S:67:GLU:OE1 | 1.90 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:421:PRO:HB3 | 3:S:62:GLU:C | 2.11 | 0.71 |
| 1:A:503:ASN:HB3 | 4:M:59:ASP:CA | 2.07 | 0.71 |
| 2:B:14:THR:HG21 | 2:B:40:GLN:CG | 2.20 | 0.71 |
| 2:B:155:LEU:HB2 | 2:B:188:TYR:CD1 | 2.26 | 0.71 |
| 2:B:181:TYR:CZ | 2:B:185:LYS:HE2 | 2.26 | 0.71 |
| 2:B:347:VAL:HG22 | 2:B:359:LEU:CG | 2.20 | 0.71 |
| 2:B:472:VAL:CG1 | 2:B:510:GLY:CA | 2.68 | 0.71 |
| 3:S:75:ILE:CG2 | 3:S:77:TYR:CE1 | 2.74 | 0.71 |
| 4:M:16:PHE:CZ | 4:M:18:TYR:HB2 | 2.24 | 0.71 |
| 1:A:379:VAL:CG1 | 1:A:441:TYR:OH | 2.38 | 0.71 |
| 1:A:638:LEU:CD1 | 2:B:557:SER:CA | 2.68 | 0.71 |
| 2:B:18:ILE:CG2 | 2:B:36:THR:C | 2.36 | 0.71 |
| 2:B:226:LEU:CD2 | 2:B:255:TYR:HD1 | 1.83 | 0.71 |
| 2:B:545:ARG:HD2 | 2:B:602:ASP:OD2 | 1.91 | 0.71 |
| 3:S:57:LEU:CA | 3:S:58:LEU:O | 2.30 | 0.71 |
| 4:M:78:ALA:HB1 | 4:M:89:CYS:SG | 2.30 | 0.71 |
| 4:M:244:VAL:O | 4:M:299:LEU:HB3 | 1.90 | 0.71 |
| 4:M:275:CYS:O | 4:M:291:ILE:HG22 | 1.91 | 0.71 |
| 4:M:347:PHE:CE2 | 4:M:350:VAL:O | 2.43 | 0.71 |
| 1:A:384:LEU:HG | 1:A:385:LYS:N | 2.05 | 0.71 |
| 1:A:578:LEU:HD23 | 1:A:607:LEU:CD2 | 2.19 | 0.71 |
| 2:B:1:MET:CG | 4:M:39:PRO:CG | 2.68 | 0.71 |
| 2:B:212:VAL:CG2 | 2:B:233:TYR:CD1 | 2.74 | 0.71 |
| 2:B:216:LYS:NZ | 2:B:250:GLU:OE2 | 2.23 | 0.71 |
| 4:M:378:ILE:O | 4:M:413:GLY:CA | 2.39 | 0.71 |
| 2:B:73:ASP:H | 4:M:19:LEU:HB3 | 1.55 | 0.71 |
| 2:B:336:ASN:HB3 | 2:B:339:PHE:CD2 | 2.25 | 0.71 |
| 2:B:396:ILE:HG12 | 2:B:418:TYR:HE2 | 1.56 | 0.71 |
| 3:S:89:VAL:HG11 | 3:S:98:ILE:HG21 | 1.71 | 0.71 |
| 4:M:244:VAL:CG1 | 4:M:472:TYR:CE2 | 2.74 | 0.71 |
| 2:B:337:THR:OG1 | 2:B:373:LEU:CD1 | 2.27 | 0.70 |
| 2:B:566:ALA:CA | 2:B:574:ASN:HB3 | 2.19 | 0.70 |
| 4:M:74:TYR:HB2 | 4:M:114:ILE:CD1 | 2.20 | 0.70 |
| 1:A:71:VAL:HG12 | 1:A:105:VAL:HG12 | 1.71 | 0.70 |
| 1:A:206:LYS:HE2 | 1:A:206:LYS:HA | 1.73 | 0.70 |
| 1:A:316:LEU:HD13 | 1:A:348:PHE:CD2 | 2.26 | 0.70 |
| 2:B:80:GLN:N | 2:B:108:PHE:CE2 | 2.57 | 0.70 |
| 2:B:107:ARG:NH1 | 4:M:20:LEU:CB | 2.51 | 0.70 |
| 2:B:382:TYR:OH | 2:B:410:GLU:CB | 2.38 | 0.70 |
| 2:B:398:ILE:O | 2:B:400:SER:N | 2.24 | 0.70 |
| 2:B:457:HIS:HA | 2:B:461:HIS:CD2 | 2.25 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:475:ILE:CG2 | 2:B:489:ILE:CG2 | 2.69 | 0.70 |
| 2:B:505:ASP:O | 2:B:506:ASN:C | 2.22 | 0.70 |
| 2:B:512:VAL:HG13 | 2:B:533:LEU:HD13 | 0.72 | 0.70 |
| 2:B:513:TRP:NE1 | 2:B:517:GLU:CG | 2.53 | 0.70 |
| 2:B:559:ASP:O | 2:B:562:ASN:HB2 | 1.91 | 0.70 |
| 2:B:567:GLN:HA | 2:B:569:THR:OG1 | 1.90 | 0.70 |
| 3:S:8:PHE:CZ | 3:S:86:THR:OG1 | 2.42 | 0.70 |
| 4:M:242:GLY:CA | 4:M:444:ALA:HB2 | 2.20 | 0.70 |
| 1:A:254:ILE:HD13 | 3:S:96:LEU:HB2 | 1.72 | 0.70 |
| 1:A:277:LYS:HG3 | 1:A:277:LYS:O | 1.91 | 0.70 |
| 2:B:169:VAL:O | 2:B:173:VAL:HG23 | 1.90 | 0.70 |
| 2:B:245:GLN:CD | 2:B:309:LEU:HD12 | 1.96 | 0.70 |
| 4:M:356:LEU:HD21 | 4:M:358:ILE:CG1 | 2.20 | 0.70 |
| 1:A:121:LEU:CD1 | 1:A:153:ILE:CG2 | 2.69 | 0.70 |
| 1:A:508:LEU:HD12 | 4:M:59:ASP:CG | 2.10 | 0.70 |
| 2:B:82:TYR:O | 2:B:83:PHE:C | 2.21 | 0.70 |
| 2:B:178:ILE:HG12 | 2:B:214:ALA:CB | 2.11 | 0.70 |
| 2:B:230:PHE:CD1 | 2:B:298:ASP:CB | 2.73 | 0.70 |
| 2:B:472:VAL:HG12 | 2:B:510:GLY:HA3 | 1.73 | 0.70 |
| 4:M:334:ASP:O | 4:M:416:GLU:HA | 1.91 | 0.70 |
| 1:A:316:LEU:CD1 | 1:A:348:PHE:CE2 | 2.74 | 0.70 |
| 1:A:581:LEU:CD1 | 1:A:585:PHE:CZ | 2.73 | 0.70 |
| 2:B:100:LEU:CD2 | 4:M:123:LEU:HD22 | 2.19 | 0.70 |
| 2:B:399:LEU:HD22 | 2:B:411:ILE:HG23 | 1.74 | 0.70 |
| 1:A:384:LEU:CG | 1:A:385:LYS:N | 2.54 | 0.70 |
| 1:A:558:VAL:HG11 | 1:A:562:TRP:CZ2 | 2.26 | 0.70 |
| 1:A:585:PHE:CB | 1:A:600:SER:OG | 2.40 | 0.70 |
| 1:A:606:PHE:CE1 | 1:A:633:PHE:CB | 2.59 | 0.70 |
| 2:B:53:SER:CB | 2:B:58:GLU:OE1 | 2.40 | 0.70 |
| 2:B:73:ASP:N | 4:M:19:LEU:CG | 2.54 | 0.70 |
| 2:B:103:LEU:HD13 | 4:M:123:LEU:HD12 | 1.71 | 0.70 |
| 2:B:219:TYR:HE2 | 2:B:226:LEU:CD1 | 1.74 | 0.70 |
| 2:B:371:GLN:HG2 | 2:B:401:THR:HB | 1.72 | 0.70 |
| 4:M:78:ALA:HB3 | 4:M:89:CYS:SG | 2.31 | 0.70 |
| 4:M:243:ILE:H | 4:M:474:THR:HG21 | 1.56 | 0.70 |
| 1:A:156:PRO:O | 1:A:157:SER:C | 2.24 | 0.70 |
| 1:A:462:GLN:O | 1:A:463:ASP:C | 2.28 | 0.70 |
| 1:A:585:PHE:C | 1:A:600:SER:OG | 2.25 | 0.70 |
| 1:A:595:GLU:CD | 2:B:513:TRP:CE3 | 2.43 | 0.70 |
| 2:B:337:THR:HG1 | 2:B:373:LEU:HD13 | 1.54 | 0.70 |
| 4:M:106:LYS:O | 4:M:108:LYS:N | 2.24 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:M:215:TYR:HB2 | 4:M:467:TYR:O | 1.90 | 0.70 |
| 1:A:370:LYS:O | 1:A:374:LEU:HD13 | 1.91 | 0.70 |
| 1:A:506:LYS:O | 1:A:507:GLN:CB | 2.39 | 0.70 |
| 2:B:252:LEU:CB | 2:B:302:PHE:CD1 | 2.74 | 0.70 |
| 4:M:48:ASP:CA | 4:M:70:ASN:HD22 | 2.03 | 0.70 |
| 4:M:317:MET:HB2 | 4:M:322:LEU:N | 2.07 | 0.70 |
| 1:A:213:SER:OG | 3:S:142:ILE:HB | 1.91 | 0.70 |
| 1:A:373:GLU:CG | 1:A:427:LYS:HE2 | 2.21 | 0.70 |
| 2:B:29:LYS:HA | 2:B:30:LEU:HD23 | 1.74 | 0.70 |
| 2:B:50:LEU:HD23 | 2:B:62:ALA:CA | 2.22 | 0.70 |
| 2:B:245:GLN:OE1 | 2:B:309:LEU:CD1 | 2.28 | 0.70 |
| 2:B:337:THR:CA | 2:B:373:LEU:HD13 | 2.08 | 0.70 |
| 3:S:8:PHE:CG | 3:S:36:TYR:HE1 | 2.09 | 0.70 |
| 4:M:338:PHE:CD1 | 4:M:415:ILE:HG13 | 2.27 | 0.70 |
| 1:A:506:LYS:CE | 4:M:82:LYS:CD | 2.70 | 0.70 |
| 2:B:322:CYS:SG | 2:B:366:LEU:CG | 2.79 | 0.70 |
| 2:B:403:ILE:HG21 | 2:B:439:CYS:HB3 | 1.72 | 0.70 |
| 4:M:443:SER:OG | 4:M:448:TYR:HA | 1.92 | 0.70 |
| 1:A:462:GLN:OE1 | 4:M:60:LEU:N | 2.25 | 0.69 |
| 2:B:73:ASP:OD1 | 4:M:19:LEU:HD11 | 1.88 | 0.69 |
| 3:S:65:ASN:O | 3:S:67:GLU:HG3 | 1.91 | 0.69 |
| 1:A:186:PHE:CZ | 1:A:224:GLU:CG | 2.64 | 0.69 |
| 1:A:393:LYS:NZ | 1:A:397:ASP:OD2 | 2.25 | 0.69 |
| 2:B:285:GLU:O | 2:B:286:ILE:C | 2.27 | 0.69 |
| 2:B:472:VAL:CG1 | 2:B:511:ILE:N | 2.55 | 0.69 |
| 2:B:513:TRP:HA | 2:B:551:LEU:CD1 | 2.22 | 0.69 |
| 4:M:100:LEU:HD21 | 4:M:121:ILE:HG12 | 1.73 | 0.69 |
| 4:M:101:LEU:C | 4:M:103:TYR:O | 2.30 | 0.69 |
| 4:M:241:HIS:O | 4:M:474:THR:CG2 | 2.40 | 0.69 |
| 4:M:243:ILE:HD13 | 4:M:301:GLU:CB | 2.21 | 0.69 |
| 4:M:306:LEU:HD22 | 4:M:317:MET:HE2 | 1.73 | 0.69 |
| 1:A:329:ASN:N | 3:S:50:PHE:HE2 | 1.87 | 0.69 |
| 1:A:391:LEU:O | 1:A:392:MET:O | 2.08 | 0.69 |
| 2:B:537:PHE:CE2 | 2:B:545:ARG:CB | 2.76 | 0.69 |
| 1:A:107:TYR:CE1 | 1:A:128:LEU:CD2 | 2.75 | 0.69 |
| 2:B:213:LEU:CD1 | 4:M:135:ASN:CG | 2.52 | 0.69 |
| 1:A:67:LYS:O | 1:A:71:VAL:HG23 | 1.92 | 0.69 |
| 1:A:179:LYS:HZ3 | 3:S:142:ILE:N | 1.88 | 0.69 |
| 1:A:323:CYS:CB | 1:A:355:LEU:HD21 | 2.22 | 0.69 |
| 1:A:402:ILE:HG12 | 1:A:406:GLY:HA2 | 1.74 | 0.69 |
| 2:B:102:HIS:CE1 | 2:B:138:ALA:HA | 2.27 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:275:ARG:H | 2:B:294:VAL:HG13 | 1.57 | 0.69 |
| 2:B:468:LEU:HD13 | 2:B:503:LEU:HD21 | 1.74 | 0.69 |
| 2:B:513:TRP:CD2 | 2:B:551:LEU:HD21 | 2.28 | 0.69 |
| 4:M:108:LYS:O | 4:M:110:SER:N | 2.25 | 0.69 |
| 4:M:114:ILE:C | 4:M:116:ASN:N | 2.44 | 0.69 |
| 4:M:350:VAL:CB | 4:M:442:GLN:HG2 | 2.23 | 0.69 |
| 1:A:196:LEU:O | 1:A:197:ARG:C | 2.25 | 0.69 |
| 1:A:370:LYS:HE2 | 1:A:370:LYS:HA | 1.74 | 0.69 |
| 2:B:106:LEU:HD13 | 2:B:144:ASP:C | 2.13 | 0.69 |
| 2:B:479:VAL:HG22 | 2:B:486:HIS:CG | 2.27 | 0.69 |
| 4:M:222:PHE:HB2 | 4:M:479:PHE:CZ | 2.27 | 0.69 |
| 4:M:243:ILE:HG22 | 4:M:472:TYR:HB3 | 1.75 | 0.69 |
| 4:M:290:PHE:CZ | 4:M:297:PHE:CZ | 2.80 | 0.69 |
| 1:A:332:TYR:CE2 | 1:A:336:ILE:HD11 | 2.28 | 0.69 |
| 2:B:154:ILE:O | 2:B:158:VAL:HG23 | 1.93 | 0.69 |
| 2:B:234:CYS:HB3 | 2:B:301:LEU:HB3 | 1.75 | 0.69 |
| 2:B:518:ILE:CD1 | 2:B:518:ILE:O | 2.40 | 0.69 |
| 3:S:127:THR:CG2 | 3:S:153:VAL:CG1 | 2.70 | 0.69 |
| 4:M:65:TYR:CZ | 4:M:66:PHE:O | 2.45 | 0.69 |
| 4:M:223:HIS:HA | 4:M:479:PHE:CZ | 2.26 | 0.69 |
| 4:M:269:ILE:C | 4:M:302:TYR:CE2 | 2.66 | 0.69 |
| 1:A:461:CYS:O | 1:A:462:GLN:C | 2.22 | 0.69 |
| 1:A:462:GLN:CG | 4:M:59:ASP:CG | 2.58 | 0.69 |
| 2:B:73:ASP:CG | 4:M:19:LEU:HD22 | 2.12 | 0.69 |
| 2:B:116:THR:CG2 | 2:B:150:LEU:HD11 | 2.23 | 0.69 |
| 2:B:189:HIS:NE2 | 2:B:222:HIS:CB | 2.55 | 0.69 |
| 2:B:375:LEU:CD1 | 2:B:404:ASN:CG | 2.48 | 0.69 |
| 2:B:447:GLU:OE1 | 2:B:485:LYS:CG | 2.40 | 0.69 |
| 3:S:135:ILE:HG22 | 3:S:141:VAL:HG22 | 1.75 | 0.69 |
| 4:M:43:GLU:C | 4:M:45:SER:H | 1.96 | 0.69 |
| 4:M:323:MET:HE3 | 4:M:342:LEU:HB3 | 1.74 | 0.69 |
| 4:M:327:PHE:HE1 | 4:M:336:ASP:OD2 | 1.73 | 0.69 |
| 4:M:379:LEU:HD13 | 4:M:397:TRP:HE1 | 1.58 | 0.69 |
| 1:A:121:LEU:HD13 | 1:A:155:THR:CG2 | 2.23 | 0.69 |
| 2:B:179:LYS:HE2 | 4:M:131:ALA:O | 1.91 | 0.69 |
| 2:B:318:ILE:CD1 | 2:B:346:THR:CG2 | 2.70 | 0.69 |
| 2:B:545:ARG:HH11 | 2:B:602:ASP:CG | 1.96 | 0.69 |
| 4:M:69:ILE:O | 4:M:75:TRP:CA | 2.39 | 0.69 |
| 4:M:99:ILE:O | 4:M:99:ILE:HG22 | 1.92 | 0.69 |
| 1:A:266:VAL:O | 1:A:267:GLU:HB2 | 1.93 | 0.69 |
| 2:B:243:TRP:CH2 | 4:M:98:ARG:CZ | 2.76 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:278:PRO:C | 2:B:288:TYR:CB | 2.59 | 0.69 |
| 2:B:334:MET:O | 2:B:373:LEU:CD2 | 2.41 | 0.69 |
| 2:B:400:SER:HB2 | 2:B:435:SER:HA | 1.75 | 0.69 |
| 2:B:468:LEU:O | 2:B:472:VAL:HG23 | 1.93 | 0.69 |
| 2:B:519:ALA:O | 2:B:523:PHE:N | 2.26 | 0.69 |
| 1:A:236:LEU:C | 1:A:238:PRO:HD2 | 2.13 | 0.68 |
| 1:A:263:LEU:O | 1:A:266:VAL:O | 2.11 | 0.68 |
| 2:B:260:LEU:HD22 | 2:B:291:TYR:CZ | 2.28 | 0.68 |
| 2:B:396:ILE:HD11 | 2:B:418:TYR:CZ | 2.28 | 0.68 |
| 4:M:306:LEU:CD2 | 4:M:317:MET:HE2 | 2.23 | 0.68 |
| 1:A:555:LEU:HD13 | 1:A:581:LEU:CD1 | 2.22 | 0.68 |
| 2:B:100:LEU:CD2 | 4:M:123:LEU:CD2 | 2.71 | 0.68 |
| 2:B:139:LEU:CD1 | 2:B:176:ALA:CB | 2.71 | 0.68 |
| 2:B:253:ILE:CG1 | 2:B:324:ALA:HA | 2.22 | 0.68 |
| 2:B:260:LEU:C | 2:B:261:PRO:O | 2.22 | 0.68 |
| 2:B:346:THR:O | 2:B:349:MET:N | 2.25 | 0.68 |
| 3:S:53:THR:CB | 3:S:69:ASN:HB2 | 2.22 | 0.68 |
| 4:M:275:CYS:SG | 4:M:293:PRO:CB | 2.76 | 0.68 |
| 4:M:374:TYR:HE1 | 4:M:393:GLY:HA2 | 1.58 | 0.68 |
| 1:A:225:LEU:HD12 | 1:A:233:PHE:CE1 | 2.29 | 0.68 |
| 1:A:402:ILE:HG21 | 3:S:62:GLU:C | 2.11 | 0.68 |
| 2:B:25:VAL:CG2 | 2:B:32:GLU:HG3 | 2.16 | 0.68 |
| 2:B:97:VAL:HG12 | 2:B:101:ILE:CD1 | 2.23 | 0.68 |
| 2:B:147:MET:O | 2:B:148:SER:C | 2.30 | 0.68 |
| 2:B:310:ILE:CB | 2:B:342:ALA:HB1 | 2.22 | 0.68 |
| 2:B:403:ILE:HD11 | 2:B:439:CYS:C | 1.87 | 0.68 |
| 2:B:418:TYR:CD1 | 2:B:424:PHE:CD2 | 2.81 | 0.68 |
| 2:B:537:PHE:HB3 | 2:B:598:LEU:HD13 | 1.75 | 0.68 |
| 3:S:87:PHE:CD1 | 3:S:102:ILE:HG12 | 2.27 | 0.68 |
| 4:M:443:SER:HB3 | 4:M:447:ILE:HG12 | 1.74 | 0.68 |
| 1:A:418:ILE:HG12 | 1:A:418:ILE:O | 1.94 | 0.68 |
| 2:B:17:VAL:HG23 | 2:B:36:THR:CA | 2.23 | 0.68 |
| 2:B:231:ARG:CD | 2:B:297:PRO:HB2 | 2.24 | 0.68 |
| 2:B:566:ALA:N | 2:B:574:ASN:ND2 | 2.33 | 0.68 |
| 3:S:4:ALA:HB1 | 3:S:19:PHE:CD1 | 2.28 | 0.68 |
| 4:M:43:GLU:C | 4:M:45:SER:N | 2.44 | 0.68 |
| 1:A:117:ASP:OD2 | 1:A:120:ILE:HG12 | 1.92 | 0.68 |
| 1:A:237:SER:N | 1:A:238:PRO:HD2 | 2.08 | 0.68 |
| 2:B:80:GLN:HG3 | 2:B:108:PHE:CZ | 2.27 | 0.68 |
| 2:B:280:PRO:HG2 | 2:B:283:TYR:CG | 2.28 | 0.68 |
| 2:B:293:VAL:HA | 2:B:299:LEU:HG | 1.75 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:340:ILE:CG2 | 2:B:374:PHE:HA | 2.24 | 0.68 |
| 2:B:378:THR:HG23 | 2:B:379:LYS:H | 1.56 | 0.68 |
| 2:B:550:VAL:O | 2:B:553:ALA:HB3 | 1.93 | 0.68 |
| 4:M:220:GLU:OE2 | 4:M:350:VAL:HG11 | 1.93 | 0.68 |
| 1:A:137:ASN:C | 1:A:139:ASP:H | 1.79 | 0.68 |
| 2:B:29:LYS:HB3 | 2:B:58:GLU:CD | 2.14 | 0.68 |
| 2:B:106:LEU:HD11 | 2:B:144:ASP:O | 1.86 | 0.68 |
| 2:B:107:ARG:NH2 | 4:M:20:LEU:HD21 | 1.86 | 0.68 |
| 2:B:132:SER:HB2 | 2:B:169:VAL:HG23 | 1.74 | 0.68 |
| 2:B:193:LEU:O | 2:B:195:ILE:N | 2.26 | 0.68 |
| 2:B:580:TYR:HB3 | 2:B:582:ASP:OD2 | 1.93 | 0.68 |
| 4:M:65:TYR:CG | 4:M:66:PHE:N | 2.60 | 0.68 |
| 4:M:288:ILE:CD1 | 4:M:300:LEU:CD2 | 2.69 | 0.68 |
| 1:A:64:LEU:HG | 1:A:102:GLN:HE22 | 1.56 | 0.68 |
| 1:A:95:MET:C | 1:A:127:LEU:HD21 | 2.14 | 0.68 |
| 1:A:370:LYS:O | 1:A:374:LEU:CD1 | 2.42 | 0.68 |
| 1:A:398:GLU:HA | 1:A:418:ILE:HG13 | 1.76 | 0.68 |
| 2:B:73:ASP:CB | 4:M:24:ALA:HB1 | 2.24 | 0.68 |
| 2:B:396:ILE:HG23 | 2:B:432:ALA:HA | 1.66 | 0.68 |
| 3:S:54:PRO:CD | 3:S:57:LEU:HB2 | 2.24 | 0.68 |
| 4:M:114:ILE:O | 4:M:116:ASN:N | 2.27 | 0.68 |
| 4:M:235:LEU:HD11 | 4:M:306:LEU:HD13 | 1.74 | 0.68 |
| 4:M:246:VAL:HB | 4:M:297:PHE:CZ | 2.29 | 0.68 |
| 1:A:101:GLN:HE22 | 3:S:167:ILE:HD11 | 1.59 | 0.68 |
| 1:A:450:TYR:HD2 | 1:A:480:LEU:HG | 1.58 | 0.68 |
| 1:A:609:LEU:HD21 | 1:A:628:VAL:HG21 | 1.76 | 0.68 |
| 2:B:73:ASP:OD1 | 4:M:19:LEU:CD2 | 2.42 | 0.68 |
| 2:B:230:PHE:CD1 | 2:B:298:ASP:CA | 2.76 | 0.68 |
| 2:B:381:PHE:O | 2:B:382:TYR:C | 2.26 | 0.68 |
| 2:B:508:ARG:O | 2:B:509:ALA:C | 2.21 | 0.68 |
| 2:B:513:TRP:CE3 | 2:B:551:LEU:HD21 | 2.29 | 0.68 |
| 4:M:51:LEU:CB | 4:M:68:VAL:CG2 | 2.70 | 0.68 |
| 4:M:59:ASP:O | 4:M:60:LEU:C | 2.05 | 0.68 |
| 4:M:290:PHE:CZ | 4:M:297:PHE:CE1 | 2.81 | 0.68 |
| 1:A:186:PHE:CE2 | 1:A:224:GLU:HB3 | 2.23 | 0.68 |
| 1:A:438:ALA:O | 1:A:441:TYR:CD1 | 2.47 | 0.68 |
| 2:B:28:SER:CA | 2:B:30:LEU:O | 2.40 | 0.68 |
| 2:B:181:TYR:CD1 | 2:B:222:HIS:HD2 | 2.12 | 0.68 |
| 2:B:363:ILE:HD12 | 2:B:374:PHE:CE1 | 2.29 | 0.68 |
| 2:B:383:VAL:HG23 | 2:B:395:LYS:HG3 | 1.75 | 0.68 |
| 3:S:71:GLU:C | 3:S:73:ILE:H | 1.96 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:S:130:SER:HB2 | 3:S:156:LEU:CD1 | 2.23 | 0.68 |
| 2:B:387:ASP:HB3 | 2:B:388:PRO:CD | 2.24 | 0.68 |
| 4:M:69:ILE:HG21 | 4:M:97:ASP:OD2 | 1.94 | 0.68 |
| 4:M:224:VAL:N | 4:M:479:PHE:HA | 2.09 | 0.68 |
| 4:M:240:ILE:HG21 | 4:M:444:ALA:O | 1.93 | 0.68 |
| 1:A:515:CYS:O | 1:A:519:LEU:HG | 1.94 | 0.67 |
| 1:A:516:ILE:HG23 | 1:A:554:ALA:HB3 | 1.75 | 0.67 |
| 2:B:340:ILE:CB | 2:B:373:LEU:HG | 2.23 | 0.67 |
| 3:S:71:GLU:C | 3:S:73:ILE:N | 2.47 | 0.67 |
| 4:M:316:ARG:CG | 4:M:322:LEU:HD13 | 2.24 | 0.67 |
| 4:M:320:ILE:HA | 4:M:323:MET:HE2 | 1.75 | 0.67 |
| 1:A:429:VAL:CG1 | 1:A:473:ILE:HG12 | 2.23 | 0.67 |
| 1:A:488:ARG:CD | 1:A:522:PHE:CE2 | 2.77 | 0.67 |
| 1:A:638:LEU:HD23 | 2:B:561:ASP:OD2 | 1.93 | 0.67 |
| 2:B:14:THR:HA | 2:B:17:VAL:CG2 | 2.25 | 0.67 |
| 2:B:17:VAL:CG2 | 2:B:35:TYR:CE2 | 2.54 | 0.67 |
| 2:B:396:ILE:HD13 | 2:B:432:ALA:N | 2.08 | 0.67 |
| 2:B:433:VAL:C | 2:B:474:VAL:HG21 | 2.14 | 0.67 |
| 3:S:74:GLN:NE2 | 3:S:95:GLU:OE2 | 2.27 | 0.67 |
| 4:M:284:SER:O | 4:M:286:SER:N | 2.27 | 0.67 |
| 1:A:436:CYS:SG | 1:A:450:TYR:CE2 | 2.85 | 0.67 |
| 1:A:530:ASN:O | 1:A:534:LYS:O | 2.12 | 0.67 |
| 2:B:14:THR:CA | 2:B:17:VAL:HG22 | 2.24 | 0.67 |
| 2:B:34:SER:O | 2:B:42:ILE:HD12 | 1.94 | 0.67 |
| 2:B:37:TYR:CD2 | 2:B:38:TYR:CD1 | 2.81 | 0.67 |
| 2:B:106:LEU:CD1 | 2:B:144:ASP:C | 2.62 | 0.67 |
| 2:B:230:PHE:HD1 | 2:B:298:ASP:CA | 2.08 | 0.67 |
| 2:B:296:ASP:OD1 | 2:B:297:PRO:N | 2.26 | 0.67 |
| 4:M:43:GLU:O | 4:M:44:ASP:C | 2.31 | 0.67 |
| 4:M:220:GLU:CD | 4:M:222:PHE:CE1 | 2.67 | 0.67 |
| 4:M:405:THR:O | 4:M:407:THR:N | 2.27 | 0.67 |
| 1:A:605:GLU:HG3 | 1:A:632:PHE:CD2 | 2.28 | 0.67 |
| 2:B:216:LYS:HZ3 | 4:M:136:VAL:HG21 | 1.59 | 0.67 |
| 2:B:596:LEU:CD1 | 2:B:611:ALA:HB1 | 2.24 | 0.67 |
| 1:A:411:GLU:CD | 3:S:46:PHE:CZ | 2.68 | 0.67 |
| 1:A:424:TYR:HD1 | 3:S:63:ASN:HD21 | 1.36 | 0.67 |
| 2:B:340:ILE:CG1 | 2:B:373:LEU:HG | 2.25 | 0.67 |
| 4:M:331:LEU:HD12 | 4:M:331:LEU:O | 1.93 | 0.67 |
| 4:M:421:GLY:O | 4:M:422:PRO:C | 2.22 | 0.67 |
| 1:A:628:VAL:O | 1:A:631:SER:N | 2.28 | 0.67 |
| 2:B:116:THR:O | 2:B:120:ILE:HG12 | 1.93 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:184:GLY:O | 2:B:188:TYR:CD2 | 2.39 | 0.67 |
| 2:B:200:MET:CE | 2:B:229:HIS:C | 2.56 | 0.67 |
| 2:B:311:TYR:O | 2:B:312:SER:C | 2.28 | 0.67 |
| 2:B:348:THR:HB | 4:M:305:ASP:OD2 | 1.93 | 0.67 |
| 2:B:497:LEU:HD22 | 2:B:511:ILE:CG2 | 2.24 | 0.67 |
| 2:B:599:ALA:C | 2:B:601:TYR:H | 1.98 | 0.67 |
| 3:S:50:PHE:HA | 3:S:77:TYR:HD1 | 1.60 | 0.67 |
| 4:M:126:ASN:O | 4:M:129:VAL:N | 2.22 | 0.67 |
| 4:M:374:TYR:HB3 | 4:M:417:TYR:HD1 | 1.58 | 0.67 |
| 1:A:88:ASN:HB3 | 1:A:120:ILE:CG2 | 2.25 | 0.67 |
| 1:A:207:LEU:O | 1:A:243:ILE:HD11 | 1.93 | 0.67 |
| 1:A:533:ILE:CG1 | 1:A:562:TRP:CH2 | 2.78 | 0.67 |
| 2:B:106:LEU:HB3 | 4:M:130:GLU:CG | 2.25 | 0.67 |
| 2:B:127:LEU:HD13 | 2:B:157:THR:CG2 | 2.17 | 0.67 |
| 2:B:193:LEU:HD21 | 2:B:225:LEU:CB | 2.10 | 0.67 |
| 2:B:266:VAL:HA | 2:B:289:PRO:HB2 | 1.75 | 0.67 |
| 2:B:341:GLU:HA | 2:B:377:TYR:CD1 | 2.28 | 0.67 |
| 2:B:556:LEU:HB3 | 2:B:588:ILE:CD1 | 2.24 | 0.67 |
| 2:B:559:ASP:O | 2:B:562:ASN:C | 2.32 | 0.67 |
| 3:S:4:ALA:CB | 3:S:19:PHE:HD1 | 2.05 | 0.67 |
| 1:A:279:LEU:O | 1:A:280:GLU:C | 2.29 | 0.67 |
| 1:A:397:ASP:O | 1:A:418:ILE:CG1 | 2.43 | 0.67 |
| 1:A:581:LEU:CG | 1:A:607:LEU:HD11 | 2.25 | 0.67 |
| 2:B:17:VAL:HG23 | 2:B:36:THR:N | 2.10 | 0.67 |
| 2:B:193:LEU:C | 2:B:195:ILE:H | 1.98 | 0.67 |
| 2:B:313:SER:OG | 4:M:269:ILE:C | 2.33 | 0.67 |
| 4:M:48:ASP:HA | 4:M:70:ASN:ND2 | 2.09 | 0.67 |
| 4:M:121:ILE:CG2 | 4:M:125:PHE:CE1 | 2.78 | 0.67 |
| 4:M:472:TYR:CD1 | 4:M:472:TYR:N | 2.57 | 0.67 |
| 1:A:179:LYS:HE3 | 3:S:140:MET:CG | 2.24 | 0.67 |
| 1:A:261:THR:HG1 | 1:A:297:CYS:HG | 1.21 | 0.67 |
| 1:A:503:ASN:OD1 | 4:M:60:LEU:CB | 2.42 | 0.67 |
| 1:A:529:GLY:HA3 | 1:A:562:TRP:CZ2 | 2.30 | 0.67 |
| 1:A:638:LEU:CD2 | 2:B:561:ASP:N | 2.38 | 0.67 |
| 2:B:10:SER:C | 2:B:40:GLN:HE22 | 1.98 | 0.67 |
| 2:B:106:LEU:CD2 | 4:M:131:ALA:N | 2.57 | 0.67 |
| 2:B:226:LEU:CD2 | 2:B:255:TYR:CE1 | 2.61 | 0.67 |
| 2:B:513:TRP:CA | 2:B:551:LEU:CD1 | 2.72 | 0.67 |
| 4:M:47:SER:HB2 | 4:M:50:TYR:CE1 | 2.29 | 0.67 |
| 4:M:219:LEU:HG | 4:M:440:ILE:HG12 | 1.76 | 0.67 |
| 2:B:344:VAL:CG2 | 2:B:377:TYR:HB3 | 2.24 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:588:ILE:CG2 | 2:B:618:PHE:CE1 | 2.78 | 0.67 |
| 3:S:157:ASN:O | 3:S:161:GLU:HG3 | 1.94 | 0.67 |
| 4:M:258:VAL:HG22 | 4:M:452:ILE:HG23 | 1.76 | 0.67 |
| 4:M:321:GLY:O | 4:M:323:MET:N | 2.29 | 0.67 |
| 1:A:99:LYS:HG2 | 1:A:101:GLN:N | 2.09 | 0.66 |
| 1:A:395:PHE:CE2 | 1:A:428:MET:HE3 | 2.29 | 0.66 |
| 1:A:460:LEU:HA | 4:M:58:ARG:HH21 | 1.60 | 0.66 |
| 2:B:247:TYR:CE1 | 4:M:136:VAL:HG12 | 2.30 | 0.66 |
| 2:B:408:VAL:CG1 | 2:B:412:PHE:CE2 | 2.78 | 0.66 |
| 2:B:588:ILE:CG2 | 2:B:618:PHE:CZ | 2.77 | 0.66 |
| 4:M:69:ILE:CD1 | 4:M:94:GLU:HA | 2.24 | 0.66 |
| 4:M:244:VAL:N | 4:M:300:LEU:O | 2.22 | 0.66 |
| 4:M:351:SER:CB | 4:M:440:ILE:O | 2.42 | 0.66 |
| 1:A:244:LEU:CD1 | 1:A:281:LEU:CD1 | 2.73 | 0.66 |
| 2:B:34:SER:CB | 2:B:65:ARG:CZ | 2.71 | 0.66 |
| 2:B:67:ILE:O | 4:M:18:TYR:CE1 | 2.46 | 0.66 |
| 2:B:106:LEU:CD2 | 2:B:144:ASP:HB3 | 2.16 | 0.66 |
| 2:B:314:ASN:ND2 | 4:M:271:SER:OG | 2.27 | 0.66 |
| 2:B:340:ILE:CG1 | 2:B:373:LEU:CG | 2.74 | 0.66 |
| 4:M:260:LEU:HD21 | 4:M:449:VAL:HG22 | 1.75 | 0.66 |
| 4:M:309:GLN:O | 4:M:313:SER:N | 2.26 | 0.66 |
| 1:A:570:LYS:CD | 1:A:618:THR:HG22 | 2.25 | 0.66 |
| 2:B:310:ILE:CG2 | 2:B:318:ILE:HG23 | 2.23 | 0.66 |
| 2:B:344:VAL:HA | 2:B:381:PHE:CZ | 2.31 | 0.66 |
| 2:B:375:LEU:CD2 | 2:B:404:ASN:HB2 | 2.25 | 0.66 |
| 2:B:563:PHE:HD1 | 2:B:584:SER:CA | 2.05 | 0.66 |
| 4:M:376:ILE:CG2 | 4:M:379:LEU:HD11 | 2.26 | 0.66 |
| 4:M:376:ILE:HG21 | 4:M:379:LEU:CD1 | 2.25 | 0.66 |
| 1:A:147:LEU:HD22 | 1:A:166:LEU:CD2 | 2.26 | 0.66 |
| 1:A:233:PHE:C | 1:A:235:GLN:N | 2.46 | 0.66 |
| 1:A:638:LEU:HD23 | 2:B:561:ASP:OD1 | 1.96 | 0.66 |
| 3:S:16:LEU:CD1 | 3:S:129:GLU:HG2 | 2.25 | 0.66 |
| 3:S:55:PRO:O | 3:S:58:LEU:HB3 | 1.94 | 0.66 |
| 4:M:51:LEU:HB2 | 4:M:68:VAL:HB | 1.76 | 0.66 |
| 4:M:133:GLU:O | 4:M:134:PRO:C | 2.25 | 0.66 |
| 4:M:212:ASN:O | 4:M:465:LYS:HB2 | 1.95 | 0.66 |
| 4:M:437:TYR:HB3 | 4:M:439:TYR:CE1 | 2.30 | 0.66 |
| 1:A:215:VAL:CG1 | 1:A:243:ILE:HG23 | 2.09 | 0.66 |
| 1:A:342:GLY:O | 1:A:343:LYS:C | 2.31 | 0.66 |
| 1:A:516:ILE:HG22 | 1:A:554:ALA:HB2 | 1.76 | 0.66 |
| 2:B:63:MET:HG2 | 2:B:100:LEU:CB | 2.24 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:144:ASP:N | 2:B:179:LYS:HD3 | 2.08 | 0.66 |
| 2:B:219:TYR:OH | 2:B:226:LEU:CA | 2.33 | 0.66 |
| 2:B:230:PHE:CZ | 2:B:234:CYS:SG | 2.87 | 0.66 |
| 2:B:392:SER:CB | 2:B:424:PHE:HE1 | 2.08 | 0.66 |
| 2:B:397:GLN:CG | 2:B:431:MET:SD | 2.84 | 0.66 |
| 2:B:594:ALA:O | 2:B:598:LEU:HG | 1.94 | 0.66 |
| 3:S:8:PHE:CD2 | 3:S:36:TYR:CE1 | 2.84 | 0.66 |
| 3:S:135:ILE:O | 3:S:141:VAL:HG22 | 1.95 | 0.66 |
| 4:M:213:GLU:O | 4:M:248:SER:HA | 1.95 | 0.66 |
| 4:M:243:ILE:HG13 | 4:M:473:LYS:O | 1.95 | 0.66 |
| 4:M:247:ARG:HG3 | 4:M:470:ALA:HA | 1.77 | 0.66 |
| 4:M:437:TYR:HD1 | 4:M:437:TYR:N | 1.91 | 0.66 |
| 1:A:107:TYR:CE1 | 1:A:128:LEU:HD21 | 2.31 | 0.66 |
| 1:A:397:ASP:O | 1:A:418:ILE:CD1 | 2.44 | 0.66 |
| 1:A:503:ASN:OD1 | 4:M:59:ASP:O | 2.13 | 0.66 |
| 1:A:563:CYS:HA | 1:A:566:PHE:HD2 | 1.61 | 0.66 |
| 2:B:17:VAL:CG1 | 2:B:35:TYR:CE2 | 2.75 | 0.66 |
| 2:B:278:PRO:HB3 | 2:B:288:TYR:C | 2.14 | 0.66 |
| 2:B:313:SER:N | 4:M:269:ILE:CD1 | 2.56 | 0.66 |
| 2:B:390:VAL:O | 2:B:393:ILE:HB | 1.95 | 0.66 |
| 2:B:396:ILE:HD11 | 2:B:418:TYR:OH | 1.96 | 0.66 |
| 2:B:508:ARG:O | 2:B:512:VAL:HG23 | 1.95 | 0.66 |
| 2:B:559:ASP:O | 2:B:562:ASN:CA | 2.44 | 0.66 |
| 2:B:589:SER:HA | 2:B:592:TYR:CD2 | 2.31 | 0.66 |
| 4:M:224:VAL:HG22 | 4:M:306:LEU:CD1 | 2.25 | 0.66 |
| 4:M:257:ALA:HB3 | 4:M:453:ASP:OD1 | 1.96 | 0.66 |
| 4:M:379:LEU:CD2 | 4:M:411:LEU:HG | 2.20 | 0.66 |
| 1:A:96:SER:N | 1:A:127:LEU:HD21 | 2.11 | 0.66 |
| 1:A:225:LEU:HB2 | 1:A:233:PHE:CE2 | 2.28 | 0.66 |
| 1:A:273:LYS:O | 1:A:276:PRO:HD2 | 1.96 | 0.66 |
| 2:B:151:ALA:HA | 2:B:180:LEU:CD1 | 2.26 | 0.66 |
| 2:B:155:LEU:HG | 2:B:188:TYR:HD1 | 1.59 | 0.66 |
| 2:B:278:PRO:CB | 2:B:288:TYR:C | 2.63 | 0.66 |
| 2:B:344:VAL:CG1 | 2:B:381:PHE:HE2 | 2.06 | 0.66 |
| 2:B:458:MET:HA | 2:B:463:LEU:HD12 | 1.78 | 0.66 |
| 2:B:559:ASP:HB2 | 2:B:563:PHE:CE2 | 2.31 | 0.66 |
| 3:S:118:GLU:O | 3:S:122:ILE:HG13 | 1.95 | 0.66 |
| 4:M:5:PHE:HE2 | 4:M:20:LEU:CD1 | 2.09 | 0.66 |
| 4:M:217:ASP:CG | 4:M:471:LYS:HA | 2.16 | 0.66 |
| 4:M:224:VAL:HG23 | 4:M:479:PHE:CD2 | 2.30 | 0.66 |
| 4:M:347:PHE:HE1 | 4:M:439:TYR:CG | 2.12 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:481:MET:SD | 1:A:518:CYS:SG | 2.94 | 0.66 |
| 2:B:13:ASP:O | 2:B:17:VAL:CG1 | 2.43 | 0.66 |
| 2:B:234:CYS:SG | 2:B:298:ASP:O | 2.49 | 0.66 |
| 2:B:243:TRP:CZ3 | 4:M:98:ARG:NE | 2.63 | 0.66 |
| 2:B:403:ILE:HD11 | 2:B:439:CYS:HA | 1.49 | 0.66 |
| 2:B:559:ASP:HB3 | 2:B:563:PHE:CD2 | 2.31 | 0.66 |
| 3:S:38:LEU:HB3 | 3:S:51:LEU:CD1 | 2.26 | 0.66 |
| 4:M:220:GLU:O | 4:M:439:TYR:N | 2.19 | 0.66 |
| 4:M:222:PHE:HB2 | 4:M:479:PHE:HZ | 1.60 | 0.66 |
| 2:B:24:ALA:N | 2:B:32:GLU:OE1 | 2.06 | 0.66 |
| 2:B:180:LEU:HD23 | 2:B:192:LEU:HD21 | 1.78 | 0.66 |
| 2:B:197:LYS:CA | 2:B:229:HIS:CD2 | 2.77 | 0.66 |
| 2:B:549:LEU:CD1 | 2:B:595:VAL:CG1 | 2.74 | 0.66 |
| 3:S:16:LEU:HA | 3:S:125:TRP:CZ2 | 2.31 | 0.66 |
| 4:M:120:ARG:O | 4:M:124:ILE:CG1 | 2.44 | 0.66 |
| 2:B:142:LEU:O | 2:B:143:SER:C | 2.28 | 0.66 |
| 2:B:205:PRO:O | 2:B:206:LYS:C | 2.28 | 0.66 |
| 4:M:16:PHE:HA | 4:M:118:TYR:CE2 | 2.31 | 0.66 |
| 4:M:223:HIS:CE1 | 4:M:476:THR:H | 2.14 | 0.66 |
| 4:M:436:GLU:HA | 4:M:479:PHE:HE1 | 1.57 | 0.66 |
| 1:A:390:THR:O | 1:A:394:GLN:HG2 | 1.96 | 0.65 |
| 2:B:120:ILE:HD12 | 2:B:142:LEU:CD2 | 2.26 | 0.65 |
| 2:B:136:CYS:SG | 2:B:168:MET:C | 2.75 | 0.65 |
| 2:B:139:LEU:HD23 | 2:B:173:VAL:CA | 2.24 | 0.65 |
| 2:B:227:HIS:O | 2:B:229:HIS:N | 2.29 | 0.65 |
| 2:B:243:TRP:HH2 | 4:M:98:ARG:CZ | 2.08 | 0.65 |
| 2:B:360:LEU:HB3 | 2:B:394:TRP:CB | 2.25 | 0.65 |
| 2:B:398:ILE:CG2 | 2:B:402:LEU:CD1 | 2.69 | 0.65 |
| 2:B:408:VAL:HG11 | 2:B:446:TRP:CB | 2.25 | 0.65 |
| 2:B:433:VAL:HG22 | 2:B:471:TYR:CE2 | 2.31 | 0.65 |
| 2:B:456:ASP:O | 2:B:460:SER:HB2 | 1.96 | 0.65 |
| 4:M:56:VAL:N | 4:M:64:LYS:HG3 | 2.09 | 0.65 |
| 4:M:253:ASN:HA | 4:M:292:PRO:CG | 2.26 | 0.65 |
| 4:M:320:ILE:O | 4:M:322:LEU:N | 2.29 | 0.65 |
| 4:M:350:VAL:HG13 | 4:M:442:GLN:HG2 | 1.78 | 0.65 |
| 1:A:196:LEU:HD22 | 1:A:196:LEU:C | 2.16 | 0.65 |
| 1:A:200:PHE:CE1 | 1:A:236:LEU:HD21 | 2.30 | 0.65 |
| 2:B:378:THR:CG2 | 2:B:379:LYS:N | 2.59 | 0.65 |
| 2:B:549:LEU:HD12 | 2:B:595:VAL:HG11 | 1.78 | 0.65 |
| 3:S:89:VAL:CG1 | 3:S:98:ILE:HG21 | 2.26 | 0.65 |
| 4:M:247:ARG:N | 4:M:470:ALA:HB2 | 2.10 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:M:304:VAL:CG1 | 4:M:445:SER:HA | 2.25 | 0.65 |
| 4:M:351:SER:OG | 4:M:441:GLY:O | 2.10 | 0.65 |
| 2:B:567:GLN:CA | 2:B:569:THR:OG1 | 2.43 | 0.65 |
| 3:S:8:PHE:HB2 | 3:S:36:TYR:HE1 | 1.61 | 0.65 |
| 3:S:164:ASP:HA | 3:S:167:ILE:HB | 1.79 | 0.65 |
| 4:M:120:ARG:O | 4:M:124:ILE:HG13 | 1.96 | 0.65 |
| 4:M:250:LEU:HD13 | 4:M:254:PRO:HG2 | 1.79 | 0.65 |
| 1:A:320:HIS:HB2 | 1:A:352:PHE:CE1 | 2.31 | 0.65 |
| 1:A:365:VAL:O | 1:A:366:SER:C | 2.23 | 0.65 |
| 1:A:408:ILE:N | 3:S:64:ASN:HD22 | 1.92 | 0.65 |
| 1:A:503:ASN:CG | 4:M:59:ASP:C | 2.51 | 0.65 |
| 1:A:585:PHE:HA | 1:A:600:SER:OG | 1.95 | 0.65 |
| 2:B:9:ALA:C | 4:M:14:LEU:HB2 | 2.16 | 0.65 |
| 2:B:251:LEU:C | 2:B:253:ILE:H | 1.99 | 0.65 |
| 2:B:307:ASN:ND2 | 2:B:338:LYS:HB3 | 2.11 | 0.65 |
| 2:B:403:ILE:HB | 2:B:408:VAL:HG22 | 1.79 | 0.65 |
| 2:B:465:ALA:HB1 | 2:B:504:ALA:HB2 | 1.77 | 0.65 |
| 2:B:509:ALA:HB1 | 2:B:547:GLN:HG3 | 1.78 | 0.65 |
| 2:B:522:GLU:O | 2:B:522:GLU:CG | 2.33 | 0.65 |
| 2:B:534:ILE:C | 2:B:536:ASN:N | 2.48 | 0.65 |
| 2:B:564:LYS:HE3 | 2:B:621:GLY:O | 1.96 | 0.65 |
| 4:M:5:PHE:HA | 4:M:77:LEU:O | 1.97 | 0.65 |
| 4:M:46:SER:O | 4:M:47:SER:C | 2.19 | 0.65 |
| 4:M:219:LEU:HA | 4:M:440:ILE:HA | 1.77 | 0.65 |
| 4:M:220:GLU:CD | 4:M:222:PHE:CZ | 2.70 | 0.65 |
| 4:M:317:MET:CB | 4:M:322:LEU:H | 2.08 | 0.65 |
| 1:A:68:THR:N | 3:S:166:LYS:HD3 | 2.11 | 0.65 |
| 1:A:582:ILE:HG23 | 1:A:604:LEU:CG | 2.19 | 0.65 |
| 2:B:252:LEU:HD12 | 2:B:302:PHE:CD1 | 2.30 | 0.65 |
| 2:B:373:LEU:C | 2:B:375:LEU:N | 2.50 | 0.65 |
| 4:M:71:LYS:CB | 4:M:74:TYR:CZ | 2.70 | 0.65 |
| 4:M:220:GLU:OE2 | 4:M:350:VAL:CG1 | 2.44 | 0.65 |
| 4:M:278:ILE:HG23 | 4:M:278:ILE:O | 1.95 | 0.65 |
| 4:M:353:VAL:HA | 4:M:439:TYR:HA | 1.76 | 0.65 |
| 1:A:170:LEU:HD22 | 1:A:181:ALA:HB1 | 1.77 | 0.65 |
| 1:A:219:VAL:HG11 | 1:A:256:LEU:HD23 | 1.79 | 0.65 |
| 1:A:257:LEU:HD22 | 1:A:278:ILE:HG23 | 1.78 | 0.65 |
| 1:A:516:ILE:CG2 | 1:A:554:ALA:CB | 2.74 | 0.65 |
| 1:A:609:LEU:CD2 | 1:A:628:VAL:HG11 | 2.27 | 0.65 |
| 2:B:28:SER:HB3 | 2:B:61:ASP:OD2 | 1.96 | 0.65 |
| 2:B:37:TYR:CD2 | 2:B:38:TYR:HD1 | 2.13 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:S:39:ILE:HD11 | 3:S:77:TYR:CD2 | 2.32 | 0.65 |
| 4:M:69:ILE:CD1 | 4:M:94:GLU:CA | 2.75 | 0.65 |
| 4:M:432:THR:HG23 | 4:M:432:THR:O | 1.97 | 0.65 |
| 1:A:304:LEU:HD23 | 1:A:306:GLU:H | 1.61 | 0.65 |
| 1:A:438:ALA:O | 1:A:440:ASN:N | 2.30 | 0.65 |
| 2:B:22:ALA:HB2 | 2:B:33:SER:HG | 1.59 | 0.65 |
| 2:B:72:SER:O | 2:B:73:ASP:CB | 2.43 | 0.65 |
| 2:B:73:ASP:N | 4:M:19:LEU:HB2 | 2.04 | 0.65 |
| 2:B:223:LEU:CD1 | 2:B:258:GLN:HB2 | 2.17 | 0.65 |
| 2:B:540:GLU:OE1 | 2:B:548:ILE:HD11 | 1.96 | 0.65 |
| 3:S:32:LEU:C | 3:S:35:VAL:HG22 | 2.14 | 0.65 |
| 4:M:121:ILE:HG22 | 4:M:125:PHE:CE1 | 2.31 | 0.65 |
| 4:M:222:PHE:CB | 4:M:479:PHE:CZ | 2.80 | 0.65 |
| 4:M:353:VAL:O | 4:M:401:LYS:CA | 2.42 | 0.65 |
| 1:A:83:ASP:CG | 1:A:85:ALA:H | 1.99 | 0.65 |
| 2:B:211:ALA:O | 2:B:214:ALA:HB3 | 1.96 | 0.65 |
| 2:B:456:ASP:O | 2:B:460:SER:CB | 2.45 | 0.65 |
| 2:B:513:TRP:CA | 2:B:551:LEU:HD13 | 2.27 | 0.65 |
| 2:B:513:TRP:HE1 | 2:B:517:GLU:HG3 | 1.62 | 0.65 |
| 2:B:574:ASN:C | 2:B:576:GLN:H | 1.98 | 0.65 |
| 4:M:306:LEU:CD2 | 4:M:317:MET:HE3 | 2.13 | 0.65 |
| 1:A:137:ASN:HA | 1:A:139:ASP:HB3 | 1.79 | 0.65 |
| 1:A:151:SER:O | 1:A:152:THR:C | 2.28 | 0.65 |
| 1:A:240:LEU:O | 1:A:242:GLU:O | 2.15 | 0.65 |
| 1:A:638:LEU:HD12 | 2:B:558:TYR:N | 2.09 | 0.65 |
| 2:B:87:VAL:O | 2:B:88:LYS:C | 2.33 | 0.65 |
| 3:S:39:ILE:HG23 | 3:S:47:GLN:OE1 | 1.97 | 0.65 |
| 4:M:225:VAL:HG22 | 4:M:480:GLN:HB3 | 1.78 | 0.65 |
| 4:M:306:LEU:CD2 | 4:M:317:MET:HE1 | 2.23 | 0.65 |
| 4:M:433:VAL:HG13 | 4:M:433:VAL:O | 1.97 | 0.65 |
| 1:A:179:LYS:HZ3 | 3:S:141:VAL:CA | 2.05 | 0.65 |
| 1:A:260:PHE:CD1 | 1:A:274:LEU:HG | 2.31 | 0.65 |
| 1:A:462:GLN:HG2 | 4:M:59:ASP:OD1 | 1.97 | 0.65 |
| 1:A:496:ILE:HD11 | 1:A:532:LEU:HG | 1.79 | 0.65 |
| 2:B:106:LEU:HD13 | 2:B:144:ASP:O | 1.91 | 0.65 |
| 2:B:120:ILE:HG21 | 2:B:150:LEU:HD22 | 1.79 | 0.65 |
| 2:B:486:HIS:CE1 | 2:B:518:ILE:CG1 | 2.79 | 0.65 |
| 4:M:15:ILE:HG22 | 4:M:114:ILE:HG22 | 1.79 | 0.65 |
| 4:M:100:LEU:O | 4:M:103:TYR:O | 2.14 | 0.65 |
| 4:M:443:SER:OG | 4:M:448:TYR:CA | 2.45 | 0.65 |
| 1:A:189:PHE:HD2 | 1:A:225:LEU:HD11 | 1.60 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:588:LEU:O | 1:A:590:TYR:N | 2.29 | 0.64 |
| 2:B:61:ASP:O | 2:B:64:LYS:HB2 | 1.97 | 0.64 |
| 2:B:227:HIS:CE1 | 2:B:292:GLU:CG | 2.80 | 0.64 |
| 2:B:290:SER:C | 2:B:292:GLU:N | 2.41 | 0.64 |
| 2:B:397:GLN:NE2 | 2:B:431:MET:HE1 | 2.11 | 0.64 |
| 2:B:566:ALA:CA | 2:B:574:ASN:CG | 2.64 | 0.64 |
| 3:S:75:ILE:HG21 | 3:S:77:TYR:CZ | 2.32 | 0.64 |
| 4:M:443:SER:HB3 | 4:M:447:ILE:CA | 2.27 | 0.64 |
| 1:A:464:ILE:HG23 | 1:A:465:SER:HA | 1.79 | 0.64 |
| 1:A:496:ILE:CD1 | 1:A:532:LEU:HG | 2.27 | 0.64 |
| 2:B:253:ILE:HG23 | 2:B:327:GLN:HB2 | 1.78 | 0.64 |
| 2:B:253:ILE:CD1 | 2:B:324:ALA:HA | 2.28 | 0.64 |
| 2:B:375:LEU:HB2 | 2:B:376:PRO:HD3 | 1.79 | 0.64 |
| 2:B:537:PHE:C | 2:B:537:PHE:CD1 | 2.71 | 0.64 |
| 3:S:89:VAL:HG11 | 3:S:98:ILE:CD1 | 2.28 | 0.64 |
| 1:A:143:VAL:O | 1:A:147:LEU:HG | 1.96 | 0.64 |
| 1:A:529:GLY:CA | 1:A:562:TRP:CZ2 | 2.80 | 0.64 |
| 2:B:35:TYR:O | 2:B:42:ILE:HD11 | 1.97 | 0.64 |
| 2:B:106:LEU:CD1 | 2:B:144:ASP:HB2 | 1.97 | 0.64 |
| 2:B:216:LYS:HZ1 | 4:M:136:VAL:CG2 | 2.09 | 0.64 |
| 2:B:231:ARG:CZ | 2:B:297:PRO:HG2 | 2.26 | 0.64 |
| 2:B:278:PRO:HD3 | 2:B:290:SER:HA | 1.79 | 0.64 |
| 2:B:472:VAL:CG1 | 2:B:510:GLY:C | 2.66 | 0.64 |
| 4:M:7:ILE:HD12 | 4:M:121:ILE:HG21 | 1.79 | 0.64 |
| 4:M:7:ILE:HD11 | 4:M:121:ILE:HG21 | 1.78 | 0.64 |
| 4:M:230:LYS:O | 4:M:232:HIS:N | 2.29 | 0.64 |
| 4:M:363:ASN:HB2 | 4:M:431:GLN:HB2 | 1.80 | 0.64 |
| 1:A:244:LEU:HD11 | 1:A:281:LEU:HD13 | 1.79 | 0.64 |
| 2:B:249:ILE:HD13 | 2:B:321:CYS:SG | 2.36 | 0.64 |
| 4:M:65:TYR:CE2 | 4:M:86:PRO:CA | 2.80 | 0.64 |
| 4:M:118:TYR:HA | 4:M:121:ILE:HD12 | 1.78 | 0.64 |
| 1:A:528:ASN:O | 1:A:529:GLY:O | 2.15 | 0.64 |
| 1:A:588:LEU:O | 1:A:589:SER:C | 2.26 | 0.64 |
| 2:B:143:SER:HB2 | 2:B:179:LYS:CG | 2.27 | 0.64 |
| 3:S:6:LEU:HA | 3:S:16:LEU:O | 1.98 | 0.64 |
| 4:M:5:PHE:CZ | 4:M:92:PHE:CD1 | 2.84 | 0.64 |
| 4:M:269:ILE:C | 4:M:302:TYR:CD2 | 2.71 | 0.64 |
| 1:A:581:LEU:CG | 1:A:585:PHE:CE2 | 2.80 | 0.64 |
| 2:B:73:ASP:HB3 | 4:M:25:PRO:C | 2.17 | 0.64 |
| 2:B:219:TYR:CB | 2:B:226:LEU:HD22 | 2.28 | 0.64 |
| 2:B:418:TYR:CD1 | 2:B:419:VAL:N | 2.65 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:457:HIS:ND1 | 2:B:461:HIS:CD2 | 2.65 | 0.64 |
| 1:A:438:ALA:C | 1:A:439:ASP:O | 2.17 | 0.64 |
| 2:B:212:VAL:HG11 | 2:B:248:LEU:HD23 | 1.79 | 0.64 |
| 2:B:299:LEU:O | 2:B:302:PHE:CB | 2.42 | 0.64 |
| 2:B:340:ILE:CG1 | 2:B:373:LEU:CD2 | 2.70 | 0.64 |
| 2:B:429:VAL:CG1 | 2:B:467:VAL:HG11 | 2.27 | 0.64 |
| 2:B:430:ILE:CD1 | 2:B:466:SER:HB3 | 2.27 | 0.64 |
| 2:B:542:PRO:O | 2:B:607:ILE:CD1 | 2.41 | 0.64 |
| 2:B:553:ALA:HB2 | 2:B:614:ILE:CD1 | 2.28 | 0.64 |
| 1:A:215:VAL:HG12 | 1:A:243:ILE:HG21 | 1.78 | 0.64 |
| 1:A:272:ALA:O | 1:A:276:PRO:HD3 | 1.97 | 0.64 |
| 4:M:9:ASP:HB3 | 4:M:111:ILE:CG2 | 2.28 | 0.64 |
| 4:M:219:LEU:CD1 | 4:M:440:ILE:HG12 | 2.27 | 0.64 |
| 4:M:222:PHE:CE2 | 4:M:439:TYR:CE2 | 2.85 | 0.64 |
| 4:M:360:LEU:HD13 | 4:M:433:VAL:CG2 | 2.27 | 0.64 |
| 4:M:458:LEU:HD13 | 4:M:464:THR:HG21 | 1.80 | 0.64 |
| 1:A:260:PHE:O | 1:A:262:ASN:N | 2.29 | 0.64 |
| 1:A:323:CYS:SG | 1:A:355:LEU:HD21 | 2.38 | 0.64 |
| 1:A:599:ARG:NE | 2:B:610:ARG:NH2 | 2.39 | 0.64 |
| 2:B:43:ASN:HB3 | 2:B:44:PRO:HD2 | 1.79 | 0.64 |
| 2:B:73:ASP:HA | 4:M:19:LEU:HD23 | 1.60 | 0.64 |
| 2:B:98:LYS:NZ | 2:B:134:LEU:HD22 | 2.12 | 0.64 |
| 2:B:181:TYR:CB | 2:B:218:CYS:SG | 2.85 | 0.64 |
| 2:B:223:LEU:HD21 | 2:B:258:GLN:HB2 | 1.80 | 0.64 |
| 2:B:237:ILE:HG23 | 2:B:238:LYS:H | 1.50 | 0.64 |
| 2:B:251:LEU:O | 2:B:254:LYS:N | 2.30 | 0.64 |
| 2:B:433:VAL:HG22 | 2:B:471:TYR:CZ | 2.32 | 0.64 |
| 2:B:457:HIS:O | 2:B:458:MET:C | 2.30 | 0.64 |
| 2:B:570:GLY:C | 2:B:571:SER:O | 2.19 | 0.64 |
| 4:M:252:ASP:O | 4:M:254:PRO:HD2 | 1.97 | 0.64 |
| 1:A:125:THR:OG1 | 1:A:158:LEU:CD1 | 2.37 | 0.64 |
| 1:A:403:LEU:O | 1:A:404:GLN:C | 2.27 | 0.64 |
| 2:B:35:TYR:O | 2:B:42:ILE:CD1 | 2.46 | 0.64 |
| 2:B:37:TYR:O | 2:B:40:GLN:O | 2.15 | 0.64 |
| 2:B:80:GLN:HG2 | 2:B:108:PHE:HZ | 1.58 | 0.64 |
| 2:B:351:GLU:OE1 | 4:M:241:HIS:HB2 | 1.98 | 0.64 |
| 2:B:452:LYS:NZ | 2:B:456:ASP:OD2 | 2.30 | 0.64 |
| 2:B:545:ARG:CD | 2:B:602:ASP:OD2 | 2.46 | 0.64 |
| 3:S:80:TYR:OH | 3:S:110:ASP:CG | 2.36 | 0.64 |
| 4:M:44:ASP:C | 4:M:47:SER:H | 2.02 | 0.64 |
| 1:A:117:ASP:CG | 1:A:120:ILE:HG12 | 2.19 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:150:LEU:HB3 | 1:A:162:ILE:CD1 | 2.27 | 0.63 |
| 1:A:609:LEU:HD13 | 1:A:609:LEU:C | 2.18 | 0.63 |
| 2:B:212:VAL:HG22 | 2:B:233:TYR:CD1 | 2.32 | 0.63 |
| 2:B:249:ILE:HD11 | 2:B:321:CYS:SG | 2.38 | 0.63 |
| 2:B:398:ILE:C | 2:B:400:SER:N | 2.50 | 0.63 |
| 4:M:63:TYR:HB3 | 4:M:81:SER:O | 1.97 | 0.63 |
| 4:M:221:THR:HG23 | 4:M:437:TYR:O | 1.98 | 0.63 |
| 1:A:384:LEU:HD22 | 1:A:441:TYR:CE2 | 2.33 | 0.63 |
| 1:A:436:CYS:HB3 | 1:A:476:GLN:HE21 | 1.63 | 0.63 |
| 2:B:35:TYR:HE1 | 4:M:118:TYR:HH | 1.44 | 0.63 |
| 2:B:178:ILE:CD1 | 2:B:218:CYS:H | 2.07 | 0.63 |
| 2:B:279:LEU:H | 2:B:288:TYR:CB | 2.02 | 0.63 |
| 2:B:313:SER:HB3 | 4:M:269:ILE:O | 1.96 | 0.63 |
| 2:B:386:LYS:CE | 4:M:480:GLN:HB2 | 2.27 | 0.63 |
| 2:B:433:VAL:O | 2:B:474:VAL:HG21 | 1.97 | 0.63 |
| 2:B:517:GLU:O | 2:B:519:ALA:N | 2.31 | 0.63 |
| 4:M:68:VAL:CA | 4:M:76:CYS:O | 2.44 | 0.63 |
| 4:M:364:VAL:C | 4:M:367:ALA:O | 2.36 | 0.63 |
| 1:A:68:THR:OG1 | 3:S:166:LYS:HD3 | 1.99 | 0.63 |
| 1:A:132:LEU:HD11 | 1:A:150:LEU:CD1 | 2.27 | 0.63 |
| 1:A:462:GLN:OE1 | 4:M:58:ARG:HB2 | 1.94 | 0.63 |
| 2:B:104:TYR:O | 2:B:107:ARG:CA | 2.45 | 0.63 |
| 2:B:371:GLN:C | 2:B:373:LEU:H | 2.01 | 0.63 |
| 2:B:585:GLY:O | 2:B:589:SER:OG | 2.17 | 0.63 |
| 3:S:65:ASN:O | 3:S:67:GLU:N | 2.32 | 0.63 |
| 4:M:44:ASP:OD2 | 4:M:50:TYR:HE2 | 1.80 | 0.63 |
| 4:M:254:PRO:HB3 | 4:M:454:ILE:HD11 | 1.79 | 0.63 |
| 1:A:250:ASN:OD1 | 1:A:285:THR:HB | 1.98 | 0.63 |
| 1:A:289:SER:O | 1:A:290:VAL:O | 2.17 | 0.63 |
| 1:A:492:ILE:HD11 | 1:A:522:PHE:CB | 2.29 | 0.63 |
| 2:B:13:ASP:O | 2:B:17:VAL:CB | 2.46 | 0.63 |
| 2:B:249:ILE:HG12 | 2:B:306:LEU:HD23 | 1.80 | 0.63 |
| 2:B:314:ASN:O | 2:B:318:ILE:HG13 | 1.98 | 0.63 |
| 2:B:378:THR:CG2 | 2:B:379:LYS:H | 2.11 | 0.63 |
| 2:B:436:LEU:HD12 | 2:B:454:LEU:HD23 | 1.79 | 0.63 |
| 2:B:530:LEU:CD2 | 2:B:591:MET:HB3 | 2.28 | 0.63 |
| 3:S:149:ILE:O | 3:S:153:VAL:HG23 | 1.99 | 0.63 |
| 4:M:51:LEU:HB2 | 4:M:68:VAL:HG11 | 1.81 | 0.63 |
| 4:M:131:ALA:C | 4:M:133:GLU:N | 2.39 | 0.63 |
| 4:M:443:SER:CA | 4:M:447:ILE:HG13 | 2.28 | 0.63 |
| 1:A:140:VAL:HG22 | 1:A:177:ILE:HG13 | 1.79 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:433:ILE:HD11 | 1:A:473:ILE:HA | 1.80 | 0.63 |
| 1:A:435:ILE:HG23 | 1:A:441:TYR:CE2 | 2.33 | 0.63 |
| 1:A:495:ILE:HG21 | 1:A:515:CYS:CB | 2.27 | 0.63 |
| 1:A:503:ASN:CG | 4:M:59:ASP:O | 2.37 | 0.63 |
| 1:A:506:LYS:HZ1 | 4:M:82:LYS:HD2 | 0.58 | 0.63 |
| 2:B:73:ASP:N | 4:M:19:LEU:HB3 | 2.03 | 0.63 |
| 2:B:157:THR:O | 2:B:161:LEU:HD13 | 1.99 | 0.63 |
| 2:B:186:ASN:C | 2:B:188:TYR:H | 2.00 | 0.63 |
| 2:B:497:LEU:HD22 | 2:B:511:ILE:HG21 | 1.79 | 0.63 |
| 2:B:589:SER:HG | 2:B:618:PHE:HE2 | 1.44 | 0.63 |
| 3:S:127:THR:HG23 | 3:S:153:VAL:HG13 | 1.80 | 0.63 |
| 4:M:55:MET:O | 4:M:56:VAL:C | 2.24 | 0.63 |
| 4:M:374:TYR:CB | 4:M:417:TYR:HD1 | 2.12 | 0.63 |
| 4:M:376:ILE:HG22 | 4:M:379:LEU:HD12 | 1.79 | 0.63 |
| 1:A:420:ILE:HG22 | 1:A:421:PRO:O | 1.99 | 0.63 |
| 1:A:480:LEU:C | 1:A:480:LEU:HD13 | 2.19 | 0.63 |
| 2:B:136:CYS:SG | 2:B:169:VAL:N | 2.71 | 0.63 |
| 2:B:212:VAL:CG1 | 2:B:248:LEU:HD23 | 2.29 | 0.63 |
| 2:B:237:ILE:HG22 | 2:B:238:LYS:H | 1.64 | 0.63 |
| 2:B:250:GLU:HA | 2:B:253:ILE:HD12 | 1.81 | 0.63 |
| 2:B:270:SER:O | 2:B:273:SER:HB2 | 1.98 | 0.63 |
| 3:S:57:LEU:O | 3:S:67:GLU:O | 2.16 | 0.63 |
| 4:M:5:PHE:O | 4:M:17:GLN:HA | 1.97 | 0.63 |
| 4:M:223:HIS:CG | 4:M:478:ASN:HA | 2.33 | 0.63 |
| 4:M:271:SER:HB3 | 4:M:301:GLU:HG2 | 1.80 | 0.63 |
| 4:M:407:THR:O | 4:M:409:PRO:HD3 | 1.99 | 0.63 |
| 1:A:111:SER:HB2 | 1:A:152:THR:HG1 | 1.63 | 0.63 |
| 2:B:124:GLN:OE1 | 2:B:153:ILE:HG23 | 1.99 | 0.63 |
| 4:M:65:TYR:CE2 | 4:M:86:PRO:O | 2.52 | 0.63 |
| 4:M:265:ASN:HB3 | 4:M:309:GLN:CG | 2.26 | 0.63 |
| 1:A:450:TYR:OH | 1:A:476:GLN:NE2 | 2.31 | 0.63 |
| 2:B:25:VAL:HG23 | 2:B:32:GLU:CA | 2.29 | 0.63 |
| 2:B:252:LEU:HD13 | 2:B:302:PHE:CG | 2.30 | 0.63 |
| 2:B:295:ASN:C | 2:B:300:ASP:HB2 | 2.01 | 0.63 |
| 2:B:511:ILE:O | 2:B:512:VAL:C | 2.35 | 0.63 |
| 2:B:513:TRP:HA | 2:B:551:LEU:HD13 | 1.81 | 0.63 |
| 3:S:126:GLN:NE2 | 3:S:127:THR:OG1 | 2.32 | 0.63 |
| 4:M:356:LEU:C | 4:M:356:LEU:HD23 | 2.19 | 0.63 |
| 1:A:185:LEU:CD1 | 1:A:203:PHE:CE1 | 2.82 | 0.63 |
| 2:B:12:LEU:HD22 | 4:M:13:LYS:CD | 2.28 | 0.63 |
| 2:B:120:ILE:CD1 | 2:B:142:LEU:HD23 | 2.29 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:306:LEU:HD12 | 2:B:325:LEU:CD2 | 2.28 | 0.63 |
| 2:B:322:CYS:SG | 2:B:366:LEU:HG | 2.39 | 0.63 |
| 3:S:87:PHE:CG | 3:S:102:ILE:HG12 | 2.34 | 0.63 |
| 1:A:71:VAL:HG21 | 1:A:94:VAL:HG11 | 1.81 | 0.62 |
| 2:B:72:SER:HB3 | 4:M:17:GLN:CD | 2.17 | 0.62 |
| 2:B:136:CYS:SG | 2:B:168:MET:HG2 | 2.39 | 0.62 |
| 2:B:271:GLU:O | 2:B:272:GLY:C | 2.29 | 0.62 |
| 2:B:360:LEU:HD13 | 2:B:391:ALA:O | 1.99 | 0.62 |
| 2:B:418:TYR:CD1 | 2:B:419:VAL:HA | 2.33 | 0.62 |
| 2:B:560:ILE:CA | 2:B:563:PHE:HB2 | 2.27 | 0.62 |
| 2:B:597:TYR:O | 2:B:601:TYR:CE2 | 2.51 | 0.62 |
| 4:M:220:GLU:OE1 | 4:M:222:PHE:CZ | 2.51 | 0.62 |
| 1:A:211:ASP:OD1 | 1:A:213:SER:N | 2.29 | 0.62 |
| 1:A:224:GLU:O | 1:A:225:LEU:C | 2.30 | 0.62 |
| 1:A:364:ASP:HB3 | 1:A:367:ILE:HD12 | 1.80 | 0.62 |
| 3:S:107:GLU:O | 3:S:111:ARG:HG2 | 1.99 | 0.62 |
| 3:S:127:THR:HG22 | 3:S:153:VAL:HG13 | 1.77 | 0.62 |
| 4:M:214:LEU:N | 4:M:465:LYS:O | 2.31 | 0.62 |
| 4:M:350:VAL:CG1 | 4:M:442:GLN:HG2 | 2.30 | 0.62 |
| 1:A:150:LEU:O | 1:A:153:ILE:N | 2.32 | 0.62 |
| 1:A:260:PHE:CZ | 1:A:274:LEU:HD11 | 2.34 | 0.62 |
| 2:B:243:TRP:HH2 | 4:M:98:ARG:NE | 1.95 | 0.62 |
| 2:B:315:PRO:HG3 | 2:B:350:THR:HG22 | 1.82 | 0.62 |
| 2:B:566:ALA:CB | 2:B:581:TYR:HB3 | 2.30 | 0.62 |
| 3:S:70:ASN:O | 3:S:71:GLU:C | 2.35 | 0.62 |
| 4:M:265:ASN:O | 4:M:267:ILE:N | 2.32 | 0.62 |
| 4:M:276:VAL:CG2 | 4:M:299:LEU:HD12 | 2.29 | 0.62 |
| 4:M:376:ILE:HG22 | 4:M:379:LEU:CD1 | 2.27 | 0.62 |
| 2:B:127:LEU:HB3 | 2:B:157:THR:CG2 | 2.30 | 0.62 |
| 2:B:328:LEU:HB2 | 2:B:333:GLN:NE2 | 2.14 | 0.62 |
| 2:B:437:SER:HB2 | 2:B:474:VAL:CG2 | 2.29 | 0.62 |
| 2:B:574:ASN:C | 2:B:576:GLN:N | 2.52 | 0.62 |
| 2:B:596:LEU:HD13 | 2:B:611:ALA:C | 2.20 | 0.62 |
| 3:S:48:SER:HG | 3:S:50:PHE:H | 1.44 | 0.62 |
| 4:M:269:ILE:O | 4:M:302:TYR:CD2 | 2.51 | 0.62 |
| 4:M:319:SER:CB | 4:M:343:ASN:O | 2.47 | 0.62 |
| 4:M:445:SER:HG | 4:M:447:ILE:HG23 | 1.61 | 0.62 |
| 1:A:121:LEU:HD11 | 1:A:155:THR:H | 1.63 | 0.62 |
| 1:A:289:SER:O | 1:A:291:ILE:N | 2.31 | 0.62 |
| 1:A:319:LEU:O | 1:A:320:HIS:O | 2.17 | 0.62 |
| 2:B:10:SER:N | 4:M:14:LEU:HD13 | 2.13 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:68:SER:HA | 4:M:18:TYR:CD1 | 2.34 | 0.62 |
| 2:B:151:ALA:CB | 2:B:180:LEU:HD11 | 2.29 | 0.62 |
| 2:B:566:ALA:HA | 2:B:574:ASN:CB | 2.25 | 0.62 |
| 4:M:224:VAL:HG23 | 4:M:479:PHE:CE2 | 2.34 | 0.62 |
| 4:M:290:PHE:HZ | 4:M:293:PRO:HD3 | 1.61 | 0.62 |
| 1:A:421:PRO:HA | 3:S:62:GLU:O | 2.00 | 0.62 |
| 1:A:429:VAL:CG1 | 1:A:469:LEU:HD11 | 2.29 | 0.62 |
| 1:A:536:MET:HB3 | 1:A:551:LEU:HD11 | 1.80 | 0.62 |
| 2:B:200:MET:HE2 | 2:B:229:HIS:HA | 1.81 | 0.62 |
| 2:B:291:TYR:CE2 | 2:B:294:VAL:HB | 2.34 | 0.62 |
| 4:M:15:ILE:HG21 | 4:M:114:ILE:HG22 | 1.79 | 0.62 |
| 4:M:290:PHE:CE1 | 4:M:297:PHE:CD2 | 2.88 | 0.62 |
| 4:M:300:LEU:O | 4:M:300:LEU:HD12 | 2.00 | 0.62 |
| 1:A:402:ILE:HB | 1:A:421:PRO:HA | 1.81 | 0.62 |
| 1:A:517:TRP:NE1 | 2:B:605:PHE:CE2 | 2.65 | 0.62 |
| 2:B:310:ILE:HG21 | 2:B:342:ALA:CB | 2.28 | 0.62 |
| 4:M:65:TYR:CE2 | 4:M:86:PRO:HB3 | 2.33 | 0.62 |
| 1:A:297:CYS:O | 1:A:298:ILE:C | 2.38 | 0.62 |
| 2:B:158:VAL:CG1 | 2:B:177:ILE:CD1 | 2.77 | 0.62 |
| 2:B:403:ILE:HD11 | 2:B:439:CYS:CA | 2.01 | 0.62 |
| 2:B:416:LYS:HA | 2:B:457:HIS:HE2 | 1.63 | 0.62 |
| 2:B:568:VAL:O | 2:B:574:ASN:ND2 | 2.32 | 0.62 |
| 2:B:596:LEU:HD13 | 2:B:611:ALA:O | 1.99 | 0.62 |
| 3:S:16:LEU:CB | 3:S:125:TRP:NE1 | 2.50 | 0.62 |
| 4:M:19:LEU:CD2 | 4:M:24:ALA:CB | 2.77 | 0.62 |
| 4:M:101:LEU:O | 4:M:103:TYR:O | 2.18 | 0.62 |
| 4:M:217:ASP:OD1 | 4:M:217:ASP:O | 2.17 | 0.62 |
| 4:M:243:ILE:N | 4:M:474:THR:HG21 | 2.14 | 0.62 |
| 4:M:261:ASN:CB | 4:M:450:GLU:CG | 2.71 | 0.62 |
| 4:M:306:LEU:HD21 | 4:M:317:MET:HE1 | 1.80 | 0.62 |
| 4:M:316:ARG:HG3 | 4:M:322:LEU:HD13 | 1.80 | 0.62 |
| 4:M:356:LEU:HD21 | 4:M:358:ILE:HG12 | 1.80 | 0.62 |
| 1:A:244:LEU:HA | 1:A:256:LEU:HD13 | 1.80 | 0.62 |
| 1:A:438:ALA:O | 1:A:439:ASP:HB2 | 1.99 | 0.62 |
| 1:A:495:ILE:CG2 | 1:A:515:CYS:SG | 2.87 | 0.62 |
| 2:B:14:THR:CA | 2:B:36:THR:HA | 2.26 | 0.62 |
| 2:B:73:ASP:H | 4:M:19:LEU:CG | 2.13 | 0.62 |
| 2:B:107:ARG:NH2 | 4:M:126:ASN:HA | 2.14 | 0.62 |
| 2:B:306:LEU:HD12 | 2:B:325:LEU:HD21 | 1.81 | 0.62 |
| 2:B:310:ILE:HG23 | 2:B:318:ILE:CG2 | 2.25 | 0.62 |
| 2:B:436:LEU:CD1 | 2:B:454:LEU:HD23 | 2.29 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:M:44:ASP:OD2 | 4:M:50:TYR:CE2 | 2.53 | 0.62 |
| 4:M:215:TYR:CB | 4:M:467:TYR:O | 2.47 | 0.62 |
| 4:M:373:ALA:O | 4:M:418:GLU:N | 2.33 | 0.62 |
| 4:M:442:GLN:HG3 | 4:M:443:SER:N | 2.14 | 0.62 |
| 1:A:244:LEU:CG | 1:A:281:LEU:HD11 | 2.29 | 0.62 |
| 1:A:609:LEU:HG | 1:A:628:VAL:CB | 2.30 | 0.62 |
| 2:B:25:VAL:HG23 | 2:B:32:GLU:CB | 2.29 | 0.62 |
| 2:B:50:LEU:HG | 2:B:62:ALA:HB2 | 1.82 | 0.62 |
| 2:B:220:ALA:CA | 2:B:258:GLN:HG3 | 2.27 | 0.62 |
| 2:B:276:SER:O | 2:B:295:ASN:CG | 2.37 | 0.62 |
| 3:S:1:MET:H2 | 3:S:93:GLU:CB | 2.13 | 0.62 |
| 4:M:69:ILE:CD1 | 4:M:94:GLU:N | 2.63 | 0.62 |
| 4:M:70:ASN:CG | 4:M:75:TRP:CE2 | 2.72 | 0.62 |
| 4:M:245:ASP:OD1 | 4:M:297:PHE:C | 2.38 | 0.62 |
| 4:M:341:SER:HG | 4:M:343:ASN:HD21 | 1.44 | 0.62 |
| 4:M:360:LEU:HD23 | 4:M:362:PHE:CE2 | 2.35 | 0.62 |
| 1:A:402:ILE:CG2 | 1:A:421:PRO:HA | 2.29 | 0.61 |
| 1:A:433:ILE:CG2 | 1:A:476:GLN:HB2 | 2.30 | 0.61 |
| 1:A:495:ILE:CG2 | 1:A:515:CYS:CB | 2.77 | 0.61 |
| 2:B:73:ASP:C | 2:B:75:ASP:N | 2.53 | 0.61 |
| 2:B:343:LEU:HD23 | 2:B:366:LEU:HD12 | 1.82 | 0.61 |
| 2:B:363:ILE:HG21 | 2:B:398:ILE:HD13 | 1.82 | 0.61 |
| 2:B:367:SER:HB2 | 2:B:401:THR:OG1 | 1.94 | 0.61 |
| 4:M:42:LEU:HD23 | 4:M:51:LEU:CD2 | 2.30 | 0.61 |
| 4:M:51:LEU:HB2 | 4:M:68:VAL:CG1 | 2.30 | 0.61 |
| 4:M:243:ILE:O | 4:M:472:TYR:HD2 | 1.76 | 0.61 |
| 4:M:245:ASP:C | 4:M:472:TYR:HE1 | 1.87 | 0.61 |
| 4:M:354:ASP:HB2 | 4:M:440:ILE:HD11 | 1.79 | 0.61 |
| 1:A:179:LYS:HD3 | 3:S:142:ILE:HD13 | 1.81 | 0.61 |
| 1:A:213:SER:CB | 3:S:142:ILE:O | 2.42 | 0.61 |
| 1:A:402:ILE:HG21 | 1:A:421:PRO:HA | 1.82 | 0.61 |
| 2:B:90:ILE:CA | 2:B:101:ILE:HD13 | 2.29 | 0.61 |
| 2:B:193:LEU:C | 2:B:195:ILE:N | 2.51 | 0.61 |
| 2:B:381:PHE:O | 2:B:395:LYS:HD2 | 2.00 | 0.61 |
| 2:B:435:SER:O | 2:B:437:SER:N | 2.33 | 0.61 |
| 2:B:588:ILE:HG23 | 2:B:618:PHE:CE1 | 2.34 | 0.61 |
| 3:S:1:MET:H2 | 3:S:93:GLU:CG | 2.13 | 0.61 |
| 3:S:29:LYS:O | 3:S:32:LEU:N | 2.32 | 0.61 |
| 3:S:136:VAL:O | 3:S:140:MET:N | 2.33 | 0.61 |
| 4:M:212:ASN:CB | 4:M:250:LEU:HD23 | 2.30 | 0.61 |
| 4:M:222:PHE:CD2 | 4:M:439:TYR:CE2 | 2.85 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:363:ILE:HG13 | 2:B:381:PHE:CZ | 2.35 | 0.61 |
| 2:B:513:TRP:NE1 | 2:B:517:GLU:HG3 | 2.15 | 0.61 |
| 4:M:69:ILE:HB | 4:M:97:ASP:OD2 | 2.00 | 0.61 |
| 4:M:223:HIS:HB2 | 4:M:476:THR:OG1 | 1.99 | 0.61 |
| 4:M:223:HIS:NE2 | 4:M:436:GLU:HB2 | 2.15 | 0.61 |
| 1:A:158:LEU:HG | 1:A:162:ILE:HD12 | 1.82 | 0.61 |
| 2:B:34:SER:HB3 | 2:B:65:ARG:CZ | 2.30 | 0.61 |
| 2:B:83:PHE:CE1 | 2:B:87:VAL:HG21 | 2.35 | 0.61 |
| 2:B:162:VAL:HG23 | 2:B:173:VAL:CG1 | 2.30 | 0.61 |
| 2:B:219:TYR:CG | 2:B:226:LEU:CB | 2.79 | 0.61 |
| 2:B:382:TYR:OH | 2:B:410:GLU:C | 2.39 | 0.61 |
| 3:S:49:SER:O | 3:S:77:TYR:O | 2.18 | 0.61 |
| 4:M:88:ASP:OD2 | 4:M:134:PRO:HG3 | 2.01 | 0.61 |
| 4:M:224:VAL:H | 4:M:479:PHE:CA | 2.12 | 0.61 |
| 4:M:270:PRO:HB2 | 4:M:288:ILE:HD11 | 1.83 | 0.61 |
| 1:A:429:VAL:CG1 | 1:A:473:ILE:CG1 | 2.78 | 0.61 |
| 2:B:12:LEU:HD22 | 4:M:13:LYS:CE | 2.31 | 0.61 |
| 2:B:216:LYS:NZ | 4:M:136:VAL:CG2 | 2.64 | 0.61 |
| 2:B:231:ARG:CG | 2:B:297:PRO:HB2 | 2.30 | 0.61 |
| 2:B:382:TYR:OH | 2:B:411:ILE:N | 2.33 | 0.61 |
| 2:B:429:VAL:CG1 | 2:B:467:VAL:CG1 | 2.78 | 0.61 |
| 4:M:45:SER:HA | 4:M:75:TRP:CH2 | 2.35 | 0.61 |
| 4:M:216:VAL:O | 4:M:216:VAL:HG23 | 1.98 | 0.61 |
| 4:M:222:PHE:HD1 | 4:M:240:ILE:HG23 | 1.53 | 0.61 |
| 4:M:250:LEU:HD11 | 4:M:254:PRO:HG2 | 1.82 | 0.61 |
| 1:A:204:VAL:HG13 | 1:A:239:LEU:HD11 | 1.82 | 0.61 |
| 1:A:217:ALA:HB2 | 3:S:140:MET:SD | 2.40 | 0.61 |
| 1:A:233:PHE:O | 1:A:234:ILE:O | 2.15 | 0.61 |
| 1:A:567:GLN:O | 1:A:568:GLU:C | 2.35 | 0.61 |
| 2:B:200:MET:CG | 2:B:232:ARG:HB3 | 2.28 | 0.61 |
| 2:B:260:LEU:HD23 | 2:B:293:VAL:HG11 | 1.82 | 0.61 |
| 2:B:292:GLU:HG3 | 2:B:296:ASP:HB2 | 1.78 | 0.61 |
| 2:B:325:LEU:HD13 | 2:B:339:PHE:CD1 | 2.36 | 0.61 |
| 2:B:347:VAL:CG2 | 2:B:381:PHE:HE1 | 2.12 | 0.61 |
| 4:M:114:ILE:C | 4:M:116:ASN:H | 2.01 | 0.61 |
| 1:A:251:TRP:CH2 | 3:S:97:ALA:C | 2.74 | 0.61 |
| 1:A:438:ALA:O | 1:A:441:TYR:CE1 | 2.54 | 0.61 |
| 1:A:441:TYR:HB3 | 1:A:444:VAL:HG23 | 1.83 | 0.61 |
| 1:A:453:VAL:O | 1:A:457:LEU:HG | 2.00 | 0.61 |
| 2:B:103:LEU:CD1 | 4:M:127:CYS:SG | 2.88 | 0.61 |
| 2:B:237:ILE:HB | 2:B:248:LEU:HD13 | 1.81 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:322:CYS:SG | 2:B:343:LEU:HD22 | 2.41 | 0.61 |
| 2:B:382:TYR:OH | 2:B:410:GLU:HB3 | 1.99 | 0.61 |
| 2:B:400:SER:HB3 | 2:B:435:SER:HA | 1.65 | 0.61 |
| 4:M:65:TYR:CE1 | 4:M:66:PHE:O | 2.53 | 0.61 |
| 4:M:212:ASN:CB | 4:M:250:LEU:HA | 2.29 | 0.61 |
| 4:M:302:TYR:HE1 | 4:M:304:VAL:HB | 1.65 | 0.61 |
| 1:A:255:ARG:O | 1:A:258:LYS:N | 2.33 | 0.61 |
| 1:A:609:LEU:CG | 1:A:628:VAL:HG11 | 2.31 | 0.61 |
| 2:B:9:ALA:CB | 4:M:14:LEU:CB | 2.53 | 0.61 |
| 2:B:73:ASP:O | 2:B:75:ASP:N | 2.34 | 0.61 |
| 4:M:117:ASN:O | 4:M:121:ILE:HG13 | 2.00 | 0.61 |
| 4:M:405:THR:O | 4:M:405:THR:HG22 | 2.01 | 0.61 |
| 4:M:443:SER:CB | 4:M:447:ILE:N | 2.62 | 0.61 |
| 1:A:154:ILE:HB | 1:A:191:GLN:HG3 | 1.82 | 0.61 |
| 1:A:450:TYR:CD2 | 1:A:480:LEU:HG | 2.36 | 0.61 |
| 1:A:637:GLU:OE2 | 2:B:554:LYS:HG3 | 2.00 | 0.61 |
| 2:B:196:LEU:CB | 2:B:215:TYR:CE1 | 2.76 | 0.61 |
| 2:B:344:VAL:CG1 | 2:B:381:PHE:CE2 | 2.74 | 0.61 |
| 2:B:397:GLN:HG3 | 2:B:431:MET:CG | 2.31 | 0.61 |
| 2:B:534:ILE:O | 2:B:536:ASN:N | 2.34 | 0.61 |
| 3:S:89:VAL:HG11 | 3:S:98:ILE:HD12 | 1.82 | 0.61 |
| 1:A:318:ARG:O | 1:A:322:PHE:CD2 | 2.53 | 0.61 |
| 1:A:323:CYS:SG | 1:A:334:SER:HB2 | 2.39 | 0.61 |
| 1:A:372:ILE:HG22 | 1:A:431:VAL:HG21 | 1.82 | 0.61 |
| 2:B:38:TYR:OH | 2:B:43:ASN:O | 2.18 | 0.61 |
| 2:B:178:ILE:CD1 | 2:B:218:CYS:CB | 2.78 | 0.61 |
| 2:B:239:GLN:OE1 | 4:M:280:ASP:OD1 | 2.09 | 0.61 |
| 2:B:247:TYR:CD1 | 4:M:136:VAL:CG1 | 2.77 | 0.61 |
| 2:B:408:VAL:HG11 | 2:B:446:TRP:HB3 | 1.83 | 0.61 |
| 2:B:464:SER:OG | 2:B:467:VAL:HG23 | 2.01 | 0.61 |
| 2:B:549:LEU:HD13 | 2:B:595:VAL:CG1 | 2.31 | 0.61 |
| 4:M:350:VAL:CA | 4:M:442:GLN:HB2 | 2.25 | 0.61 |
| 1:A:103:LYS:O | 1:A:104:ARG:C | 2.29 | 0.60 |
| 2:B:216:LYS:CD | 2:B:251:LEU:HA | 2.30 | 0.60 |
| 2:B:251:LEU:C | 2:B:253:ILE:N | 2.54 | 0.60 |
| 2:B:599:ALA:O | 2:B:602:ASP:N | 2.30 | 0.60 |
| 4:M:435:LEU:H | 4:M:479:PHE:HB2 | 1.65 | 0.60 |
| 1:A:132:LEU:HD11 | 1:A:150:LEU:HD12 | 1.82 | 0.60 |
| 1:A:185:LEU:HD13 | 1:A:203:PHE:CE1 | 2.36 | 0.60 |
| 1:A:231:GLN:HB2 | 1:A:232:PRO:HD3 | 1.81 | 0.60 |
| 1:A:422:GLU:HB2 | 3:S:62:GLU:CD | 2.21 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:625:LEU:O | 1:A:627:GLU:N | 2.34 | 0.60 |
| 2:B:1:MET:HG3 | 4:M:39:PRO:CG | 2.27 | 0.60 |
| 2:B:12:LEU:CD2 | 4:M:13:LYS:HE3 | 2.31 | 0.60 |
| 2:B:230:PHE:HD1 | 2:B:298:ASP:HA | 1.66 | 0.60 |
| 3:S:137:GLN:C | 3:S:140:MET:H | 2.04 | 0.60 |
| 4:M:437:TYR:CE1 | 4:M:479:PHE:CE2 | 2.89 | 0.60 |
| 1:A:68:THR:OG1 | 3:S:166:LYS:CD | 2.50 | 0.60 |
| 1:A:163:ALA:HB1 | 1:A:199:ASN:HD21 | 1.66 | 0.60 |
| 1:A:232:PRO:O | 1:A:235:GLN:HB2 | 2.00 | 0.60 |
| 2:B:14:THR:CB | 2:B:36:THR:HG23 | 2.16 | 0.60 |
| 2:B:252:LEU:CB | 2:B:302:PHE:CG | 2.83 | 0.60 |
| 2:B:279:LEU:HD12 | 2:B:285:GLU:CG | 2.31 | 0.60 |
| 3:S:54:PRO:O | 3:S:69:ASN:HB2 | 2.01 | 0.60 |
| 3:S:99:LEU:O | 3:S:102:ILE:HB | 2.00 | 0.60 |
| 4:M:7:ILE:HG12 | 4:M:76:CYS:SG | 2.42 | 0.60 |
| 4:M:76:CYS:HB3 | 4:M:93:LEU:HD22 | 1.83 | 0.60 |
| 4:M:213:GLU:OE1 | 4:M:467:TYR:HD1 | 1.84 | 0.60 |
| 4:M:221:THR:N | 4:M:474:THR:HG1 | 1.73 | 0.60 |
| 4:M:252:ASP:C | 4:M:254:PRO:HD2 | 2.20 | 0.60 |
| 4:M:323:MET:HB3 | 4:M:340:LEU:CD1 | 2.27 | 0.60 |
| 1:A:200:PHE:HZ | 1:A:236:LEU:HD21 | 1.60 | 0.60 |
| 1:A:318:ARG:O | 1:A:322:PHE:HD2 | 1.84 | 0.60 |
| 1:A:436:CYS:HB2 | 1:A:450:TYR:CE1 | 2.36 | 0.60 |
| 2:B:161:LEU:CB | 2:B:173:VAL:HG22 | 2.26 | 0.60 |
| 2:B:560:ILE:HG22 | 2:B:561:ASP:N | 2.16 | 0.60 |
| 4:M:118:TYR:CD1 | 4:M:118:TYR:C | 2.72 | 0.60 |
| 4:M:290:PHE:HZ | 4:M:293:PRO:CD | 2.14 | 0.60 |
| 4:M:360:LEU:CD2 | 4:M:362:PHE:CE2 | 2.84 | 0.60 |
| 1:A:64:LEU:CB | 1:A:102:GLN:HE22 | 2.14 | 0.60 |
| 2:B:18:ILE:HG22 | 2:B:36:THR:C | 1.90 | 0.60 |
| 2:B:34:SER:OG | 2:B:35:TYR:N | 2.34 | 0.60 |
| 2:B:106:LEU:HD21 | 2:B:144:ASP:CG | 2.21 | 0.60 |
| 2:B:139:LEU:HD11 | 2:B:176:ALA:HB1 | 1.83 | 0.60 |
| 2:B:206:LYS:O | 2:B:210:CYS:SG | 2.53 | 0.60 |
| 2:B:374:PHE:O | 2:B:374:PHE:CG | 2.50 | 0.60 |
| 2:B:436:LEU:HB2 | 2:B:454:LEU:HD21 | 1.83 | 0.60 |
| 2:B:588:ILE:HG21 | 2:B:618:PHE:HE1 | 1.66 | 0.60 |
| 3:S:17:VAL:HG21 | 3:S:19:PHE:HZ | 1.61 | 0.60 |
| 3:S:89:VAL:CG1 | 3:S:98:ILE:HD12 | 2.31 | 0.60 |
| 3:S:93:GLU:HA | 3:S:93:GLU:OE1 | 2.00 | 0.60 |
| 4:M:344:ILE:H | 4:M:408:VAL:HG22 | 1.67 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:M:356:LEU:HD23 | 4:M:358:ILE:HG13 | 1.82 | 0.60 |
| 4:M:442:GLN:CG | 4:M:443:SER:H | 2.12 | 0.60 |
| 1:A:189:PHE:CB | 1:A:225:LEU:CD2 | 2.80 | 0.60 |
| 1:A:375:VAL:O | 1:A:376:GLU:C | 2.39 | 0.60 |
| 2:B:20:ARG:HD3 | 4:M:115:VAL:O | 2.02 | 0.60 |
| 2:B:193:LEU:O | 2:B:229:HIS:HE1 | 1.83 | 0.60 |
| 2:B:515:PHE:HD2 | 2:B:529:VAL:HG21 | 1.64 | 0.60 |
| 2:B:523:PHE:CD2 | 2:B:559:ASP:OD1 | 2.54 | 0.60 |
| 2:B:546:CYS:CB | 2:B:607:ILE:HG12 | 2.32 | 0.60 |
| 4:M:219:LEU:HB2 | 4:M:472:TYR:C | 2.16 | 0.60 |
| 4:M:219:LEU:H | 4:M:472:TYR:HB2 | 1.67 | 0.60 |
| 4:M:225:VAL:HA | 4:M:480:GLN:O | 2.01 | 0.60 |
| 4:M:260:LEU:HD23 | 4:M:449:VAL:HG22 | 1.81 | 0.60 |
| 1:A:253:ILE:O | 1:A:257:LEU:HG | 2.02 | 0.60 |
| 1:A:328:PRO:O | 3:S:50:PHE:CZ | 2.46 | 0.60 |
| 1:A:537:THR:O | 1:A:540:ILE:HG22 | 2.01 | 0.60 |
| 1:A:589:SER:C | 1:A:597:GLN:HG3 | 1.87 | 0.60 |
| 2:B:144:ASP:OD2 | 4:M:131:ALA:N | 2.33 | 0.60 |
| 2:B:399:LEU:HB3 | 2:B:411:ILE:CG2 | 2.32 | 0.60 |
| 1:A:178:ARG:HD3 | 1:A:209:ASP:OD2 | 2.01 | 0.60 |
| 1:A:609:LEU:HG | 1:A:628:VAL:HB | 1.84 | 0.60 |
| 2:B:189:HIS:CE1 | 2:B:222:HIS:HB3 | 2.36 | 0.60 |
| 2:B:220:ALA:O | 2:B:258:GLN:OE1 | 2.19 | 0.60 |
| 3:S:53:THR:HG21 | 3:S:67:GLU:O | 2.02 | 0.60 |
| 4:M:6:TYR:HA | 4:M:17:GLN:HA | 1.82 | 0.60 |
| 4:M:80:THR:HG23 | 4:M:89:CYS:SG | 2.41 | 0.60 |
| 4:M:360:LEU:HD13 | 4:M:433:VAL:HG23 | 1.83 | 0.60 |
| 4:M:374:TYR:OH | 4:M:394:GLN:CA | 2.50 | 0.60 |
| 2:B:182:ARG:HD2 | 2:B:217:GLU:HB3 | 1.84 | 0.60 |
| 2:B:280:PRO:CG | 2:B:283:TYR:HD2 | 2.07 | 0.60 |
| 2:B:336:ASN:O | 2:B:373:LEU:CD2 | 2.43 | 0.60 |
| 2:B:418:TYR:HD1 | 2:B:424:PHE:CE2 | 2.20 | 0.60 |
| 2:B:497:LEU:HD13 | 2:B:503:LEU:HD12 | 1.83 | 0.60 |
| 2:B:500:GLN:HB3 | 2:B:503:LEU:HG | 1.83 | 0.60 |
| 4:M:6:TYR:CD1 | 4:M:6:TYR:N | 2.68 | 0.60 |
| 4:M:257:ALA:HB3 | 4:M:453:ASP:CG | 2.22 | 0.60 |
| 1:A:441:TYR:HB3 | 1:A:444:VAL:CG2 | 2.32 | 0.60 |
| 1:A:480:LEU:O | 1:A:483:LYS:O | 2.20 | 0.60 |
| 1:A:632:PHE:O | 1:A:635:ALA:N | 2.34 | 0.60 |
| 2:B:216:LYS:HD3 | 2:B:251:LEU:HA | 1.84 | 0.60 |
| 2:B:231:ARG:NE | 2:B:297:PRO:HB2 | 2.17 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:374:PHE:CZ | 2:B:381:PHE:HD2 | 2.06 | 0.60 |
| 4:M:46:SER:O | 4:M:48:ASP:N | 2.34 | 0.60 |
| 4:M:217:ASP:HB3 | 4:M:470:ALA:C | 2.22 | 0.60 |
| 4:M:220:GLU:OE1 | 4:M:222:PHE:CE1 | 2.55 | 0.60 |
| 4:M:315:VAL:O | 4:M:315:VAL:HG12 | 2.02 | 0.60 |
| 2:B:72:SER:CB | 4:M:17:GLN:NE2 | 2.65 | 0.59 |
| 2:B:89:ASN:C | 2:B:101:ILE:CD1 | 2.70 | 0.59 |
| 2:B:302:PHE:CD2 | 2:B:328:LEU:HD11 | 2.36 | 0.59 |
| 2:B:374:PHE:HE2 | 2:B:402:LEU:HD11 | 0.95 | 0.59 |
| 2:B:392:SER:HG | 2:B:424:PHE:HE1 | 1.50 | 0.59 |
| 2:B:466:SER:O | 2:B:469:ASP:HB2 | 2.02 | 0.59 |
| 2:B:513:TRP:HE1 | 2:B:517:GLU:CG | 2.15 | 0.59 |
| 4:M:6:TYR:CA | 4:M:16:PHE:O | 2.49 | 0.59 |
| 4:M:65:TYR:HE2 | 4:M:86:PRO:O | 1.85 | 0.59 |
| 4:M:374:TYR:CB | 4:M:417:TYR:CD1 | 2.85 | 0.59 |
| 4:M:429:ASP:O | 4:M:430:LEU:C | 2.40 | 0.59 |
| 1:A:64:LEU:CG | 1:A:102:GLN:HE22 | 2.14 | 0.59 |
| 1:A:460:LEU:HA | 4:M:58:ARG:NH2 | 2.17 | 0.59 |
| 2:B:5:ILE:CD1 | 4:M:39:PRO:CD | 2.80 | 0.59 |
| 2:B:252:LEU:CB | 2:B:302:PHE:CD2 | 2.69 | 0.59 |
| 2:B:340:ILE:CD1 | 2:B:366:LEU:HB3 | 2.32 | 0.59 |
| 2:B:347:VAL:HB | 2:B:381:PHE:CE1 | 2.36 | 0.59 |
| 2:B:495:ASP:O | 2:B:499:VAL:HG23 | 2.02 | 0.59 |
| 4:M:19:LEU:HD12 | 4:M:20:LEU:H | 1.66 | 0.59 |
| 4:M:226:PHE:CE2 | 4:M:321:GLY:O | 2.55 | 0.59 |
| 4:M:410:VAL:HG12 | 4:M:412:ARG:HG3 | 1.83 | 0.59 |
| 1:A:384:LEU:HD12 | 1:A:385:LYS:N | 2.17 | 0.59 |
| 1:A:397:ASP:O | 1:A:418:ILE:HD12 | 2.03 | 0.59 |
| 1:A:450:TYR:HE2 | 1:A:480:LEU:HB2 | 1.66 | 0.59 |
| 2:B:107:ARG:HD3 | 4:M:130:GLU:OE2 | 2.03 | 0.59 |
| 2:B:343:LEU:O | 2:B:346:THR:HB | 2.01 | 0.59 |
| 2:B:344:VAL:HA | 2:B:381:PHE:HZ | 1.67 | 0.59 |
| 2:B:355:ASN:O | 2:B:359:LEU:HD23 | 2.02 | 0.59 |
| 2:B:430:ILE:HG12 | 2:B:467:VAL:CA | 2.31 | 0.59 |
| 4:M:114:ILE:O | 4:M:117:ASN:N | 2.35 | 0.59 |
| 4:M:224:VAL:N | 4:M:479:PHE:CA | 2.65 | 0.59 |
| 4:M:241:HIS:O | 4:M:474:THR:HG21 | 2.01 | 0.59 |
| 4:M:269:ILE:N | 4:M:302:TYR:CE2 | 2.70 | 0.59 |
| 4:M:437:TYR:HD1 | 4:M:437:TYR:H | 1.49 | 0.59 |
| 1:A:402:ILE:CB | 1:A:421:PRO:HA | 2.32 | 0.59 |
| 3:S:47:GLN:O | 3:S:48:SER:C | 2.34 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:M:96:ILE:HD12 | 4:M:125:PHE:CE1 | 2.36 | 0.59 |
| 4:M:240:ILE:HG21 | 4:M:444:ALA:CA | 2.26 | 0.59 |
| 4:M:290:PHE:CZ | 4:M:293:PRO:CD | 2.85 | 0.59 |
| 1:A:300:LYS:O | 1:A:301:GLY:C | 2.38 | 0.59 |
| 1:A:559:PHE:CD2 | 1:A:581:LEU:HD22 | 2.37 | 0.59 |
| 1:A:625:LEU:O | 1:A:626:SER:C | 2.32 | 0.59 |
| 2:B:120:ILE:HG13 | 2:B:150:LEU:HD22 | 1.84 | 0.59 |
| 2:B:177:ILE:HG21 | 2:B:196:LEU:HG | 1.84 | 0.59 |
| 2:B:178:ILE:CD1 | 2:B:218:CYS:HB2 | 2.28 | 0.59 |
| 2:B:181:TYR:CZ | 2:B:222:HIS:CD2 | 2.88 | 0.59 |
| 2:B:261:PRO:HG2 | 2:B:292:GLU:CB | 2.32 | 0.59 |
| 2:B:436:LEU:HD13 | 2:B:454:LEU:CD2 | 2.31 | 0.59 |
| 4:M:20:LEU:HD13 | 4:M:129:VAL:HG21 | 1.84 | 0.59 |
| 4:M:42:LEU:CD2 | 4:M:51:LEU:HD21 | 2.32 | 0.59 |
| 1:A:395:PHE:CD2 | 1:A:428:MET:HE3 | 2.37 | 0.59 |
| 1:A:435:ILE:CG2 | 1:A:441:TYR:CE2 | 2.85 | 0.59 |
| 2:B:80:GLN:CA | 2:B:108:PHE:HE2 | 2.16 | 0.59 |
| 2:B:170:ARG:HA | 2:B:199:LEU:HD22 | 1.85 | 0.59 |
| 2:B:216:LYS:HZ1 | 4:M:136:VAL:HG21 | 1.66 | 0.59 |
| 2:B:378:THR:C | 2:B:380:LYS:H | 2.05 | 0.59 |
| 2:B:493:LEU:HD23 | 2:B:514:LEU:HD23 | 1.83 | 0.59 |
| 3:S:73:ILE:HG21 | 3:S:88:ILE:HG23 | 1.76 | 0.59 |
| 4:M:16:PHE:HB2 | 4:M:118:TYR:CD2 | 2.38 | 0.59 |
| 4:M:243:ILE:C | 4:M:472:TYR:HB3 | 2.22 | 0.59 |
| 1:A:605:GLU:HB2 | 1:A:636:TYR:CE2 | 2.38 | 0.59 |
| 2:B:73:ASP:OD1 | 4:M:24:ALA:HB2 | 1.96 | 0.59 |
| 2:B:217:GLU:OE2 | 4:M:133:GLU:CD | 2.40 | 0.59 |
| 2:B:399:LEU:HD12 | 2:B:415:LEU:CD2 | 2.33 | 0.59 |
| 4:M:70:ASN:HB2 | 4:M:75:TRP:CZ3 | 2.37 | 0.59 |
| 4:M:110:SER:O | 4:M:113:LYS:N | 2.27 | 0.59 |
| 4:M:129:VAL:O | 4:M:133:GLU:O | 2.21 | 0.59 |
| 4:M:374:TYR:HB2 | 4:M:417:TYR:CD1 | 2.38 | 0.59 |
| 1:A:121:LEU:CD1 | 1:A:155:THR:HG23 | 2.32 | 0.59 |
| 1:A:189:PHE:CD2 | 1:A:225:LEU:HD11 | 2.37 | 0.59 |
| 1:A:508:LEU:HD12 | 4:M:59:ASP:OD1 | 2.03 | 0.59 |
| 1:A:562:TRP:CE3 | 1:A:574:ILE:HD12 | 2.37 | 0.59 |
| 2:B:268:LYS:C | 2:B:273:SER:OG | 2.40 | 0.59 |
| 2:B:559:ASP:O | 2:B:562:ASN:CB | 2.50 | 0.59 |
| 2:B:585:GLY:O | 2:B:589:SER:CB | 2.50 | 0.59 |
| 2:B:592:TYR:C | 2:B:592:TYR:CD1 | 2.76 | 0.59 |
| 4:M:224:VAL:N | 4:M:479:PHE:CB | 2.55 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:M:235:LEU:HD11 | 4:M:306:LEU:CD1 | 2.33 | 0.59 |
| 4:M:244:VAL:O | 4:M:299:LEU:CB | 2.51 | 0.59 |
| 4:M:338:PHE:CZ | 4:M:379:LEU:HD21 | 2.37 | 0.59 |
| 4:M:386:PHE:CD2 | 4:M:386:PHE:O | 2.56 | 0.59 |
| 1:A:185:LEU:HB3 | 1:A:203:PHE:HE1 | 1.67 | 0.59 |
| 2:B:13:ASP:O | 2:B:17:VAL:N | 2.30 | 0.59 |
| 2:B:90:ILE:N | 2:B:101:ILE:CD1 | 2.65 | 0.59 |
| 2:B:178:ILE:CD1 | 2:B:214:ALA:C | 2.71 | 0.59 |
| 3:S:89:VAL:CG1 | 3:S:98:ILE:CG2 | 2.80 | 0.59 |
| 4:M:217:ASP:CB | 4:M:470:ALA:C | 2.71 | 0.59 |
| 4:M:240:ILE:HB | 4:M:304:VAL:HG12 | 1.84 | 0.59 |
| 4:M:271:SER:C | 4:M:272:LEU:HD12 | 2.23 | 0.59 |
| 4:M:283:PHE:HE2 | 4:M:289:THR:HB | 1.65 | 0.59 |
| 1:A:186:PHE:CD1 | 1:A:186:PHE:C | 2.76 | 0.59 |
| 1:A:516:ILE:CG2 | 1:A:554:ALA:HB3 | 2.32 | 0.59 |
| 2:B:69:ILE:CG2 | 2:B:74:ASP:HB3 | 2.32 | 0.59 |
| 2:B:78:ASP:O | 2:B:79:VAL:C | 2.25 | 0.59 |
| 2:B:106:LEU:HD22 | 2:B:144:ASP:HB2 | 1.83 | 0.59 |
| 2:B:193:LEU:CB | 2:B:225:LEU:CD1 | 2.81 | 0.59 |
| 2:B:299:LEU:C | 2:B:299:LEU:HD13 | 2.24 | 0.59 |
| 2:B:334:MET:O | 2:B:373:LEU:HD22 | 2.03 | 0.59 |
| 2:B:360:LEU:HD21 | 2:B:395:LYS:CE | 2.33 | 0.59 |
| 2:B:360:LEU:HD21 | 2:B:395:LYS:CD | 2.32 | 0.59 |
| 2:B:396:ILE:HD11 | 2:B:418:TYR:CE2 | 2.38 | 0.59 |
| 2:B:549:LEU:HD12 | 2:B:595:VAL:CG1 | 2.32 | 0.59 |
| 4:M:235:LEU:HD23 | 4:M:235:LEU:C | 2.23 | 0.59 |
| 4:M:290:PHE:CZ | 4:M:291:ILE:O | 2.55 | 0.59 |
| 4:M:347:PHE:CE1 | 4:M:439:TYR:CG | 2.90 | 0.59 |
| 1:A:125:THR:CB | 1:A:158:LEU:HD13 | 2.33 | 0.58 |
| 1:A:186:PHE:HD1 | 1:A:187:LYS:N | 2.00 | 0.58 |
| 1:A:225:LEU:HB3 | 1:A:233:PHE:HE2 | 1.62 | 0.58 |
| 1:A:383:ASN:O | 1:A:387:ILE:HG12 | 2.03 | 0.58 |
| 1:A:621:LEU:HD13 | 1:A:621:LEU:C | 2.23 | 0.58 |
| 2:B:211:ALA:HB3 | 2:B:233:TYR:CZ | 2.37 | 0.58 |
| 2:B:223:LEU:CD1 | 2:B:258:GLN:CA | 2.78 | 0.58 |
| 2:B:284:ASN:O | 2:B:285:GLU:C | 2.34 | 0.58 |
| 2:B:343:LEU:CD2 | 2:B:363:ILE:CD1 | 2.74 | 0.58 |
| 2:B:537:PHE:CE2 | 2:B:545:ARG:HG2 | 2.38 | 0.58 |
| 2:B:537:PHE:CE1 | 2:B:598:LEU:HB3 | 2.38 | 0.58 |
| 4:M:9:ASP:HB3 | 4:M:111:ILE:HG22 | 1.84 | 0.58 |
| 4:M:244:VAL:HG13 | 4:M:472:TYR:HE2 | 1.65 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:M:354:ASP:CB | 4:M:440:ILE:CD1 | 2.77 | 0.58 |
| 1:A:509:PRO:O | 1:A:512:LEU:HB2 | 2.03 | 0.58 |
| 1:A:555:LEU:HD13 | 1:A:581:LEU:HD11 | 1.84 | 0.58 |
| 2:B:37:TYR:HD2 | 2:B:38:TYR:CE1 | 2.20 | 0.58 |
| 2:B:200:MET:CE | 2:B:229:HIS:HA | 2.33 | 0.58 |
| 2:B:364:HIS:O | 2:B:368:ILE:HG12 | 2.03 | 0.58 |
| 2:B:526:CYS:N | 2:B:527:PRO:HD3 | 2.17 | 0.58 |
| 2:B:580:TYR:O | 2:B:582:ASP:CG | 2.41 | 0.58 |
| 3:S:65:ASN:O | 3:S:66:ASP:C | 2.39 | 0.58 |
| 4:M:293:PRO:CB | 4:M:294:ASP:O | 2.49 | 0.58 |
| 4:M:405:THR:O | 4:M:407:THR:CG2 | 2.48 | 0.58 |
| 1:A:125:THR:CG2 | 1:A:158:LEU:HD13 | 2.34 | 0.58 |
| 1:A:185:LEU:CB | 1:A:203:PHE:HE1 | 2.16 | 0.58 |
| 1:A:224:GLU:O | 1:A:227:LYS:N | 2.36 | 0.58 |
| 2:B:67:ILE:HG23 | 4:M:18:TYR:OH | 2.03 | 0.58 |
| 2:B:80:GLN:CA | 2:B:108:PHE:CE2 | 2.86 | 0.58 |
| 2:B:155:LEU:O | 2:B:158:VAL:N | 2.37 | 0.58 |
| 2:B:204:ASP:HB3 | 2:B:207:VAL:CG2 | 2.34 | 0.58 |
| 2:B:219:TYR:CD1 | 2:B:226:LEU:CB | 2.82 | 0.58 |
| 2:B:344:VAL:CB | 2:B:377:TYR:HB3 | 2.33 | 0.58 |
| 1:A:179:LYS:CE | 3:S:140:MET:CB | 2.66 | 0.58 |
| 1:A:291:ILE:HG21 | 1:A:322:PHE:CE2 | 2.37 | 0.58 |
| 1:A:585:PHE:HE2 | 1:A:603:VAL:HG12 | 1.49 | 0.58 |
| 2:B:430:ILE:CD1 | 2:B:466:SER:CB | 2.81 | 0.58 |
| 3:S:15:ARG:O | 3:S:125:TRP:CE2 | 2.57 | 0.58 |
| 1:A:97:SER:C | 1:A:98:ASN:O | 2.16 | 0.58 |
| 1:A:529:GLY:C | 1:A:562:TRP:CZ2 | 2.76 | 0.58 |
| 2:B:143:SER:C | 2:B:179:LYS:HD2 | 2.23 | 0.58 |
| 2:B:241:ASP:OD1 | 2:B:241:ASP:O | 2.20 | 0.58 |
| 2:B:333:GLN:O | 2:B:336:ASN:HB2 | 2.03 | 0.58 |
| 2:B:556:LEU:C | 2:B:588:ILE:HD11 | 2.24 | 0.58 |
| 3:S:55:PRO:HG3 | 3:S:71:GLU:HG2 | 1.85 | 0.58 |
| 4:M:220:GLU:HB2 | 4:M:222:PHE:HE1 | 1.66 | 0.58 |
| 1:A:405:THR:CB | 2:B:7:ARG:HE | 2.16 | 0.58 |
| 1:A:562:TRP:HE3 | 1:A:574:ILE:HD12 | 1.69 | 0.58 |
| 2:B:34:SER:OG | 2:B:65:ARG:NE | 2.37 | 0.58 |
| 2:B:260:LEU:HD22 | 2:B:291:TYR:CE1 | 2.37 | 0.58 |
| 2:B:404:ASN:O | 2:B:408:VAL:HG23 | 2.04 | 0.58 |
| 2:B:563:PHE:O | 2:B:564:LYS:O | 2.21 | 0.58 |
| 3:S:5:VAL:HB | 3:S:132:LEU:HD21 | 1.84 | 0.58 |
| 3:S:87:PHE:CE1 | 3:S:102:ILE:HG12 | 2.39 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:244:LEU:CA | 1:A:256:LEU:HD13 | 2.33 | 0.58 |
| 1:A:412:LYS:O | 1:A:413:SER:C | 2.34 | 0.58 |
| 1:A:462:GLN:CD | 4:M:59:ASP:C | 2.34 | 0.58 |
| 2:B:102:HIS:CE1 | 2:B:138:ALA:N | 2.72 | 0.58 |
| 2:B:329:ALA:CB | 2:B:334:MET:HG2 | 2.30 | 0.58 |
| 2:B:479:VAL:CG1 | 2:B:486:HIS:CG | 2.70 | 0.58 |
| 2:B:519:ALA:O | 2:B:523:PHE:CA | 2.52 | 0.58 |
| 4:M:218:LEU:N | 4:M:218:LEU:HD12 | 2.18 | 0.58 |
| 4:M:338:PHE:CE1 | 4:M:415:ILE:HG13 | 2.38 | 0.58 |
| 1:A:429:VAL:HG21 | 1:A:469:LEU:HD11 | 1.86 | 0.58 |
| 1:A:487:MET:O | 1:A:488:ARG:C | 2.38 | 0.58 |
| 2:B:2:VAL:CG1 | 4:M:54:SER:HG | 2.14 | 0.58 |
| 2:B:120:ILE:HG13 | 2:B:150:LEU:CD2 | 2.33 | 0.58 |
| 2:B:127:LEU:HD11 | 2:B:142:LEU:HD11 | 1.83 | 0.58 |
| 2:B:139:LEU:CG | 2:B:176:ALA:CB | 2.80 | 0.58 |
| 2:B:256:CYS:O | 2:B:257:LYS:C | 2.38 | 0.58 |
| 2:B:334:MET:C | 2:B:336:ASN:N | 2.44 | 0.58 |
| 2:B:378:THR:C | 2:B:380:LYS:N | 2.54 | 0.58 |
| 2:B:479:VAL:CB | 2:B:486:HIS:CD2 | 2.86 | 0.58 |
| 2:B:553:ALA:HA | 2:B:556:LEU:HD12 | 1.86 | 0.58 |
| 3:S:6:LEU:HD11 | 3:S:14:PRO:CB | 2.32 | 0.58 |
| 3:S:35:VAL:HG12 | 3:S:75:ILE:HD13 | 1.85 | 0.58 |
| 4:M:4:SER:HB3 | 4:M:79:SER:OG | 2.03 | 0.58 |
| 4:M:6:TYR:CD2 | 4:M:17:GLN:HG3 | 2.38 | 0.58 |
| 4:M:70:ASN:HB2 | 4:M:75:TRP:CD2 | 2.39 | 0.58 |
| 4:M:222:PHE:CG | 4:M:240:ILE:HG12 | 2.38 | 0.58 |
| 4:M:235:LEU:CD1 | 4:M:306:LEU:HD13 | 2.34 | 0.58 |
| 4:M:258:VAL:CG1 | 4:M:449:VAL:HG13 | 2.31 | 0.58 |
| 4:M:306:LEU:O | 4:M:307:SER:O | 2.22 | 0.58 |
| 1:A:436:CYS:SG | 1:A:450:TYR:CZ | 2.97 | 0.58 |
| 2:B:28:SER:CA | 2:B:58:GLU:CG | 2.80 | 0.58 |
| 2:B:100:LEU:HD23 | 4:M:123:LEU:CD1 | 2.34 | 0.58 |
| 2:B:226:LEU:O | 2:B:226:LEU:HD12 | 2.04 | 0.58 |
| 2:B:418:TYR:HD1 | 2:B:418:TYR:O | 1.86 | 0.58 |
| 2:B:493:LEU:O | 2:B:496:LEU:N | 2.34 | 0.58 |
| 2:B:534:ILE:HD11 | 2:B:591:MET:O | 2.04 | 0.58 |
| 1:A:229:ASN:O | 1:A:230:PRO:C | 2.33 | 0.58 |
| 1:A:274:LEU:O | 1:A:277:LYS:N | 2.36 | 0.58 |
| 1:A:581:LEU:HD11 | 1:A:585:PHE:HZ | 1.66 | 0.58 |
| 2:B:9:ALA:CB | 4:M:14:LEU:HD12 | 2.33 | 0.58 |
| 2:B:28:SER:HA | 2:B:58:GLU:HG3 | 1.86 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:103:LEU:CD2 | 4:M:127:CYS:SG | 2.92 | 0.58 |
| 2:B:351:GLU:HB2 | 4:M:476:THR:HG22 | 1.86 | 0.58 |
| 2:B:546:CYS:HB2 | 2:B:607:ILE:HG12 | 1.85 | 0.58 |
| 4:M:241:HIS:HB2 | 4:M:476:THR:CG2 | 2.34 | 0.58 |
| 4:M:243:ILE:CD1 | 4:M:301:GLU:HB3 | 2.31 | 0.58 |
| 1:A:64:LEU:HG | 1:A:102:GLN:NE2 | 2.18 | 0.57 |
| 1:A:140:VAL:O | 1:A:141:VAL:C | 2.38 | 0.57 |
| 1:A:186:PHE:CD1 | 1:A:187:LYS:N | 2.72 | 0.57 |
| 1:A:278:ILE:O | 1:A:280:GLU:N | 2.36 | 0.57 |
| 1:A:293:GLU:OE1 | 3:S:94:SER:HB3 | 2.04 | 0.57 |
| 1:A:529:GLY:C | 1:A:562:TRP:CH2 | 2.78 | 0.57 |
| 1:A:556:VAL:CG2 | 1:A:603:VAL:CG1 | 2.76 | 0.57 |
| 2:B:104:TYR:O | 2:B:107:ARG:CG | 2.51 | 0.57 |
| 2:B:364:HIS:CE1 | 2:B:368:ILE:HD11 | 2.38 | 0.57 |
| 2:B:472:VAL:HG11 | 2:B:511:ILE:H | 1.68 | 0.57 |
| 2:B:513:TRP:CD1 | 2:B:517:GLU:HG2 | 2.39 | 0.57 |
| 2:B:519:ALA:O | 2:B:523:PHE:CG | 2.55 | 0.57 |
| 4:M:250:LEU:HD13 | 4:M:254:PRO:CG | 2.34 | 0.57 |
| 4:M:479:PHE:CD1 | 4:M:479:PHE:N | 2.57 | 0.57 |
| 2:B:306:LEU:CD1 | 2:B:325:LEU:CD2 | 2.83 | 0.57 |
| 2:B:310:ILE:HB | 2:B:342:ALA:HB1 | 1.83 | 0.57 |
| 2:B:347:VAL:O | 2:B:348:THR:C | 2.40 | 0.57 |
| 2:B:396:ILE:CD1 | 2:B:418:TYR:OH | 2.52 | 0.57 |
| 2:B:566:ALA:CA | 2:B:574:ASN:CB | 2.82 | 0.57 |
| 3:S:51:LEU:HB2 | 3:S:77:TYR:CE1 | 2.40 | 0.57 |
| 3:S:75:ILE:HG21 | 3:S:77:TYR:OH | 2.04 | 0.57 |
| 3:S:98:ILE:O | 3:S:102:ILE:HG13 | 2.04 | 0.57 |
| 4:M:243:ILE:HG12 | 4:M:474:THR:HG22 | 1.84 | 0.57 |
| 4:M:362:PHE:HE1 | 4:M:374:TYR:CZ | 2.21 | 0.57 |
| 4:M:379:LEU:CA | 4:M:412:ARG:O | 2.49 | 0.57 |
| 1:A:151:SER:C | 1:A:153:ILE:N | 2.52 | 0.57 |
| 2:B:219:TYR:OH | 2:B:226:LEU:N | 2.37 | 0.57 |
| 2:B:223:LEU:CD2 | 2:B:258:GLN:HB2 | 2.33 | 0.57 |
| 1:A:281:LEU:O | 1:A:282:MET:O | 2.21 | 0.57 |
| 1:A:316:LEU:HD21 | 1:A:341:ILE:HG13 | 1.85 | 0.57 |
| 1:A:323:CYS:SG | 1:A:338:PHE:HE2 | 2.27 | 0.57 |
| 1:A:462:GLN:NE2 | 4:M:60:LEU:O | 2.37 | 0.57 |
| 1:A:558:VAL:CG1 | 1:A:562:TRP:CZ2 | 2.87 | 0.57 |
| 1:A:579:LYS:HA | 1:A:582:ILE:HD12 | 1.85 | 0.57 |
| 1:A:638:LEU:HD13 | 2:B:557:SER:HG | 1.65 | 0.57 |
| 2:B:245:GLN:CG | 2:B:309:LEU:HD11 | 2.35 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:278:PRO:CA | 2:B:288:TYR:HB3 | 2.26 | 0.57 |
| 2:B:363:ILE:CG2 | 2:B:398:ILE:HG12 | 2.34 | 0.57 |
| 2:B:386:LYS:NZ | 4:M:479:PHE:O | 2.37 | 0.57 |
| 2:B:437:SER:OG | 2:B:474:VAL:HA | 2.04 | 0.57 |
| 2:B:540:GLU:OE1 | 2:B:548:ILE:HD12 | 2.04 | 0.57 |
| 4:M:374:TYR:HH | 4:M:394:GLN:C | 2.08 | 0.57 |
| 4:M:433:VAL:O | 4:M:435:LEU:HD12 | 2.04 | 0.57 |
| 1:A:92:LEU:HD13 | 1:A:123:LEU:CD1 | 2.35 | 0.57 |
| 2:B:20:ARG:NH2 | 4:M:118:TYR:CG | 2.71 | 0.57 |
| 2:B:102:HIS:CE1 | 2:B:138:ALA:CA | 2.87 | 0.57 |
| 2:B:251:LEU:O | 2:B:253:ILE:N | 2.38 | 0.57 |
| 2:B:393:ILE:HG12 | 2:B:428:VAL:HA | 1.86 | 0.57 |
| 2:B:559:ASP:CB | 2:B:563:PHE:CE2 | 2.88 | 0.57 |
| 3:S:17:VAL:CG2 | 3:S:19:PHE:CE1 | 2.87 | 0.57 |
| 4:M:104:PHE:CE2 | 4:M:117:ASN:CB | 2.86 | 0.57 |
| 4:M:354:ASP:CB | 4:M:440:ILE:HD11 | 2.33 | 0.57 |
| 1:A:189:PHE:HB3 | 1:A:225:LEU:CD2 | 2.35 | 0.57 |
| 1:A:260:PHE:CE2 | 1:A:274:LEU:HD11 | 2.40 | 0.57 |
| 2:B:116:THR:HG22 | 2:B:150:LEU:HD11 | 1.86 | 0.57 |
| 2:B:476:ARG:CB | 2:B:514:LEU:HD13 | 2.35 | 0.57 |
| 2:B:588:ILE:HG21 | 2:B:618:PHE:CE1 | 2.40 | 0.57 |
| 4:M:66:PHE:CE1 | 4:M:79:SER:HB3 | 2.40 | 0.57 |
| 4:M:224:VAL:CG1 | 4:M:226:PHE:CE2 | 2.88 | 0.57 |
| 2:B:141:ALA:O | 2:B:142:LEU:C | 2.42 | 0.57 |
| 2:B:161:LEU:HB3 | 2:B:173:VAL:HG21 | 1.82 | 0.57 |
| 2:B:170:ARG:HA | 2:B:199:LEU:CD2 | 2.35 | 0.57 |
| 2:B:347:VAL:CA | 2:B:359:LEU:HG | 2.33 | 0.57 |
| 3:S:64:ASN:C | 3:S:66:ASP:H | 2.08 | 0.57 |
| 3:S:167:ILE:HG22 | 3:S:168:GLY:HA2 | 1.84 | 0.57 |
| 4:M:41:LEU:CB | 4:M:51:LEU:HA | 2.34 | 0.57 |
| 4:M:56:VAL:H | 4:M:64:LYS:CG | 2.13 | 0.57 |
| 4:M:302:TYR:CE1 | 4:M:304:VAL:HB | 2.40 | 0.57 |
| 4:M:383:HIS:HB2 | 4:M:403:THR:OG1 | 2.02 | 0.57 |
| 1:A:222:ILE:CG2 | 1:A:240:LEU:HD11 | 2.31 | 0.57 |
| 1:A:609:LEU:O | 1:A:612:GLU:N | 2.34 | 0.57 |
| 2:B:123:LEU:HD12 | 2:B:142:LEU:CD2 | 2.35 | 0.57 |
| 2:B:259:TYR:O | 2:B:293:VAL:HG21 | 2.03 | 0.57 |
| 2:B:347:VAL:CG2 | 2:B:381:PHE:CZ | 2.87 | 0.57 |
| 2:B:386:LYS:NZ | 4:M:478:ASN:N | 2.53 | 0.57 |
| 2:B:436:LEU:CB | 2:B:454:LEU:HD21 | 2.34 | 0.57 |
| 2:B:451:MET:HG3 | 2:B:489:ILE:CG1 | 2.22 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:S:75:ILE:CG2 | 3:S:77:TYR:CZ | 2.88 | 0.57 |
| 3:S:130:SER:HB2 | 3:S:156:LEU:HD13 | 1.83 | 0.57 |
| 4:M:271:SER:O | 4:M:300:LEU:CA | 2.48 | 0.57 |
| 4:M:273:HIS:CB | 4:M:298:ARG:O | 2.42 | 0.57 |
| 4:M:344:ILE:HD12 | 4:M:407:THR:O | 2.03 | 0.57 |
| 1:A:216:SER:HB2 | 1:A:252:ILE:HG12 | 1.87 | 0.57 |
| 1:A:433:ILE:HG23 | 1:A:476:GLN:CB | 2.33 | 0.57 |
| 1:A:565:ASN:O | 1:A:567:GLN:N | 2.38 | 0.57 |
| 2:B:34:SER:HB3 | 2:B:65:ARG:HH12 | 1.65 | 0.57 |
| 4:M:5:PHE:HE2 | 4:M:20:LEU:HD13 | 1.68 | 0.57 |
| 1:A:492:ILE:HD13 | 1:A:526:VAL:CG2 | 2.34 | 0.57 |
| 1:A:517:TRP:NE1 | 2:B:605:PHE:CD2 | 2.71 | 0.57 |
| 2:B:144:ASP:OD1 | 4:M:131:ALA:C | 2.44 | 0.57 |
| 2:B:162:VAL:HG22 | 2:B:199:LEU:HG | 1.86 | 0.57 |
| 4:M:270:PRO:O | 4:M:272:LEU:CD1 | 2.53 | 0.57 |
| 4:M:358:ILE:O | 4:M:397:TRP:HE3 | 1.88 | 0.57 |
| 1:A:91:ILE:HG23 | 1:A:106:GLY:HA2 | 1.86 | 0.56 |
| 1:A:268:PRO:HA | 1:A:271:ARG:HE | 1.69 | 0.56 |
| 1:A:291:ILE:O | 1:A:295:VAL:HG23 | 2.05 | 0.56 |
| 1:A:322:PHE:HB3 | 1:A:330:LEU:HD21 | 1.87 | 0.56 |
| 2:B:147:MET:HB2 | 2:B:150:LEU:HG | 1.87 | 0.56 |
| 2:B:227:HIS:C | 2:B:229:HIS:N | 2.58 | 0.56 |
| 2:B:256:CYS:HG | 2:B:328:LEU:HD21 | 1.69 | 0.56 |
| 2:B:371:GLN:CB | 2:B:401:THR:O | 2.48 | 0.56 |
| 2:B:414:GLU:O | 2:B:417:TYR:HB3 | 2.05 | 0.56 |
| 3:S:17:VAL:HG22 | 3:S:19:PHE:CZ | 2.36 | 0.56 |
| 4:M:372:ILE:O | 4:M:372:ILE:HG22 | 2.04 | 0.56 |
| 1:A:103:LYS:C | 1:A:107:TYR:CD2 | 2.77 | 0.56 |
| 1:A:147:LEU:HD13 | 1:A:181:ALA:HA | 1.87 | 0.56 |
| 1:A:215:VAL:HG13 | 1:A:243:ILE:CG2 | 2.13 | 0.56 |
| 1:A:257:LEU:CD2 | 1:A:278:ILE:HG22 | 2.33 | 0.56 |
| 2:B:340:ILE:HG13 | 2:B:373:LEU:CG | 2.35 | 0.56 |
| 2:B:397:GLN:HG3 | 2:B:431:MET:HG2 | 1.85 | 0.56 |
| 2:B:527:PRO:HB3 | 2:B:587:ARG:HG3 | 1.85 | 0.56 |
| 3:S:8:PHE:CD2 | 3:S:36:TYR:HE1 | 2.22 | 0.56 |
| 4:M:290:PHE:CE2 | 4:M:297:PHE:CE1 | 2.93 | 0.56 |
| 4:M:424:PHE:CE1 | 4:M:428:VAL:HG22 | 2.40 | 0.56 |
| 1:A:113:SER:O | 1:A:115:TYR:N | 2.38 | 0.56 |
| 1:A:150:LEU:HD22 | 1:A:158:LEU:HD11 | 1.86 | 0.56 |
| 1:A:359:LEU:HB3 | 1:A:367:ILE:CG2 | 2.35 | 0.56 |
| 1:A:503:ASN:CA | 4:M:59:ASP:C | 2.55 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:606:PHE:HE1 | 1:A:633:PHE:CA | 2.19 | 0.56 |
| 1:A:634:ASN:O | 1:A:638:LEU:HB2 | 2.05 | 0.56 |
| 2:B:38:TYR:CE1 | 2:B:43:ASN:N | 2.64 | 0.56 |
| 2:B:55:ASN:O | 2:B:58:GLU:HB2 | 2.05 | 0.56 |
| 2:B:97:VAL:HG12 | 2:B:101:ILE:HD11 | 1.87 | 0.56 |
| 2:B:144:ASP:N | 2:B:179:LYS:CD | 2.66 | 0.56 |
| 2:B:260:LEU:O | 2:B:261:PRO:C | 2.37 | 0.56 |
| 2:B:293:VAL:HA | 2:B:299:LEU:CB | 2.35 | 0.56 |
| 2:B:306:LEU:HD13 | 2:B:325:LEU:HG | 1.88 | 0.56 |
| 2:B:340:ILE:HG13 | 2:B:373:LEU:CB | 2.33 | 0.56 |
| 2:B:440:GLY:C | 2:B:442:LEU:N | 2.56 | 0.56 |
| 2:B:513:TRP:CG | 2:B:551:LEU:HD21 | 2.40 | 0.56 |
| 2:B:566:ALA:HB1 | 2:B:581:TYR:HB3 | 1.87 | 0.56 |
| 3:S:53:THR:CB | 3:S:69:ASN:N | 2.67 | 0.56 |
| 4:M:235:LEU:HD13 | 4:M:306:LEU:HB3 | 1.86 | 0.56 |
| 4:M:260:LEU:HD23 | 4:M:449:VAL:HA | 1.85 | 0.56 |
| 4:M:358:ILE:O | 4:M:397:TRP:CE3 | 2.58 | 0.56 |
| 4:M:405:THR:CG2 | 4:M:406:GLY:N | 2.68 | 0.56 |
| 1:A:80:TYR:HB2 | 1:A:82:PHE:CD2 | 2.41 | 0.56 |
| 1:A:95:MET:SD | 1:A:107:TYR:HD1 | 2.27 | 0.56 |
| 1:A:110:ALA:O | 1:A:111:SER:C | 2.34 | 0.56 |
| 1:A:166:LEU:HD12 | 1:A:185:LEU:HD23 | 1.87 | 0.56 |
| 1:A:196:LEU:O | 1:A:197:ARG:O | 2.22 | 0.56 |
| 1:A:204:VAL:HG13 | 1:A:239:LEU:HD13 | 1.85 | 0.56 |
| 1:A:477:PHE:CZ | 1:A:491:THR:HB | 2.40 | 0.56 |
| 2:B:73:ASP:OD1 | 4:M:19:LEU:HD22 | 2.04 | 0.56 |
| 2:B:212:VAL:CG2 | 2:B:248:LEU:HD23 | 2.36 | 0.56 |
| 2:B:329:ALA:O | 2:B:330:SER:C | 2.33 | 0.56 |
| 2:B:481:LYS:C | 2:B:483:PRO:HD3 | 2.25 | 0.56 |
| 3:S:16:LEU:HD13 | 3:S:129:GLU:HG2 | 1.88 | 0.56 |
| 4:M:5:PHE:CE2 | 4:M:20:LEU:HD11 | 2.38 | 0.56 |
| 4:M:66:PHE:HB3 | 4:M:77:LEU:HD11 | 1.88 | 0.56 |
| 1:A:92:LEU:HD23 | 1:A:95:MET:CE | 2.33 | 0.56 |
| 1:A:128:LEU:HD13 | 1:A:150:LEU:CG | 2.35 | 0.56 |
| 1:A:594:PHE:CZ | 2:B:477:MET:HE1 | 2.40 | 0.56 |
| 2:B:83:PHE:HE1 | 2:B:87:VAL:HG21 | 1.69 | 0.56 |
| 2:B:123:LEU:HD22 | 2:B:138:ALA:HA | 1.87 | 0.56 |
| 2:B:132:SER:HB2 | 2:B:169:VAL:CG2 | 2.36 | 0.56 |
| 2:B:252:LEU:HB3 | 2:B:302:PHE:CD1 | 2.40 | 0.56 |
| 2:B:497:LEU:HB2 | 2:B:511:ILE:HG21 | 1.88 | 0.56 |
| 3:S:8:PHE:CD1 | 3:S:84:TYR:O | 2.58 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:M:223:HIS:CD2 | 4:M:478:ASN:CA | 2.87 | 0.56 |
| 4:M:242:GLY:HA3 | 4:M:444:ALA:HB2 | 1.86 | 0.56 |
| 1:A:63:ASP:OD1 | 1:A:64:LEU:N | 2.39 | 0.56 |
| 2:B:68:SER:HA | 4:M:18:TYR:CE1 | 2.41 | 0.56 |
| 2:B:72:SER:HA | 4:M:17:GLN:CD | 2.18 | 0.56 |
| 2:B:325:LEU:CD1 | 2:B:339:PHE:CD1 | 2.88 | 0.56 |
| 2:B:560:ILE:O | 2:B:563:PHE:N | 2.35 | 0.56 |
| 3:S:1:MET:SD | 3:S:20:TYR:CD2 | 2.99 | 0.56 |
| 3:S:55:PRO:O | 3:S:58:LEU:HB2 | 2.06 | 0.56 |
| 4:M:121:ILE:HG23 | 4:M:125:PHE:CE1 | 2.41 | 0.56 |
| 4:M:270:PRO:N | 4:M:302:TYR:CD2 | 2.74 | 0.56 |
| 1:A:213:SER:HB3 | 3:S:142:ILE:C | 2.26 | 0.56 |
| 1:A:481:MET:HE2 | 1:A:518:CYS:HB3 | 1.88 | 0.56 |
| 2:B:347:VAL:HG11 | 2:B:381:PHE:CD1 | 2.40 | 0.56 |
| 2:B:349:MET:CG | 4:M:305:ASP:HB2 | 2.33 | 0.56 |
| 3:S:55:PRO:HB3 | 3:S:71:GLU:HG3 | 1.88 | 0.56 |
| 4:M:256:VAL:O | 4:M:289:THR:HA | 2.05 | 0.56 |
| 1:A:88:ASN:HB2 | 1:A:120:ILE:CD1 | 2.36 | 0.56 |
| 1:A:499:ILE:HG12 | 1:A:512:LEU:HD23 | 1.88 | 0.56 |
| 1:A:638:LEU:HD11 | 2:B:557:SER:O | 2.05 | 0.56 |
| 2:B:50:LEU:CG | 2:B:62:ALA:HB2 | 2.36 | 0.56 |
| 2:B:124:GLN:OE1 | 2:B:153:ILE:CG2 | 2.53 | 0.56 |
| 2:B:400:SER:CB | 2:B:435:SER:CB | 2.56 | 0.56 |
| 3:S:8:PHE:CE1 | 3:S:84:TYR:O | 2.59 | 0.56 |
| 4:M:214:LEU:C | 4:M:467:TYR:HB3 | 2.26 | 0.56 |
| 4:M:360:LEU:CD1 | 4:M:433:VAL:HB | 2.36 | 0.56 |
| 1:A:140:VAL:HA | 1:A:177:ILE:CG1 | 2.36 | 0.56 |
| 1:A:200:PHE:HZ | 1:A:236:LEU:CD2 | 2.14 | 0.56 |
| 1:A:353:ASP:OD1 | 1:A:378:ILE:HD12 | 2.05 | 0.56 |
| 1:A:485:PRO:O | 1:A:488:ARG:HG3 | 2.06 | 0.56 |
| 1:A:513:ARG:CG | 1:A:547:VAL:HG22 | 2.36 | 0.56 |
| 1:A:638:LEU:CD2 | 2:B:561:ASP:CB | 2.83 | 0.56 |
| 2:B:109:ALA:C | 2:B:111:ASN:N | 2.55 | 0.56 |
| 2:B:256:CYS:SG | 2:B:299:LEU:HD21 | 2.45 | 0.56 |
| 2:B:304:GLN:O | 2:B:307:ASN:HB2 | 2.06 | 0.56 |
| 2:B:475:ILE:CG2 | 2:B:489:ILE:HG22 | 2.34 | 0.56 |
| 3:S:53:THR:C | 3:S:69:ASN:HB2 | 2.26 | 0.56 |
| 4:M:20:LEU:C | 4:M:21:GLY:O | 2.37 | 0.56 |
| 4:M:74:TYR:CG | 4:M:114:ILE:HD11 | 2.40 | 0.56 |
| 4:M:347:PHE:CD2 | 4:M:350:VAL:HB | 2.41 | 0.56 |
| 1:A:329:ASN:H | 3:S:50:PHE:HE2 | 1.48 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:505:ASN:O | 1:A:506:LYS:C | 2.38 | 0.56 |
| 1:A:606:PHE:CE1 | 1:A:633:PHE:CA | 2.88 | 0.56 |
| 2:B:73:ASP:OD1 | 4:M:19:LEU:CG | 2.53 | 0.56 |
| 2:B:79:VAL:C | 2:B:108:PHE:CE2 | 2.75 | 0.56 |
| 2:B:106:LEU:HG | 4:M:130:GLU:CD | 2.25 | 0.56 |
| 2:B:596:LEU:HA | 2:B:611:ALA:HB1 | 1.88 | 0.56 |
| 3:S:49:SER:O | 3:S:77:TYR:N | 2.39 | 0.56 |
| 4:M:15:ILE:CG2 | 4:M:114:ILE:CG2 | 2.79 | 0.56 |
| 4:M:462:LYS:O | 4:M:464:THR:N | 2.31 | 0.56 |
| 1:A:220:SER:O | 1:A:223:CYS:CB | 2.48 | 0.55 |
| 1:A:566:PHE:O | 1:A:569:ASP:O | 2.23 | 0.55 |
| 1:A:582:ILE:HG12 | 1:A:607:LEU:HB2 | 1.88 | 0.55 |
| 2:B:162:VAL:CG2 | 2:B:199:LEU:CD1 | 2.77 | 0.55 |
| 2:B:189:HIS:CD2 | 2:B:222:HIS:CG | 2.93 | 0.55 |
| 2:B:344:VAL:CG2 | 2:B:374:PHE:CE1 | 2.83 | 0.55 |
| 2:B:392:SER:HB3 | 2:B:424:PHE:HE1 | 1.71 | 0.55 |
| 2:B:476:ARG:HD2 | 2:B:513:TRP:CD1 | 2.41 | 0.55 |
| 4:M:319:SER:OG | 4:M:345:GLU:N | 2.39 | 0.55 |
| 4:M:434:SER:HB3 | 4:M:478:ASN:CG | 2.27 | 0.55 |
| 1:A:84:MET:HB3 | 1:A:113:SER:CB | 2.36 | 0.55 |
| 1:A:260:PHE:O | 1:A:261:THR:O | 2.21 | 0.55 |
| 1:A:594:PHE:CZ | 2:B:477:MET:SD | 2.93 | 0.55 |
| 2:B:12:LEU:HD22 | 4:M:13:LYS:HG3 | 1.88 | 0.55 |
| 2:B:67:ILE:CG2 | 4:M:18:TYR:OH | 2.54 | 0.55 |
| 2:B:68:SER:O | 4:M:18:TYR:HD1 | 1.88 | 0.55 |
| 2:B:83:PHE:CZ | 2:B:105:LEU:HG | 2.40 | 0.55 |
| 2:B:437:SER:HB2 | 2:B:474:VAL:HG22 | 1.88 | 0.55 |
| 2:B:534:ILE:HG21 | 2:B:594:ALA:CB | 2.37 | 0.55 |
| 4:M:240:ILE:HB | 4:M:304:VAL:CG1 | 2.35 | 0.55 |
| 4:M:323:MET:CB | 4:M:340:LEU:HD11 | 2.30 | 0.55 |
| 1:A:403:LEU:HD23 | 1:A:422:GLU:HG3 | 1.87 | 0.55 |
| 1:A:581:LEU:CG | 1:A:585:PHE:CZ | 2.90 | 0.55 |
| 2:B:123:LEU:HD22 | 2:B:138:ALA:CA | 2.36 | 0.55 |
| 2:B:399:LEU:HB3 | 2:B:411:ILE:HG23 | 1.88 | 0.55 |
| 4:M:69:ILE:CB | 4:M:97:ASP:OD2 | 2.54 | 0.55 |
| 4:M:114:ILE:O | 4:M:115:VAL:C | 2.45 | 0.55 |
| 4:M:224:VAL:O | 4:M:479:PHE:CB | 2.54 | 0.55 |
| 4:M:327:PHE:HE1 | 4:M:336:ASP:CB | 2.17 | 0.55 |
| 1:A:170:LEU:O | 1:A:206:LYS:HD2 | 2.07 | 0.55 |
| 1:A:219:VAL:CG1 | 1:A:256:LEU:HD23 | 2.36 | 0.55 |
| 1:A:605:GLU:HB2 | 1:A:636:TYR:HE2 | 1.72 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:29:LYS:HG3 | 2:B:29:LYS:O | 2.06 | 0.55 |
| 2:B:107:ARG:CZ | 4:M:20:LEU:CD2 | 2.33 | 0.55 |
| 2:B:309:LEU:HD12 | 2:B:317:VAL:HG11 | 1.88 | 0.55 |
| 2:B:363:ILE:HD12 | 2:B:374:PHE:CD1 | 2.41 | 0.55 |
| 2:B:490:ILE:HG13 | 2:B:518:ILE:HG12 | 1.88 | 0.55 |
| 3:S:35:VAL:O | 3:S:39:ILE:HG12 | 2.06 | 0.55 |
| 4:M:243:ILE:CG1 | 4:M:473:LYS:O | 2.54 | 0.55 |
| 4:M:478:ASN:C | 4:M:479:PHE:O | 2.44 | 0.55 |
| 1:A:107:TYR:CE1 | 1:A:128:LEU:HD23 | 2.40 | 0.55 |
| 1:A:121:LEU:HD23 | 1:A:121:LEU:C | 2.27 | 0.55 |
| 1:A:233:PHE:O | 1:A:235:GLN:N | 2.36 | 0.55 |
| 1:A:240:LEU:C | 1:A:242:GLU:O | 2.44 | 0.55 |
| 1:A:320:HIS:O | 1:A:322:PHE:N | 2.39 | 0.55 |
| 1:A:488:ARG:HD2 | 1:A:522:PHE:CD2 | 2.41 | 0.55 |
| 3:S:53:THR:CG2 | 3:S:67:GLU:O | 2.55 | 0.55 |
| 4:M:45:SER:O | 4:M:75:TRP:HZ2 | 1.89 | 0.55 |
| 4:M:253:ASN:N | 4:M:254:PRO:CD | 2.69 | 0.55 |
| 4:M:316:ARG:HG3 | 4:M:322:LEU:CD1 | 2.36 | 0.55 |
| 4:M:424:PHE:CZ | 4:M:428:VAL:CG2 | 2.89 | 0.55 |
| 4:M:424:PHE:HZ | 4:M:428:VAL:HG23 | 1.70 | 0.55 |
| 1:A:121:LEU:HG | 1:A:158:LEU:HD22 | 1.87 | 0.55 |
| 1:A:132:LEU:O | 1:A:133:LYS:C | 2.43 | 0.55 |
| 1:A:477:PHE:CE2 | 1:A:491:THR:HB | 2.42 | 0.55 |
| 1:A:625:LEU:CD1 | 1:A:629:LEU:HB2 | 2.36 | 0.55 |
| 2:B:12:LEU:HB3 | 4:M:13:LYS:CE | 2.36 | 0.55 |
| 2:B:37:TYR:O | 2:B:38:TYR:C | 2.44 | 0.55 |
| 2:B:317:VAL:O | 2:B:321:CYS:SG | 2.59 | 0.55 |
| 2:B:377:TYR:O | 2:B:380:LYS:CB | 2.53 | 0.55 |
| 4:M:69:ILE:HD12 | 4:M:94:GLU:N | 2.21 | 0.55 |
| 1:A:275:LEU:O | 1:A:277:LYS:N | 2.38 | 0.55 |
| 1:A:405:THR:O | 2:B:7:ARG:NH2 | 2.39 | 0.55 |
| 1:A:405:THR:C | 2:B:7:ARG:NH2 | 2.58 | 0.55 |
| 2:B:5:ILE:HD13 | 4:M:42:LEU:CD1 | 2.25 | 0.55 |
| 2:B:64:LYS:HZ2 | 4:M:120:ARG:HH12 | 1.45 | 0.55 |
| 2:B:219:TYR:CE2 | 2:B:226:LEU:CA | 2.77 | 0.55 |
| 2:B:347:VAL:CB | 2:B:381:PHE:HE1 | 2.13 | 0.55 |
| 2:B:390:VAL:HG12 | 2:B:394:TRP:CD1 | 2.41 | 0.55 |
| 2:B:418:TYR:CZ | 2:B:432:ALA:CB | 2.88 | 0.55 |
| 3:S:38:LEU:HB3 | 3:S:51:LEU:HD13 | 1.89 | 0.55 |
| 4:M:65:TYR:CD2 | 4:M:86:PRO:HA | 2.42 | 0.55 |
| 4:M:69:ILE:HG12 | 4:M:90:PHE:CE1 | 2.42 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:M:92:PHE:CE2 | 4:M:128:CYS:CB | 2.90 | 0.55 |
| 4:M:258:VAL:CG1 | 4:M:449:VAL:HG22 | 2.37 | 0.55 |
| 1:A:158:LEU:HG | 1:A:162:ILE:HD11 | 1.87 | 0.55 |
| 1:A:180:LYS:HZ3 | 3:S:137:GLN:HB2 | 1.71 | 0.55 |
| 1:A:185:LEU:CB | 1:A:203:PHE:CE1 | 2.89 | 0.55 |
| 1:A:203:PHE:CE2 | 1:A:221:VAL:HG11 | 2.41 | 0.55 |
| 1:A:244:LEU:HD13 | 1:A:256:LEU:HB2 | 1.87 | 0.55 |
| 2:B:185:LYS:CE | 2:B:221:ASP:OD2 | 2.54 | 0.55 |
| 2:B:276:SER:C | 2:B:295:ASN:CB | 2.72 | 0.55 |
| 2:B:308:CYS:O | 2:B:311:TYR:N | 2.40 | 0.55 |
| 2:B:472:VAL:HG11 | 2:B:510:GLY:C | 2.26 | 0.55 |
| 3:S:48:SER:HG | 3:S:50:PHE:N | 2.00 | 0.55 |
| 4:M:244:VAL:CB | 4:M:472:TYR:CE2 | 2.90 | 0.55 |
| 4:M:305:ASP:O | 4:M:307:SER:N | 2.39 | 0.55 |
| 4:M:386:PHE:HB2 | 4:M:397:TRP:CD1 | 2.42 | 0.55 |
| 1:A:104:ARG:HG3 | 1:A:145:ILE:HG13 | 1.89 | 0.55 |
| 1:A:245:VAL:O | 1:A:245:VAL:HG22 | 2.07 | 0.55 |
| 2:B:318:ILE:CD1 | 2:B:346:THR:HG23 | 2.37 | 0.55 |
| 2:B:418:TYR:HD1 | 2:B:424:PHE:CD2 | 2.25 | 0.55 |
| 2:B:453:TRP:HA | 2:B:453:TRP:CE3 | 2.42 | 0.55 |
| 2:B:518:ILE:O | 2:B:518:ILE:CG1 | 2.54 | 0.55 |
| 3:S:15:ARG:CZ | 3:S:122:ILE:HD11 | 2.37 | 0.55 |
| 3:S:53:THR:HG1 | 3:S:68:VAL:C | 2.09 | 0.55 |
| 4:M:16:PHE:HD1 | 4:M:118:TYR:CE2 | 2.25 | 0.55 |
| 4:M:262:THR:C | 4:M:264:GLY:N | 2.44 | 0.55 |
| 4:M:316:ARG:HG2 | 4:M:322:LEU:HD13 | 1.88 | 0.55 |
| 1:A:244:LEU:HD23 | 1:A:277:LYS:HG3 | 1.88 | 0.55 |
| 1:A:408:ILE:HA | 3:S:64:ASN:HB2 | 1.87 | 0.55 |
| 1:A:581:LEU:HB3 | 1:A:607:LEU:CD1 | 2.35 | 0.55 |
| 2:B:120:ILE:CD1 | 2:B:142:LEU:CD2 | 2.84 | 0.55 |
| 2:B:291:TYR:CD2 | 2:B:294:VAL:HB | 2.42 | 0.55 |
| 2:B:346:THR:O | 2:B:349:MET:HB2 | 2.06 | 0.55 |
| 2:B:563:PHE:CD1 | 2:B:584:SER:HB3 | 2.31 | 0.55 |
| 3:S:4:ALA:CA | 3:S:18:LYS:O | 2.50 | 0.55 |
| 4:M:220:GLU:CD | 4:M:439:TYR:CD2 | 2.57 | 0.55 |
| 4:M:260:LEU:CD2 | 4:M:449:VAL:CG2 | 2.81 | 0.55 |
| 4:M:290:PHE:HZ | 4:M:293:PRO:CG | 2.20 | 0.55 |
| 1:A:292:TYR:CD1 | 1:A:292:TYR:C | 2.79 | 0.54 |
| 1:A:516:ILE:HG21 | 1:A:551:LEU:HA | 1.88 | 0.54 |
| 1:A:581:LEU:CD2 | 1:A:607:LEU:HD21 | 2.32 | 0.54 |
| 2:B:20:ARG:NH1 | 4:M:118:TYR:CA | 2.57 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:171:GLY:HA3 | 2:B:207:VAL:HA | 1.89 | 0.54 |
| 2:B:398:ILE:HG23 | 2:B:402:LEU:HD11 | 1.87 | 0.54 |
| 3:S:7:ILE:O | 3:S:15:ARG:N | 2.38 | 0.54 |
| 4:M:54:SER:HB2 | 4:M:66:PHE:HE2 | 1.71 | 0.54 |
| 4:M:219:LEU:CG | 4:M:440:ILE:HG12 | 2.36 | 0.54 |
| 4:M:262:THR:HG23 | 4:M:265:ASN:O | 2.07 | 0.54 |
| 4:M:435:LEU:O | 4:M:437:TYR:CE1 | 2.60 | 0.54 |
| 1:A:102:GLN:HE22 | 3:S:166:LYS:NZ | 2.05 | 0.54 |
| 1:A:373:GLU:HG2 | 1:A:427:LYS:NZ | 2.22 | 0.54 |
| 1:A:436:CYS:HB3 | 1:A:476:GLN:NE2 | 2.22 | 0.54 |
| 1:A:484:VAL:O | 1:A:486:SER:O | 2.25 | 0.54 |
| 1:A:584:PHE:O | 1:A:587:ASN:N | 2.40 | 0.54 |
| 2:B:17:VAL:HG23 | 2:B:36:THR:HA | 1.88 | 0.54 |
| 2:B:28:SER:HA | 2:B:58:GLU:CG | 2.37 | 0.54 |
| 2:B:38:TYR:CE2 | 2:B:43:ASN:H | 1.61 | 0.54 |
| 2:B:537:PHE:CD1 | 2:B:598:LEU:HB3 | 2.42 | 0.54 |
| 2:B:537:PHE:HE2 | 2:B:545:ARG:HB3 | 1.67 | 0.54 |
| 2:B:563:PHE:CE2 | 2:B:588:ILE:HD12 | 2.42 | 0.54 |
| 3:S:17:VAL:HG21 | 3:S:19:PHE:CE1 | 2.39 | 0.54 |
| 3:S:50:PHE:O | 3:S:51:LEU:HD23 | 2.07 | 0.54 |
| 3:S:60:SER:O | 3:S:66:ASP:HB2 | 2.07 | 0.54 |
| 4:M:7:ILE:HG13 | 4:M:16:PHE:HD2 | 1.72 | 0.54 |
| 4:M:242:GLY:O | 4:M:302:TYR:N | 2.38 | 0.54 |
| 4:M:469:GLY:O | 4:M:470:ALA:C | 2.44 | 0.54 |
| 1:A:150:LEU:HB3 | 1:A:162:ILE:HD13 | 1.89 | 0.54 |
| 1:A:438:ALA:O | 1:A:441:TYR:HD1 | 1.91 | 0.54 |
| 2:B:79:VAL:CG2 | 2:B:108:PHE:CE2 | 2.81 | 0.54 |
| 2:B:188:TYR:HB3 | 2:B:192:LEU:HD13 | 1.87 | 0.54 |
| 2:B:375:LEU:CG | 2:B:404:ASN:HB2 | 2.37 | 0.54 |
| 2:B:453:TRP:HA | 2:B:453:TRP:HE3 | 1.72 | 0.54 |
| 3:S:53:THR:CB | 3:S:68:VAL:CA | 2.82 | 0.54 |
| 4:M:45:SER:HB2 | 4:M:75:TRP:CE2 | 2.42 | 0.54 |
| 1:A:288:THR:CG2 | 3:S:96:LEU:HD21 | 2.27 | 0.54 |
| 1:A:462:GLN:HG3 | 4:M:59:ASP:CG | 1.94 | 0.54 |
| 2:B:106:LEU:HB3 | 4:M:130:GLU:HG3 | 1.88 | 0.54 |
| 2:B:392:SER:HB3 | 2:B:424:PHE:CE1 | 2.42 | 0.54 |
| 2:B:408:VAL:CG1 | 2:B:446:TRP:HB3 | 2.38 | 0.54 |
| 2:B:439:CYS:C | 2:B:441:GLN:N | 2.60 | 0.54 |
| 2:B:578:PRO:CD | 2:B:581:TYR:CD2 | 2.73 | 0.54 |
| 4:M:259:LYS:O | 4:M:450:GLU:N | 2.41 | 0.54 |
| 4:M:352:GLN:CG | 4:M:440:ILE:HB | 2.36 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:585:PHE:CD2 | 1:A:603:VAL:HG12 | 2.40 | 0.54 |
| 1:A:594:PHE:CZ | 2:B:477:MET:CE | 2.90 | 0.54 |
| 2:B:230:PHE:HD1 | 2:B:298:ASP:CB | 2.18 | 0.54 |
| 2:B:310:ILE:CG1 | 2:B:321:CYS:HB2 | 2.38 | 0.54 |
| 2:B:522:GLU:C | 2:B:524:LYS:H | 2.09 | 0.54 |
| 4:M:51:LEU:HD22 | 4:M:68:VAL:HG11 | 1.88 | 0.54 |
| 4:M:325:LEU:HD23 | 4:M:325:LEU:O | 2.07 | 0.54 |
| 4:M:436:GLU:HA | 4:M:479:PHE:CD1 | 2.42 | 0.54 |
| 1:A:71:VAL:HG11 | 1:A:105:VAL:HG12 | 1.88 | 0.54 |
| 1:A:244:LEU:CD1 | 1:A:281:LEU:HD11 | 2.36 | 0.54 |
| 1:A:532:LEU:O | 1:A:533:ILE:O | 2.25 | 0.54 |
| 2:B:24:ALA:CB | 2:B:32:GLU:CG | 2.72 | 0.54 |
| 2:B:73:ASP:HA | 2:B:75:ASP:OD1 | 2.08 | 0.54 |
| 2:B:73:ASP:HA | 4:M:24:ALA:HB3 | 1.89 | 0.54 |
| 2:B:83:PHE:CE2 | 2:B:105:LEU:HA | 2.43 | 0.54 |
| 2:B:97:VAL:HG12 | 2:B:101:ILE:HD12 | 1.89 | 0.54 |
| 2:B:191:GLU:C | 2:B:193:LEU:H | 2.11 | 0.54 |
| 2:B:313:SER:HB3 | 4:M:269:ILE:CA | 2.36 | 0.54 |
| 2:B:351:GLU:CB | 4:M:476:THR:HG22 | 2.32 | 0.54 |
| 2:B:374:PHE:O | 2:B:374:PHE:CD2 | 2.60 | 0.54 |
| 4:M:96:ILE:HG23 | 4:M:125:PHE:HE1 | 1.61 | 0.54 |
| 4:M:213:GLU:CB | 4:M:467:TYR:HB2 | 2.37 | 0.54 |
| 4:M:319:SER:O | 4:M:323:MET:SD | 2.65 | 0.54 |
| 1:A:488:ARG:HG2 | 1:A:522:PHE:CE2 | 2.43 | 0.54 |
| 1:A:606:PHE:HE1 | 1:A:633:PHE:N | 2.06 | 0.54 |
| 2:B:293:VAL:HA | 2:B:299:LEU:HB2 | 1.88 | 0.54 |
| 2:B:343:LEU:HD21 | 2:B:363:ILE:N | 2.23 | 0.54 |
| 2:B:398:ILE:HG22 | 2:B:402:LEU:HD12 | 1.89 | 0.54 |
| 3:S:46:PHE:O | 3:S:47:GLN:C | 2.24 | 0.54 |
| 4:M:215:TYR:O | 4:M:246:VAL:CG1 | 2.54 | 0.54 |
| 4:M:253:ASN:OD1 | 4:M:292:PRO:CD | 2.56 | 0.54 |
| 4:M:279:ASN:ND2 | 4:M:283:PHE:CE2 | 2.76 | 0.54 |
| 1:A:323:CYS:HG | 1:A:338:PHE:HE2 | 1.54 | 0.54 |
| 1:A:416:ILE:O | 1:A:417:PRO:C | 2.41 | 0.54 |
| 2:B:86:VAL:CG1 | 2:B:101:ILE:HG23 | 2.31 | 0.54 |
| 2:B:170:ARG:HH12 | 2:B:198:GLU:HG2 | 1.73 | 0.54 |
| 2:B:214:ALA:O | 2:B:216:LYS:N | 2.41 | 0.54 |
| 2:B:418:TYR:CD1 | 2:B:419:VAL:CA | 2.91 | 0.54 |
| 2:B:430:ILE:HD13 | 2:B:466:SER:HB3 | 1.89 | 0.54 |
| 3:S:112:CYS:HB2 | 3:S:113:PHE:CE1 | 2.43 | 0.54 |
| 4:M:19:LEU:CD2 | 4:M:24:ALA:HB3 | 2.37 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:M:47:SER:C | 4:M:49:ASP:H | 2.06 | 0.54 |
| 4:M:137:SER:O | 4:M:138:ASP:C | 2.45 | 0.54 |
| 4:M:270:PRO:CA | 4:M:302:TYR:HD2 | 2.21 | 0.54 |
| 4:M:272:LEU:HD12 | 4:M:272:LEU:N | 2.22 | 0.54 |
| 1:A:365:VAL:HG11 | 3:S:63:ASN:HB3 | 1.90 | 0.54 |
| 1:A:455:MET:HG2 | 1:A:498:LEU:HD11 | 1.90 | 0.54 |
| 1:A:628:VAL:O | 1:A:631:SER:OG | 2.07 | 0.54 |
| 2:B:155:LEU:HD13 | 2:B:155:LEU:C | 2.28 | 0.54 |
| 2:B:422:ALA:HB3 | 2:B:424:PHE:CZ | 2.39 | 0.54 |
| 2:B:429:VAL:HG11 | 2:B:467:VAL:HG11 | 1.89 | 0.54 |
| 2:B:522:GLU:C | 2:B:524:LYS:N | 2.60 | 0.54 |
| 2:B:566:ALA:HB2 | 2:B:581:TYR:CG | 2.42 | 0.54 |
| 3:S:8:PHE:CZ | 3:S:84:TYR:HB3 | 2.41 | 0.54 |
| 3:S:57:LEU:HD23 | 3:S:66:ASP:HA | 1.90 | 0.54 |
| 4:M:20:LEU:CD1 | 4:M:129:VAL:HG21 | 2.37 | 0.54 |
| 4:M:41:LEU:CD1 | 4:M:52:ASP:HB2 | 2.38 | 0.54 |
| 4:M:338:PHE:CE1 | 4:M:415:ILE:CG1 | 2.90 | 0.54 |
| 4:M:390:ILE:O | 4:M:393:GLY:N | 2.41 | 0.54 |
| 1:A:306:GLU:O | 1:A:307:ASP:C | 2.38 | 0.54 |
| 1:A:552:ILE:O | 1:A:556:VAL:HG23 | 2.08 | 0.54 |
| 2:B:87:VAL:O | 2:B:90:ILE:HG22 | 2.07 | 0.54 |
| 2:B:106:LEU:HD21 | 4:M:131:ALA:N | 2.23 | 0.54 |
| 2:B:120:ILE:HG23 | 2:B:142:LEU:HD22 | 1.90 | 0.54 |
| 2:B:285:GLU:C | 2:B:286:ILE:O | 2.24 | 0.54 |
| 2:B:292:GLU:HG3 | 2:B:296:ASP:CB | 2.37 | 0.54 |
| 2:B:340:ILE:HD11 | 2:B:366:LEU:HB3 | 1.90 | 0.54 |
| 2:B:549:LEU:HD22 | 2:B:607:ILE:O | 2.07 | 0.54 |
| 4:M:100:LEU:HD11 | 4:M:121:ILE:HG23 | 1.90 | 0.54 |
| 4:M:270:PRO:CB | 4:M:288:ILE:HD11 | 2.38 | 0.54 |
| 1:A:155:THR:O | 1:A:158:LEU:HB3 | 2.08 | 0.53 |
| 1:A:312:ALA:O | 1:A:315:CYS:HB2 | 2.08 | 0.53 |
| 2:B:16:LYS:NZ | 4:M:111:ILE:HG13 | 2.12 | 0.53 |
| 2:B:154:ILE:O | 2:B:157:THR:HB | 2.08 | 0.53 |
| 2:B:398:ILE:O | 2:B:399:LEU:C | 2.46 | 0.53 |
| 2:B:482:ASN:N | 2:B:483:PRO:HD3 | 2.23 | 0.53 |
| 2:B:494:ALA:HB2 | 2:B:515:PHE:CE2 | 2.44 | 0.53 |
| 2:B:534:ILE:O | 2:B:535:GLN:C | 2.46 | 0.53 |
| 2:B:562:ASN:ND2 | 2:B:580:TYR:HD2 | 2.06 | 0.53 |
| 3:S:58:LEU:HD22 | 3:S:70:ASN:HA | 1.89 | 0.53 |
| 4:M:104:PHE:N | 4:M:104:PHE:CD1 | 2.64 | 0.53 |
| 4:M:223:HIS:NE2 | 4:M:436:GLU:CB | 2.71 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:M:323:MET:CE | 4:M:437:TYR:HE2 | 2.21 | 0.53 |
| 1:A:223:CYS:HB2 | 1:A:259:LEU:HD12 | 1.90 | 0.53 |
| 1:A:332:TYR:CE2 | 1:A:336:ILE:CD1 | 2.91 | 0.53 |
| 1:A:562:TRP:O | 1:A:566:PHE:N | 2.41 | 0.53 |
| 1:A:638:LEU:O | 2:B:558:TYR:HA | 2.08 | 0.53 |
| 2:B:191:GLU:O | 2:B:193:LEU:N | 2.40 | 0.53 |
| 2:B:234:CYS:HB3 | 2:B:301:LEU:CB | 2.37 | 0.53 |
| 2:B:254:LYS:O | 2:B:257:LYS:N | 2.41 | 0.53 |
| 2:B:330:SER:O | 2:B:332:LEU:N | 2.41 | 0.53 |
| 2:B:349:MET:HG2 | 4:M:305:ASP:CB | 2.37 | 0.53 |
| 2:B:472:VAL:HG12 | 2:B:510:GLY:CA | 2.36 | 0.53 |
| 4:M:45:SER:O | 4:M:75:TRP:CZ2 | 2.61 | 0.53 |
| 4:M:218:LEU:HD21 | 4:M:449:VAL:HG23 | 1.91 | 0.53 |
| 1:A:264:SER:CB | 1:A:271:ARG:CG | 2.87 | 0.53 |
| 1:A:364:ASP:OD1 | 3:S:65:ASN:ND2 | 2.41 | 0.53 |
| 1:A:384:LEU:CD1 | 1:A:385:LYS:N | 2.71 | 0.53 |
| 1:A:395:PHE:CD2 | 1:A:428:MET:CE | 2.92 | 0.53 |
| 1:A:395:PHE:O | 1:A:396:VAL:C | 2.40 | 0.53 |
| 1:A:513:ARG:HG2 | 1:A:547:VAL:HA | 1.90 | 0.53 |
| 2:B:38:TYR:CD1 | 2:B:38:TYR:N | 2.74 | 0.53 |
| 2:B:132:SER:O | 2:B:133:GLU:C | 2.34 | 0.53 |
| 2:B:193:LEU:O | 2:B:229:HIS:CE1 | 2.61 | 0.53 |
| 2:B:367:SER:HB3 | 2:B:401:THR:OG1 | 2.08 | 0.53 |
| 2:B:513:TRP:CD1 | 2:B:517:GLU:CG | 2.91 | 0.53 |
| 2:B:523:PHE:O | 2:B:524:LYS:C | 2.42 | 0.53 |
| 3:S:6:LEU:HD21 | 3:S:36:TYR:CE2 | 2.43 | 0.53 |
| 3:S:68:VAL:O | 3:S:75:ILE:HD12 | 2.08 | 0.53 |
| 4:M:240:ILE:CG2 | 4:M:444:ALA:O | 2.55 | 0.53 |
| 4:M:347:PHE:CZ | 4:M:350:VAL:CG1 | 2.63 | 0.53 |
| 1:A:174:ARG:O | 1:A:177:ILE:HB | 2.09 | 0.53 |
| 1:A:481:MET:CE | 1:A:518:CYS:HB3 | 2.38 | 0.53 |
| 2:B:191:GLU:C | 2:B:193:LEU:N | 2.59 | 0.53 |
| 2:B:196:LEU:CB | 2:B:215:TYR:OH | 2.57 | 0.53 |
| 2:B:344:VAL:HG22 | 2:B:374:PHE:CD1 | 2.42 | 0.53 |
| 2:B:546:CYS:HA | 2:B:607:ILE:HG12 | 1.91 | 0.53 |
| 4:M:3:LEU:HA | 4:M:79:SER:O | 2.08 | 0.53 |
| 4:M:5:PHE:O | 4:M:18:TYR:N | 2.42 | 0.53 |
| 4:M:222:PHE:C | 4:M:479:PHE:HZ | 2.05 | 0.53 |
| 4:M:224:VAL:CG2 | 4:M:306:LEU:CD1 | 2.86 | 0.53 |
| 4:M:300:LEU:HD12 | 4:M:300:LEU:C | 2.29 | 0.53 |
| 1:A:338:PHE:HE1 | 1:A:352:PHE:CZ | 2.26 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:20:ARG:HH12 | 4:M:118:TYR:HB3 | 0.71 | 0.53 |
| 2:B:29:LYS:HB3 | 2:B:58:GLU:OE2 | 2.09 | 0.53 |
| 2:B:172:GLU:O | 2:B:174:ALA:N | 2.41 | 0.53 |
| 2:B:364:HIS:ND1 | 2:B:397:GLN:HB3 | 2.24 | 0.53 |
| 2:B:437:SER:HA | 2:B:474:VAL:HG13 | 1.83 | 0.53 |
| 2:B:469:ASP:CG | 2:B:506:ASN:CB | 2.67 | 0.53 |
| 2:B:513:TRP:NE1 | 2:B:517:GLU:HG2 | 2.23 | 0.53 |
| 3:S:35:VAL:CG1 | 3:S:75:ILE:HD13 | 2.39 | 0.53 |
| 4:M:5:PHE:CE2 | 4:M:92:PHE:CE1 | 2.97 | 0.53 |
| 4:M:6:TYR:N | 4:M:77:LEU:O | 2.33 | 0.53 |
| 4:M:15:ILE:CG2 | 4:M:115:VAL:HG23 | 2.34 | 0.53 |
| 4:M:71:LYS:O | 4:M:74:TYR:CE2 | 2.61 | 0.53 |
| 4:M:78:ALA:HB2 | 4:M:93:LEU:HG | 1.90 | 0.53 |
| 1:A:536:MET:HB3 | 1:A:555:LEU:HD21 | 1.89 | 0.53 |
| 2:B:178:ILE:HA | 2:B:218:CYS:HB2 | 1.91 | 0.53 |
| 2:B:374:PHE:HZ | 2:B:381:PHE:CG | 2.13 | 0.53 |
| 2:B:566:ALA:O | 2:B:574:ASN:HB3 | 2.08 | 0.53 |
| 4:M:12:ASN:OD1 | 4:M:42:LEU:HB3 | 2.09 | 0.53 |
| 4:M:93:LEU:O | 4:M:96:ILE:HB | 2.08 | 0.53 |
| 4:M:374:TYR:O | 4:M:390:ILE:CD1 | 2.48 | 0.53 |
| 4:M:424:PHE:CZ | 4:M:428:VAL:HG22 | 2.43 | 0.53 |
| 4:M:443:SER:CB | 4:M:447:ILE:C | 2.76 | 0.53 |
| 1:A:301:GLY:O | 1:A:302:ASN:CB | 2.53 | 0.53 |
| 1:A:446:ASP:CG | 1:A:448:GLU:O | 2.47 | 0.53 |
| 2:B:230:PHE:HZ | 2:B:302:PHE:HB2 | 1.72 | 0.53 |
| 2:B:260:LEU:CD2 | 2:B:293:VAL:HG11 | 2.39 | 0.53 |
| 2:B:309:LEU:O | 2:B:312:SER:HB3 | 2.08 | 0.53 |
| 2:B:310:ILE:CD1 | 2:B:321:CYS:CB | 2.78 | 0.53 |
| 2:B:344:VAL:HG22 | 2:B:381:PHE:HE2 | 1.74 | 0.53 |
| 3:S:16:LEU:HA | 3:S:125:TRP:HZ2 | 1.70 | 0.53 |
| 3:S:38:LEU:HB3 | 3:S:51:LEU:HD11 | 1.89 | 0.53 |
| 3:S:109:LEU:CD1 | 3:S:113:PHE:CD1 | 2.88 | 0.53 |
| 4:M:69:ILE:HD12 | 4:M:94:GLU:HA | 1.90 | 0.53 |
| 4:M:92:PHE:HZ | 4:M:125:PHE:O | 1.91 | 0.53 |
| 4:M:217:ASP:O | 4:M:472:TYR:CG | 2.62 | 0.53 |
| 4:M:221:THR:CA | 4:M:474:THR:OG1 | 2.55 | 0.53 |
| 4:M:262:THR:CG2 | 4:M:265:ASN:O | 2.57 | 0.53 |
| 4:M:443:SER:HA | 4:M:447:ILE:HG13 | 1.90 | 0.53 |
| 1:A:114:PHE:CE2 | 1:A:153:ILE:HA | 2.39 | 0.53 |
| 1:A:149:GLY:O | 1:A:152:THR:N | 2.42 | 0.53 |
| 1:A:516:ILE:CG2 | 1:A:554:ALA:HB2 | 2.39 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:532:LEU:O | 1:A:533:ILE:C | 2.30 | 0.53 |
| 2:B:17:VAL:CB | 2:B:35:TYR:CE2 | 2.91 | 0.53 |
| 2:B:127:LEU:HD22 | 2:B:157:THR:HG21 | 1.91 | 0.53 |
| 2:B:136:CYS:HB3 | 2:B:172:GLU:HG2 | 1.87 | 0.53 |
| 2:B:266:VAL:CG1 | 2:B:275:ARG:HB3 | 2.39 | 0.53 |
| 2:B:534:ILE:HG21 | 2:B:594:ALA:HB3 | 1.91 | 0.53 |
| 2:B:546:CYS:CA | 2:B:607:ILE:HG12 | 2.38 | 0.53 |
| 2:B:577:ASN:O | 2:B:578:PRO:C | 2.39 | 0.53 |
| 4:M:245:ASP:N | 4:M:472:TYR:CD2 | 2.71 | 0.53 |
| 4:M:261:ASN:CB | 4:M:450:GLU:HG2 | 2.34 | 0.53 |
| 1:A:379:VAL:HG11 | 1:A:441:TYR:HH | 1.74 | 0.53 |
| 1:A:566:PHE:HZ | 1:A:618:THR:O | 1.91 | 0.53 |
| 2:B:105:LEU:HB3 | 2:B:145:MET:CE | 2.39 | 0.53 |
| 2:B:253:ILE:HD11 | 2:B:324:ALA:HB2 | 1.90 | 0.53 |
| 2:B:371:GLN:OE1 | 2:B:442:LEU:HD11 | 2.08 | 0.53 |
| 2:B:408:VAL:HB | 2:B:446:TRP:CG | 2.44 | 0.53 |
| 2:B:435:SER:C | 2:B:437:SER:N | 2.60 | 0.53 |
| 4:M:5:PHE:CE2 | 4:M:20:LEU:HD13 | 2.43 | 0.53 |
| 4:M:432:THR:CB | 4:M:480:GLN:HG3 | 2.24 | 0.53 |
| 1:A:185:LEU:HD13 | 1:A:203:PHE:HE1 | 1.73 | 0.53 |
| 2:B:14:THR:OG1 | 2:B:40:GLN:CG | 2.57 | 0.53 |
| 2:B:34:SER:O | 2:B:37:TYR:CA | 2.57 | 0.53 |
| 2:B:103:LEU:CB | 4:M:126:ASN:HD22 | 1.95 | 0.53 |
| 2:B:151:ALA:HB1 | 2:B:188:TYR:CD2 | 2.43 | 0.53 |
| 2:B:174:ALA:HB3 | 2:B:211:ALA:HA | 1.83 | 0.53 |
| 2:B:177:ILE:HB | 2:B:196:LEU:HD21 | 1.91 | 0.53 |
| 2:B:293:VAL:HA | 2:B:299:LEU:CG | 2.37 | 0.53 |
| 3:S:131:VAL:O | 3:S:135:ILE:HG13 | 2.08 | 0.53 |
| 4:M:217:ASP:C | 4:M:472:TYR:CZ | 2.82 | 0.53 |
| 4:M:229:LYS:HG2 | 4:M:230:LYS:HG3 | 1.90 | 0.53 |
| 4:M:317:MET:CB | 4:M:320:ILE:O | 2.56 | 0.53 |
| 1:A:68:THR:CB | 3:S:166:LYS:CB | 2.71 | 0.52 |
| 1:A:95:MET:CB | 1:A:127:LEU:HD23 | 2.39 | 0.52 |
| 1:A:219:VAL:HG13 | 1:A:259:LEU:HD13 | 1.92 | 0.52 |
| 1:A:399:ASP:N | 1:A:418:ILE:CG1 | 2.72 | 0.52 |
| 2:B:38:TYR:C | 2:B:40:GLN:N | 2.62 | 0.52 |
| 2:B:100:LEU:HD23 | 4:M:123:LEU:HD11 | 1.91 | 0.52 |
| 2:B:133:GLU:HA | 2:B:168:MET:SD | 2.49 | 0.52 |
| 2:B:267:ASP:N | 2:B:276:SER:HB3 | 2.25 | 0.52 |
| 2:B:393:ILE:HG23 | 2:B:431:MET:CB | 2.39 | 0.52 |
| 2:B:416:LYS:HG3 | 2:B:457:HIS:CE1 | 2.43 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:515:PHE:HA | 2:B:518:ILE:HG22 | 1.92 | 0.52 |
| 3:S:131:VAL:HG22 | 3:S:153:VAL:CG2 | 2.36 | 0.52 |
| 4:M:51:LEU:CB | 4:M:68:VAL:CB | 2.87 | 0.52 |
| 4:M:96:ILE:CD1 | 4:M:125:PHE:CD1 | 2.83 | 0.52 |
| 4:M:224:VAL:O | 4:M:479:PHE:CA | 2.57 | 0.52 |
| 4:M:347:PHE:CE1 | 4:M:439:TYR:CD1 | 2.96 | 0.52 |
| 4:M:373:ALA:O | 4:M:417:TYR:HA | 2.08 | 0.52 |
| 4:M:428:VAL:O | 4:M:430:LEU:HA | 2.08 | 0.52 |
| 4:M:449:VAL:CG1 | 4:M:452:ILE:CG1 | 2.82 | 0.52 |
| 1:A:68:THR:CB | 3:S:166:LYS:CD | 2.87 | 0.52 |
| 1:A:104:ARG:HG3 | 1:A:145:ILE:CG1 | 2.39 | 0.52 |
| 1:A:104:ARG:HG3 | 1:A:145:ILE:HD12 | 1.90 | 0.52 |
| 1:A:301:GLY:O | 1:A:302:ASN:HB3 | 2.09 | 0.52 |
| 2:B:35:TYR:C | 2:B:37:TYR:N | 2.63 | 0.52 |
| 2:B:37:TYR:O | 2:B:40:GLN:C | 2.48 | 0.52 |
| 2:B:89:ASN:C | 2:B:101:ILE:HD11 | 2.29 | 0.52 |
| 2:B:236:ILE:O | 2:B:239:GLN:HB2 | 2.09 | 0.52 |
| 2:B:259:TYR:HD1 | 2:B:261:PRO:CB | 2.21 | 0.52 |
| 2:B:303:LEU:HD22 | 2:B:339:PHE:HZ | 1.63 | 0.52 |
| 2:B:307:ASN:ND2 | 2:B:338:LYS:CB | 2.72 | 0.52 |
| 2:B:328:LEU:O | 2:B:330:SER:N | 2.42 | 0.52 |
| 2:B:592:TYR:CD2 | 2:B:618:PHE:CE2 | 2.97 | 0.52 |
| 3:S:49:SER:O | 3:S:77:TYR:CA | 2.57 | 0.52 |
| 4:M:222:PHE:HA | 4:M:240:ILE:HA | 1.91 | 0.52 |
| 4:M:277:GLU:N | 4:M:289:THR:O | 2.38 | 0.52 |
| 4:M:374:TYR:HE1 | 4:M:393:GLY:CA | 2.21 | 0.52 |
| 1:A:326:GLN:O | 1:A:328:PRO:HD3 | 2.09 | 0.52 |
| 1:A:409:VAL:HG22 | 1:A:410:TYR:N | 2.25 | 0.52 |
| 2:B:14:THR:HB | 2:B:40:GLN:HE21 | 1.74 | 0.52 |
| 2:B:143:SER:O | 2:B:179:LYS:HD3 | 2.06 | 0.52 |
| 2:B:158:VAL:CG1 | 2:B:177:ILE:HD11 | 2.39 | 0.52 |
| 2:B:302:PHE:HE1 | 2:B:306:LEU:HD21 | 1.74 | 0.52 |
| 2:B:374:PHE:CZ | 2:B:398:ILE:HG21 | 2.44 | 0.52 |
| 2:B:429:VAL:O | 2:B:433:VAL:HG23 | 2.09 | 0.52 |
| 2:B:437:SER:CB | 2:B:474:VAL:CG1 | 2.40 | 0.52 |
| 2:B:537:PHE:CZ | 2:B:545:ARG:HG2 | 2.45 | 0.52 |
| 3:S:49:SER:O | 3:S:77:TYR:CB | 2.57 | 0.52 |
| 4:M:6:TYR:HD2 | 4:M:17:GLN:CG | 2.19 | 0.52 |
| 4:M:48:ASP:O | 4:M:70:ASN:CB | 2.44 | 0.52 |
| 1:A:69:ASN:OD1 | 3:S:166:LYS:O | 2.27 | 0.52 |
| 1:A:92:LEU:HD13 | 1:A:123:LEU:HD13 | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:24:ALA:O | 2:B:27:THR:OG1 | 2.25 | 0.52 |
| 2:B:25:VAL:CG2 | 2:B:30:LEU:O | 2.33 | 0.52 |
| 2:B:195:ILE:C | 2:B:197:LYS:N | 2.60 | 0.52 |
| 2:B:215:TYR:HB3 | 2:B:226:LEU:CD1 | 2.40 | 0.52 |
| 2:B:383:VAL:O | 2:B:383:VAL:HG13 | 2.09 | 0.52 |
| 2:B:527:PRO:HB3 | 2:B:587:ARG:CG | 2.38 | 0.52 |
| 2:B:553:ALA:O | 2:B:556:LEU:HB2 | 2.09 | 0.52 |
| 4:M:267:ILE:HG23 | 4:M:445:SER:OG | 2.10 | 0.52 |
| 1:A:185:LEU:CD1 | 1:A:203:PHE:HE1 | 2.22 | 0.52 |
| 1:A:516:ILE:HD13 | 1:A:551:LEU:HB2 | 1.91 | 0.52 |
| 2:B:178:ILE:HD11 | 2:B:215:TYR:CA | 2.37 | 0.52 |
| 2:B:212:VAL:C | 2:B:214:ALA:N | 2.57 | 0.52 |
| 2:B:230:PHE:CZ | 2:B:302:PHE:HB2 | 2.45 | 0.52 |
| 2:B:234:CYS:CB | 2:B:301:LEU:CB | 2.88 | 0.52 |
| 2:B:239:GLN:HA | 4:M:279:ASN:C | 2.30 | 0.52 |
| 2:B:252:LEU:O | 2:B:328:LEU:HD21 | 2.10 | 0.52 |
| 2:B:293:VAL:O | 2:B:299:LEU:HD11 | 1.94 | 0.52 |
| 2:B:310:ILE:HG22 | 2:B:342:ALA:CB | 2.31 | 0.52 |
| 2:B:333:GLN:O | 2:B:336:ASN:N | 2.33 | 0.52 |
| 4:M:245:ASP:O | 4:M:472:TYR:OH | 2.28 | 0.52 |
| 4:M:333:LYS:NZ | 4:M:334:ASP:OD2 | 2.32 | 0.52 |
| 4:M:360:LEU:HD13 | 4:M:433:VAL:HB | 1.91 | 0.52 |
| 4:M:435:LEU:HB2 | 4:M:437:TYR:HE1 | 1.71 | 0.52 |
| 1:A:64:LEU:HA | 1:A:102:GLN:HE22 | 1.73 | 0.52 |
| 1:A:395:PHE:CE2 | 1:A:420:ILE:CD1 | 2.92 | 0.52 |
| 1:A:462:GLN:CD | 4:M:60:LEU:N | 2.63 | 0.52 |
| 2:B:35:TYR:O | 2:B:37:TYR:N | 2.42 | 0.52 |
| 2:B:176:ALA:C | 2:B:178:ILE:N | 2.62 | 0.52 |
| 2:B:253:ILE:CG1 | 2:B:324:ALA:CA | 2.82 | 0.52 |
| 2:B:294:VAL:CA | 2:B:299:LEU:HD12 | 2.39 | 0.52 |
| 2:B:318:ILE:HD12 | 2:B:346:THR:CG2 | 2.40 | 0.52 |
| 2:B:456:ASP:O | 2:B:460:SER:OG | 2.28 | 0.52 |
| 4:M:5:PHE:CD2 | 4:M:20:LEU:HD11 | 2.44 | 0.52 |
| 4:M:71:LYS:CG | 4:M:74:TYR:OH | 2.57 | 0.52 |
| 4:M:342:LEU:HD12 | 4:M:342:LEU:N | 2.24 | 0.52 |
| 4:M:356:LEU:HD23 | 4:M:356:LEU:O | 2.07 | 0.52 |
| 2:B:14:THR:CB | 2:B:40:GLN:CG | 2.88 | 0.52 |
| 2:B:16:LYS:NZ | 4:M:111:ILE:HB | 2.25 | 0.52 |
| 2:B:29:LYS:HB3 | 2:B:58:GLU:OE1 | 2.09 | 0.52 |
| 2:B:120:ILE:HD12 | 2:B:142:LEU:HD23 | 1.89 | 0.52 |
| 2:B:143:SER:O | 2:B:145:MET:N | 2.42 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:209:SER:O | 2:B:212:VAL:HB | 2.09 | 0.52 |
| 2:B:249:ILE:HG22 | 2:B:324:ALA:HB2 | 1.91 | 0.52 |
| 2:B:302:PHE:CE1 | 2:B:306:LEU:HD11 | 2.45 | 0.52 |
| 2:B:313:SER:OG | 4:M:269:ILE:HG22 | 2.10 | 0.52 |
| 2:B:318:ILE:HD12 | 2:B:346:THR:HG23 | 1.91 | 0.52 |
| 3:S:1:MET:SD | 3:S:20:TYR:CE2 | 3.03 | 0.52 |
| 4:M:288:ILE:HD12 | 4:M:300:LEU:HD23 | 1.92 | 0.52 |
| 4:M:334:ASP:O | 4:M:416:GLU:CA | 2.57 | 0.52 |
| 1:A:258:LYS:NZ | 3:S:94:SER:N | 2.58 | 0.52 |
| 1:A:536:MET:SD | 1:A:551:LEU:HD12 | 2.50 | 0.52 |
| 1:A:566:PHE:CD1 | 1:A:566:PHE:C | 2.83 | 0.52 |
| 2:B:83:PHE:HE1 | 2:B:87:VAL:CG2 | 2.20 | 0.52 |
| 2:B:267:ASP:HB3 | 2:B:289:PRO:HG3 | 1.90 | 0.52 |
| 2:B:318:ILE:HG21 | 2:B:346:THR:HB | 1.91 | 0.52 |
| 2:B:454:LEU:O | 2:B:457:HIS:HB2 | 2.09 | 0.52 |
| 4:M:2:TYR:CZ | 4:M:64:LYS:NZ | 2.75 | 0.52 |
| 4:M:390:ILE:C | 4:M:393:GLY:H | 2.13 | 0.52 |
| 4:M:458:LEU:HD13 | 4:M:464:THR:CG2 | 2.39 | 0.52 |
| 1:A:451:ASN:OD1 | 1:A:480:LEU:HD12 | 2.10 | 0.52 |
| 1:A:536:MET:HG2 | 1:A:551:LEU:HD13 | 1.91 | 0.52 |
| 1:A:563:CYS:O | 1:A:566:PHE:CD2 | 2.62 | 0.52 |
| 2:B:14:THR:OG1 | 2:B:40:GLN:NE2 | 2.43 | 0.52 |
| 2:B:170:ARG:HG2 | 2:B:199:LEU:HD23 | 1.92 | 0.52 |
| 2:B:375:LEU:HB2 | 2:B:376:PRO:CD | 2.40 | 0.52 |
| 2:B:566:ALA:C | 2:B:574:ASN:ND2 | 2.63 | 0.52 |
| 3:S:105:PHE:CZ | 3:S:128:LEU:HD11 | 2.45 | 0.52 |
| 4:M:214:LEU:O | 4:M:214:LEU:CD2 | 2.49 | 0.52 |
| 4:M:248:SER:C | 4:M:249:TYR:CD1 | 2.84 | 0.52 |
| 4:M:275:CYS:HG | 4:M:293:PRO:HB3 | 1.68 | 0.52 |
| 4:M:353:VAL:CG2 | 4:M:438:SER:O | 2.56 | 0.52 |
| 4:M:379:LEU:HD13 | 4:M:397:TRP:NE1 | 2.23 | 0.52 |
| 1:A:226:SER:O | 1:A:227:LYS:C | 2.45 | 0.52 |
| 1:A:384:LEU:HB2 | 1:A:441:TYR:HE2 | 1.75 | 0.52 |
| 1:A:441:TYR:O | 1:A:442:SER:C | 2.46 | 0.52 |
| 2:B:22:ALA:N | 2:B:33:SER:N | 2.56 | 0.52 |
| 2:B:127:LEU:HD22 | 2:B:157:THR:CG2 | 2.40 | 0.52 |
| 2:B:176:ALA:O | 2:B:178:ILE:N | 2.43 | 0.52 |
| 2:B:256:CYS:O | 2:B:258:GLN:N | 2.42 | 0.52 |
| 3:S:83:LEU:HD13 | 3:S:121:LEU:HD22 | 1.90 | 0.52 |
| 4:M:20:LEU:O | 4:M:21:GLY:O | 2.28 | 0.52 |
| 4:M:65:TYR:CE2 | 4:M:66:PHE:O | 2.62 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:M:74:TYR:CD2 | 4:M:109:LEU:HB2 | 2.45 | 0.52 |
| 4:M:213:GLU:HB3 | 4:M:467:TYR:HB2 | 1.92 | 0.52 |
| 4:M:221:THR:HG22 | 4:M:223:HIS:CE1 | 2.45 | 0.52 |
| 4:M:272:LEU:HD22 | 4:M:278:ILE:HB | 1.90 | 0.52 |
| 1:A:104:ARG:HG3 | 1:A:145:ILE:CD1 | 2.40 | 0.51 |
| 1:A:140:VAL:HA | 1:A:177:ILE:HG12 | 1.92 | 0.51 |
| 1:A:406:GLY:O | 3:S:64:ASN:CG | 2.45 | 0.51 |
| 1:A:516:ILE:HG22 | 1:A:554:ALA:CB | 2.39 | 0.51 |
| 1:A:533:ILE:HG12 | 1:A:562:TRP:HH2 | 1.71 | 0.51 |
| 1:A:544:SER:OG | 1:A:547:VAL:HG23 | 2.10 | 0.51 |
| 1:A:585:PHE:CD2 | 1:A:603:VAL:CG1 | 2.92 | 0.51 |
| 2:B:63:MET:HB3 | 2:B:100:LEU:HD13 | 1.92 | 0.51 |
| 2:B:63:MET:HG3 | 2:B:100:LEU:HB3 | 1.92 | 0.51 |
| 2:B:107:ARG:NH2 | 4:M:18:TYR:CZ | 2.79 | 0.51 |
| 2:B:215:TYR:CD1 | 2:B:219:TYR:CE2 | 2.81 | 0.51 |
| 2:B:215:TYR:O | 2:B:219:TYR:HD2 | 1.93 | 0.51 |
| 2:B:279:LEU:HB3 | 2:B:280:PRO:HD2 | 1.91 | 0.51 |
| 2:B:416:LYS:HG3 | 2:B:457:HIS:NE2 | 2.25 | 0.51 |
| 2:B:440:GLY:C | 2:B:442:LEU:H | 2.12 | 0.51 |
| 2:B:493:LEU:CD2 | 2:B:514:LEU:HD23 | 2.39 | 0.51 |
| 2:B:585:GLY:O | 2:B:589:SER:N | 2.40 | 0.51 |
| 3:S:53:THR:HG22 | 3:S:54:PRO:O | 2.10 | 0.51 |
| 3:S:127:THR:HG21 | 3:S:153:VAL:CG1 | 2.39 | 0.51 |
| 4:M:20:LEU:HD22 | 4:M:129:VAL:HB | 1.90 | 0.51 |
| 4:M:250:LEU:CD1 | 4:M:254:PRO:CG | 2.88 | 0.51 |
| 4:M:340:LEU:HG | 4:M:342:LEU:HD11 | 1.91 | 0.51 |
| 4:M:379:LEU:HB3 | 4:M:411:LEU:HD11 | 1.91 | 0.51 |
| 1:A:162:ILE:O | 1:A:165:ASP:N | 2.44 | 0.51 |
| 1:A:274:LEU:O | 1:A:275:LEU:O | 2.28 | 0.51 |
| 1:A:438:ALA:O | 1:A:439:ASP:CB | 2.53 | 0.51 |
| 2:B:70:MET:HE1 | 2:B:107:ARG:HB2 | 1.88 | 0.51 |
| 2:B:178:ILE:HG23 | 2:B:218:CYS:H | 1.76 | 0.51 |
| 2:B:227:HIS:CE1 | 2:B:292:GLU:HG2 | 2.46 | 0.51 |
| 2:B:253:ILE:HG12 | 2:B:324:ALA:HB1 | 1.92 | 0.51 |
| 2:B:563:PHE:CE1 | 2:B:584:SER:CA | 2.93 | 0.51 |
| 3:S:1:MET:N | 3:S:93:GLU:HB2 | 2.25 | 0.51 |
| 3:S:8:PHE:N | 3:S:8:PHE:HD1 | 2.04 | 0.51 |
| 3:S:87:PHE:HB2 | 3:S:102:ILE:HD11 | 1.91 | 0.51 |
| 4:M:218:LEU:HG | 4:M:244:VAL:CG2 | 2.38 | 0.51 |
| 1:A:496:ILE:HD11 | 1:A:519:LEU:CD1 | 2.40 | 0.51 |
| 2:B:38:TYR:HD1 | 2:B:38:TYR:N | 2.09 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:181:TYR:CD1 | 2:B:222:HIS:CD2 | 2.89 | 0.51 |
| 2:B:284:ASN:O | 2:B:284:ASN:CG | 2.47 | 0.51 |
| 2:B:343:LEU:HD22 | 2:B:366:LEU:HD11 | 1.90 | 0.51 |
| 2:B:439:CYS:C | 2:B:441:GLN:H | 2.14 | 0.51 |
| 2:B:565:GLN:CB | 2:B:581:TYR:CZ | 2.93 | 0.51 |
| 4:M:424:PHE:HZ | 4:M:428:VAL:CG2 | 2.23 | 0.51 |
| 1:A:249:ASN:HB3 | 1:A:252:ILE:HD12 | 1.91 | 0.51 |
| 1:A:253:ILE:HG23 | 1:A:281:LEU:HD13 | 1.92 | 0.51 |
| 2:B:234:CYS:CB | 2:B:301:LEU:HB3 | 2.40 | 0.51 |
| 2:B:307:ASN:OD1 | 2:B:339:PHE:HD1 | 1.92 | 0.51 |
| 2:B:348:THR:HG23 | 2:B:380:LYS:HB3 | 1.86 | 0.51 |
| 2:B:404:ASN:O | 2:B:405:GLU:O | 2.29 | 0.51 |
| 2:B:437:SER:CB | 2:B:474:VAL:HA | 2.40 | 0.51 |
| 2:B:483:PRO:HA | 2:B:486:HIS:CB | 2.40 | 0.51 |
| 2:B:566:ALA:C | 2:B:574:ASN:HB3 | 2.30 | 0.51 |
| 4:M:65:TYR:OH | 4:M:86:PRO:HB3 | 2.08 | 0.51 |
| 4:M:95:THR:O | 4:M:99:ILE:HG13 | 2.09 | 0.51 |
| 4:M:235:LEU:HD22 | 4:M:307:SER:HA | 1.92 | 0.51 |
| 1:A:88:ASN:CB | 1:A:120:ILE:CG2 | 2.89 | 0.51 |
| 1:A:509:PRO:HA | 1:A:512:LEU:HD12 | 1.92 | 0.51 |
| 1:A:509:PRO:HB3 | 1:A:547:VAL:HG21 | 1.92 | 0.51 |
| 2:B:279:LEU:CD1 | 2:B:285:GLU:HG2 | 2.40 | 0.51 |
| 2:B:556:LEU:HA | 2:B:588:ILE:HD12 | 1.84 | 0.51 |
| 2:B:563:PHE:O | 2:B:566:ALA:CA | 2.58 | 0.51 |
| 4:M:55:MET:O | 4:M:56:VAL:O | 2.28 | 0.51 |
| 4:M:80:THR:HG21 | 4:M:89:CYS:HB2 | 1.93 | 0.51 |
| 4:M:222:PHE:CE2 | 4:M:240:ILE:HD13 | 2.45 | 0.51 |
| 4:M:327:PHE:CE1 | 4:M:336:ASP:CB | 2.89 | 0.51 |
| 4:M:357:LYS:O | 4:M:436:GLU:HG2 | 2.10 | 0.51 |
| 1:A:91:ILE:O | 1:A:94:VAL:HB | 2.10 | 0.51 |
| 1:A:129:LYS:HG2 | 1:A:165:ASP:OD2 | 2.10 | 0.51 |
| 1:A:288:THR:O | 1:A:291:ILE:HB | 2.10 | 0.51 |
| 1:A:373:GLU:CG | 1:A:427:LYS:CE | 2.89 | 0.51 |
| 2:B:12:LEU:CB | 4:M:13:LYS:HG2 | 2.21 | 0.51 |
| 2:B:13:ASP:OD1 | 4:M:14:LEU:CB | 2.59 | 0.51 |
| 2:B:162:VAL:O | 2:B:163:THR:C | 2.46 | 0.51 |
| 2:B:170:ARG:CA | 2:B:199:LEU:HD22 | 2.40 | 0.51 |
| 2:B:204:ASP:HB3 | 2:B:207:VAL:HG23 | 1.91 | 0.51 |
| 2:B:306:LEU:HD22 | 2:B:321:CYS:HA | 1.91 | 0.51 |
| 2:B:486:HIS:NE2 | 2:B:518:ILE:HB | 2.25 | 0.51 |
| 2:B:563:PHE:CE1 | 2:B:584:SER:HA | 2.45 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:599:ALA:HB1 | 2:B:607:ILE:HG22 | 1.91 | 0.51 |
| 4:M:15:ILE:CG2 | 4:M:115:VAL:CG2 | 2.79 | 0.51 |
| 1:A:421:PRO:CB | 3:S:63:ASN:N | 2.70 | 0.51 |
| 1:A:504:ILE:O | 1:A:505:ASN:O | 2.28 | 0.51 |
| 1:A:514:GLU:HA | 1:A:514:GLU:OE1 | 2.11 | 0.51 |
| 1:A:566:PHE:C | 1:A:568:GLU:N | 2.57 | 0.51 |
| 2:B:28:SER:CB | 2:B:61:ASP:OD2 | 2.59 | 0.51 |
| 2:B:68:SER:O | 4:M:18:TYR:CD1 | 2.63 | 0.51 |
| 2:B:144:ASP:CG | 4:M:131:ALA:CA | 2.45 | 0.51 |
| 2:B:217:GLU:O | 2:B:218:CYS:C | 2.48 | 0.51 |
| 2:B:340:ILE:HD13 | 2:B:366:LEU:HD13 | 1.91 | 0.51 |
| 2:B:344:VAL:HG21 | 2:B:377:TYR:HB2 | 1.87 | 0.51 |
| 2:B:424:PHE:HD1 | 2:B:428:VAL:HG11 | 1.74 | 0.51 |
| 2:B:474:VAL:C | 2:B:476:ARG:N | 2.64 | 0.51 |
| 4:M:18:TYR:CD1 | 4:M:19:LEU:N | 2.78 | 0.51 |
| 4:M:290:PHE:CZ | 4:M:297:PHE:CE2 | 2.99 | 0.51 |
| 1:A:217:ALA:CB | 3:S:140:MET:SD | 2.98 | 0.51 |
| 1:A:241:TYR:C | 1:A:242:GLU:O | 2.27 | 0.51 |
| 2:B:307:ASN:OD1 | 2:B:339:PHE:CD1 | 2.64 | 0.51 |
| 4:M:343:ASN:ND2 | 4:M:343:ASN:H | 2.04 | 0.51 |
| 1:A:275:LEU:HA | 1:A:278:ILE:CG1 | 2.41 | 0.51 |
| 1:A:316:LEU:HD11 | 1:A:341:ILE:HG21 | 1.92 | 0.51 |
| 1:A:398:GLU:CA | 1:A:418:ILE:HG13 | 2.41 | 0.51 |
| 1:A:485:PRO:C | 1:A:486:SER:O | 2.42 | 0.51 |
| 1:A:503:ASN:OD1 | 4:M:60:LEU:CG | 2.58 | 0.51 |
| 1:A:594:PHE:HZ | 2:B:477:MET:HE1 | 1.74 | 0.51 |
| 2:B:38:TYR:CD1 | 2:B:42:ILE:CD1 | 2.91 | 0.51 |
| 2:B:517:GLU:C | 2:B:519:ALA:H | 2.14 | 0.51 |
| 1:A:158:LEU:CG | 1:A:162:ILE:HD11 | 2.41 | 0.51 |
| 1:A:170:LEU:HD13 | 1:A:181:ALA:HB3 | 1.93 | 0.51 |
| 1:A:189:PHE:O | 1:A:190:LEU:C | 2.48 | 0.51 |
| 2:B:215:TYR:O | 2:B:219:TYR:CD2 | 2.64 | 0.51 |
| 2:B:237:ILE:HD12 | 2:B:248:LEU:HB2 | 1.92 | 0.51 |
| 2:B:246:SER:O | 2:B:249:ILE:HB | 2.10 | 0.51 |
| 4:M:8:THR:HG22 | 4:M:14:LEU:HA | 1.93 | 0.51 |
| 4:M:70:ASN:ND2 | 4:M:75:TRP:CZ2 | 2.79 | 0.51 |
| 4:M:212:ASN:HB3 | 4:M:250:LEU:HD23 | 1.93 | 0.51 |
| 4:M:276:VAL:HG21 | 4:M:299:LEU:HD12 | 1.92 | 0.51 |
| 4:M:280:ASP:OD2 | 4:M:282:VAL:HG23 | 2.10 | 0.51 |
| 1:A:450:TYR:OH | 1:A:476:GLN:CD | 2.48 | 0.50 |
| 2:B:197:LYS:CA | 2:B:229:HIS:NE2 | 2.74 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:284:ASN:C | 2:B:285:GLU:O | 2.31 | 0.50 |
| 2:B:400:SER:HB2 | 2:B:435:SER:O | 2.11 | 0.50 |
| 2:B:426:GLU:O | 2:B:430:ILE:HG13 | 2.11 | 0.50 |
| 2:B:468:LEU:HD13 | 2:B:503:LEU:HD22 | 1.93 | 0.50 |
| 4:M:213:GLU:C | 4:M:467:TYR:HB2 | 2.31 | 0.50 |
| 4:M:276:VAL:HG22 | 4:M:299:LEU:HD12 | 1.94 | 0.50 |
| 1:A:180:LYS:NZ | 3:S:137:GLN:CB | 2.75 | 0.50 |
| 1:A:251:TRP:HA | 1:A:254:ILE:HD12 | 1.93 | 0.50 |
| 1:A:253:ILE:CD1 | 1:A:285:THR:HG21 | 2.41 | 0.50 |
| 1:A:258:LYS:HZ2 | 3:S:93:GLU:HA | 1.63 | 0.50 |
| 2:B:44:PRO:HG3 | 2:B:77:ILE:CD1 | 2.42 | 0.50 |
| 2:B:64:LYS:HZ2 | 4:M:120:ARG:NH1 | 1.99 | 0.50 |
| 2:B:120:ILE:HG13 | 2:B:150:LEU:CD1 | 2.41 | 0.50 |
| 2:B:146:LYS:O | 2:B:147:MET:SD | 2.69 | 0.50 |
| 2:B:155:LEU:CB | 2:B:188:TYR:CD1 | 2.93 | 0.50 |
| 2:B:231:ARG:C | 2:B:233:TYR:N | 2.62 | 0.50 |
| 2:B:334:MET:O | 2:B:373:LEU:HD23 | 2.11 | 0.50 |
| 2:B:564:LYS:HE3 | 2:B:621:GLY:C | 2.32 | 0.50 |
| 3:S:47:GLN:O | 3:S:49:SER:N | 2.44 | 0.50 |
| 3:S:109:LEU:O | 3:S:111:ARG:N | 2.44 | 0.50 |
| 4:M:323:MET:SD | 4:M:342:LEU:CB | 2.99 | 0.50 |
| 4:M:386:PHE:CB | 4:M:397:TRP:CD1 | 2.94 | 0.50 |
| 1:A:64:LEU:CB | 1:A:102:GLN:NE2 | 2.74 | 0.50 |
| 1:A:237:SER:N | 1:A:238:PRO:CD | 2.74 | 0.50 |
| 1:A:253:ILE:HD12 | 1:A:285:THR:HG21 | 1.93 | 0.50 |
| 1:A:288:THR:CG2 | 3:S:96:LEU:CD2 | 2.84 | 0.50 |
| 1:A:535:ILE:O | 1:A:536:MET:HG3 | 2.11 | 0.50 |
| 2:B:5:ILE:CD1 | 4:M:39:PRO:CA | 2.88 | 0.50 |
| 2:B:17:VAL:CG2 | 2:B:36:THR:HA | 2.41 | 0.50 |
| 2:B:64:LYS:HD3 | 4:M:119:ASP:HB3 | 1.92 | 0.50 |
| 2:B:106:LEU:CD1 | 2:B:144:ASP:CA | 2.78 | 0.50 |
| 2:B:108:PHE:HE1 | 2:B:112:ASP:CB | 2.24 | 0.50 |
| 2:B:120:ILE:HD12 | 2:B:150:LEU:HD13 | 1.92 | 0.50 |
| 2:B:120:ILE:HD13 | 2:B:142:LEU:HD23 | 1.93 | 0.50 |
| 2:B:271:GLU:C | 2:B:273:SER:N | 2.54 | 0.50 |
| 2:B:336:ASN:C | 2:B:373:LEU:HD22 | 2.24 | 0.50 |
| 2:B:437:SER:HB2 | 2:B:474:VAL:CA | 2.40 | 0.50 |
| 2:B:580:TYR:CB | 2:B:582:ASP:CG | 2.75 | 0.50 |
| 3:S:14:PRO:HA | 3:S:36:TYR:OH | 2.11 | 0.50 |
| 3:S:125:TRP:CD1 | 3:S:129:GLU:HG3 | 2.46 | 0.50 |
| 4:M:278:ILE:O | 4:M:278:ILE:HG12 | 2.12 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:254:ILE:CG2 | 3:S:94:SER:CB | 2.90 | 0.50 |
| 1:A:429:VAL:HG11 | 1:A:473:ILE:HD11 | 1.92 | 0.50 |
| 1:A:582:ILE:CG1 | 1:A:607:LEU:HB2 | 2.41 | 0.50 |
| 1:A:589:SER:HA | 1:A:597:GLN:CG | 2.38 | 0.50 |
| 2:B:155:LEU:HB2 | 2:B:188:TYR:CE1 | 2.47 | 0.50 |
| 2:B:243:TRP:HH2 | 4:M:98:ARG:HD3 | 0.92 | 0.50 |
| 2:B:262:LYS:O | 2:B:290:SER:HB2 | 2.12 | 0.50 |
| 2:B:537:PHE:CE2 | 2:B:545:ARG:CG | 2.95 | 0.50 |
| 2:B:563:PHE:O | 2:B:567:GLN:N | 2.45 | 0.50 |
| 4:M:125:PHE:O | 4:M:128:CYS:HB2 | 2.11 | 0.50 |
| 4:M:235:LEU:HD23 | 4:M:235:LEU:O | 2.12 | 0.50 |
| 4:M:304:VAL:HB | 4:M:445:SER:CB | 2.42 | 0.50 |
| 1:A:117:ASP:OD2 | 1:A:120:ILE:CG1 | 2.59 | 0.50 |
| 1:A:251:TRP:HE3 | 3:S:97:ALA:CA | 1.91 | 0.50 |
| 1:A:268:PRO:HG3 | 1:A:271:ARG:HH21 | 1.76 | 0.50 |
| 1:A:581:LEU:HG | 1:A:585:PHE:CZ | 2.47 | 0.50 |
| 2:B:352:ASN:O | 2:B:355:ASN:HB2 | 2.12 | 0.50 |
| 2:B:564:LYS:HG2 | 2:B:565:GLN:N | 2.27 | 0.50 |
| 3:S:8:PHE:HZ | 3:S:86:THR:HG1 | 1.46 | 0.50 |
| 3:S:57:LEU:HA | 3:S:58:LEU:O | 2.11 | 0.50 |
| 3:S:83:LEU:HD11 | 3:S:116:VAL:CG2 | 2.41 | 0.50 |
| 3:S:100:ASP:O | 3:S:104:THR:OG1 | 2.18 | 0.50 |
| 4:M:136:VAL:CG1 | 4:M:137:SER:N | 2.74 | 0.50 |
| 4:M:243:ILE:CG2 | 4:M:472:TYR:HB3 | 2.41 | 0.50 |
| 4:M:371:GLU:O | 4:M:419:ASN:OD1 | 2.29 | 0.50 |
| 1:A:128:LEU:HB2 | 1:A:150:LEU:HD21 | 1.93 | 0.50 |
| 1:A:384:LEU:HD12 | 1:A:384:LEU:C | 2.30 | 0.50 |
| 2:B:9:ALA:HB3 | 4:M:14:LEU:HD12 | 1.94 | 0.50 |
| 2:B:68:SER:O | 2:B:71:ALA:HB3 | 2.12 | 0.50 |
| 2:B:178:ILE:HG13 | 2:B:214:ALA:HA | 1.82 | 0.50 |
| 2:B:382:TYR:OH | 2:B:410:GLU:HB2 | 2.12 | 0.50 |
| 2:B:400:SER:HB2 | 2:B:435:SER:CA | 2.32 | 0.50 |
| 3:S:8:PHE:HE1 | 3:S:86:THR:N | 2.09 | 0.50 |
| 4:M:242:GLY:N | 4:M:444:ALA:CB | 2.75 | 0.50 |
| 4:M:447:ILE:O | 4:M:448:TYR:C | 2.48 | 0.50 |
| 1:A:182:ILE:CG2 | 1:A:221:VAL:CG2 | 2.81 | 0.50 |
| 1:A:341:ILE:O | 1:A:344:ILE:HB | 2.11 | 0.50 |
| 1:A:426:ILE:CD1 | 1:A:466:ASP:OD2 | 2.58 | 0.50 |
| 1:A:429:VAL:HG11 | 1:A:473:ILE:CD1 | 2.41 | 0.50 |
| 1:A:488:ARG:CG | 1:A:522:PHE:CE2 | 2.94 | 0.50 |
| 1:A:638:LEU:HD12 | 2:B:557:SER:OG | 2.11 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:20:ARG:NH2 | 4:M:118:TYR:HB3 | 2.23 | 0.50 |
| 2:B:151:ALA:HB3 | 2:B:188:TYR:HE2 | 1.73 | 0.50 |
| 2:B:162:VAL:HG22 | 2:B:199:LEU:HD21 | 1.93 | 0.50 |
| 2:B:181:TYR:CG | 2:B:218:CYS:SG | 2.99 | 0.50 |
| 2:B:185:LYS:HE2 | 2:B:221:ASP:OD2 | 2.12 | 0.50 |
| 2:B:513:TRP:CA | 2:B:551:LEU:CD2 | 2.83 | 0.50 |
| 1:A:92:LEU:HD13 | 1:A:123:LEU:CB | 2.42 | 0.50 |
| 1:A:223:CYS:HB2 | 1:A:259:LEU:CD1 | 2.41 | 0.50 |
| 1:A:613:ALA:HB3 | 1:A:621:LEU:HD23 | 1.93 | 0.50 |
| 2:B:230:PHE:HB3 | 2:B:298:ASP:OD2 | 2.12 | 0.50 |
| 2:B:232:ARG:CG | 2:B:236:ILE:HD11 | 2.33 | 0.50 |
| 2:B:568:VAL:C | 2:B:574:ASN:ND2 | 2.65 | 0.50 |
| 2:B:596:LEU:O | 2:B:599:ALA:N | 2.32 | 0.50 |
| 3:S:3:HIS:O | 3:S:19:PHE:HA | 2.12 | 0.50 |
| 4:M:220:GLU:CG | 4:M:439:TYR:CB | 2.85 | 0.50 |
| 4:M:306:LEU:CG | 4:M:317:MET:CE | 2.90 | 0.50 |
| 4:M:316:ARG:O | 4:M:317:MET:C | 2.45 | 0.50 |
| 4:M:343:ASN:HB3 | 4:M:345:GLU:HG3 | 1.94 | 0.50 |
| 1:A:263:LEU:O | 1:A:266:VAL:C | 2.51 | 0.50 |
| 1:A:341:ILE:O | 1:A:345:ASN:N | 2.45 | 0.50 |
| 1:A:379:VAL:CG1 | 1:A:441:TYR:HH | 2.24 | 0.50 |
| 1:A:433:ILE:HD13 | 1:A:472:LYS:O | 2.12 | 0.50 |
| 1:A:516:ILE:HD13 | 1:A:551:LEU:CA | 2.42 | 0.50 |
| 1:A:556:VAL:HG22 | 1:A:603:VAL:HG13 | 1.90 | 0.50 |
| 2:B:38:TYR:O | 2:B:40:GLN:N | 2.45 | 0.50 |
| 2:B:143:SER:HB2 | 2:B:179:LYS:CD | 2.42 | 0.50 |
| 2:B:189:HIS:CE1 | 2:B:222:HIS:CG | 2.99 | 0.50 |
| 2:B:241:ASP:OD1 | 2:B:243:TRP:HB2 | 2.12 | 0.50 |
| 2:B:476:ARG:O | 2:B:480:GLN:HG3 | 2.11 | 0.50 |
| 2:B:479:VAL:CG2 | 2:B:486:HIS:HD2 | 2.09 | 0.50 |
| 2:B:565:GLN:HB2 | 2:B:581:TYR:CZ | 2.46 | 0.50 |
| 4:M:68:VAL:HG23 | 4:M:77:LEU:HD12 | 1.94 | 0.50 |
| 4:M:364:VAL:CA | 4:M:367:ALA:O | 2.60 | 0.50 |
| 1:A:151:SER:O | 1:A:153:ILE:N | 2.45 | 0.49 |
| 1:A:158:LEU:CD1 | 1:A:162:ILE:HG13 | 2.42 | 0.49 |
| 1:A:254:ILE:HG12 | 1:A:290:VAL:HA | 1.93 | 0.49 |
| 1:A:508:LEU:CD1 | 4:M:59:ASP:OD1 | 2.60 | 0.49 |
| 2:B:131:ASN:O | 2:B:135:ARG:HG3 | 2.12 | 0.49 |
| 2:B:162:VAL:HG22 | 2:B:199:LEU:CD2 | 2.42 | 0.49 |
| 2:B:189:HIS:NE2 | 2:B:222:HIS:CG | 2.80 | 0.49 |
| 2:B:333:GLN:O | 2:B:336:ASN:CB | 2.60 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:M:212:ASN:CG | 4:M:250:LEU:HD23 | 2.32 | 0.49 |
| 4:M:223:HIS:CA | 4:M:479:PHE:CG | 2.92 | 0.49 |
| 4:M:379:LEU:HB3 | 4:M:411:LEU:CD1 | 2.42 | 0.49 |
| 1:A:119:ASP:O | 1:A:123:LEU:HG | 2.11 | 0.49 |
| 2:B:17:VAL:CG1 | 2:B:35:TYR:CD2 | 2.95 | 0.49 |
| 2:B:97:VAL:CG1 | 2:B:101:ILE:HD11 | 2.42 | 0.49 |
| 2:B:260:LEU:CD2 | 2:B:291:TYR:OH | 2.54 | 0.49 |
| 2:B:279:LEU:N | 2:B:288:TYR:CB | 2.49 | 0.49 |
| 2:B:390:VAL:HA | 2:B:393:ILE:HD12 | 1.94 | 0.49 |
| 4:M:51:LEU:N | 4:M:51:LEU:HD12 | 2.28 | 0.49 |
| 4:M:92:PHE:CE2 | 4:M:128:CYS:HB3 | 2.47 | 0.49 |
| 4:M:223:HIS:CB | 4:M:476:THR:OG1 | 2.60 | 0.49 |
| 4:M:293:PRO:CA | 4:M:294:ASP:O | 2.60 | 0.49 |
| 1:A:460:LEU:O | 1:A:463:ASP:N | 2.37 | 0.49 |
| 1:A:496:ILE:HG13 | 1:A:532:LEU:HD11 | 1.93 | 0.49 |
| 2:B:37:TYR:CD2 | 2:B:38:TYR:CE1 | 3.00 | 0.49 |
| 2:B:83:PHE:CD1 | 2:B:87:VAL:HG23 | 2.47 | 0.49 |
| 2:B:162:VAL:HG11 | 2:B:195:ILE:HG23 | 1.92 | 0.49 |
| 2:B:195:ILE:O | 2:B:197:LYS:N | 2.44 | 0.49 |
| 2:B:215:TYR:CZ | 2:B:229:HIS:HB3 | 2.47 | 0.49 |
| 2:B:223:LEU:HD22 | 2:B:255:TYR:CD1 | 2.48 | 0.49 |
| 2:B:335:LYS:O | 2:B:373:LEU:HD22 | 2.12 | 0.49 |
| 2:B:365:PHE:O | 2:B:368:ILE:HB | 2.12 | 0.49 |
| 2:B:497:LEU:CD1 | 2:B:503:LEU:HD12 | 2.41 | 0.49 |
| 2:B:563:PHE:CD2 | 2:B:588:ILE:HD12 | 2.47 | 0.49 |
| 3:S:135:ILE:O | 3:S:141:VAL:CG2 | 2.59 | 0.49 |
| 4:M:212:ASN:CA | 4:M:249:TYR:O | 2.55 | 0.49 |
| 4:M:214:LEU:N | 4:M:467:TYR:H | 2.11 | 0.49 |
| 4:M:280:ASP:OD1 | 4:M:280:ASP:N | 2.44 | 0.49 |
| 4:M:290:PHE:CD2 | 4:M:297:PHE:CZ | 2.99 | 0.49 |
| 4:M:291:ILE:HG12 | 4:M:292:PRO:CD | 2.42 | 0.49 |
| 1:A:244:LEU:O | 1:A:245:VAL:C | 2.47 | 0.49 |
| 2:B:6:HIS:NE2 | 4:M:77:LEU:HD21 | 2.27 | 0.49 |
| 2:B:9:ALA:C | 4:M:14:LEU:HD13 | 2.32 | 0.49 |
| 2:B:14:THR:HA | 2:B:36:THR:CA | 2.26 | 0.49 |
| 2:B:25:VAL:HA | 2:B:30:LEU:O | 2.12 | 0.49 |
| 2:B:79:VAL:HG23 | 2:B:108:PHE:CD2 | 2.43 | 0.49 |
| 2:B:567:GLN:O | 2:B:569:THR:HB | 2.00 | 0.49 |
| 3:S:25:LEU:O | 3:S:27:LYS:N | 2.45 | 0.49 |
| 3:S:146:VAL:O | 3:S:150:VAL:HG23 | 2.12 | 0.49 |
| 4:M:270:PRO:O | 4:M:272:LEU:HD12 | 2.11 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:M:372:ILE:CD1 | 4:M:428:VAL:HG22 | 2.42 | 0.49 |
| 1:A:264:SER:HB3 | 1:A:271:ARG:CG | 2.42 | 0.49 |
| 1:A:329:ASN:O | 1:A:333:ILE:HG13 | 2.13 | 0.49 |
| 1:A:429:VAL:HG11 | 1:A:473:ILE:HG13 | 1.91 | 0.49 |
| 1:A:516:ILE:HG23 | 1:A:554:ALA:CB | 2.37 | 0.49 |
| 1:A:588:LEU:C | 1:A:590:TYR:N | 2.63 | 0.49 |
| 2:B:309:LEU:CG | 2:B:317:VAL:HG11 | 2.42 | 0.49 |
| 2:B:512:VAL:C | 2:B:551:LEU:CD1 | 2.67 | 0.49 |
| 2:B:537:PHE:CZ | 2:B:545:ARG:CG | 2.96 | 0.49 |
| 2:B:564:LYS:CE | 2:B:621:GLY:C | 2.79 | 0.49 |
| 3:S:25:LEU:HA | 3:S:28:GLN:CG | 2.41 | 0.49 |
| 4:M:276:VAL:CG2 | 4:M:290:PHE:HD1 | 2.15 | 0.49 |
| 4:M:362:PHE:O | 4:M:364:VAL:HG13 | 2.12 | 0.49 |
| 1:A:78:GLU:O | 1:A:80:TYR:O | 2.30 | 0.49 |
| 1:A:186:PHE:HE1 | 1:A:187:LYS:HD3 | 1.78 | 0.49 |
| 1:A:316:LEU:O | 1:A:319:LEU:N | 2.44 | 0.49 |
| 2:B:175:LEU:O | 2:B:178:ILE:HB | 2.13 | 0.49 |
| 2:B:216:LYS:HB2 | 2:B:251:LEU:CG | 2.37 | 0.49 |
| 2:B:513:TRP:CZ2 | 2:B:554:LYS:NZ | 2.79 | 0.49 |
| 4:M:219:LEU:N | 4:M:472:TYR:CD2 | 2.79 | 0.49 |
| 1:A:64:LEU:CA | 1:A:102:GLN:HE22 | 2.25 | 0.49 |
| 1:A:134:TYR:O | 1:A:135:ASP:C | 2.47 | 0.49 |
| 1:A:170:LEU:HD12 | 1:A:206:LYS:HG3 | 1.94 | 0.49 |
| 1:A:179:LYS:NZ | 3:S:142:ILE:H | 2.08 | 0.49 |
| 1:A:190:LEU:HD12 | 1:A:228:LYS:HG3 | 1.94 | 0.49 |
| 1:A:241:TYR:C | 1:A:241:TYR:CD1 | 2.86 | 0.49 |
| 1:A:293:GLU:OE1 | 3:S:94:SER:CB | 2.59 | 0.49 |
| 1:A:573:GLU:O | 1:A:577:VAL:HG23 | 2.12 | 0.49 |
| 1:A:638:LEU:CD1 | 2:B:557:SER:CB | 2.91 | 0.49 |
| 2:B:85:ASP:O | 2:B:89:ASN:ND2 | 2.46 | 0.49 |
| 2:B:120:ILE:HG13 | 2:B:150:LEU:HD13 | 1.94 | 0.49 |
| 2:B:231:ARG:HG2 | 2:B:298:ASP:OD1 | 2.11 | 0.49 |
| 2:B:294:VAL:HA | 2:B:299:LEU:CD1 | 2.43 | 0.49 |
| 2:B:483:PRO:O | 2:B:486:HIS:HB3 | 2.13 | 0.49 |
| 3:S:131:VAL:CG2 | 3:S:153:VAL:CG2 | 2.84 | 0.49 |
| 4:M:226:PHE:CE2 | 4:M:321:GLY:C | 2.86 | 0.49 |
| 4:M:323:MET:HG2 | 4:M:437:TYR:OH | 2.13 | 0.49 |
| 1:A:136:GLY:O | 1:A:139:ASP:HA | 2.12 | 0.49 |
| 2:B:162:VAL:CG1 | 2:B:195:ILE:HG23 | 2.42 | 0.49 |
| 2:B:189:HIS:CE1 | 2:B:222:HIS:ND1 | 2.81 | 0.49 |
| 2:B:219:TYR:CG | 2:B:226:LEU:CD2 | 2.83 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:325:LEU:O | 2:B:326:TYR:C | 2.38 | 0.49 |
| 2:B:412:PHE:HB3 | 2:B:453:TRP:CD1 | 2.48 | 0.49 |
| 2:B:430:ILE:HG13 | 2:B:467:VAL:HG22 | 1.94 | 0.49 |
| 4:M:340:LEU:HG | 4:M:342:LEU:CD1 | 2.43 | 0.49 |
| 4:M:480:GLN:OE1 | 4:M:482:ARG:NE | 2.38 | 0.49 |
| 1:A:206:LYS:C | 1:A:208:ASP:N | 2.65 | 0.49 |
| 1:A:261:THR:O | 1:A:264:SER:OG | 2.18 | 0.49 |
| 2:B:10:SER:O | 2:B:40:GLN:NE2 | 2.45 | 0.49 |
| 2:B:278:PRO:CD | 2:B:292:GLU:CA | 2.90 | 0.49 |
| 2:B:430:ILE:HG23 | 2:B:470:ALA:HB2 | 1.94 | 0.49 |
| 2:B:486:HIS:NE2 | 2:B:490:ILE:HD11 | 2.27 | 0.49 |
| 2:B:494:ALA:O | 2:B:498:THR:HG23 | 2.12 | 0.49 |
| 3:S:129:GLU:O | 3:S:132:LEU:N | 2.45 | 0.49 |
| 4:M:6:TYR:O | 4:M:76:CYS:HA | 2.13 | 0.49 |
| 4:M:67:SER:O | 4:M:93:LEU:HD11 | 2.13 | 0.49 |
| 4:M:379:LEU:HD22 | 4:M:397:TRP:CE2 | 2.48 | 0.49 |
| 1:A:264:SER:HB2 | 1:A:271:ARG:CG | 2.43 | 0.49 |
| 1:A:292:TYR:O | 1:A:292:TYR:HD1 | 1.93 | 0.49 |
| 1:A:486:SER:O | 1:A:487:MET:HB2 | 2.12 | 0.49 |
| 1:A:610:SER:OG | 1:A:625:LEU:HD13 | 2.13 | 0.49 |
| 2:B:28:SER:OG | 2:B:30:LEU:O | 0.49 | 0.49 |
| 2:B:140:SER:O | 2:B:143:SER:N | 2.45 | 0.49 |
| 2:B:214:ALA:C | 2:B:216:LYS:N | 2.65 | 0.49 |
| 4:M:69:ILE:HD12 | 4:M:93:LEU:C | 2.33 | 0.49 |
| 4:M:338:PHE:HZ | 4:M:379:LEU:HD21 | 1.78 | 0.49 |
| 4:M:437:TYR:CE1 | 4:M:479:PHE:CD2 | 3.01 | 0.49 |
| 1:A:261:THR:O | 1:A:264:SER:N | 2.45 | 0.48 |
| 1:A:638:LEU:HD13 | 2:B:557:SER:CB | 2.42 | 0.48 |
| 2:B:86:VAL:HG13 | 2:B:101:ILE:HG12 | 1.93 | 0.48 |
| 2:B:98:LYS:HZ2 | 2:B:134:LEU:HD22 | 1.78 | 0.48 |
| 2:B:178:ILE:CG1 | 2:B:214:ALA:O | 2.53 | 0.48 |
| 2:B:275:ARG:HG2 | 2:B:294:VAL:HG11 | 1.95 | 0.48 |
| 2:B:295:ASN:O | 2:B:296:ASP:O | 2.30 | 0.48 |
| 3:S:1:MET:N | 3:S:93:GLU:CD | 2.66 | 0.48 |
| 3:S:24:ASP:HB3 | 3:S:26:PRO:HD2 | 1.93 | 0.48 |
| 4:M:44:ASP:CG | 4:M:50:TYR:CE2 | 2.86 | 0.48 |
| 1:A:169:MET:C | 1:A:171:ASN:N | 2.65 | 0.48 |
| 1:A:185:LEU:HB2 | 1:A:203:PHE:CZ | 2.47 | 0.48 |
| 1:A:190:LEU:CD1 | 1:A:228:LYS:HE3 | 2.37 | 0.48 |
| 1:A:581:LEU:CD2 | 1:A:585:PHE:CE2 | 2.96 | 0.48 |
| 3:S:53:THR:CG2 | 3:S:69:ASN:N | 2.77 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:S:64:ASN:C | 3:S:66:ASP:N | 2.66 | 0.48 |
| 1:A:76:TYR:O | 1:A:80:TYR:CD2 | 2.67 | 0.48 |
| 1:A:213:SER:HB2 | 3:S:142:ILE:CG2 | 2.44 | 0.48 |
| 1:A:441:TYR:C | 1:A:443:SER:N | 2.56 | 0.48 |
| 1:A:498:LEU:HB3 | 1:A:504:ILE:HG13 | 1.95 | 0.48 |
| 2:B:98:LYS:HZ1 | 2:B:134:LEU:HD22 | 1.78 | 0.48 |
| 2:B:212:VAL:HG13 | 2:B:251:LEU:HD23 | 1.95 | 0.48 |
| 2:B:267:ASP:O | 2:B:268:LYS:C | 2.46 | 0.48 |
| 3:S:25:LEU:HA | 3:S:28:GLN:HG2 | 1.95 | 0.48 |
| 3:S:33:GLU:O | 3:S:36:TYR:HB2 | 2.12 | 0.48 |
| 1:A:71:VAL:CG1 | 1:A:105:VAL:CG1 | 2.89 | 0.48 |
| 1:A:186:PHE:CE1 | 1:A:187:LYS:HD3 | 2.48 | 0.48 |
| 1:A:304:LEU:HD23 | 1:A:304:LEU:C | 2.34 | 0.48 |
| 2:B:249:ILE:CG2 | 2:B:324:ALA:HB2 | 2.43 | 0.48 |
| 2:B:297:PRO:O | 2:B:301:LEU:CB | 2.61 | 0.48 |
| 2:B:325:LEU:O | 2:B:334:MET:SD | 2.71 | 0.48 |
| 2:B:366:LEU:O | 2:B:368:ILE:N | 2.46 | 0.48 |
| 2:B:425:PRO:HD2 | 2:B:428:VAL:HG21 | 1.95 | 0.48 |
| 2:B:556:LEU:O | 2:B:588:ILE:CD1 | 2.61 | 0.48 |
| 2:B:586:SER:O | 2:B:590:GLN:HG3 | 2.13 | 0.48 |
| 2:B:599:ALA:O | 2:B:600:LYS:C | 2.52 | 0.48 |
| 3:S:49:SER:C | 3:S:77:TYR:HB2 | 2.33 | 0.48 |
| 4:M:4:SER:HA | 4:M:18:TYR:O | 2.14 | 0.48 |
| 4:M:6:TYR:HD2 | 4:M:17:GLN:HG3 | 1.76 | 0.48 |
| 4:M:54:SER:N | 4:M:66:PHE:CD2 | 2.68 | 0.48 |
| 4:M:467:TYR:CG | 4:M:468:LYS:N | 2.82 | 0.48 |
| 1:A:140:VAL:O | 1:A:141:VAL:O | 2.30 | 0.48 |
| 2:B:20:ARG:NH1 | 4:M:118:TYR:N | 2.61 | 0.48 |
| 2:B:92:THR:HG22 | 2:B:94:ASP:H | 1.78 | 0.48 |
| 2:B:112:ASP:C | 2:B:112:ASP:OD1 | 2.51 | 0.48 |
| 2:B:219:TYR:C | 2:B:221:ASP:N | 2.59 | 0.48 |
| 2:B:227:HIS:CG | 2:B:298:ASP:OD2 | 2.67 | 0.48 |
| 2:B:307:ASN:OD1 | 2:B:339:PHE:HA | 2.13 | 0.48 |
| 3:S:4:ALA:HB2 | 3:S:19:PHE:CD1 | 2.36 | 0.48 |
| 3:S:5:VAL:HG13 | 3:S:87:PHE:CE2 | 2.48 | 0.48 |
| 4:M:20:LEU:O | 4:M:21:GLY:C | 2.44 | 0.48 |
| 4:M:350:VAL:HA | 4:M:442:GLN:CG | 2.43 | 0.48 |
| 1:A:207:LEU:HD23 | 1:A:239:LEU:HB3 | 1.95 | 0.48 |
| 1:A:536:MET:CB | 1:A:555:LEU:HD21 | 2.44 | 0.48 |
| 1:A:581:LEU:HD23 | 1:A:607:LEU:CG | 2.43 | 0.48 |
| 2:B:120:ILE:HD11 | 2:B:145:MET:HG3 | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:426:GLU:O | 2:B:467:VAL:HG22 | 2.14 | 0.48 |
| 2:B:559:ASP:O | 2:B:562:ASN:N | 2.46 | 0.48 |
| 2:B:559:ASP:CA | 2:B:562:ASN:HB2 | 2.40 | 0.48 |
| 3:S:54:PRO:O | 3:S:69:ASN:CB | 2.62 | 0.48 |
| 4:M:4:SER:OG | 4:M:18:TYR:O | 2.15 | 0.48 |
| 4:M:101:LEU:HG | 4:M:106:LYS:HG3 | 1.94 | 0.48 |
| 4:M:222:PHE:CD1 | 4:M:222:PHE:N | 2.79 | 0.48 |
| 4:M:336:ASP:OD2 | 4:M:415:ILE:HB | 2.14 | 0.48 |
| 1:A:182:ILE:HG23 | 1:A:203:PHE:CE2 | 2.49 | 0.48 |
| 1:A:222:ILE:HD12 | 1:A:240:LEU:HD21 | 1.96 | 0.48 |
| 1:A:339:TYR:HB2 | 1:A:374:LEU:HD11 | 1.95 | 0.48 |
| 2:B:155:LEU:CG | 2:B:188:TYR:HD1 | 2.26 | 0.48 |
| 4:M:8:THR:N | 4:M:75:TRP:O | 2.43 | 0.48 |
| 4:M:133:GLU:O | 4:M:135:ASN:N | 2.47 | 0.48 |
| 4:M:379:LEU:HD22 | 4:M:411:LEU:HD21 | 1.96 | 0.48 |
| 1:A:99:LYS:O | 1:A:103:LYS:HG3 | 2.14 | 0.48 |
| 1:A:263:LEU:O | 1:A:264:SER:C | 2.48 | 0.48 |
| 1:A:264:SER:CB | 1:A:271:ARG:HG3 | 2.43 | 0.48 |
| 1:A:454:ILE:HG23 | 1:A:473:ILE:HG23 | 1.96 | 0.48 |
| 1:A:528:ASN:O | 1:A:530:ASN:N | 2.46 | 0.48 |
| 2:B:83:PHE:HE2 | 2:B:105:LEU:HA | 1.79 | 0.48 |
| 2:B:178:ILE:HG21 | 2:B:217:GLU:CB | 2.32 | 0.48 |
| 2:B:261:PRO:CB | 2:B:290:SER:HB3 | 2.32 | 0.48 |
| 2:B:312:SER:CA | 4:M:269:ILE:CG1 | 2.92 | 0.48 |
| 2:B:399:LEU:O | 2:B:403:ILE:HG23 | 2.14 | 0.48 |
| 2:B:497:LEU:CD2 | 2:B:511:ILE:HG21 | 2.44 | 0.48 |
| 3:S:58:LEU:HD12 | 3:S:58:LEU:HA | 1.83 | 0.48 |
| 4:M:310:VAL:HG13 | 4:M:315:VAL:O | 2.13 | 0.48 |
| 4:M:376:ILE:HD12 | 4:M:415:ILE:HG12 | 1.95 | 0.48 |
| 1:A:121:LEU:HG | 1:A:153:ILE:HG21 | 1.96 | 0.48 |
| 1:A:436:CYS:CB | 1:A:450:TYR:CE1 | 2.97 | 0.48 |
| 1:A:462:GLN:CG | 4:M:59:ASP:OD1 | 2.60 | 0.48 |
| 1:A:484:VAL:HG12 | 1:A:486:SER:O | 2.13 | 0.48 |
| 2:B:325:LEU:HD22 | 2:B:339:PHE:CE1 | 2.49 | 0.48 |
| 2:B:389:ILE:HG23 | 2:B:428:VAL:CG2 | 2.43 | 0.48 |
| 3:S:73:ILE:HG23 | 3:S:88:ILE:HG22 | 1.93 | 0.48 |
| 4:M:16:PHE:CD1 | 4:M:118:TYR:CE2 | 3.01 | 0.48 |
| 4:M:19:LEU:HD12 | 4:M:20:LEU:N | 2.29 | 0.48 |
| 4:M:126:ASN:C | 4:M:128:CYS:N | 2.66 | 0.48 |
| 4:M:275:CYS:HB2 | 4:M:290:PHE:HE1 | 1.78 | 0.48 |
| 4:M:290:PHE:CZ | 4:M:297:PHE:CD1 | 3.01 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:341:ILE:CG2 | 1:A:348:PHE:HD2 | 2.26 | 0.48 |
| 1:A:531:ASP:C | 1:A:534:LYS:O | 2.52 | 0.48 |
| 2:B:83:PHE:CE2 | 2:B:108:PHE:HB3 | 2.48 | 0.48 |
| 2:B:253:ILE:CD1 | 2:B:324:ALA:CA | 2.91 | 0.48 |
| 2:B:522:GLU:O | 2:B:524:LYS:N | 2.47 | 0.48 |
| 4:M:45:SER:CA | 4:M:75:TRP:CH2 | 2.97 | 0.48 |
| 4:M:45:SER:CB | 4:M:75:TRP:CH2 | 2.94 | 0.48 |
| 4:M:354:ASP:O | 4:M:438:SER:HB2 | 2.14 | 0.48 |
| 4:M:376:ILE:HD13 | 4:M:415:ILE:HG23 | 1.95 | 0.48 |
| 4:M:405:THR:O | 4:M:406:GLY:C | 2.48 | 0.48 |
| 1:A:162:ILE:O | 1:A:165:ASP:HB2 | 2.14 | 0.47 |
| 1:A:449:TRP:O | 1:A:453:VAL:HG23 | 2.14 | 0.47 |
| 1:A:609:LEU:HD23 | 1:A:628:VAL:HG11 | 1.96 | 0.47 |
| 2:B:83:PHE:CE1 | 2:B:87:VAL:HG23 | 2.47 | 0.47 |
| 2:B:291:TYR:HE2 | 2:B:294:VAL:HB | 1.79 | 0.47 |
| 2:B:355:ASN:O | 2:B:359:LEU:CD2 | 2.62 | 0.47 |
| 2:B:374:PHE:CE2 | 2:B:398:ILE:HG22 | 2.47 | 0.47 |
| 2:B:437:SER:HG | 2:B:477:MET:HB2 | 1.78 | 0.47 |
| 3:S:51:LEU:HD12 | 3:S:77:TYR:CZ | 2.49 | 0.47 |
| 4:M:217:ASP:OD1 | 4:M:471:LYS:HA | 2.14 | 0.47 |
| 1:A:114:PHE:CG | 1:A:153:ILE:HG23 | 2.42 | 0.47 |
| 1:A:250:ASN:O | 1:A:254:ILE:HG13 | 2.14 | 0.47 |
| 2:B:25:VAL:CG2 | 2:B:31:GLY:CA | 2.92 | 0.47 |
| 2:B:367:SER:OG | 2:B:401:THR:CG2 | 2.61 | 0.47 |
| 2:B:405:GLU:O | 2:B:446:TRP:CD1 | 2.67 | 0.47 |
| 2:B:572:GLU:C | 2:B:574:ASN:N | 2.66 | 0.47 |
| 4:M:51:LEU:CD2 | 4:M:68:VAL:HG21 | 2.44 | 0.47 |
| 4:M:218:LEU:N | 4:M:472:TYR:CE2 | 2.82 | 0.47 |
| 4:M:233:LEU:HD22 | 4:M:324:SER:HA | 1.95 | 0.47 |
| 4:M:245:ASP:N | 4:M:472:TYR:CE2 | 2.82 | 0.47 |
| 4:M:386:PHE:CB | 4:M:397:TRP:HD1 | 2.27 | 0.47 |
| 1:A:84:MET:HB3 | 1:A:113:SER:HB2 | 1.95 | 0.47 |
| 1:A:395:PHE:CZ | 1:A:428:MET:CG | 2.96 | 0.47 |
| 1:A:504:ILE:N | 4:M:59:ASP:OD2 | 2.47 | 0.47 |
| 1:A:529:GLY:O | 1:A:532:LEU:HB2 | 2.14 | 0.47 |
| 1:A:581:LEU:HD21 | 1:A:585:PHE:CE2 | 2.49 | 0.47 |
| 2:B:161:LEU:C | 2:B:173:VAL:HG21 | 2.34 | 0.47 |
| 2:B:177:ILE:HD11 | 2:B:195:ILE:HG21 | 1.95 | 0.47 |
| 2:B:249:ILE:HG23 | 2:B:306:LEU:HD21 | 1.94 | 0.47 |
| 2:B:389:ILE:O | 2:B:390:VAL:O | 2.32 | 0.47 |
| 4:M:223:HIS:CA | 4:M:479:PHE:CZ | 2.94 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:M:226:PHE:CE1 | 4:M:235:LEU:HB2 | 2.49 | 0.47 |
| 4:M:331:LEU:HA | 4:M:335:SER:O | 2.15 | 0.47 |
| 1:A:136:GLY:O | 1:A:139:ASP:N | 2.47 | 0.47 |
| 1:A:192:TYR:CE2 | 1:A:194:GLU:HB2 | 2.49 | 0.47 |
| 1:A:254:ILE:CG1 | 1:A:290:VAL:HG22 | 2.43 | 0.47 |
| 1:A:350:SER:O | 1:A:352:PHE:N | 2.46 | 0.47 |
| 2:B:100:LEU:CD2 | 4:M:123:LEU:CD1 | 2.92 | 0.47 |
| 2:B:162:VAL:HB | 2:B:195:ILE:HG23 | 1.93 | 0.47 |
| 2:B:211:ALA:C | 2:B:233:TYR:CZ | 2.85 | 0.47 |
| 2:B:213:LEU:CD2 | 4:M:136:VAL:CB | 2.90 | 0.47 |
| 2:B:215:TYR:HB3 | 2:B:226:LEU:HD13 | 1.96 | 0.47 |
| 2:B:415:LEU:HD13 | 2:B:436:LEU:HG | 1.97 | 0.47 |
| 4:M:41:LEU:HD13 | 4:M:52:ASP:HB2 | 1.96 | 0.47 |
| 4:M:347:PHE:O | 4:M:350:VAL:N | 2.42 | 0.47 |
| 4:M:351:SER:HB2 | 4:M:441:GLY:CA | 2.44 | 0.47 |
| 4:M:360:LEU:HD13 | 4:M:433:VAL:CB | 2.44 | 0.47 |
| 1:A:187:LYS:O | 1:A:190:LEU:HB3 | 2.14 | 0.47 |
| 1:A:316:LEU:O | 1:A:319:LEU:HB2 | 2.14 | 0.47 |
| 2:B:16:LYS:NZ | 4:M:111:ILE:CB | 2.78 | 0.47 |
| 2:B:25:VAL:CG2 | 2:B:31:GLY:C | 2.82 | 0.47 |
| 2:B:35:TYR:CZ | 4:M:118:TYR:CE2 | 3.03 | 0.47 |
| 2:B:47:LEU:HD22 | 2:B:66:ILE:HG13 | 1.96 | 0.47 |
| 2:B:486:HIS:CD2 | 2:B:490:ILE:HG12 | 2.48 | 0.47 |
| 2:B:566:ALA:HB2 | 2:B:581:TYR:HB3 | 1.96 | 0.47 |
| 4:M:51:LEU:HD12 | 4:M:51:LEU:H | 1.79 | 0.47 |
| 1:A:91:ILE:HG21 | 1:A:106:GLY:O | 2.15 | 0.47 |
| 1:A:135:ASP:O | 1:A:136:GLY:O | 2.32 | 0.47 |
| 1:A:422:GLU:OE1 | 3:S:62:GLU:CB | 2.61 | 0.47 |
| 1:A:423:ASN:N | 3:S:62:GLU:OE1 | 2.48 | 0.47 |
| 1:A:570:LYS:O | 1:A:571:ARG:CB | 2.54 | 0.47 |
| 1:A:572:PHE:O | 1:A:575:LYS:HB3 | 2.13 | 0.47 |
| 1:A:599:ARG:NH2 | 2:B:550:VAL:HG22 | 2.29 | 0.47 |
| 2:B:106:LEU:HG | 4:M:130:GLU:HB3 | 1.75 | 0.47 |
| 2:B:270:SER:C | 2:B:273:SER:HB2 | 2.34 | 0.47 |
| 2:B:360:LEU:HD22 | 2:B:395:LYS:HD3 | 1.97 | 0.47 |
| 2:B:494:ALA:HB2 | 2:B:515:PHE:HZ | 1.74 | 0.47 |
| 2:B:563:PHE:CA | 2:B:566:ALA:HB3 | 2.45 | 0.47 |
| 2:B:592:TYR:CG | 2:B:593:ASN:N | 2.83 | 0.47 |
| 4:M:76:CYS:CB | 4:M:93:LEU:HD22 | 2.44 | 0.47 |
| 4:M:263:MET:HG2 | 4:M:263:MET:O | 2.14 | 0.47 |
| 4:M:332:GLY:O | 4:M:426:LYS:HE3 | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:68:THR:HB | 3:S:166:LYS:HD3 | 1.95 | 0.47 |
| 1:A:72:LEU:O | 1:A:76:TYR:CD2 | 2.68 | 0.47 |
| 1:A:231:GLN:N | 1:A:232:PRO:CD | 2.78 | 0.47 |
| 1:A:292:TYR:O | 1:A:295:VAL:HB | 2.15 | 0.47 |
| 1:A:447:PHE:O | 1:A:450:TYR:HB3 | 2.15 | 0.47 |
| 1:A:578:LEU:CD2 | 1:A:607:LEU:CD2 | 2.91 | 0.47 |
| 1:A:638:LEU:HA | 2:B:557:SER:OG | 2.14 | 0.47 |
| 2:B:5:ILE:CD1 | 4:M:39:PRO:HG3 | 2.40 | 0.47 |
| 2:B:231:ARG:HH21 | 2:B:279:LEU:HD21 | 1.64 | 0.47 |
| 2:B:237:ILE:HD12 | 2:B:248:LEU:CB | 2.43 | 0.47 |
| 2:B:253:ILE:CG1 | 2:B:324:ALA:HB2 | 2.44 | 0.47 |
| 2:B:266:VAL:HG22 | 2:B:291:TYR:H | 1.79 | 0.47 |
| 2:B:325:LEU:HB3 | 2:B:334:MET:CE | 2.44 | 0.47 |
| 2:B:325:LEU:CB | 2:B:334:MET:SD | 2.95 | 0.47 |
| 2:B:389:ILE:HG23 | 2:B:428:VAL:HG23 | 1.97 | 0.47 |
| 2:B:399:LEU:CD1 | 2:B:415:LEU:CD2 | 2.93 | 0.47 |
| 2:B:439:CYS:O | 2:B:441:GLN:N | 2.48 | 0.47 |
| 3:S:53:THR:O | 3:S:69:ASN:ND2 | 2.48 | 0.47 |
| 3:S:76:ILE:O | 3:S:86:THR:HA | 2.14 | 0.47 |
| 4:M:16:PHE:HA | 4:M:118:TYR:HE2 | 1.78 | 0.47 |
| 4:M:106:LYS:O | 4:M:107:ASP:O | 2.31 | 0.47 |
| 4:M:223:HIS:CD2 | 4:M:478:ASN:CB | 2.98 | 0.47 |
| 4:M:246:VAL:HA | 4:M:470:ALA:HB2 | 1.96 | 0.47 |
| 4:M:257:ALA:HB3 | 4:M:453:ASP:OD2 | 2.15 | 0.47 |
| 4:M:290:PHE:CE1 | 4:M:297:PHE:CE2 | 3.03 | 0.47 |
| 1:A:84:MET:SD | 1:A:112:GLN:O | 2.73 | 0.47 |
| 1:A:134:TYR:CD2 | 1:A:136:GLY:N | 2.81 | 0.47 |
| 1:A:291:ILE:HG12 | 1:A:322:PHE:CE2 | 2.50 | 0.47 |
| 1:A:319:LEU:O | 1:A:321:THR:N | 2.47 | 0.47 |
| 1:A:586:GLU:HB2 | 1:A:604:LEU:CD1 | 2.45 | 0.47 |
| 2:B:12:LEU:HD22 | 4:M:13:LYS:CG | 2.45 | 0.47 |
| 2:B:219:TYR:O | 2:B:223:LEU:CG | 2.63 | 0.47 |
| 2:B:267:ASP:CB | 2:B:289:PRO:HG3 | 2.45 | 0.47 |
| 2:B:313:SER:O | 2:B:315:PRO:HD3 | 2.14 | 0.47 |
| 2:B:334:MET:HG3 | 2:B:369:LEU:HD23 | 1.97 | 0.47 |
| 3:S:38:LEU:CB | 3:S:51:LEU:HD13 | 2.44 | 0.47 |
| 4:M:99:ILE:O | 4:M:103:TYR:CD1 | 2.68 | 0.47 |
| 4:M:217:ASP:O | 4:M:472:TYR:CD1 | 2.67 | 0.47 |
| 4:M:221:THR:CB | 4:M:474:THR:OG1 | 2.62 | 0.47 |
| 4:M:347:PHE:CD2 | 4:M:350:VAL:O | 2.68 | 0.47 |
| 4:M:435:LEU:CB | 4:M:437:TYR:CE1 | 2.94 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:95:MET:HB2 | 1:A:127:LEU:HD23 | 1.96 | 0.47 |
| 1:A:166:LEU:O | 1:A:170:LEU:CD2 | 2.63 | 0.47 |
| 1:A:219:VAL:CG2 | 1:A:256:LEU:HD21 | 2.40 | 0.47 |
| 2:B:327:GLN:O | 2:B:328:LEU:C | 2.51 | 0.47 |
| 2:B:335:LYS:C | 2:B:373:LEU:HD22 | 2.35 | 0.47 |
| 2:B:403:ILE:O | 2:B:403:ILE:HG13 | 2.15 | 0.47 |
| 2:B:471:TYR:O | 2:B:474:VAL:HB | 2.14 | 0.47 |
| 2:B:549:LEU:HD23 | 2:B:610:ARG:HB2 | 1.96 | 0.47 |
| 2:B:592:TYR:CE2 | 2:B:618:PHE:CE2 | 3.03 | 0.47 |
| 3:S:151:ALA:O | 3:S:154:ASP:N | 2.41 | 0.47 |
| 4:M:374:TYR:CE1 | 4:M:393:GLY:HA2 | 2.44 | 0.47 |
| 1:A:322:PHE:HD1 | 1:A:330:LEU:HD21 | 1.75 | 0.47 |
| 2:B:83:PHE:CD2 | 2:B:108:PHE:CB | 2.97 | 0.47 |
| 2:B:181:TYR:CB | 2:B:218:CYS:HG | 2.27 | 0.47 |
| 2:B:230:PHE:CD1 | 2:B:234:CYS:SG | 3.00 | 0.47 |
| 2:B:238:LYS:HG3 | 2:B:305:SER:OG | 2.15 | 0.47 |
| 2:B:306:LEU:CD1 | 2:B:325:LEU:HD21 | 2.44 | 0.47 |
| 3:S:7:ILE:HD13 | 3:S:16:LEU:HD23 | 1.96 | 0.47 |
| 4:M:41:LEU:HD13 | 4:M:52:ASP:CB | 2.45 | 0.47 |
| 4:M:100:LEU:O | 4:M:109:LEU:HD21 | 2.15 | 0.47 |
| 4:M:218:LEU:HG | 4:M:472:TYR:HE2 | 1.80 | 0.47 |
| 4:M:433:VAL:HG13 | 4:M:435:LEU:HD11 | 1.96 | 0.47 |
| 2:B:35:TYR:O | 2:B:42:ILE:HG13 | 2.15 | 0.46 |
| 2:B:120:ILE:HD12 | 2:B:142:LEU:HD22 | 1.95 | 0.46 |
| 2:B:246:SER:HA | 2:B:249:ILE:HD12 | 1.97 | 0.46 |
| 2:B:274:PRO:HG3 | 2:B:295:ASN:CA | 2.33 | 0.46 |
| 2:B:278:PRO:CG | 2:B:292:GLU:HB2 | 2.37 | 0.46 |
| 2:B:315:PRO:HA | 2:B:318:ILE:HD12 | 1.97 | 0.46 |
| 2:B:337:THR:CA | 2:B:373:LEU:CG | 2.49 | 0.46 |
| 2:B:399:LEU:CD1 | 2:B:415:LEU:HD21 | 2.38 | 0.46 |
| 2:B:424:PHE:CE1 | 2:B:428:VAL:HG11 | 2.49 | 0.46 |
| 3:S:53:THR:HG23 | 3:S:57:LEU:HB3 | 1.97 | 0.46 |
| 3:S:102:ILE:O | 3:S:105:PHE:HB3 | 2.15 | 0.46 |
| 4:M:2:TYR:HB3 | 4:M:23:THR:O | 2.15 | 0.46 |
| 4:M:45:SER:HB2 | 4:M:75:TRP:CZ3 | 2.50 | 0.46 |
| 4:M:69:ILE:HD12 | 4:M:94:GLU:CA | 2.44 | 0.46 |
| 4:M:222:PHE:CB | 4:M:479:PHE:HZ | 2.22 | 0.46 |
| 4:M:240:ILE:HG21 | 4:M:444:ALA:C | 2.36 | 0.46 |
| 4:M:280:ASP:OD1 | 4:M:282:VAL:HB | 2.15 | 0.46 |
| 4:M:311:LYS:O | 4:M:312:GLN:C | 2.51 | 0.46 |
| 4:M:338:PHE:CD1 | 4:M:415:ILE:CD1 | 2.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:294:SER:O | 1:A:298:ILE:HG12 | 2.15 | 0.46 |
| 1:A:461:CYS:HB2 | 1:A:469:LEU:HD23 | 1.96 | 0.46 |
| 1:A:533:ILE:HD12 | 1:A:555:LEU:HD22 | 1.97 | 0.46 |
| 1:A:565:ASN:O | 1:A:567:GLN:HG2 | 2.15 | 0.46 |
| 2:B:90:ILE:HB | 2:B:101:ILE:HG21 | 1.96 | 0.46 |
| 2:B:123:LEU:HD12 | 2:B:142:LEU:HD23 | 1.95 | 0.46 |
| 2:B:178:ILE:HG23 | 2:B:218:CYS:N | 2.29 | 0.46 |
| 2:B:219:TYR:O | 2:B:223:LEU:HG | 2.15 | 0.46 |
| 2:B:267:ASP:H | 2:B:289:PRO:CB | 2.28 | 0.46 |
| 2:B:396:ILE:HG21 | 2:B:431:MET:C | 2.36 | 0.46 |
| 4:M:19:LEU:HD11 | 4:M:24:ALA:HB2 | 1.96 | 0.46 |
| 4:M:121:ILE:HG22 | 4:M:125:PHE:CZ | 2.50 | 0.46 |
| 4:M:222:PHE:CA | 4:M:479:PHE:CZ | 2.97 | 0.46 |
| 4:M:244:VAL:O | 4:M:299:LEU:CA | 2.63 | 0.46 |
| 4:M:374:TYR:OH | 4:M:395:GLY:N | 2.47 | 0.46 |
| 1:A:219:VAL:HG22 | 1:A:240:LEU:HD22 | 1.98 | 0.46 |
| 1:A:300:LYS:O | 1:A:302:ASN:N | 2.48 | 0.46 |
| 1:A:355:LEU:O | 1:A:359:LEU:HG | 2.15 | 0.46 |
| 1:A:399:ASP:H | 1:A:418:ILE:CD1 | 2.23 | 0.46 |
| 1:A:581:LEU:HG | 1:A:607:LEU:HD11 | 1.95 | 0.46 |
| 1:A:605:GLU:CD | 1:A:636:TYR:OH | 2.52 | 0.46 |
| 1:A:625:LEU:HD11 | 1:A:629:LEU:HD12 | 1.98 | 0.46 |
| 2:B:106:LEU:CG | 2:B:144:ASP:HB2 | 2.40 | 0.46 |
| 2:B:120:ILE:CG1 | 2:B:150:LEU:HD13 | 2.44 | 0.46 |
| 2:B:158:VAL:CG1 | 2:B:173:VAL:HG12 | 2.36 | 0.46 |
| 2:B:198:GLU:O | 2:B:201:ALA:HB3 | 2.15 | 0.46 |
| 2:B:396:ILE:HD13 | 2:B:432:ALA:HA | 1.91 | 0.46 |
| 2:B:450:VAL:O | 2:B:453:TRP:HB2 | 2.16 | 0.46 |
| 2:B:557:SER:O | 2:B:560:ILE:N | 2.48 | 0.46 |
| 2:B:596:LEU:CD1 | 2:B:611:ALA:C | 2.83 | 0.46 |
| 4:M:226:PHE:CD1 | 4:M:235:LEU:HA | 2.50 | 0.46 |
| 4:M:359:ASP:HA | 4:M:395:GLY:O | 2.15 | 0.46 |
| 4:M:364:VAL:HA | 4:M:367:ALA:O | 2.15 | 0.46 |
| 1:A:128:LEU:CD1 | 1:A:150:LEU:CD2 | 2.94 | 0.46 |
| 1:A:215:VAL:O | 1:A:219:VAL:HG23 | 2.16 | 0.46 |
| 1:A:408:ILE:CG2 | 3:S:41:GLN:HB3 | 2.09 | 0.46 |
| 1:A:422:GLU:H | 3:S:62:GLU:HB3 | 1.80 | 0.46 |
| 1:A:462:GLN:O | 1:A:464:ILE:N | 2.49 | 0.46 |
| 2:B:185:LYS:O | 2:B:186:ASN:C | 2.31 | 0.46 |
| 2:B:253:ILE:CG1 | 2:B:324:ALA:HB1 | 2.44 | 0.46 |
| 2:B:316:THR:C | 2:B:318:ILE:N | 2.66 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:M:8:THR:HA | 4:M:15:ILE:HG12 | 1.98 | 0.46 |
| 4:M:283:PHE:HE2 | 4:M:289:THR:CB | 2.25 | 0.46 |
| 1:A:244:LEU:CG | 1:A:281:LEU:CD1 | 2.94 | 0.46 |
| 1:A:401:VAL:HG23 | 1:A:418:ILE:O | 2.16 | 0.46 |
| 1:A:461:CYS:SG | 1:A:464:ILE:HG22 | 2.55 | 0.46 |
| 2:B:43:ASN:HB3 | 2:B:44:PRO:CD | 2.45 | 0.46 |
| 2:B:71:ALA:CB | 4:M:19:LEU:N | 2.76 | 0.46 |
| 2:B:136:CYS:CB | 2:B:172:GLU:CG | 2.77 | 0.46 |
| 2:B:212:VAL:N | 2:B:233:TYR:OH | 2.45 | 0.46 |
| 2:B:213:LEU:HD22 | 4:M:136:VAL:CG2 | 2.46 | 0.46 |
| 2:B:227:HIS:C | 2:B:229:HIS:H | 2.19 | 0.46 |
| 2:B:250:GLU:OE2 | 4:M:136:VAL:HG22 | 2.15 | 0.46 |
| 2:B:348:THR:O | 2:B:349:MET:C | 2.50 | 0.46 |
| 3:S:53:THR:C | 3:S:69:ASN:CG | 2.73 | 0.46 |
| 4:M:223:HIS:HE1 | 4:M:476:THR:H | 1.62 | 0.46 |
| 4:M:224:VAL:HG11 | 4:M:226:PHE:CE2 | 2.49 | 0.46 |
| 4:M:306:LEU:CG | 4:M:317:MET:HE3 | 2.46 | 0.46 |
| 1:A:91:ILE:CG2 | 1:A:106:GLY:O | 2.64 | 0.46 |
| 1:A:409:VAL:CG2 | 1:A:410:TYR:N | 2.78 | 0.46 |
| 1:A:471:SER:HA | 1:A:510:THR:HG21 | 1.96 | 0.46 |
| 2:B:321:CYS:O | 2:B:325:LEU:HG | 2.15 | 0.46 |
| 2:B:399:LEU:HD13 | 2:B:415:LEU:HG | 1.97 | 0.46 |
| 2:B:477:MET:O | 2:B:480:GLN:N | 2.46 | 0.46 |
| 4:M:347:PHE:HA | 4:M:350:VAL:CG2 | 2.46 | 0.46 |
| 1:A:67:LYS:HB2 | 3:S:166:LYS:NZ | 2.31 | 0.46 |
| 1:A:179:LYS:NZ | 3:S:141:VAL:CA | 2.71 | 0.46 |
| 1:A:247:ILE:HG21 | 1:A:252:ILE:CG2 | 2.45 | 0.46 |
| 1:A:254:ILE:CD1 | 3:S:96:LEU:HB2 | 2.44 | 0.46 |
| 1:A:395:PHE:CZ | 1:A:428:MET:HB2 | 2.51 | 0.46 |
| 1:A:554:ALA:O | 1:A:557:LYS:HB2 | 2.15 | 0.46 |
| 1:A:594:PHE:HZ | 2:B:477:MET:CE | 2.28 | 0.46 |
| 2:B:27:THR:CB | 2:B:57:ARG:HD2 | 2.38 | 0.46 |
| 2:B:66:ILE:HG22 | 2:B:104:TYR:CE1 | 2.51 | 0.46 |
| 2:B:105:LEU:HB3 | 2:B:145:MET:HE1 | 1.97 | 0.46 |
| 2:B:293:VAL:CA | 2:B:299:LEU:CG | 2.87 | 0.46 |
| 2:B:437:SER:C | 2:B:439:CYS:N | 2.69 | 0.46 |
| 3:S:87:PHE:CD2 | 3:S:102:ILE:HG12 | 2.51 | 0.46 |
| 4:M:5:PHE:CD2 | 4:M:20:LEU:CD1 | 2.98 | 0.46 |
| 4:M:215:TYR:HB3 | 4:M:470:ALA:H | 1.81 | 0.46 |
| 4:M:222:PHE:CZ | 4:M:439:TYR:CE2 | 3.04 | 0.46 |
| 4:M:222:PHE:CG | 4:M:439:TYR:HE2 | 2.31 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:M:246:VAL:HA | 4:M:470:ALA:CB | 2.45 | 0.46 |
| 4:M:300:LEU:HD11 | 4:M:447:ILE:HD12 | 1.98 | 0.46 |
| 4:M:322:LEU:O | 4:M:322:LEU:HD23 | 2.16 | 0.46 |
| 4:M:435:LEU:O | 4:M:437:TYR:HE1 | 1.99 | 0.46 |
| 1:A:200:PHE:CZ | 1:A:236:LEU:CG | 2.98 | 0.46 |
| 1:A:204:VAL:O | 1:A:206:LYS:N | 2.48 | 0.46 |
| 1:A:280:GLU:O | 1:A:283:GLU:HB3 | 2.15 | 0.46 |
| 1:A:558:VAL:HG12 | 1:A:562:TRP:CD2 | 2.50 | 0.46 |
| 2:B:9:ALA:HB1 | 4:M:14:LEU:HD12 | 1.97 | 0.46 |
| 2:B:256:CYS:HB3 | 2:B:328:LEU:CD2 | 2.35 | 0.46 |
| 2:B:549:LEU:CD2 | 2:B:610:ARG:HB2 | 2.46 | 0.46 |
| 3:S:2:ILE:CD1 | 3:S:101:LEU:HD22 | 2.45 | 0.46 |
| 3:S:80:TYR:HH | 3:S:110:ASP:CG | 2.18 | 0.46 |
| 4:M:121:ILE:HG23 | 4:M:125:PHE:HE1 | 1.81 | 0.46 |
| 4:M:376:ILE:CD1 | 4:M:415:ILE:HG23 | 2.46 | 0.46 |
| 4:M:435:LEU:HD12 | 4:M:435:LEU:N | 2.31 | 0.46 |
| 1:A:170:LEU:HD13 | 1:A:170:LEU:HA | 1.80 | 0.46 |
| 1:A:219:VAL:HG22 | 1:A:240:LEU:CD2 | 2.46 | 0.46 |
| 1:A:244:LEU:CB | 1:A:256:LEU:HD13 | 2.46 | 0.46 |
| 1:A:275:LEU:C | 1:A:275:LEU:HD23 | 2.36 | 0.46 |
| 1:A:275:LEU:HD12 | 1:A:303:MET:SD | 2.55 | 0.46 |
| 1:A:405:THR:CA | 2:B:7:ARG:CZ | 2.89 | 0.46 |
| 2:B:21:GLU:HA | 2:B:21:GLU:OE1 | 2.16 | 0.46 |
| 2:B:127:LEU:CG | 2:B:157:THR:HG21 | 2.46 | 0.46 |
| 2:B:169:VAL:HG12 | 2:B:173:VAL:CG2 | 2.46 | 0.46 |
| 2:B:285:GLU:O | 2:B:286:ILE:O | 2.31 | 0.46 |
| 2:B:359:LEU:O | 2:B:363:ILE:HG12 | 2.16 | 0.46 |
| 2:B:378:THR:OG1 | 2:B:411:ILE:HG12 | 2.16 | 0.46 |
| 2:B:399:LEU:O | 2:B:400:SER:C | 2.53 | 0.46 |
| 2:B:408:VAL:CG1 | 2:B:446:TRP:CB | 2.93 | 0.46 |
| 2:B:500:GLN:CB | 2:B:503:LEU:HG | 2.46 | 0.46 |
| 2:B:591:MET:O | 2:B:595:VAL:HG23 | 2.16 | 0.46 |
| 3:S:50:PHE:HA | 3:S:77:TYR:CD1 | 2.45 | 0.46 |
| 4:M:51:LEU:H | 4:M:51:LEU:CD1 | 2.28 | 0.46 |
| 4:M:374:TYR:CD2 | 4:M:376:ILE:HD11 | 2.51 | 0.46 |
| 4:M:442:GLN:CG | 4:M:443:SER:N | 2.76 | 0.46 |
| 1:A:166:LEU:O | 1:A:170:LEU:HD22 | 2.16 | 0.46 |
| 1:A:197:ARG:O | 1:A:198:ASP:C | 2.49 | 0.46 |
| 1:A:244:LEU:HD22 | 1:A:260:PHE:HE2 | 1.81 | 0.46 |
| 1:A:316:LEU:HD11 | 1:A:348:PHE:CE2 | 2.48 | 0.46 |
| 1:A:436:CYS:CB | 1:A:450:TYR:CZ | 2.99 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:47:LEU:HD21 | 2:B:65:ARG:HB3 | 1.97 | 0.46 |
| 2:B:278:PRO:HD2 | 2:B:292:GLU:CD | 2.33 | 0.46 |
| 3:S:83:LEU:HD12 | 3:S:116:VAL:HG11 | 1.97 | 0.46 |
| 3:S:132:LEU:O | 3:S:136:VAL:HG23 | 2.16 | 0.46 |
| 4:M:9:ASP:C | 4:M:9:ASP:OD1 | 2.54 | 0.46 |
| 4:M:118:TYR:O | 4:M:121:ILE:HB | 2.16 | 0.46 |
| 4:M:242:GLY:N | 4:M:444:ALA:HB2 | 2.31 | 0.46 |
| 4:M:304:VAL:CB | 4:M:445:SER:HA | 2.46 | 0.46 |
| 4:M:436:GLU:HG3 | 4:M:436:GLU:O | 2.16 | 0.46 |
| 4:M:437:TYR:CB | 4:M:439:TYR:CZ | 2.99 | 0.46 |
| 1:A:103:LYS:O | 1:A:104:ARG:O | 2.34 | 0.45 |
| 1:A:104:ARG:CG | 1:A:145:ILE:HG13 | 2.46 | 0.45 |
| 1:A:182:ILE:HG23 | 1:A:221:VAL:HG21 | 1.93 | 0.45 |
| 2:B:35:TYR:CE1 | 4:M:118:TYR:CZ | 3.04 | 0.45 |
| 2:B:279:LEU:O | 2:B:280:PRO:C | 2.52 | 0.45 |
| 2:B:310:ILE:HG23 | 2:B:318:ILE:HG12 | 1.98 | 0.45 |
| 2:B:344:VAL:HG22 | 2:B:381:PHE:CE2 | 2.51 | 0.45 |
| 2:B:386:LYS:CE | 4:M:478:ASN:OD1 | 2.62 | 0.45 |
| 2:B:418:TYR:OH | 2:B:432:ALA:HB3 | 2.07 | 0.45 |
| 2:B:418:TYR:CE1 | 2:B:419:VAL:HG22 | 2.52 | 0.45 |
| 2:B:447:GLU:O | 2:B:450:VAL:HB | 2.16 | 0.45 |
| 2:B:577:ASN:C | 2:B:578:PRO:O | 2.53 | 0.45 |
| 3:S:68:VAL:O | 3:S:75:ILE:CD1 | 2.65 | 0.45 |
| 4:M:67:SER:OG | 4:M:90:PHE:CD1 | 2.54 | 0.45 |
| 4:M:437:TYR:HD1 | 4:M:479:PHE:CE1 | 2.33 | 0.45 |
| 1:A:185:LEU:HB3 | 1:A:203:PHE:CE1 | 2.48 | 0.45 |
| 1:A:256:LEU:O | 1:A:260:PHE:CD2 | 2.69 | 0.45 |
| 1:A:399:ASP:HA | 1:A:420:ILE:HB | 1.98 | 0.45 |
| 1:A:450:TYR:O | 1:A:454:ILE:HG12 | 2.16 | 0.45 |
| 1:A:617:ASP:OD1 | 1:A:618:THR:N | 2.46 | 0.45 |
| 1:A:638:LEU:HD21 | 2:B:561:ASP:CB | 2.45 | 0.45 |
| 2:B:75:ASP:CG | 4:M:24:ALA:CB | 2.58 | 0.45 |
| 2:B:276:SER:OG | 2:B:289:PRO:HG3 | 2.17 | 0.45 |
| 2:B:577:ASN:O | 2:B:578:PRO:O | 2.35 | 0.45 |
| 4:M:229:LYS:HE2 | 4:M:230:LYS:HE3 | 1.98 | 0.45 |
| 4:M:350:VAL:N | 4:M:442:GLN:HE21 | 2.15 | 0.45 |
| 4:M:480:GLN:OE1 | 4:M:482:ARG:NH2 | 2.46 | 0.45 |
| 1:A:366:SER:O | 1:A:370:LYS:HG2 | 2.17 | 0.45 |
| 1:A:503:ASN:CG | 4:M:60:LEU:CG | 2.83 | 0.45 |
| 2:B:106:LEU:HG | 4:M:130:GLU:CB | 2.41 | 0.45 |
| 2:B:123:LEU:CD1 | 2:B:142:LEU:CD2 | 2.94 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:155:LEU:HD21 | 2:B:192:LEU:CD1 | 2.10 | 0.45 |
| 2:B:574:ASN:O | 2:B:576:GLN:N | 2.49 | 0.45 |
| 4:M:253:ASN:O | 4:M:254:PRO:C | 2.53 | 0.45 |
| 4:M:291:ILE:HG12 | 4:M:292:PRO:HD2 | 1.98 | 0.45 |
| 4:M:338:PHE:CD1 | 4:M:415:ILE:CG1 | 2.97 | 0.45 |
| 4:M:410:VAL:HG11 | 4:M:412:ARG:CZ | 2.47 | 0.45 |
| 1:A:186:PHE:CB | 1:A:221:VAL:HG13 | 2.45 | 0.45 |
| 1:A:356:ILE:HD11 | 1:A:374:LEU:HD23 | 1.99 | 0.45 |
| 1:A:497:LYS:O | 1:A:500:SER:N | 2.41 | 0.45 |
| 1:A:604:LEU:HD23 | 1:A:604:LEU:C | 2.37 | 0.45 |
| 2:B:143:SER:CA | 2:B:179:LYS:HB2 | 2.43 | 0.45 |
| 2:B:261:PRO:HB2 | 2:B:290:SER:OG | 2.17 | 0.45 |
| 4:M:212:ASN:CG | 4:M:250:LEU:HA | 2.37 | 0.45 |
| 4:M:220:GLU:OE1 | 4:M:222:PHE:HZ | 1.99 | 0.45 |
| 4:M:290:PHE:CE2 | 4:M:291:ILE:O | 2.70 | 0.45 |
| 1:A:87:CYS:O | 1:A:91:ILE:HG12 | 2.17 | 0.45 |
| 1:A:213:SER:HB3 | 3:S:142:ILE:CA | 2.46 | 0.45 |
| 1:A:395:PHE:CG | 1:A:428:MET:HE2 | 2.51 | 0.45 |
| 1:A:476:GLN:OE1 | 1:A:476:GLN:HA | 2.16 | 0.45 |
| 2:B:103:LEU:HD22 | 4:M:127:CYS:HA | 1.97 | 0.45 |
| 2:B:319:LEU:HD22 | 2:B:358:MET:HB3 | 1.96 | 0.45 |
| 2:B:341:GLU:N | 2:B:377:TYR:CE2 | 2.84 | 0.45 |
| 2:B:374:PHE:CE1 | 2:B:381:PHE:HE2 | 2.20 | 0.45 |
| 2:B:458:MET:SD | 2:B:471:TYR:CB | 2.98 | 0.45 |
| 2:B:474:VAL:O | 2:B:476:ARG:N | 2.49 | 0.45 |
| 2:B:560:ILE:C | 2:B:563:PHE:H | 2.19 | 0.45 |
| 2:B:592:TYR:CE2 | 2:B:618:PHE:CD2 | 3.04 | 0.45 |
| 3:S:30:LEU:O | 3:S:34:GLN:HG3 | 2.16 | 0.45 |
| 4:M:20:LEU:CD2 | 4:M:129:VAL:CG2 | 2.71 | 0.45 |
| 4:M:42:LEU:HD23 | 4:M:51:LEU:CG | 2.46 | 0.45 |
| 4:M:57:GLY:O | 4:M:58:ARG:HG3 | 2.17 | 0.45 |
| 4:M:223:HIS:CD2 | 4:M:479:PHE:CE1 | 3.04 | 0.45 |
| 4:M:245:ASP:HA | 4:M:297:PHE:O | 2.16 | 0.45 |
| 4:M:261:ASN:N | 4:M:448:TYR:O | 2.42 | 0.45 |
| 4:M:374:TYR:CE2 | 4:M:376:ILE:HD11 | 2.51 | 0.45 |
| 1:A:258:LYS:HZ1 | 3:S:93:GLU:CA | 1.88 | 0.45 |
| 1:A:364:ASP:O | 1:A:367:ILE:HB | 2.17 | 0.45 |
| 1:A:413:SER:O | 1:A:415:ARG:O | 2.35 | 0.45 |
| 1:A:492:ILE:HD13 | 1:A:526:VAL:HG21 | 1.99 | 0.45 |
| 1:A:566:PHE:HD1 | 1:A:570:LYS:HA | 1.76 | 0.45 |
| 1:A:623:MET:O | 1:A:627:GLU:HG3 | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:5:ILE:HD11 | 4:M:39:PRO:CB | 2.46 | 0.45 |
| 2:B:27:THR:HB | 2:B:57:ARG:CD | 2.40 | 0.45 |
| 2:B:100:LEU:CD2 | 4:M:123:LEU:HD13 | 2.46 | 0.45 |
| 2:B:120:ILE:HA | 2:B:142:LEU:CD2 | 2.44 | 0.45 |
| 2:B:143:SER:CA | 2:B:179:LYS:HD2 | 2.46 | 0.45 |
| 2:B:354:GLY:HA2 | 4:M:49:ASP:OD1 | 2.17 | 0.45 |
| 2:B:364:HIS:NE2 | 2:B:368:ILE:HD11 | 2.32 | 0.45 |
| 2:B:416:LYS:HA | 2:B:457:HIS:NE2 | 2.30 | 0.45 |
| 2:B:549:LEU:HD21 | 2:B:611:ALA:H | 1.80 | 0.45 |
| 2:B:566:ALA:C | 2:B:574:ASN:CB | 2.84 | 0.45 |
| 2:B:602:ASP:OD1 | 2:B:603:ASP:N | 2.50 | 0.45 |
| 4:M:16:PHE:HA | 4:M:118:TYR:CD2 | 2.52 | 0.45 |
| 4:M:215:TYR:CD2 | 4:M:469:GLY:N | 2.80 | 0.45 |
| 4:M:376:ILE:HB | 4:M:388:ASN:OD1 | 2.17 | 0.45 |
| 1:A:158:LEU:HD12 | 1:A:162:ILE:HG13 | 1.98 | 0.45 |
| 1:A:259:LEU:O | 1:A:262:ASN:HB2 | 2.16 | 0.45 |
| 1:A:496:ILE:HG13 | 1:A:532:LEU:CD1 | 2.47 | 0.45 |
| 2:B:9:ALA:CB | 4:M:14:LEU:CD1 | 2.94 | 0.45 |
| 2:B:18:ILE:O | 2:B:33:SER:HA | 2.16 | 0.45 |
| 2:B:144:ASP:OD2 | 4:M:131:ALA:CB | 2.65 | 0.45 |
| 2:B:318:ILE:CG2 | 2:B:346:THR:OG1 | 2.62 | 0.45 |
| 2:B:327:GLN:O | 2:B:329:ALA:N | 2.50 | 0.45 |
| 2:B:396:ILE:CG1 | 2:B:418:TYR:HE2 | 2.25 | 0.45 |
| 2:B:408:VAL:HG11 | 2:B:446:TRP:HB2 | 1.95 | 0.45 |
| 3:S:53:THR:CG2 | 3:S:57:LEU:CB | 2.95 | 0.45 |
| 4:M:7:ILE:HD11 | 4:M:121:ILE:CG2 | 2.45 | 0.45 |
| 4:M:65:TYR:CE2 | 4:M:86:PRO:CB | 2.95 | 0.45 |
| 4:M:70:ASN:CG | 4:M:75:TRP:CZ2 | 2.90 | 0.45 |
| 4:M:281:GLY:N | 4:M:283:PHE:O | 2.50 | 0.45 |
| 1:A:97:SER:O | 1:A:98:ASN:C | 2.46 | 0.45 |
| 1:A:333:ILE:HD11 | 3:S:95:GLU:CD | 2.29 | 0.45 |
| 1:A:498:LEU:O | 1:A:501:ASN:O | 2.35 | 0.45 |
| 2:B:170:ARG:O | 2:B:171:GLY:C | 2.54 | 0.45 |
| 2:B:208:ILE:HG21 | 2:B:236:ILE:HG21 | 1.98 | 0.45 |
| 2:B:394:TRP:CZ3 | 2:B:397:GLN:OE1 | 2.70 | 0.45 |
| 2:B:418:TYR:O | 2:B:419:VAL:O | 2.32 | 0.45 |
| 2:B:564:LYS:HG2 | 2:B:565:GLN:H | 1.82 | 0.45 |
| 3:S:5:VAL:O | 3:S:17:VAL:HG23 | 2.16 | 0.45 |
| 4:M:372:ILE:CD1 | 4:M:428:VAL:HG13 | 2.47 | 0.45 |
| 1:A:128:LEU:HD13 | 1:A:150:LEU:CD2 | 2.47 | 0.45 |
| 1:A:206:LYS:C | 1:A:208:ASP:H | 2.20 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:215:VAL:O | 1:A:216:SER:O | 2.34 | 0.45 |
| 1:A:219:VAL:HG11 | 1:A:256:LEU:CD2 | 2.47 | 0.45 |
| 1:A:316:LEU:HD12 | 1:A:348:PHE:CE2 | 2.49 | 0.45 |
| 1:A:422:GLU:OE1 | 3:S:62:GLU:CD | 2.55 | 0.45 |
| 1:A:563:CYS:CB | 1:A:621:LEU:HD11 | 2.18 | 0.45 |
| 3:S:60:SER:O | 3:S:66:ASP:CB | 2.65 | 0.45 |
| 3:S:136:VAL:O | 3:S:139:GLY:C | 2.56 | 0.45 |
| 3:S:155:GLU:HA | 3:S:158:LYS:HE2 | 1.99 | 0.45 |
| 4:M:372:ILE:HD12 | 4:M:428:VAL:CG2 | 2.47 | 0.45 |
| 4:M:453:ASP:OD1 | 4:M:453:ASP:O | 2.35 | 0.45 |
| 1:A:399:ASP:OD2 | 1:A:403:LEU:HD12 | 2.17 | 0.45 |
| 1:A:450:TYR:CE1 | 1:A:454:ILE:HD11 | 2.52 | 0.45 |
| 1:A:499:ILE:HG12 | 1:A:512:LEU:CD2 | 2.47 | 0.45 |
| 1:A:638:LEU:HD21 | 2:B:561:ASP:CA | 2.35 | 0.45 |
| 1:A:638:LEU:HD12 | 2:B:558:TYR:CA | 2.46 | 0.45 |
| 2:B:17:VAL:HG23 | 2:B:35:TYR:CD2 | 2.27 | 0.45 |
| 2:B:87:VAL:HG11 | 2:B:118:LEU:HG | 1.99 | 0.45 |
| 2:B:199:LEU:O | 2:B:200:MET:C | 2.50 | 0.45 |
| 2:B:226:LEU:HD21 | 2:B:255:TYR:CG | 2.50 | 0.45 |
| 2:B:247:TYR:HD1 | 4:M:136:VAL:CG1 | 2.22 | 0.45 |
| 2:B:343:LEU:HG | 2:B:363:ILE:CD1 | 2.47 | 0.45 |
| 2:B:344:VAL:CG2 | 2:B:374:PHE:CD1 | 3.00 | 0.45 |
| 2:B:396:ILE:HD11 | 2:B:432:ALA:HB2 | 1.90 | 0.45 |
| 2:B:433:VAL:CG2 | 2:B:471:TYR:CG | 3.00 | 0.45 |
| 2:B:447:GLU:OE1 | 2:B:485:LYS:CB | 2.64 | 0.45 |
| 3:S:57:LEU:N | 3:S:58:LEU:O | 2.47 | 0.45 |
| 3:S:65:ASN:O | 3:S:67:GLU:CG | 2.62 | 0.45 |
| 4:M:69:ILE:HD13 | 4:M:94:GLU:HA | 1.95 | 0.45 |
| 4:M:92:PHE:HE2 | 4:M:128:CYS:C | 2.20 | 0.45 |
| 4:M:242:GLY:CA | 4:M:444:ALA:CB | 2.93 | 0.45 |
| 4:M:261:ASN:CB | 4:M:450:GLU:HG3 | 2.30 | 0.45 |
| 4:M:271:SER:N | 4:M:301:GLU:O | 2.35 | 0.45 |
| 1:A:166:LEU:CD1 | 1:A:185:LEU:HD23 | 2.47 | 0.44 |
| 1:A:216:SER:HB3 | 3:S:140:MET:CG | 2.47 | 0.44 |
| 2:B:107:ARG:CZ | 4:M:18:TYR:OH | 2.65 | 0.44 |
| 2:B:116:THR:HG21 | 2:B:150:LEU:HD11 | 1.98 | 0.44 |
| 2:B:262:LYS:O | 2:B:263:PRO:C | 2.50 | 0.44 |
| 2:B:346:THR:O | 2:B:350:THR:N | 2.49 | 0.44 |
| 2:B:509:ALA:CB | 2:B:547:GLN:HG3 | 2.45 | 0.44 |
| 2:B:546:CYS:HB2 | 2:B:607:ILE:CG1 | 2.47 | 0.44 |
| 2:B:565:GLN:CB | 2:B:581:TYR:OH | 2.65 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:S:151:ALA:O | 3:S:154:ASP:HB2 | 2.17 | 0.44 |
| 4:M:270:PRO:CA | 4:M:302:TYR:CD2 | 3.00 | 0.44 |
| 4:M:338:PHE:CD1 | 4:M:415:ILE:HD11 | 2.52 | 0.44 |
| 4:M:344:ILE:HG22 | 4:M:344:ILE:O | 2.17 | 0.44 |
| 1:A:189:PHE:C | 1:A:191:GLN:N | 2.68 | 0.44 |
| 1:A:625:LEU:C | 1:A:627:GLU:N | 2.70 | 0.44 |
| 2:B:13:ASP:OD1 | 4:M:14:LEU:CA | 2.63 | 0.44 |
| 2:B:14:THR:CB | 2:B:40:GLN:HE21 | 2.30 | 0.44 |
| 2:B:106:LEU:HD11 | 2:B:144:ASP:CB | 2.00 | 0.44 |
| 2:B:107:ARG:HA | 4:M:130:GLU:CD | 2.37 | 0.44 |
| 2:B:181:TYR:HB2 | 2:B:218:CYS:SG | 2.57 | 0.44 |
| 2:B:234:CYS:CB | 2:B:301:LEU:HB2 | 2.46 | 0.44 |
| 2:B:252:LEU:CA | 2:B:302:PHE:CE2 | 3.01 | 0.44 |
| 2:B:270:SER:O | 2:B:273:SER:CB | 2.64 | 0.44 |
| 2:B:371:GLN:O | 2:B:373:LEU:N | 2.50 | 0.44 |
| 2:B:396:ILE:CD1 | 2:B:418:TYR:CE2 | 3.00 | 0.44 |
| 2:B:418:TYR:CE2 | 2:B:432:ALA:HB2 | 2.51 | 0.44 |
| 2:B:431:MET:O | 2:B:434:LYS:N | 2.50 | 0.44 |
| 2:B:562:ASN:HB3 | 2:B:580:TYR:HB2 | 2.00 | 0.44 |
| 2:B:565:GLN:HB3 | 2:B:581:TYR:CZ | 2.51 | 0.44 |
| 4:M:217:ASP:O | 4:M:472:TYR:CD2 | 2.71 | 0.44 |
| 4:M:434:SER:CB | 4:M:479:PHE:O | 2.65 | 0.44 |
| 1:A:92:LEU:CD1 | 1:A:123:LEU:CD1 | 2.96 | 0.44 |
| 1:A:180:LYS:HZ3 | 3:S:137:GLN:CB | 2.30 | 0.44 |
| 1:A:290:VAL:O | 1:A:293:GLU:HB3 | 2.16 | 0.44 |
| 1:A:435:ILE:HG22 | 1:A:441:TYR:CE2 | 2.53 | 0.44 |
| 1:A:595:GLU:OE2 | 2:B:513:TRP:CE2 | 2.70 | 0.44 |
| 2:B:268:LYS:HA | 2:B:276:SER:CB | 2.40 | 0.44 |
| 2:B:361:GLN:O | 2:B:364:HIS:HB3 | 2.17 | 0.44 |
| 2:B:440:GLY:O | 2:B:442:LEU:N | 2.51 | 0.44 |
| 2:B:520:SER:O | 2:B:523:PHE:HE1 | 2.01 | 0.44 |
| 2:B:566:ALA:O | 2:B:574:ASN:CB | 2.65 | 0.44 |
| 3:S:93:GLU:CG | 3:S:98:ILE:HD11 | 2.48 | 0.44 |
| 4:M:9:ASP:OD2 | 4:M:13:LYS:HB3 | 2.17 | 0.44 |
| 4:M:214:LEU:CD2 | 4:M:466:LEU:HG | 2.47 | 0.44 |
| 4:M:223:HIS:CD2 | 4:M:479:PHE:CD1 | 3.05 | 0.44 |
| 4:M:252:ASP:C | 4:M:254:PRO:CD | 2.85 | 0.44 |
| 4:M:320:ILE:HA | 4:M:323:MET:CE | 2.46 | 0.44 |
| 4:M:432:THR:O | 4:M:432:THR:CG2 | 2.65 | 0.44 |
| 4:M:443:SER:CB | 4:M:447:ILE:CG1 | 2.63 | 0.44 |
| 4:M:446:GLY:C | 4:M:448:TYR:H | 2.19 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:68:THR:O | 1:A:72:LEU:HG | 2.17 | 0.44 |
| 1:A:264:SER:HB2 | 1:A:271:ARG:HD3 | 2.00 | 0.44 |
| 2:B:141:ALA:O | 2:B:145:MET:HG2 | 2.18 | 0.44 |
| 2:B:232:ARG:HG3 | 2:B:236:ILE:CG1 | 2.47 | 0.44 |
| 2:B:310:ILE:CG2 | 2:B:342:ALA:C | 2.85 | 0.44 |
| 2:B:530:LEU:HD23 | 2:B:591:MET:CB | 2.48 | 0.44 |
| 2:B:604:GLU:O | 2:B:607:ILE:HB | 2.18 | 0.44 |
| 3:S:8:PHE:HZ | 3:S:86:THR:OG1 | 1.95 | 0.44 |
| 3:S:16:LEU:HB2 | 3:S:125:TRP:CE2 | 2.47 | 0.44 |
| 3:S:39:ILE:HG23 | 3:S:47:GLN:CD | 2.38 | 0.44 |
| 4:M:134:PRO:O | 4:M:136:VAL:HG23 | 2.17 | 0.44 |
| 4:M:323:MET:HE2 | 4:M:437:TYR:HE2 | 1.81 | 0.44 |
| 4:M:374:TYR:O | 4:M:390:ILE:CG2 | 2.65 | 0.44 |
| 1:A:244:LEU:HB2 | 1:A:256:LEU:HD13 | 1.99 | 0.44 |
| 1:A:407:SER:CA | 3:S:64:ASN:ND2 | 2.75 | 0.44 |
| 1:A:569:ASP:C | 1:A:571:ARG:N | 2.67 | 0.44 |
| 1:A:625:LEU:HD12 | 1:A:629:LEU:HB2 | 2.00 | 0.44 |
| 2:B:28:SER:C | 2:B:58:GLU:CD | 2.75 | 0.44 |
| 2:B:154:ILE:HB | 2:B:180:LEU:HD13 | 1.99 | 0.44 |
| 2:B:174:ALA:CB | 2:B:211:ALA:CA | 2.80 | 0.44 |
| 2:B:327:GLN:C | 2:B:329:ALA:N | 2.70 | 0.44 |
| 2:B:374:PHE:CE2 | 2:B:398:ILE:HG23 | 2.48 | 0.44 |
| 2:B:433:VAL:C | 2:B:474:VAL:CG2 | 2.82 | 0.44 |
| 2:B:545:ARG:HB2 | 2:B:607:ILE:HD13 | 2.00 | 0.44 |
| 3:S:16:LEU:HD11 | 3:S:129:GLU:HG2 | 1.96 | 0.44 |
| 4:M:90:PHE:O | 4:M:93:LEU:HB2 | 2.16 | 0.44 |
| 4:M:103:TYR:CB | 4:M:104:PHE:CD1 | 3.00 | 0.44 |
| 4:M:240:ILE:HG22 | 4:M:444:ALA:HA | 1.82 | 0.44 |
| 1:A:68:THR:HB | 3:S:166:LYS:CD | 2.47 | 0.44 |
| 1:A:255:ARG:CZ | 3:S:139:GLY:O | 2.66 | 0.44 |
| 2:B:35:TYR:C | 2:B:37:TYR:H | 2.21 | 0.44 |
| 2:B:103:LEU:CB | 4:M:126:ASN:ND2 | 2.60 | 0.44 |
| 2:B:107:ARG:NH2 | 4:M:18:TYR:CE2 | 2.85 | 0.44 |
| 2:B:144:ASP:OD1 | 4:M:132:GLY:N | 2.51 | 0.44 |
| 2:B:200:MET:CE | 2:B:229:HIS:CA | 2.96 | 0.44 |
| 2:B:337:THR:O | 2:B:373:LEU:HD11 | 2.16 | 0.44 |
| 4:M:217:ASP:C | 4:M:472:TYR:CE2 | 2.91 | 0.44 |
| 4:M:217:ASP:N | 4:M:472:TYR:CZ | 2.86 | 0.44 |
| 4:M:219:LEU:HD22 | 4:M:474:THR:N | 2.33 | 0.44 |
| 4:M:347:PHE:HE1 | 4:M:350:VAL:CG1 | 1.91 | 0.44 |
| 1:A:185:LEU:HB2 | 1:A:203:PHE:CE1 | 2.52 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:375:VAL:HG11 | 1:A:387:ILE:HG21 | 1.98 | 0.44 |
| 1:A:405:THR:OG1 | 1:A:406:GLY:N | 2.51 | 0.44 |
| 2:B:83:PHE:CD1 | 2:B:87:VAL:CG2 | 3.00 | 0.44 |
| 2:B:188:TYR:HB3 | 2:B:192:LEU:CD1 | 2.47 | 0.44 |
| 2:B:216:LYS:NZ | 4:M:133:GLU:OE2 | 2.49 | 0.44 |
| 2:B:266:VAL:HG12 | 2:B:275:ARG:HB3 | 1.99 | 0.44 |
| 2:B:303:LEU:HB3 | 2:B:339:PHE:CZ | 2.53 | 0.44 |
| 2:B:572:GLU:O | 2:B:575:ASN:N | 2.43 | 0.44 |
| 3:S:8:PHE:HB3 | 3:S:36:TYR:HH | 1.70 | 0.44 |
| 4:M:270:PRO:HA | 4:M:302:TYR:HD2 | 1.83 | 0.44 |
| 4:M:336:ASP:CG | 4:M:415:ILE:HB | 2.38 | 0.44 |
| 4:M:374:TYR:HB3 | 4:M:417:TYR:CD1 | 2.44 | 0.44 |
| 1:A:153:ILE:HB | 1:A:158:LEU:HD21 | 1.99 | 0.44 |
| 1:A:170:LEU:CD2 | 1:A:181:ALA:HB1 | 2.44 | 0.44 |
| 1:A:260:PHE:CE2 | 1:A:274:LEU:CD1 | 3.00 | 0.44 |
| 1:A:264:SER:HB3 | 1:A:271:ARG:HG2 | 2.00 | 0.44 |
| 1:A:495:ILE:HD12 | 1:A:515:CYS:SG | 2.58 | 0.44 |
| 1:A:506:LYS:HB3 | 4:M:61:GLU:HG3 | 0.80 | 0.44 |
| 2:B:103:LEU:CD2 | 4:M:127:CYS:HA | 2.48 | 0.44 |
| 2:B:123:LEU:CD1 | 2:B:142:LEU:HG | 2.45 | 0.44 |
| 2:B:178:ILE:HD13 | 2:B:178:ILE:HA | 1.90 | 0.44 |
| 2:B:238:LYS:HE3 | 2:B:305:SER:OG | 2.18 | 0.44 |
| 2:B:389:ILE:O | 2:B:393:ILE:HG13 | 2.17 | 0.44 |
| 2:B:392:SER:OG | 2:B:424:PHE:HE1 | 2.01 | 0.44 |
| 2:B:430:ILE:CG1 | 2:B:467:VAL:HA | 2.43 | 0.44 |
| 2:B:514:LEU:O | 2:B:517:GLU:HB2 | 2.18 | 0.44 |
| 4:M:121:ILE:CG2 | 4:M:125:PHE:CZ | 3.01 | 0.44 |
| 4:M:242:GLY:O | 4:M:301:GLU:CA | 2.60 | 0.44 |
| 1:A:638:LEU:HD13 | 2:B:557:SER:CA | 2.46 | 0.44 |
| 2:B:47:LEU:CD2 | 2:B:65:ARG:HB2 | 2.48 | 0.44 |
| 2:B:123:LEU:O | 2:B:127:LEU:HG | 2.18 | 0.44 |
| 2:B:212:VAL:HG22 | 2:B:233:TYR:CE1 | 2.51 | 0.44 |
| 2:B:239:GLN:CA | 4:M:279:ASN:O | 2.57 | 0.44 |
| 2:B:300:ASP:C | 2:B:302:PHE:N | 2.69 | 0.44 |
| 2:B:545:ARG:HD3 | 2:B:602:ASP:OD2 | 2.18 | 0.44 |
| 4:M:74:TYR:HB3 | 4:M:114:ILE:HD12 | 1.94 | 0.44 |
| 4:M:304:VAL:O | 4:M:304:VAL:HG13 | 2.18 | 0.44 |
| 4:M:357:LYS:HB2 | 4:M:436:GLU:OE2 | 2.17 | 0.44 |
| 4:M:437:TYR:HB2 | 4:M:439:TYR:CZ | 2.52 | 0.44 |
| 1:A:114:PHE:HE1 | 1:A:154:ILE:HG12 | 1.83 | 0.43 |
| 1:A:314:ALA:O | 1:A:318:ARG:HD3 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:435:ILE:O | 1:A:436:CYS:C | 2.56 | 0.43 |
| 2:B:171:GLY:CA | 2:B:207:VAL:HA | 2.48 | 0.43 |
| 2:B:224:GLU:HA | 2:B:259:TYR:OH | 0.58 | 0.43 |
| 2:B:306:LEU:HD12 | 2:B:325:LEU:HD23 | 2.00 | 0.43 |
| 2:B:329:ALA:O | 2:B:331:PRO:HD3 | 2.18 | 0.43 |
| 2:B:371:GLN:C | 2:B:373:LEU:N | 2.70 | 0.43 |
| 2:B:469:ASP:OD1 | 2:B:507:ALA:CA | 2.65 | 0.43 |
| 3:S:53:THR:HG21 | 3:S:69:ASN:N | 2.33 | 0.43 |
| 4:M:222:PHE:CG | 4:M:439:TYR:CE2 | 3.06 | 0.43 |
| 4:M:290:PHE:CE1 | 4:M:291:ILE:O | 2.70 | 0.43 |
| 4:M:376:ILE:HG21 | 4:M:379:LEU:HD13 | 1.99 | 0.43 |
| 1:A:125:THR:C | 1:A:127:LEU:N | 2.70 | 0.43 |
| 2:B:20:ARG:NH1 | 4:M:118:TYR:H | 2.16 | 0.43 |
| 2:B:396:ILE:C | 2:B:435:SER:OG | 2.56 | 0.43 |
| 2:B:563:PHE:C | 2:B:564:LYS:O | 2.57 | 0.43 |
| 3:S:70:ASN:HD22 | 3:S:73:ILE:HD12 | 1.83 | 0.43 |
| 3:S:113:PHE:CD1 | 3:S:113:PHE:N | 2.85 | 0.43 |
| 4:M:212:ASN:O | 4:M:465:LYS:N | 2.49 | 0.43 |
| 4:M:219:LEU:H | 4:M:472:TYR:CB | 2.29 | 0.43 |
| 4:M:223:HIS:HB3 | 4:M:479:PHE:N | 2.32 | 0.43 |
| 4:M:377:LYS:CE | 4:M:416:GLU:OE1 | 2.67 | 0.43 |
| 1:A:153:ILE:HB | 1:A:158:LEU:CD2 | 2.49 | 0.43 |
| 1:A:356:ILE:O | 1:A:359:LEU:HB2 | 2.17 | 0.43 |
| 1:A:460:LEU:C | 1:A:462:GLN:N | 2.71 | 0.43 |
| 2:B:38:TYR:O | 2:B:39:SER:C | 2.55 | 0.43 |
| 2:B:141:ALA:O | 2:B:144:ASP:N | 2.50 | 0.43 |
| 2:B:256:CYS:HB3 | 2:B:328:LEU:HD22 | 1.91 | 0.43 |
| 2:B:430:ILE:O | 2:B:433:VAL:HB | 2.18 | 0.43 |
| 2:B:486:HIS:CE1 | 2:B:518:ILE:HB | 2.53 | 0.43 |
| 4:M:216:VAL:O | 4:M:216:VAL:CG2 | 2.66 | 0.43 |
| 4:M:245:ASP:HB2 | 4:M:472:TYR:CD1 | 2.46 | 0.43 |
| 4:M:273:HIS:HB3 | 4:M:276:VAL:HG23 | 2.00 | 0.43 |
| 4:M:291:ILE:CG1 | 4:M:292:PRO:CD | 2.96 | 0.43 |
| 4:M:360:LEU:HD23 | 4:M:362:PHE:CZ | 2.53 | 0.43 |
| 1:A:180:LYS:NZ | 3:S:137:GLN:HB2 | 2.33 | 0.43 |
| 1:A:420:ILE:HA | 1:A:421:PRO:HD3 | 1.83 | 0.43 |
| 1:A:594:PHE:O | 1:A:597:GLN:HB3 | 2.18 | 0.43 |
| 2:B:14:THR:CG2 | 2:B:18:ILE:CG2 | 2.92 | 0.43 |
| 2:B:79:VAL:CG2 | 2:B:108:PHE:CD2 | 3.00 | 0.43 |
| 2:B:89:ASN:O | 2:B:92:THR:HB | 2.18 | 0.43 |
| 2:B:152:PRO:CA | 2:B:188:TYR:CE1 | 2.82 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:340:ILE:HG21 | 2:B:374:PHE:N | 2.33 | 0.43 |
| 2:B:515:PHE:CG | 2:B:529:VAL:HG11 | 2.54 | 0.43 |
| 2:B:526:CYS:H | 2:B:527:PRO:HD3 | 1.80 | 0.43 |
| 3:S:55:PRO:HB3 | 3:S:71:GLU:CG | 2.48 | 0.43 |
| 4:M:220:GLU:HB2 | 4:M:222:PHE:CE1 | 2.51 | 0.43 |
| 4:M:331:LEU:HD12 | 4:M:331:LEU:C | 2.38 | 0.43 |
| 1:A:349:ILE:O | 1:A:350:SER:C | 2.55 | 0.43 |
| 1:A:381:GLU:O | 1:A:382:ASP:O | 2.31 | 0.43 |
| 1:A:399:ASP:O | 1:A:420:ILE:HB | 2.18 | 0.43 |
| 1:A:606:PHE:CZ | 1:A:633:PHE:HD1 | 2.32 | 0.43 |
| 1:A:629:LEU:O | 1:A:631:SER:N | 2.50 | 0.43 |
| 2:B:217:GLU:CD | 4:M:133:GLU:OE1 | 2.54 | 0.43 |
| 2:B:292:GLU:CG | 2:B:296:ASP:CB | 2.96 | 0.43 |
| 2:B:424:PHE:HA | 2:B:425:PRO:HD3 | 1.59 | 0.43 |
| 2:B:552:SER:CB | 2:B:595:VAL:HG21 | 2.49 | 0.43 |
| 2:B:588:ILE:CG2 | 2:B:618:PHE:HZ | 2.24 | 0.43 |
| 2:B:588:ILE:HD13 | 2:B:618:PHE:HE1 | 1.83 | 0.43 |
| 2:B:596:LEU:CD1 | 2:B:611:ALA:CB | 2.89 | 0.43 |
| 2:B:602:ASP:O | 2:B:608:ARG:NE | 2.52 | 0.43 |
| 4:M:68:VAL:CG2 | 4:M:77:LEU:HD12 | 2.49 | 0.43 |
| 4:M:92:PHE:CE2 | 4:M:128:CYS:O | 2.51 | 0.43 |
| 4:M:213:GLU:HA | 4:M:465:LYS:O | 2.18 | 0.43 |
| 4:M:222:PHE:HD1 | 4:M:222:PHE:N | 2.16 | 0.43 |
| 4:M:262:THR:OG1 | 4:M:267:ILE:HG12 | 2.19 | 0.43 |
| 1:A:68:THR:OG1 | 3:S:166:LYS:HD2 | 2.19 | 0.43 |
| 1:A:88:ASN:CG | 1:A:120:ILE:CG2 | 2.84 | 0.43 |
| 1:A:132:LEU:CD1 | 1:A:150:LEU:CD1 | 2.96 | 0.43 |
| 1:A:356:ILE:HG12 | 1:A:374:LEU:HD22 | 2.00 | 0.43 |
| 1:A:509:PRO:HB3 | 1:A:547:VAL:CG2 | 2.48 | 0.43 |
| 1:A:537:THR:HB | 1:A:584:PHE:CE2 | 2.53 | 0.43 |
| 1:A:625:LEU:HD11 | 1:A:629:LEU:HB2 | 2.01 | 0.43 |
| 2:B:9:ALA:HB1 | 4:M:14:LEU:CD1 | 2.48 | 0.43 |
| 2:B:279:LEU:CG | 2:B:288:TYR:HD2 | 2.13 | 0.43 |
| 2:B:400:SER:HB2 | 2:B:435:SER:C | 2.39 | 0.43 |
| 2:B:440:GLY:HA3 | 2:B:478:LEU:HD22 | 2.00 | 0.43 |
| 3:S:93:GLU:HB3 | 3:S:98:ILE:HD11 | 2.00 | 0.43 |
| 4:M:126:ASN:C | 4:M:128:CYS:H | 2.22 | 0.43 |
| 4:M:244:VAL:HG13 | 4:M:472:TYR:OH | 2.18 | 0.43 |
| 4:M:336:ASP:OD1 | 4:M:415:ILE:HB | 2.17 | 0.43 |
| 1:A:427:LYS:O | 1:A:430:ASN:HB2 | 2.19 | 0.43 |
| 1:A:635:ALA:C | 1:A:638:LEU:H | 2.22 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:162:VAL:O | 2:B:164:ASP:N | 2.52 | 0.43 |
| 2:B:208:ILE:O | 2:B:212:VAL:HG23 | 2.18 | 0.43 |
| 2:B:223:LEU:CD1 | 2:B:259:TYR:H | 2.05 | 0.43 |
| 2:B:302:PHE:CE1 | 2:B:306:LEU:HD21 | 2.53 | 0.43 |
| 2:B:512:VAL:CG2 | 2:B:533:LEU:HD22 | 2.39 | 0.43 |
| 2:B:530:LEU:HD21 | 2:B:591:MET:HB3 | 2.00 | 0.43 |
| 2:B:592:TYR:CD2 | 2:B:618:PHE:CD2 | 3.06 | 0.43 |
| 3:S:58:LEU:HD12 | 3:S:68:VAL:HG13 | 2.00 | 0.43 |
| 4:M:243:ILE:HG21 | 4:M:298:ARG:HG2 | 2.01 | 0.43 |
| 4:M:267:ILE:HG22 | 4:M:302:TYR:CE2 | 2.53 | 0.43 |
| 4:M:290:PHE:CZ | 4:M:293:PRO:CG | 3.02 | 0.43 |
| 4:M:290:PHE:CB | 4:M:299:LEU:CD1 | 2.88 | 0.43 |
| 4:M:443:SER:OG | 4:M:447:ILE:O | 2.23 | 0.43 |
| 1:A:244:LEU:HD13 | 1:A:256:LEU:CB | 2.49 | 0.43 |
| 1:A:341:ILE:HG21 | 1:A:348:PHE:HD2 | 1.84 | 0.43 |
| 1:A:356:ILE:HD13 | 1:A:374:LEU:HB3 | 2.00 | 0.43 |
| 1:A:440:ASN:C | 1:A:442:SER:H | 2.18 | 0.43 |
| 2:B:1:MET:CG | 4:M:39:PRO:HG2 | 2.38 | 0.43 |
| 2:B:70:MET:SD | 2:B:107:ARG:CB | 3.00 | 0.43 |
| 2:B:124:GLN:O | 2:B:127:LEU:N | 2.43 | 0.43 |
| 2:B:310:ILE:O | 4:M:269:ILE:HD13 | 2.09 | 0.43 |
| 2:B:328:LEU:O | 2:B:329:ALA:C | 2.54 | 0.43 |
| 2:B:400:SER:CB | 2:B:435:SER:C | 2.87 | 0.43 |
| 2:B:589:SER:O | 2:B:592:TYR:N | 2.52 | 0.43 |
| 4:M:44:ASP:O | 4:M:46:SER:N | 2.51 | 0.43 |
| 4:M:219:LEU:HD12 | 4:M:440:ILE:HG12 | 1.98 | 0.43 |
| 4:M:269:ILE:N | 4:M:302:TYR:CZ | 2.86 | 0.43 |
| 4:M:353:VAL:O | 4:M:401:LYS:CB | 2.67 | 0.43 |
| 1:A:94:VAL:O | 1:A:95:MET:C | 2.50 | 0.43 |
| 1:A:370:LYS:O | 1:A:374:LEU:HD12 | 2.17 | 0.43 |
| 1:A:461:CYS:SG | 1:A:469:LEU:HB3 | 2.58 | 0.43 |
| 1:A:536:MET:SD | 1:A:555:LEU:HD21 | 2.59 | 0.43 |
| 2:B:44:PRO:HG3 | 2:B:77:ILE:HD12 | 2.01 | 0.43 |
| 2:B:256:CYS:C | 2:B:258:GLN:N | 2.67 | 0.43 |
| 2:B:397:GLN:O | 2:B:401:THR:HG23 | 2.18 | 0.43 |
| 2:B:451:MET:CG | 2:B:489:ILE:HG12 | 2.23 | 0.43 |
| 2:B:479:VAL:HG12 | 2:B:486:HIS:CE1 | 2.24 | 0.43 |
| 2:B:513:TRP:HB2 | 2:B:551:LEU:HD11 | 2.01 | 0.43 |
| 2:B:564:LYS:NZ | 2:B:621:GLY:O | 2.51 | 0.43 |
| 4:M:262:THR:HG23 | 4:M:265:ASN:H | 1.68 | 0.43 |
| 4:M:310:VAL:O | 4:M:314:GLY:N | 2.51 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:395:PHE:CZ | 1:A:420:ILE:HD13 | 2.54 | 0.43 |
| 1:A:573:GLU:O | 1:A:574:ILE:O | 2.29 | 0.43 |
| 1:A:594:PHE:CE2 | 2:B:477:MET:CE | 3.00 | 0.43 |
| 2:B:17:VAL:HG23 | 2:B:36:THR:OG1 | 2.19 | 0.43 |
| 2:B:73:ASP:HA | 4:M:24:ALA:CB | 2.49 | 0.43 |
| 2:B:75:ASP:C | 2:B:77:ILE:H | 2.20 | 0.43 |
| 2:B:105:LEU:O | 2:B:108:PHE:N | 2.52 | 0.43 |
| 2:B:143:SER:CB | 2:B:179:LYS:CB | 2.67 | 0.43 |
| 2:B:143:SER:O | 2:B:179:LYS:HB3 | 2.19 | 0.43 |
| 2:B:158:VAL:HG12 | 2:B:177:ILE:HD11 | 2.01 | 0.43 |
| 2:B:181:TYR:HD2 | 2:B:218:CYS:HA | 1.84 | 0.43 |
| 2:B:403:ILE:HG23 | 2:B:439:CYS:SG | 2.58 | 0.43 |
| 4:M:66:PHE:HB3 | 4:M:77:LEU:CD1 | 2.48 | 0.43 |
| 4:M:217:ASP:N | 4:M:472:TYR:OH | 2.52 | 0.43 |
| 4:M:242:GLY:HA3 | 4:M:444:ALA:CB | 2.47 | 0.43 |
| 1:A:264:SER:HB2 | 1:A:271:ARG:HG3 | 2.00 | 0.42 |
| 1:A:356:ILE:O | 1:A:359:LEU:N | 2.46 | 0.42 |
| 1:A:500:SER:HB3 | 1:A:535:ILE:HD13 | 2.01 | 0.42 |
| 1:A:571:ARG:O | 1:A:574:ILE:N | 2.47 | 0.42 |
| 2:B:107:ARG:NH2 | 4:M:126:ASN:CA | 2.79 | 0.42 |
| 2:B:112:ASP:OD2 | 2:B:115:LEU:HD23 | 2.18 | 0.42 |
| 2:B:158:VAL:CG1 | 2:B:173:VAL:CG1 | 2.92 | 0.42 |
| 2:B:241:ASP:C | 2:B:243:TRP:H | 2.21 | 0.42 |
| 2:B:396:ILE:HG22 | 2:B:435:SER:CB | 2.45 | 0.42 |
| 2:B:537:PHE:CZ | 2:B:545:ARG:HD3 | 2.54 | 0.42 |
| 2:B:564:LYS:HG3 | 2:B:568:VAL:CG2 | 2.42 | 0.42 |
| 3:S:16:LEU:HD12 | 3:S:17:VAL:N | 2.34 | 0.42 |
| 4:M:234:ARG:O | 4:M:236:LEU:N | 2.51 | 0.42 |
| 4:M:455:VAL:HG12 | 4:M:455:VAL:O | 2.19 | 0.42 |
| 1:A:140:VAL:HG22 | 1:A:177:ILE:CG1 | 2.47 | 0.42 |
| 1:A:192:TYR:CD2 | 1:A:192:TYR:O | 2.72 | 0.42 |
| 1:A:356:ILE:CD1 | 1:A:374:LEU:HD23 | 2.49 | 0.42 |
| 1:A:395:PHE:CZ | 1:A:428:MET:CB | 3.02 | 0.42 |
| 1:A:398:GLU:C | 1:A:418:ILE:HG13 | 2.39 | 0.42 |
| 1:A:581:LEU:CB | 1:A:607:LEU:HD13 | 2.41 | 0.42 |
| 2:B:38:TYR:C | 2:B:40:GLN:H | 2.23 | 0.42 |
| 2:B:43:ASN:CB | 2:B:44:PRO:CD | 2.95 | 0.42 |
| 2:B:167:ALA:C | 2:B:207:VAL:HG21 | 2.39 | 0.42 |
| 2:B:169:VAL:C | 2:B:173:VAL:HG23 | 2.39 | 0.42 |
| 2:B:343:LEU:HG | 2:B:363:ILE:HD11 | 2.00 | 0.42 |
| 4:M:103:TYR:HB2 | 4:M:104:PHE:CD1 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:M:246:VAL:HB | 4:M:297:PHE:CE2 | 2.53 | 0.42 |
| 4:M:443:SER:HB3 | 4:M:447:ILE:H | 1.80 | 0.42 |
| 4:M:479:PHE:HD1 | 4:M:479:PHE:N | 1.98 | 0.42 |
| 1:A:192:TYR:HD2 | 1:A:195:ALA:H | 1.68 | 0.42 |
| 1:A:247:ILE:HG21 | 1:A:252:ILE:HB | 2.00 | 0.42 |
| 1:A:304:LEU:HD12 | 1:A:312:ALA:HB2 | 2.01 | 0.42 |
| 1:A:372:ILE:O | 1:A:375:VAL:HB | 2.19 | 0.42 |
| 2:B:315:PRO:HG3 | 2:B:350:THR:CG2 | 2.48 | 0.42 |
| 3:S:8:PHE:CZ | 3:S:84:TYR:CB | 2.97 | 0.42 |
| 4:M:219:LEU:HG | 4:M:439:TYR:O | 2.19 | 0.42 |
| 4:M:262:THR:HG22 | 4:M:264:GLY:H | 1.81 | 0.42 |
| 4:M:469:GLY:C | 4:M:470:ALA:O | 2.56 | 0.42 |
| 1:A:63:ASP:O | 1:A:67:LYS:HG3 | 2.19 | 0.42 |
| 1:A:213:SER:CB | 3:S:142:ILE:C | 2.87 | 0.42 |
| 1:A:327:ASP:OD1 | 3:S:50:PHE:HE2 | 2.02 | 0.42 |
| 1:A:406:GLY:C | 3:S:64:ASN:CG | 2.69 | 0.42 |
| 2:B:22:ALA:HA | 2:B:32:GLU:HB2 | 1.75 | 0.42 |
| 2:B:195:ILE:C | 2:B:197:LYS:H | 2.21 | 0.42 |
| 2:B:343:LEU:CG | 2:B:363:ILE:CD1 | 2.97 | 0.42 |
| 2:B:343:LEU:HD11 | 2:B:362:ALA:HB3 | 2.00 | 0.42 |
| 2:B:464:SER:O | 2:B:468:LEU:HG | 2.19 | 0.42 |
| 2:B:513:TRP:CB | 2:B:551:LEU:HD21 | 2.50 | 0.42 |
| 2:B:537:PHE:HD1 | 2:B:538:SER:N | 2.17 | 0.42 |
| 2:B:580:TYR:CB | 2:B:582:ASP:OD2 | 2.64 | 0.42 |
| 3:S:9:ASN:ND2 | 3:S:118:GLU:OE1 | 2.53 | 0.42 |
| 4:M:69:ILE:HD11 | 4:M:94:GLU:N | 2.34 | 0.42 |
| 4:M:74:TYR:HB2 | 4:M:114:ILE:HD13 | 2.00 | 0.42 |
| 4:M:213:GLU:H | 4:M:249:TYR:HB2 | 1.84 | 0.42 |
| 4:M:290:PHE:CE2 | 4:M:297:PHE:CE2 | 3.04 | 0.42 |
| 4:M:327:PHE:HE1 | 4:M:336:ASP:CG | 2.22 | 0.42 |
| 1:A:231:GLN:N | 1:A:232:PRO:HD2 | 2.35 | 0.42 |
| 1:A:338:PHE:HE1 | 1:A:352:PHE:CE2 | 2.38 | 0.42 |
| 1:A:412:LYS:O | 1:A:414:LYS:N | 2.51 | 0.42 |
| 1:A:447:PHE:CD2 | 1:A:484:VAL:HG13 | 2.54 | 0.42 |
| 2:B:9:ALA:HB1 | 4:M:14:LEU:CG | 2.45 | 0.42 |
| 2:B:108:PHE:HE1 | 2:B:112:ASP:HB3 | 1.84 | 0.42 |
| 2:B:139:LEU:HD23 | 2:B:172:GLU:C | 2.39 | 0.42 |
| 2:B:253:ILE:HD11 | 2:B:324:ALA:CA | 2.50 | 0.42 |
| 2:B:274:PRO:CG | 2:B:295:ASN:HB3 | 2.37 | 0.42 |
| 2:B:343:LEU:CD2 | 2:B:366:LEU:CD1 | 2.81 | 0.42 |
| 2:B:418:TYR:CE1 | 2:B:419:VAL:HA | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:457:HIS:ND1 | 2:B:461:HIS:NE2 | 2.67 | 0.42 |
| 2:B:458:MET:HG3 | 2:B:471:TYR:CD1 | 2.55 | 0.42 |
| 4:M:74:TYR:CE2 | 4:M:109:LEU:HB2 | 2.55 | 0.42 |
| 4:M:323:MET:CE | 4:M:342:LEU:CB | 2.93 | 0.42 |
| 4:M:360:LEU:CD1 | 4:M:433:VAL:HG23 | 2.50 | 0.42 |
| 1:A:88:ASN:ND2 | 1:A:120:ILE:HG21 | 2.34 | 0.42 |
| 1:A:176:TYR:CD1 | 3:S:142:ILE:HD11 | 2.54 | 0.42 |
| 1:A:368:ARG:NH1 | 1:A:419:ILE:O | 2.53 | 0.42 |
| 1:A:522:PHE:C | 1:A:524:THR:N | 2.72 | 0.42 |
| 2:B:127:LEU:HD23 | 2:B:135:ARG:O | 2.20 | 0.42 |
| 2:B:374:PHE:HE2 | 2:B:398:ILE:CG2 | 2.26 | 0.42 |
| 2:B:405:GLU:HA | 2:B:446:TRP:CD1 | 2.55 | 0.42 |
| 2:B:458:MET:HA | 2:B:463:LEU:CD1 | 2.47 | 0.42 |
| 2:B:513:TRP:N | 2:B:551:LEU:HD11 | 2.33 | 0.42 |
| 2:B:513:TRP:CD1 | 2:B:517:GLU:HG3 | 2.54 | 0.42 |
| 2:B:588:ILE:HD13 | 2:B:618:PHE:CE1 | 2.54 | 0.42 |
| 4:M:223:HIS:N | 4:M:479:PHE:CZ | 2.83 | 0.42 |
| 4:M:462:LYS:HD2 | 4:M:462:LYS:HA | 2.01 | 0.42 |
| 1:A:71:VAL:HG11 | 1:A:105:VAL:CG1 | 2.50 | 0.42 |
| 1:A:353:ASP:O | 1:A:356:ILE:HB | 2.19 | 0.42 |
| 1:A:413:SER:HB3 | 1:A:415:ARG:O | 2.19 | 0.42 |
| 2:B:18:ILE:HG21 | 2:B:36:THR:C | 2.32 | 0.42 |
| 2:B:105:LEU:HB3 | 2:B:145:MET:HE3 | 2.02 | 0.42 |
| 2:B:119:SER:O | 2:B:123:LEU:CG | 2.56 | 0.42 |
| 2:B:159:LYS:HA | 2:B:195:ILE:HD13 | 2.01 | 0.42 |
| 2:B:373:LEU:O | 2:B:375:LEU:N | 2.52 | 0.42 |
| 2:B:429:VAL:HG11 | 2:B:463:LEU:HD22 | 2.00 | 0.42 |
| 2:B:510:GLY:O | 2:B:513:TRP:HB3 | 2.19 | 0.42 |
| 2:B:567:GLN:N | 2:B:574:ASN:ND2 | 2.67 | 0.42 |
| 2:B:568:VAL:C | 2:B:571:SER:OG | 2.57 | 0.42 |
| 3:S:53:THR:CG2 | 3:S:69:ASN:HB2 | 2.49 | 0.42 |
| 3:S:58:LEU:O | 3:S:59:LEU:C | 2.56 | 0.42 |
| 3:S:89:VAL:HG21 | 3:S:98:ILE:HG13 | 2.00 | 0.42 |
| 4:M:110:SER:C | 4:M:112:LYS:N | 2.73 | 0.42 |
| 4:M:120:ARG:C | 4:M:124:ILE:HD12 | 2.39 | 0.42 |
| 4:M:222:PHE:CB | 4:M:479:PHE:CE2 | 3.03 | 0.42 |
| 4:M:241:HIS:C | 4:M:474:THR:HB | 2.36 | 0.42 |
| 4:M:435:LEU:HD22 | 4:M:437:TYR:OH | 2.20 | 0.42 |
| 1:A:95:MET:HB3 | 1:A:127:LEU:HD23 | 2.01 | 0.42 |
| 1:A:225:LEU:CD1 | 1:A:233:PHE:CE1 | 2.92 | 0.42 |
| 1:A:357:ILE:O | 1:A:358:ARG:C | 2.57 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:416:ILE:HG22 | 1:A:417:PRO:O | 2.20 | 0.42 |
| 1:A:561:ASN:O | 1:A:562:TRP:C | 2.57 | 0.42 |
| 2:B:13:ASP:HB3 | 2:B:35:TYR:HE2 | 1.85 | 0.42 |
| 2:B:158:VAL:HA | 2:B:173:VAL:HG13 | 2.01 | 0.42 |
| 2:B:178:ILE:HG22 | 2:B:179:LYS:N | 2.34 | 0.42 |
| 2:B:196:LEU:CA | 2:B:215:TYR:OH | 2.66 | 0.42 |
| 2:B:405:GLU:OE2 | 2:B:445:SER:HB2 | 2.20 | 0.42 |
| 2:B:574:ASN:O | 2:B:575:ASN:C | 2.50 | 0.42 |
| 4:M:220:GLU:OE2 | 4:M:350:VAL:HG13 | 2.19 | 0.42 |
| 4:M:316:ARG:O | 4:M:318:ASN:N | 2.53 | 0.42 |
| 4:M:351:SER:HB2 | 4:M:441:GLY:C | 2.40 | 0.42 |
| 4:M:362:PHE:C | 4:M:363:ASN:O | 2.55 | 0.42 |
| 1:A:466:ASP:OD1 | 1:A:468:SER:N | 2.48 | 0.42 |
| 1:A:546:SER:O | 1:A:550:VAL:HG23 | 2.18 | 0.42 |
| 2:B:38:TYR:CZ | 2:B:43:ASN:CA | 2.98 | 0.42 |
| 2:B:40:GLN:OE1 | 2:B:40:GLN:HA | 2.20 | 0.42 |
| 2:B:176:ALA:O | 2:B:179:LYS:N | 2.52 | 0.42 |
| 2:B:310:ILE:HG21 | 2:B:342:ALA:C | 2.40 | 0.42 |
| 2:B:486:HIS:NE2 | 2:B:518:ILE:CG1 | 2.83 | 0.42 |
| 3:S:5:VAL:CG1 | 3:S:87:PHE:CE2 | 3.03 | 0.42 |
| 3:S:5:VAL:HG22 | 3:S:87:PHE:CD2 | 2.54 | 0.42 |
| 4:M:103:TYR:N | 4:M:103:TYR:HD1 | 2.18 | 0.42 |
| 4:M:215:TYR:CG | 4:M:467:TYR:O | 2.70 | 0.42 |
| 4:M:245:ASP:OD1 | 4:M:298:ARG:N | 2.53 | 0.42 |
| 4:M:292:PRO:HA | 4:M:293:PRO:HD3 | 1.55 | 0.42 |
| 4:M:379:LEU:CD2 | 4:M:411:LEU:CD2 | 2.98 | 0.42 |
| 1:A:78:GLU:C | 1:A:80:TYR:O | 2.58 | 0.42 |
| 1:A:103:LYS:O | 1:A:107:TYR:CG | 2.71 | 0.42 |
| 1:A:140:VAL:HG22 | 1:A:177:ILE:CD1 | 2.50 | 0.42 |
| 1:A:259:LEU:HD23 | 1:A:259:LEU:C | 2.40 | 0.42 |
| 1:A:512:LEU:HD13 | 1:A:543:TYR:CE1 | 2.55 | 0.42 |
| 2:B:31:GLY:HA2 | 2:B:65:ARG:HH12 | 1.85 | 0.42 |
| 2:B:83:PHE:O | 2:B:86:VAL:HB | 2.19 | 0.42 |
| 2:B:172:GLU:O | 2:B:175:LEU:N | 2.53 | 0.42 |
| 2:B:261:PRO:C | 2:B:290:SER:HB3 | 2.41 | 0.42 |
| 2:B:262:LYS:O | 2:B:264:THR:N | 2.53 | 0.42 |
| 2:B:307:ASN:HD21 | 2:B:338:LYS:HB2 | 1.85 | 0.42 |
| 2:B:393:ILE:HG23 | 2:B:431:MET:HB2 | 2.01 | 0.42 |
| 2:B:403:ILE:HB | 2:B:408:VAL:CG2 | 2.49 | 0.42 |
| 2:B:412:PHE:HB3 | 2:B:453:TRP:HD1 | 1.84 | 0.42 |
| 2:B:433:VAL:HG22 | 2:B:471:TYR:CE1 | 2.53 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:497:LEU:HB2 | 2:B:511:ILE:HD13 | 2.02 | 0.42 |
| 2:B:512:VAL:HB | 2:B:551:LEU:HD12 | 2.02 | 0.42 |
| 2:B:556:LEU:CB | 2:B:588:ILE:CD1 | 2.74 | 0.42 |
| 2:B:562:ASN:ND2 | 2:B:580:TYR:CD2 | 2.88 | 0.42 |
| 4:M:217:ASP:CG | 4:M:470:ALA:O | 2.58 | 0.42 |
| 4:M:218:LEU:HD12 | 4:M:218:LEU:H | 1.83 | 0.42 |
| 4:M:290:PHE:CZ | 4:M:293:PRO:HG3 | 2.55 | 0.42 |
| 4:M:323:MET:HE3 | 4:M:437:TYR:HE2 | 1.85 | 0.42 |
| 4:M:405:THR:HG23 | 4:M:406:GLY:N | 2.35 | 0.42 |
| 1:A:264:SER:HB2 | 1:A:271:ARG:CD | 2.49 | 0.41 |
| 1:A:356:ILE:HG12 | 1:A:374:LEU:CD2 | 2.50 | 0.41 |
| 1:A:423:ASN:CG | 3:S:62:GLU:OE1 | 2.58 | 0.41 |
| 1:A:513:ARG:O | 1:A:516:ILE:HB | 2.19 | 0.41 |
| 2:B:20:ARG:CZ | 4:M:118:TYR:CB | 2.75 | 0.41 |
| 2:B:212:VAL:O | 2:B:251:LEU:HD22 | 2.20 | 0.41 |
| 2:B:475:ILE:HG22 | 2:B:514:LEU:HD21 | 2.02 | 0.41 |
| 2:B:534:ILE:C | 2:B:536:ASN:H | 2.22 | 0.41 |
| 2:B:560:ILE:HA | 2:B:563:PHE:CB | 2.38 | 0.41 |
| 3:S:85:PHE:CZ | 3:S:109:LEU:HD23 | 2.55 | 0.41 |
| 4:M:245:ASP:HB3 | 4:M:472:TYR:CE1 | 2.54 | 0.41 |
| 4:M:304:VAL:HG11 | 4:M:444:ALA:O | 2.19 | 0.41 |
| 1:A:92:LEU:CD1 | 1:A:123:LEU:HD12 | 2.50 | 0.41 |
| 1:A:95:MET:SD | 1:A:107:TYR:CE1 | 3.13 | 0.41 |
| 1:A:189:PHE:O | 1:A:191:GLN:N | 2.53 | 0.41 |
| 1:A:617:ASP:CG | 1:A:618:THR:H | 2.19 | 0.41 |
| 2:B:90:ILE:HA | 2:B:101:ILE:CD1 | 2.50 | 0.41 |
| 2:B:108:PHE:CE1 | 2:B:112:ASP:HB3 | 2.55 | 0.41 |
| 2:B:151:ALA:N | 2:B:152:PRO:CD | 2.82 | 0.41 |
| 2:B:253:ILE:HG13 | 2:B:324:ALA:CB | 2.50 | 0.41 |
| 2:B:268:LYS:O | 2:B:273:SER:HB3 | 2.20 | 0.41 |
| 2:B:275:ARG:H | 2:B:294:VAL:CG1 | 2.27 | 0.41 |
| 2:B:395:LYS:O | 2:B:398:ILE:HB | 2.20 | 0.41 |
| 3:S:53:THR:CG2 | 3:S:68:VAL:CA | 2.90 | 0.41 |
| 4:M:424:PHE:CE1 | 4:M:427:LYS:O | 2.73 | 0.41 |
| 1:A:304:LEU:HA | 1:A:308:ASP:HB2 | 2.02 | 0.41 |
| 1:A:323:CYS:HG | 1:A:355:LEU:HD21 | 1.83 | 0.41 |
| 1:A:371:ALA:O | 1:A:374:LEU:HB2 | 2.20 | 0.41 |
| 1:A:429:VAL:HG11 | 1:A:469:LEU:HD11 | 2.00 | 0.41 |
| 2:B:10:SER:C | 2:B:40:GLN:NE2 | 2.70 | 0.41 |
| 2:B:43:ASN:HA | 2:B:44:PRO:HD3 | 1.68 | 0.41 |
| 2:B:72:SER:C | 4:M:17:GLN:NE2 | 2.59 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:120:ILE:HG23 | 2:B:142:LEU:CD2 | 2.50 | 0.41 |
| 2:B:295:ASN:C | 2:B:296:ASP:O | 2.58 | 0.41 |
| 2:B:332:LEU:HG | 2:B:332:LEU:O | 2.19 | 0.41 |
| 2:B:347:VAL:CB | 2:B:359:LEU:HB3 | 2.42 | 0.41 |
| 2:B:486:HIS:O | 2:B:489:ILE:N | 2.52 | 0.41 |
| 2:B:610:ARG:O | 2:B:614:ILE:HG13 | 2.21 | 0.41 |
| 3:S:7:ILE:HG23 | 3:S:85:PHE:CD2 | 2.55 | 0.41 |
| 4:M:5:PHE:HA | 4:M:78:ALA:HA | 2.02 | 0.41 |
| 1:A:394:GLN:O | 1:A:397:ASP:N | 2.52 | 0.41 |
| 1:A:448:GLU:HB2 | 1:A:487:MET:SD | 2.60 | 0.41 |
| 2:B:14:THR:O | 2:B:18:ILE:HG12 | 2.17 | 0.41 |
| 2:B:90:ILE:O | 2:B:98:LYS:HE2 | 2.21 | 0.41 |
| 2:B:219:TYR:CE2 | 2:B:226:LEU:HA | 2.49 | 0.41 |
| 2:B:295:ASN:O | 2:B:300:ASP:HB3 | 1.99 | 0.41 |
| 2:B:334:MET:O | 2:B:335:LYS:C | 2.56 | 0.41 |
| 3:S:87:PHE:CZ | 3:S:102:ILE:HG12 | 2.55 | 0.41 |
| 4:M:16:PHE:HD1 | 4:M:118:TYR:CD2 | 2.37 | 0.41 |
| 4:M:52:ASP:O | 4:M:53:HIS:HB3 | 2.21 | 0.41 |
| 4:M:422:PRO:C | 4:M:424:PHE:H | 2.24 | 0.41 |
| 1:A:460:LEU:C | 1:A:462:GLN:H | 2.23 | 0.41 |
| 1:A:555:LEU:CD1 | 1:A:581:LEU:HD11 | 2.48 | 0.41 |
| 1:A:556:VAL:CG2 | 1:A:603:VAL:HG22 | 2.30 | 0.41 |
| 2:B:513:TRP:CA | 2:B:551:LEU:HD11 | 2.47 | 0.41 |
| 3:S:4:ALA:HB1 | 3:S:19:PHE:CE1 | 2.55 | 0.41 |
| 3:S:16:LEU:HD13 | 3:S:129:GLU:CG | 2.50 | 0.41 |
| 3:S:51:LEU:HB2 | 3:S:77:TYR:HE1 | 1.84 | 0.41 |
| 4:M:322:LEU:HD23 | 4:M:322:LEU:C | 2.41 | 0.41 |
| 4:M:323:MET:HG3 | 4:M:342:LEU:HG | 2.01 | 0.41 |
| 4:M:341:SER:CB | 4:M:343:ASN:HD21 | 2.24 | 0.41 |
| 4:M:374:TYR:O | 4:M:390:ILE:HG23 | 2.19 | 0.41 |
| 4:M:374:TYR:H | 4:M:390:ILE:HG23 | 1.84 | 0.41 |
| 4:M:434:SER:HB3 | 4:M:478:ASN:OD1 | 2.20 | 0.41 |
| 1:A:132:LEU:O | 1:A:134:TYR:N | 2.54 | 0.41 |
| 1:A:222:ILE:HG23 | 1:A:233:PHE:CD1 | 2.55 | 0.41 |
| 1:A:516:ILE:HD13 | 1:A:551:LEU:HA | 2.02 | 0.41 |
| 1:A:530:ASN:O | 1:A:534:LYS:N | 2.54 | 0.41 |
| 2:B:34:SER:HG | 2:B:35:TYR:N | 2.19 | 0.41 |
| 2:B:115:LEU:HA | 2:B:115:LEU:HD13 | 1.85 | 0.41 |
| 2:B:123:LEU:HB2 | 2:B:142:LEU:HD21 | 2.02 | 0.41 |
| 2:B:374:PHE:HB3 | 2:B:402:LEU:HD23 | 1.02 | 0.41 |
| 2:B:430:ILE:HG12 | 2:B:467:VAL:N | 2.35 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:537:PHE:CZ | 2:B:545:ARG:HB3 | 2.50 | 0.41 |
| 4:M:119:ASP:C | 4:M:121:ILE:H | 2.24 | 0.41 |
| 4:M:220:GLU:CG | 4:M:222:PHE:CE1 | 3.04 | 0.41 |
| 4:M:222:PHE:CZ | 4:M:240:ILE:HD13 | 2.56 | 0.41 |
| 4:M:372:ILE:HD12 | 4:M:428:VAL:HG22 | 2.03 | 0.41 |
| 1:A:326:GLN:HA | 1:A:331:ARG:NH2 | 2.36 | 0.41 |
| 1:A:373:GLU:HG2 | 1:A:427:LYS:CE | 2.51 | 0.41 |
| 1:A:381:GLU:O | 1:A:383:ASN:N | 2.48 | 0.41 |
| 1:A:451:ASN:HD21 | 1:A:487:MET:HB3 | 1.85 | 0.41 |
| 2:B:75:ASP:OD1 | 4:M:19:LEU:HD21 | 2.21 | 0.41 |
| 2:B:116:THR:HG21 | 2:B:147:MET:HG3 | 2.03 | 0.41 |
| 2:B:179:LYS:HE3 | 4:M:131:ALA:O | 2.20 | 0.41 |
| 2:B:241:ASP:O | 2:B:243:TRP:N | 2.50 | 0.41 |
| 2:B:435:SER:C | 2:B:437:SER:H | 2.22 | 0.41 |
| 2:B:472:VAL:CG2 | 2:B:511:ILE:HG13 | 2.50 | 0.41 |
| 2:B:493:LEU:C | 2:B:495:ASP:N | 2.74 | 0.41 |
| 2:B:596:LEU:HD22 | 2:B:615:SER:CB | 2.50 | 0.41 |
| 3:S:7:ILE:HD13 | 3:S:16:LEU:HB3 | 2.01 | 0.41 |
| 3:S:87:PHE:CD1 | 3:S:87:PHE:N | 2.88 | 0.41 |
| 4:M:103:TYR:O | 4:M:104:PHE:HB2 | 2.21 | 0.41 |
| 4:M:119:ASP:C | 4:M:121:ILE:N | 2.74 | 0.41 |
| 4:M:212:ASN:O | 4:M:465:LYS:CB | 2.65 | 0.41 |
| 1:A:182:ILE:HG22 | 1:A:221:VAL:HG23 | 2.00 | 0.41 |
| 1:A:393:LYS:O | 1:A:394:GLN:C | 2.58 | 0.41 |
| 1:A:451:ASN:OD1 | 1:A:480:LEU:CD1 | 2.68 | 0.41 |
| 1:A:529:GLY:CA | 1:A:562:TRP:HZ2 | 2.34 | 0.41 |
| 2:B:136:CYS:SG | 2:B:168:MET:O | 2.78 | 0.41 |
| 2:B:208:ILE:O | 2:B:209:SER:C | 2.58 | 0.41 |
| 2:B:230:PHE:HB3 | 2:B:298:ASP:CG | 2.41 | 0.41 |
| 2:B:267:ASP:CA | 2:B:289:PRO:HG3 | 2.50 | 0.41 |
| 2:B:301:LEU:O | 2:B:305:SER:CB | 2.68 | 0.41 |
| 2:B:367:SER:OG | 2:B:401:THR:CB | 2.68 | 0.41 |
| 2:B:508:ARG:HD3 | 2:B:540:GLU:OE2 | 2.21 | 0.41 |
| 2:B:513:TRP:HA | 2:B:551:LEU:CG | 2.50 | 0.41 |
| 2:B:577:ASN:OD1 | 2:B:577:ASN:N | 2.53 | 0.41 |
| 2:B:588:ILE:O | 2:B:591:MET:HB2 | 2.21 | 0.41 |
| 3:S:137:GLN:O | 3:S:140:MET:HB3 | 2.20 | 0.41 |
| 4:M:103:TYR:CD1 | 4:M:103:TYR:N | 2.89 | 0.41 |
| 4:M:372:ILE:HD11 | 4:M:428:VAL:HG13 | 2.03 | 0.41 |
| 4:M:386:PHE:HB3 | 4:M:397:TRP:HD1 | 1.84 | 0.41 |
| 1:A:150:LEU:C | 1:A:153:ILE:H | 2.22 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:182:ILE:HD13 | 1:A:218:ALA:HB2 | 2.02 | 0.41 |
| 1:A:349:ILE:O | 1:A:352:PHE:N | 2.48 | 0.41 |
| 1:A:402:ILE:O | 1:A:403:LEU:C | 2.56 | 0.41 |
| 1:A:461:CYS:SG | 1:A:464:ILE:CG2 | 3.09 | 0.41 |
| 1:A:516:ILE:CD1 | 1:A:551:LEU:HB2 | 2.51 | 0.41 |
| 1:A:528:ASN:C | 1:A:530:ASN:N | 2.68 | 0.41 |
| 1:A:530:ASN:ND2 | 1:A:571:ARG:NH2 | 2.69 | 0.41 |
| 2:B:56:SER:O | 2:B:57:ARG:O | 2.35 | 0.41 |
| 2:B:75:ASP:CG | 4:M:24:ALA:N | 2.70 | 0.41 |
| 2:B:83:PHE:HZ | 2:B:105:LEU:HG | 1.85 | 0.41 |
| 2:B:120:ILE:O | 2:B:123:LEU:HB2 | 2.21 | 0.41 |
| 2:B:166:SER:O | 2:B:170:ARG:HG3 | 2.21 | 0.41 |
| 2:B:177:ILE:HD11 | 2:B:195:ILE:CG2 | 2.51 | 0.41 |
| 2:B:181:TYR:HB3 | 2:B:218:CYS:SG | 2.60 | 0.41 |
| 2:B:196:LEU:HD13 | 2:B:215:TYR:CE1 | 2.56 | 0.41 |
| 2:B:302:PHE:CZ | 2:B:306:LEU:HD11 | 2.56 | 0.41 |
| 2:B:346:THR:HA | 2:B:349:MET:CE | 2.51 | 0.41 |
| 2:B:360:LEU:HD21 | 2:B:395:LYS:HE2 | 2.03 | 0.41 |
| 2:B:524:LYS:HG2 | 2:B:524:LYS:O | 2.21 | 0.41 |
| 2:B:565:GLN:HB3 | 2:B:581:TYR:OH | 2.21 | 0.41 |
| 3:S:39:ILE:HD11 | 3:S:77:TYR:CG | 2.55 | 0.41 |
| 3:S:53:THR:CG2 | 3:S:67:GLU:C | 2.89 | 0.41 |
| 3:S:87:PHE:CE1 | 3:S:102:ILE:HG23 | 2.55 | 0.41 |
| 3:S:135:ILE:O | 3:S:140:MET:O | 2.38 | 0.41 |
| 4:M:78:ALA:HB2 | 4:M:93:LEU:CG | 2.50 | 0.41 |
| 4:M:96:ILE:O | 4:M:99:ILE:HB | 2.21 | 0.41 |
| 4:M:218:LEU:N | 4:M:218:LEU:CD1 | 2.82 | 0.41 |
| 4:M:219:LEU:HB3 | 4:M:472:TYR:HB2 | 2.02 | 0.41 |
| 4:M:221:THR:CG2 | 4:M:223:HIS:CE1 | 3.04 | 0.41 |
| 4:M:224:VAL:O | 4:M:479:PHE:HA | 2.20 | 0.41 |
| 4:M:240:ILE:O | 4:M:444:ALA:HB1 | 2.21 | 0.41 |
| 4:M:317:MET:SD | 4:M:321:GLY:HA3 | 2.61 | 0.41 |
| 4:M:319:SER:OG | 4:M:346:ASN:N | 2.45 | 0.41 |
| 4:M:356:LEU:CD2 | 4:M:356:LEU:O | 2.68 | 0.41 |
| 4:M:433:VAL:O | 4:M:435:LEU:CD1 | 2.68 | 0.41 |
| 1:A:85:ALA:C | 1:A:87:CYS:H | 2.25 | 0.41 |
| 1:A:254:ILE:HD13 | 3:S:96:LEU:CB | 2.46 | 0.41 |
| 1:A:420:ILE:HG23 | 1:A:424:TYR:CB | 2.47 | 0.41 |
| 1:A:540:ILE:HG23 | 1:A:541:SER:N | 2.35 | 0.41 |
| 2:B:35:TYR:O | 2:B:42:ILE:CG1 | 2.69 | 0.41 |
| 2:B:100:LEU:CD2 | 4:M:123:LEU:HD21 | 2.51 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:107:ARG:NH1 | 4:M:20:LEU:CG | 2.66 | 0.41 |
| 2:B:210:CYS:O | 2:B:213:LEU:N | 2.54 | 0.41 |
| 2:B:252:LEU:CG | 2:B:302:PHE:CD1 | 2.99 | 0.41 |
| 2:B:325:LEU:HD22 | 2:B:339:PHE:CD1 | 2.56 | 0.41 |
| 2:B:359:LEU:HA | 2:B:359:LEU:HD13 | 1.85 | 0.41 |
| 2:B:363:ILE:HB | 2:B:398:ILE:HD11 | 2.01 | 0.41 |
| 2:B:375:LEU:O | 2:B:376:PRO:C | 2.32 | 0.41 |
| 3:S:135:ILE:O | 3:S:141:VAL:CB | 2.69 | 0.41 |
| 4:M:96:ILE:HD13 | 4:M:124:ILE:HG22 | 2.03 | 0.41 |
| 4:M:243:ILE:CB | 4:M:472:TYR:HB3 | 2.51 | 0.41 |
| 4:M:270:PRO:HA | 4:M:302:TYR:CD2 | 2.56 | 0.41 |
| 4:M:275:CYS:HB3 | 4:M:290:PHE:CE1 | 2.56 | 0.41 |
| 4:M:293:PRO:C | 4:M:294:ASP:O | 2.34 | 0.41 |
| 1:A:101:GLN:NE2 | 3:S:167:ILE:HD11 | 2.31 | 0.40 |
| 1:A:433:ILE:HG23 | 1:A:476:GLN:CG | 2.50 | 0.40 |
| 1:A:496:ILE:O | 1:A:499:ILE:HB | 2.21 | 0.40 |
| 2:B:20:ARG:NH2 | 4:M:118:TYR:CD1 | 2.78 | 0.40 |
| 2:B:86:VAL:O | 2:B:89:ASN:HB2 | 2.20 | 0.40 |
| 2:B:279:LEU:CG | 2:B:288:TYR:CD2 | 2.94 | 0.40 |
| 2:B:396:ILE:CG2 | 2:B:432:ALA:CA | 2.45 | 0.40 |
| 2:B:437:SER:C | 2:B:439:CYS:H | 2.24 | 0.40 |
| 2:B:477:MET:O | 2:B:480:GLN:CB | 2.63 | 0.40 |
| 2:B:486:HIS:CE1 | 2:B:518:ILE:CB | 3.04 | 0.40 |
| 3:S:61:ASN:O | 3:S:62:GLU:C | 2.59 | 0.40 |
| 4:M:71:LYS:CG | 4:M:74:TYR:CZ | 3.05 | 0.40 |
| 4:M:223:HIS:HD2 | 4:M:478:ASN:HB2 | 1.86 | 0.40 |
| 4:M:280:ASP:CG | 4:M:282:VAL:HG23 | 2.42 | 0.40 |
| 4:M:351:SER:HB2 | 4:M:441:GLY:HA3 | 2.01 | 0.40 |
| 1:A:128:LEU:HD22 | 1:A:146:ALA:HB1 | 2.02 | 0.40 |
| 1:A:249:ASN:OD1 | 1:A:251:TRP:N | 2.54 | 0.40 |
| 2:B:204:ASP:HA | 2:B:205:PRO:HD3 | 1.96 | 0.40 |
| 2:B:220:ALA:HA | 2:B:258:GLN:CG | 2.35 | 0.40 |
| 2:B:309:LEU:CB | 2:B:317:VAL:HG12 | 2.25 | 0.40 |
| 2:B:347:VAL:O | 2:B:349:MET:N | 2.54 | 0.40 |
| 3:S:43:ASN:HB3 | 3:S:46:PHE:CD2 | 2.56 | 0.40 |
| 4:M:212:ASN:ND2 | 4:M:250:LEU:HA | 2.36 | 0.40 |
| 4:M:222:PHE:CZ | 4:M:439:TYR:HE2 | 2.35 | 0.40 |
| 4:M:302:TYR:HB3 | 4:M:447:ILE:HD13 | 2.03 | 0.40 |
| 4:M:360:LEU:CD1 | 4:M:433:VAL:CB | 2.98 | 0.40 |
| 4:M:450:GLU:O | 4:M:451:ALA:HB2 | 2.22 | 0.40 |
| 1:A:429:VAL:CG1 | 1:A:469:LEU:CD1 | 2.99 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:461:CYS:O | 1:A:462:GLN:O | 2.39 | 0.40 |
| 1:A:533:ILE:HG21 | 1:A:559:PHE:CZ | 2.56 | 0.40 |
| 1:A:609:LEU:CG | 1:A:628:VAL:HB | 2.49 | 0.40 |
| 2:B:43:ASN:CB | 2:B:44:PRO:HD2 | 2.50 | 0.40 |
| 2:B:127:LEU:CD2 | 2:B:139:LEU:HB2 | 2.51 | 0.40 |
| 2:B:143:SER:OG | 2:B:179:LYS:CD | 2.31 | 0.40 |
| 2:B:225:LEU:O | 2:B:227:HIS:N | 2.55 | 0.40 |
| 2:B:230:PHE:CG | 2:B:298:ASP:HB3 | 2.52 | 0.40 |
| 2:B:326:TYR:CE2 | 2:B:369:LEU:HB2 | 2.57 | 0.40 |
| 2:B:356:LYS:O | 2:B:360:LEU:HG | 2.22 | 0.40 |
| 2:B:497:LEU:CD2 | 2:B:511:ILE:CG2 | 2.99 | 0.40 |
| 4:M:20:LEU:HD21 | 4:M:126:ASN:HA | 2.03 | 0.40 |
| 4:M:100:LEU:HD21 | 4:M:121:ILE:HA | 2.03 | 0.40 |
| 4:M:443:SER:CA | 4:M:447:ILE:CG1 | 2.99 | 0.40 |
| 1:A:241:TYR:CE2 | 1:A:277:LYS:CB | 3.05 | 0.40 |
| 1:A:244:LEU:CD2 | 1:A:277:LYS:HG3 | 2.51 | 0.40 |
| 1:A:580:GLU:O | 1:A:583:GLU:N | 2.54 | 0.40 |
| 1:A:614:LEU:HD21 | 1:A:621:LEU:HG | 2.03 | 0.40 |
| 2:B:12:LEU:HB3 | 4:M:13:LYS:CD | 2.46 | 0.40 |
| 2:B:216:LYS:HD3 | 2:B:251:LEU:CA | 2.47 | 0.40 |
| 2:B:223:LEU:HD21 | 2:B:258:GLN:CB | 2.50 | 0.40 |
| 2:B:309:LEU:CD1 | 2:B:317:VAL:HG11 | 2.49 | 0.40 |
| 2:B:392:SER:O | 2:B:396:ILE:HG13 | 2.21 | 0.40 |
| 2:B:431:MET:C | 2:B:433:VAL:N | 2.73 | 0.40 |
| 2:B:537:PHE:C | 2:B:539:ASN:N | 2.75 | 0.40 |
| 3:S:37:GLU:O | 3:S:40:SER:N | 2.53 | 0.40 |
| 3:S:80:TYR:HE2 | 3:S:110:ASP:OD1 | 2.05 | 0.40 |
| 3:S:159:ALA:C | 3:S:161:GLU:N | 2.75 | 0.40 |
| 4:M:45:SER:CB | 4:M:75:TRP:CZ2 | 2.95 | 0.40 |
| 4:M:64:LYS:HE3 | 4:M:79:SER:HB2 | 2.02 | 0.40 |
| 1:A:193:PRO:O | 1:A:196:LEU:HB3 | 2.21 | 0.40 |
| 1:A:488:ARG:CD | 1:A:522:PHE:CZ | 3.04 | 0.40 |
| 1:A:488:ARG:HG2 | 1:A:522:PHE:HE2 | 1.85 | 0.40 |
| 2:B:108:PHE:HE1 | 2:B:112:ASP:HB2 | 1.87 | 0.40 |
| 2:B:231:ARG:C | 2:B:233:TYR:H | 2.25 | 0.40 |
| 2:B:249:ILE:O | 2:B:253:ILE:HG13 | 2.21 | 0.40 |
| 2:B:478:LEU:O | 2:B:480:GLN:N | 2.53 | 0.40 |
| 2:B:549:LEU:HA | 2:B:595:VAL:HG11 | 2.03 | 0.40 |
| 3:S:2:ILE:HG12 | 3:S:98:ILE:HD12 | 2.03 | 0.40 |
| 3:S:53:THR:O | 3:S:69:ASN:OD1 | 2.40 | 0.40 |
| 3:S:80:TYR:CE2 | 3:S:110:ASP:OD1 | 2.75 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|----------------|--------------------------|-------------------|
| 3:S:110:ASP:O | 3:S:114:THR:HA | 2.21 | 0.40 |
| 4:M:47:SER:O | 4:M:75:TRP:CH2 | 2.53 | 0.40 |
| 4:M:58:ARG:C | 4:M:60:LEU:O | 2.59 | 0.40 |
| 4:M:70:ASN:OD1 | 4:M:75:TRP:NE1 | 2.54 | 0.40 |
| 4:M:92:PHE:CZ | 4:M:128:CYS:CB | 2.91 | 0.40 |
| 4:M:389:SER:N | 4:M:394:GLN:O | 2.49 | 0.40 |
| 4:M:428:VAL:O | 4:M:430:LEU:N | 2.54 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 1 | A | 574/964 (60%) | 529 (92%) | 32 (6%) | 13 (2%) | 6 | 34 |
| 2 | B | 619/809 (76%) | 500 (81%) | 72 (12%) | 47 (8%) | 1 | 13 |
| 3 | S | 166/194 (86%) | 160 (96%) | 4 (2%) | 2 (1%) | 13 | 50 |
| 4 | M | 391/483 (81%) | 315 (81%) | 51 (13%) | 25 (6%) | 1 | 16 |
| All | All | 1750/2450 (71%) | 1504 (86%) | 159 (9%) | 87 (5%) | 4 | 20 |

All (87) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 86 | TRP |
| 1 | A | 267 | GLU |
| 1 | A | 278 | ILE |
| 1 | A | 305 | GLU |
| 1 | A | 306 | GLU |
| 1 | A | 449 | TRP |
| 1 | A | 566 | PHE |
| 2 | B | 26 | ALA |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | B | 70 | MET |
| 2 | B | 109 | ALA |
| 2 | B | 200 | MET |
| 2 | B | 242 | SER |
| 2 | B | 296 | ASP |
| 2 | B | 313 | SER |
| 2 | B | 436 | LEU |
| 2 | B | 523 | PHE |
| 2 | B | 558 | TYR |
| 2 | B | 560 | ILE |
| 2 | B | 561 | ASP |
| 2 | B | 564 | LYS |
| 2 | B | 565 | GLN |
| 2 | B | 568 | VAL |
| 3 | S | 72 | ASP |
| 3 | S | 164 | ASP |
| 4 | M | 51 | LEU |
| 4 | M | 84 | LYS |
| 4 | M | 104 | PHE |
| 4 | M | 106 | LYS |
| 4 | M | 280 | ASP |
| 4 | M | 306 | LEU |
| 4 | M | 405 | THR |
| 4 | M | 447 | ILE |
| 4 | M | 479 | PHE |
| 1 | A | 114 | PHE |
| 1 | A | 536 | MET |
| 2 | B | 182 | ARG |
| 2 | B | 215 | TYR |
| 2 | B | 228 | GLY |
| 2 | B | 232 | ARG |
| 2 | B | 259 | TYR |
| 2 | B | 274 | PRO |
| 2 | B | 347 | VAL |
| 2 | B | 353 | GLN |
| 2 | B | 372 | THR |
| 2 | B | 374 | PHE |
| 2 | B | 379 | LYS |
| 2 | B | 399 | LEU |
| 2 | B | 406 | SER |
| 2 | B | 600 | LYS |
| 4 | M | 231 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | M | 279 | ASN |
| 4 | M | 316 | ARG |
| 4 | M | 321 | GLY |
| 4 | M | 429 | ASP |
| 1 | A | 116 | LYS |
| 1 | A | 174 | ARG |
| 1 | A | 279 | LEU |
| 2 | B | 36 | THR |
| 2 | B | 105 | LEU |
| 2 | B | 196 | LEU |
| 2 | B | 226 | LEU |
| 2 | B | 252 | LEU |
| 2 | B | 462 | ASN |
| 2 | B | 573 | GLU |
| 4 | M | 81 | SER |
| 4 | M | 356 | LEU |
| 4 | M | 363 | ASN |
| 4 | M | 463 | ASN |
| 4 | M | 470 | ALA |
| 2 | B | 75 | ASP |
| 2 | B | 177 | ILE |
| 2 | B | 194 | ASP |
| 2 | B | 199 | LEU |
| 2 | B | 231 | ARG |
| 2 | B | 535 | GLN |
| 4 | M | 44 | ASP |
| 4 | M | 263 | MET |
| 2 | B | 227 | HIS |
| 2 | B | 376 | PRO |
| 4 | M | 12 | ASN |
| 4 | M | 48 | ASP |
| 2 | B | 440 | GLY |
| 4 | M | 253 | ASN |
| 2 | B | 69 | ILE |
| 1 | A | 406 | GLY |
| 4 | M | 406 | GLY |
| 2 | B | 518 | ILE |

5.3.2 Protein sidechains [i](#)

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

entries.

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1 | A | 536/898 (60%) | 530 (99%) | 6 (1%) | 73 | 84 |
| 2 | B | 566/738 (77%) | 561 (99%) | 5 (1%) | 78 | 87 |
| 3 | S | 159/175 (91%) | 156 (98%) | 3 (2%) | 57 | 75 |
| 4 | M | 360/441 (82%) | 351 (98%) | 9 (2%) | 47 | 68 |
| All | All | 1621/2252 (72%) | 1598 (99%) | 23 (1%) | 68 | 80 |

All (23) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 175 | PRO |
| 1 | A | 186 | PHE |
| 1 | A | 196 | LEU |
| 1 | A | 241 | TYR |
| 1 | A | 292 | TYR |
| 1 | A | 418 | ILE |
| 2 | B | 233 | TYR |
| 2 | B | 259 | TYR |
| 2 | B | 418 | TYR |
| 2 | B | 453 | TRP |
| 2 | B | 592 | TYR |
| 3 | S | 8 | PHE |
| 3 | S | 38 | LEU |
| 3 | S | 113 | PHE |
| 4 | M | 6 | TYR |
| 4 | M | 118 | TYR |
| 4 | M | 214 | LEU |
| 4 | M | 250 | LEU |
| 4 | M | 343 | ASN |
| 4 | M | 379 | LEU |
| 4 | M | 437 | TYR |
| 4 | M | 472 | TYR |
| 4 | M | 479 | PHE |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 101 | GLN |
| 1 | A | 102 | GLN |
| 1 | A | 199 | ASN |
| 1 | A | 634 | ASN |
| 2 | B | 40 | GLN |
| 2 | B | 41 | ASN |
| 2 | B | 46 | GLN |
| 2 | B | 222 | HIS |
| 2 | B | 229 | HIS |
| 2 | B | 258 | GLN |
| 2 | B | 304 | GLN |
| 2 | B | 333 | GLN |
| 2 | B | 397 | GLN |
| 2 | B | 404 | ASN |
| 2 | B | 441 | GLN |
| 2 | B | 461 | HIS |
| 2 | B | 486 | HIS |
| 2 | B | 574 | ASN |
| 3 | S | 64 | ASN |
| 3 | S | 65 | ASN |
| 3 | S | 126 | GLN |
| 4 | M | 70 | ASN |
| 4 | M | 265 | ASN |
| 4 | M | 343 | ASN |
| 4 | M | 346 | ASN |

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 |
|-----|-------|------------------|
| 4 | M | 33 |
| 3 | S | 11 |
| 1 | A | 9 |
| 2 | B | 6 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | S | 68:VAL | C | 69:ASN | N | 1.67 |
| 1 | A | 244:LEU | C | 245:VAL | N | 1.20 |
| 1 | A | 277:LYS | C | 278:ILE | N | 1.20 |
| 1 | A | 464:ILE | C | 465:SER | N | 1.20 |
| 1 | B | 259:TYR | C | 260:LEU | N | 1.20 |
| 1 | S | 60:SER | C | 61:ASN | N | 1.20 |
| 1 | S | 62:GLU | C | 63:ASN | N | 1.20 |
| 1 | S | 144:THR | C | 145:ASN | N | 1.20 |
| 1 | M | 6:TYR | C | 7:ILE | N | 1.20 |
| 1 | M | 252:ASP | C | 253:ASN | N | 1.20 |
| 1 | M | 280:ASP | C | 281:GLY | N | 1.20 |
| 1 | A | 378:ILE | C | 379:VAL | N | 1.19 |
| 1 | A | 439:ASP | C | 440:ASN | N | 1.19 |
| 1 | A | 535:ILE | C | 536:MET | N | 1.19 |
| 1 | B | 184:GLY | C | 185:LYS | N | 1.19 |
| 1 | B | 334:MET | C | 335:LYS | N | 1.19 |
| 1 | S | 113:PHE | C | 114:THR | N | 1.19 |
| 1 | M | 23:THR | C | 24:ALA | N | 1.19 |
| 1 | M | 82:LYS | C | 83:SER | N | 1.19 |
| 1 | M | 288:ILE | C | 289:THR | N | 1.19 |
| 1 | M | 377:LYS | C | 378:ILE | N | 1.19 |
| 1 | A | 289:SER | C | 290:VAL | N | 1.18 |
| 1 | A | 508:LEU | C | 509:PRO | N | 1.18 |
| 1 | S | 6:LEU | C | 7:ILE | N | 1.18 |
| 1 | S | 22:PRO | C | 23:VAL | N | 1.18 |
| 1 | S | 114:THR | C | 115:GLU | N | 1.18 |
| 1 | M | 56:VAL | C | 57:GLY | N | 1.18 |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | M | 64:LYS | C | 65:TYR | N | 1.18 |
| 1 | M | 136:VAL | C | 137:SER | N | 1.18 |
| 1 | M | 379:LEU | C | 380:ARG | N | 1.18 |
| 1 | A | 507:GLN | C | 508:LEU | N | 1.17 |
| 1 | S | 70:ASN | C | 71:GLU | N | 1.17 |
| 1 | M | 62:VAL | C | 63:TYR | N | 1.17 |
| 1 | M | 70:ASN | C | 71:LYS | N | 1.17 |
| 1 | M | 403:THR | C | 404:ALA | N | 1.17 |
| 1 | M | 450:GLU | C | 451:ALA | N | 1.17 |
| 1 | S | 8:PHE | C | 9:ASN | N | 1.16 |
| 1 | M | 134:PRO | C | 135:ASN | N | 1.16 |
| 1 | M | 279:ASN | C | 280:ASP | N | 1.16 |
| 1 | M | 319:SER | C | 320:ILE | N | 1.16 |
| 1 | M | 352:GLN | C | 353:VAL | N | 1.16 |
| 1 | M | 453:ASP | C | 454:ILE | N | 1.16 |
| 1 | M | 106:LYS | C | 107:ASP | N | 1.15 |
| 1 | B | 581:TYR | C | 582:ASP | N | 1.14 |
| 1 | M | 20:LEU | C | 21:GLY | N | 1.14 |
| 1 | M | 52:ASP | C | 53:HIS | N | 1.14 |
| 1 | M | 61:GLU | C | 62:VAL | N | 1.14 |
| 1 | M | 351:SER | C | 352:GLN | N | 1.14 |
| 1 | B | 284:ASN | C | 285:GLU | N | 1.13 |
| 1 | B | 293:VAL | C | 294:VAL | N | 1.13 |
| 1 | M | 21:GLY | C | 22:ALA | N | 1.13 |
| 1 | M | 63:TYR | C | 64:LYS | N | 1.13 |
| 1 | M | 130:GLU | C | 131:ALA | N | 1.12 |
| 1 | M | 80:THR | C | 81:SER | N | 1.11 |
| 1 | M | 105:ASP | C | 106:LYS | N | 1.10 |
| 1 | M | 3:LEU | C | 4:SER | N | 1.08 |
| 1 | M | 81:SER | C | 82:LYS | N | 1.08 |
| 1 | S | 48:SER | C | 49:SER | N | 1.03 |
| 1 | M | 135:ASN | C | 136:VAL | N | 0.93 |

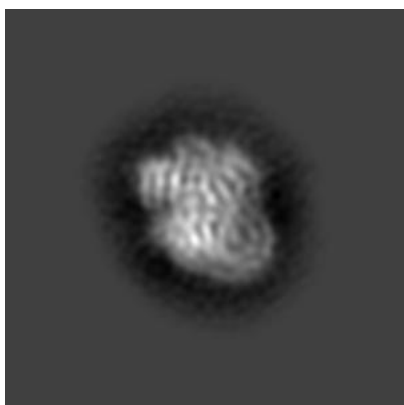
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13187. These allow visual inspection of the internal detail of the map and identification of artifacts.

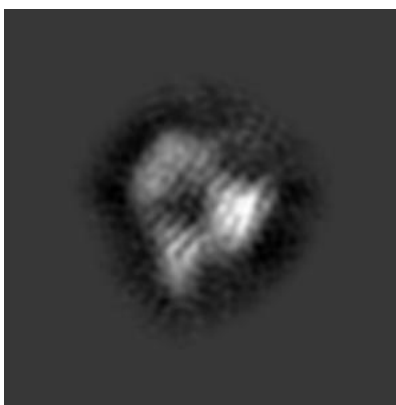
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

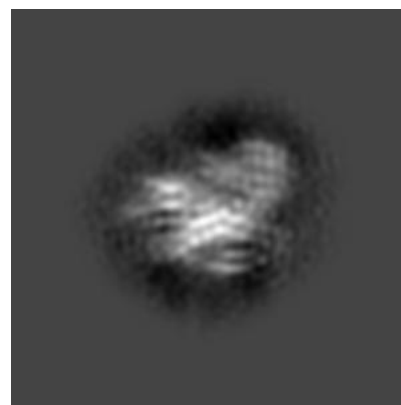
6.1.1 Primary map



X



Y

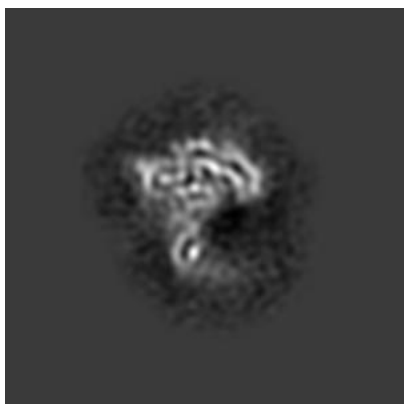


Z

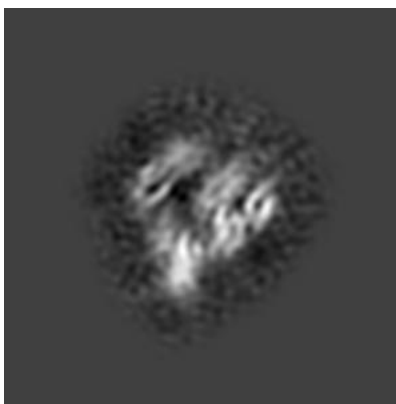
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 132



Y Index: 132

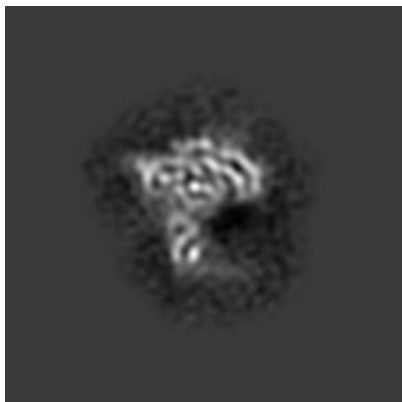


Z Index: 132

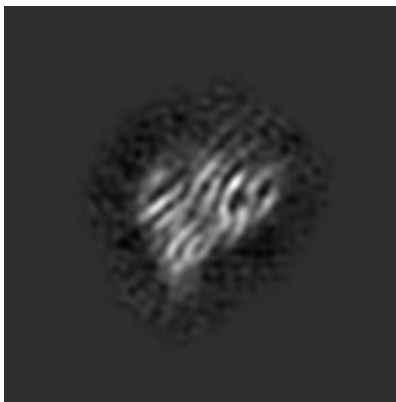
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 130



Y Index: 123

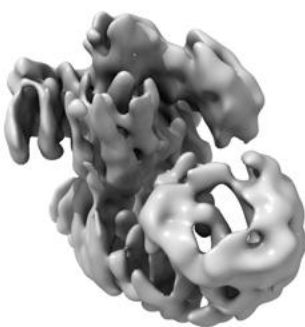


Z Index: 150

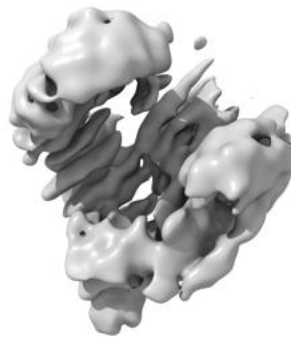
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

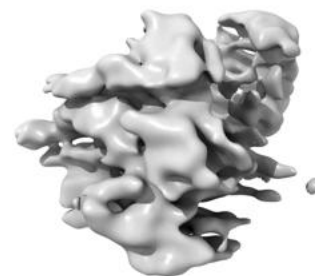
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

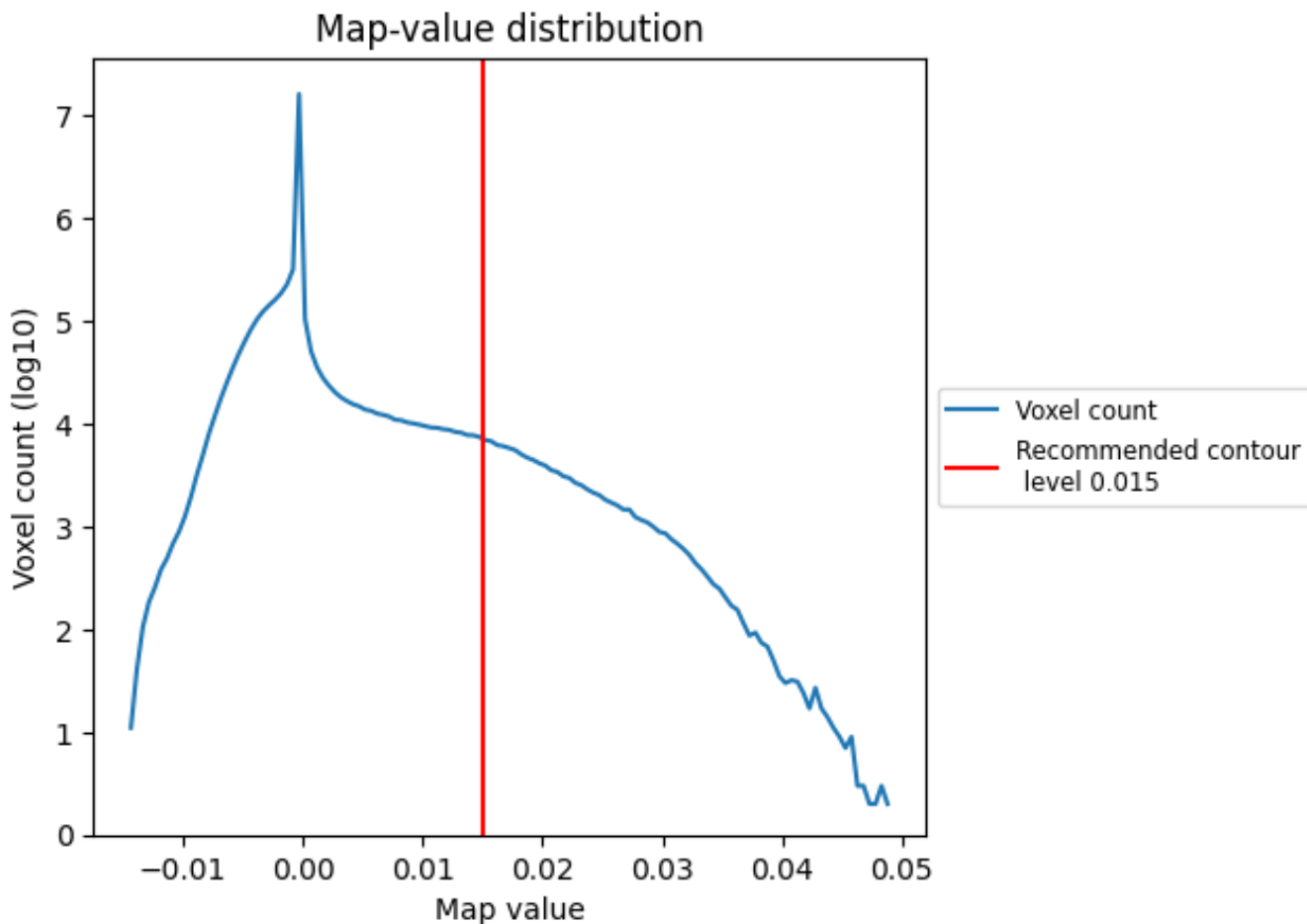
6.5 Mask visualisation

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

7 Map analysis [i](#)

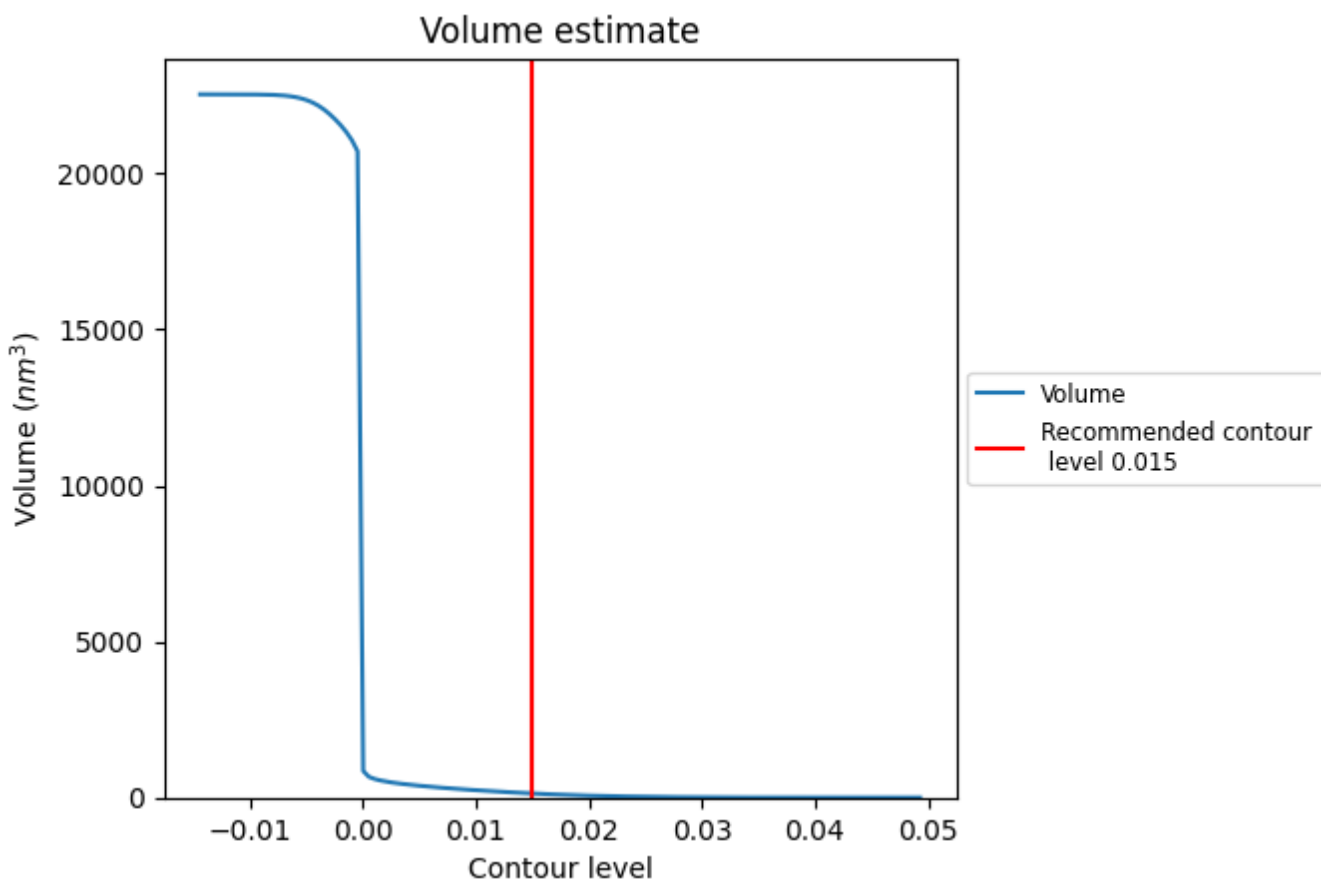
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

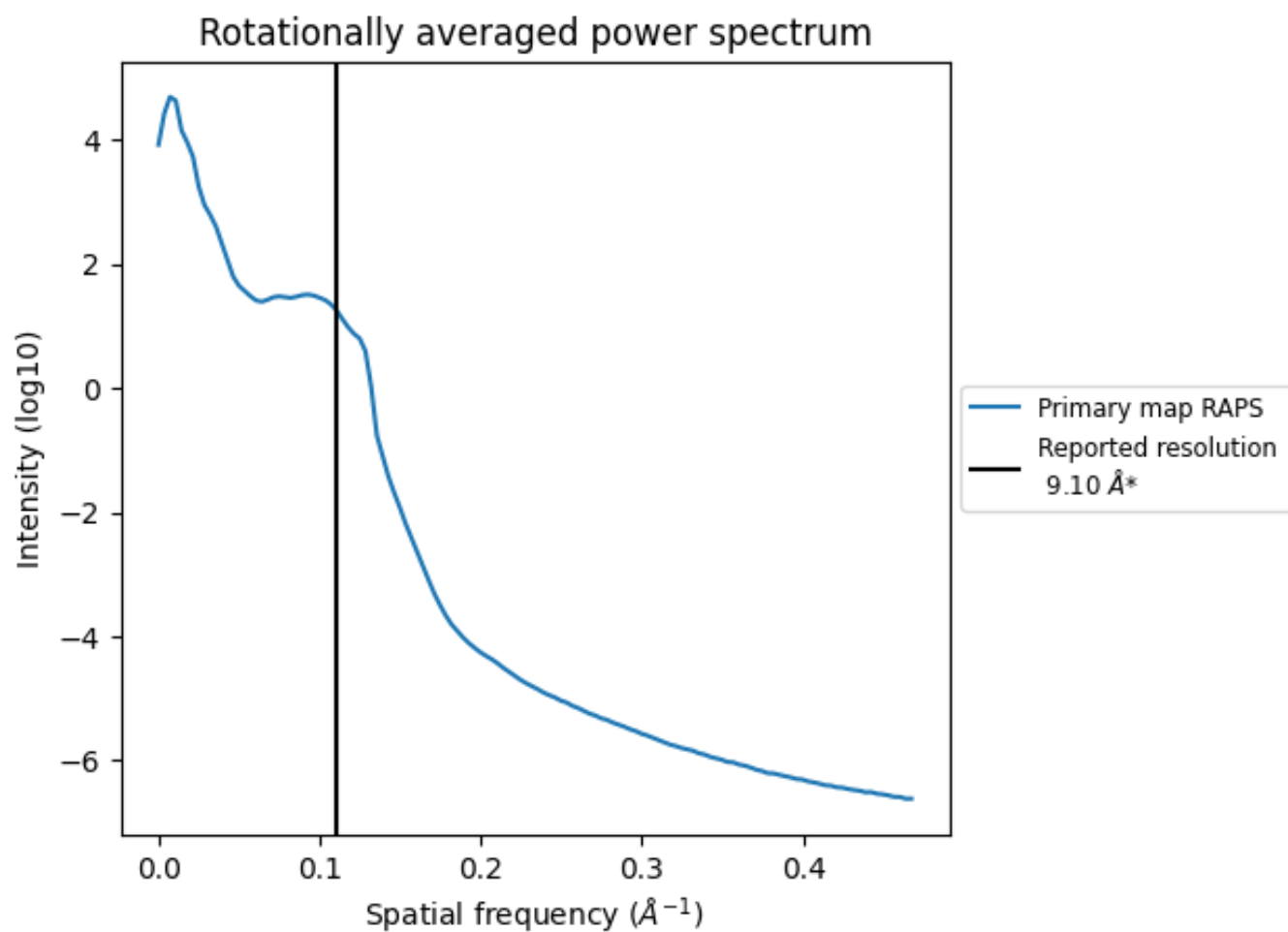
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 131 nm³; this corresponds to an approximate mass of 119 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum i



*Reported resolution corresponds to spatial frequency of 0.110 Å⁻¹

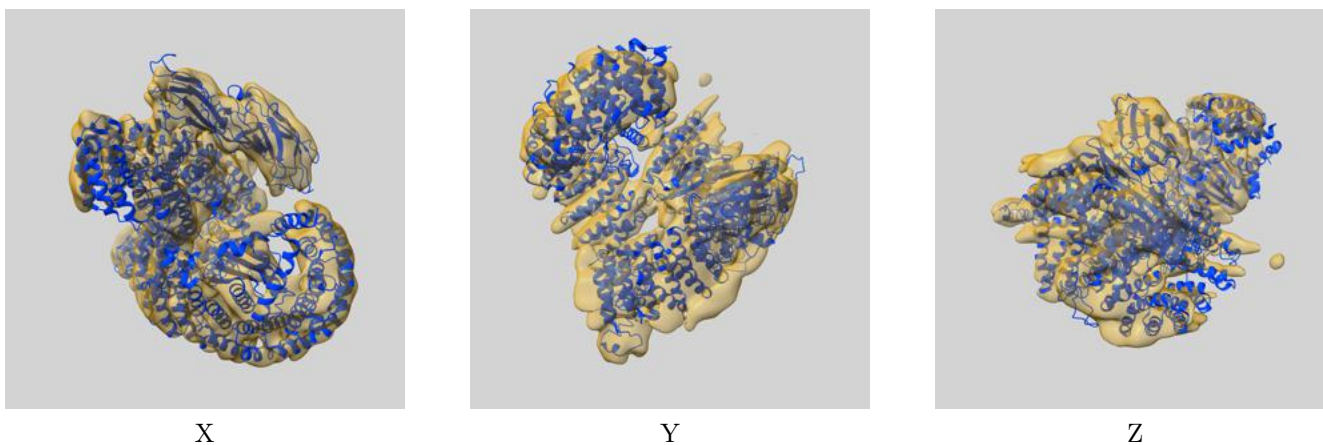
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

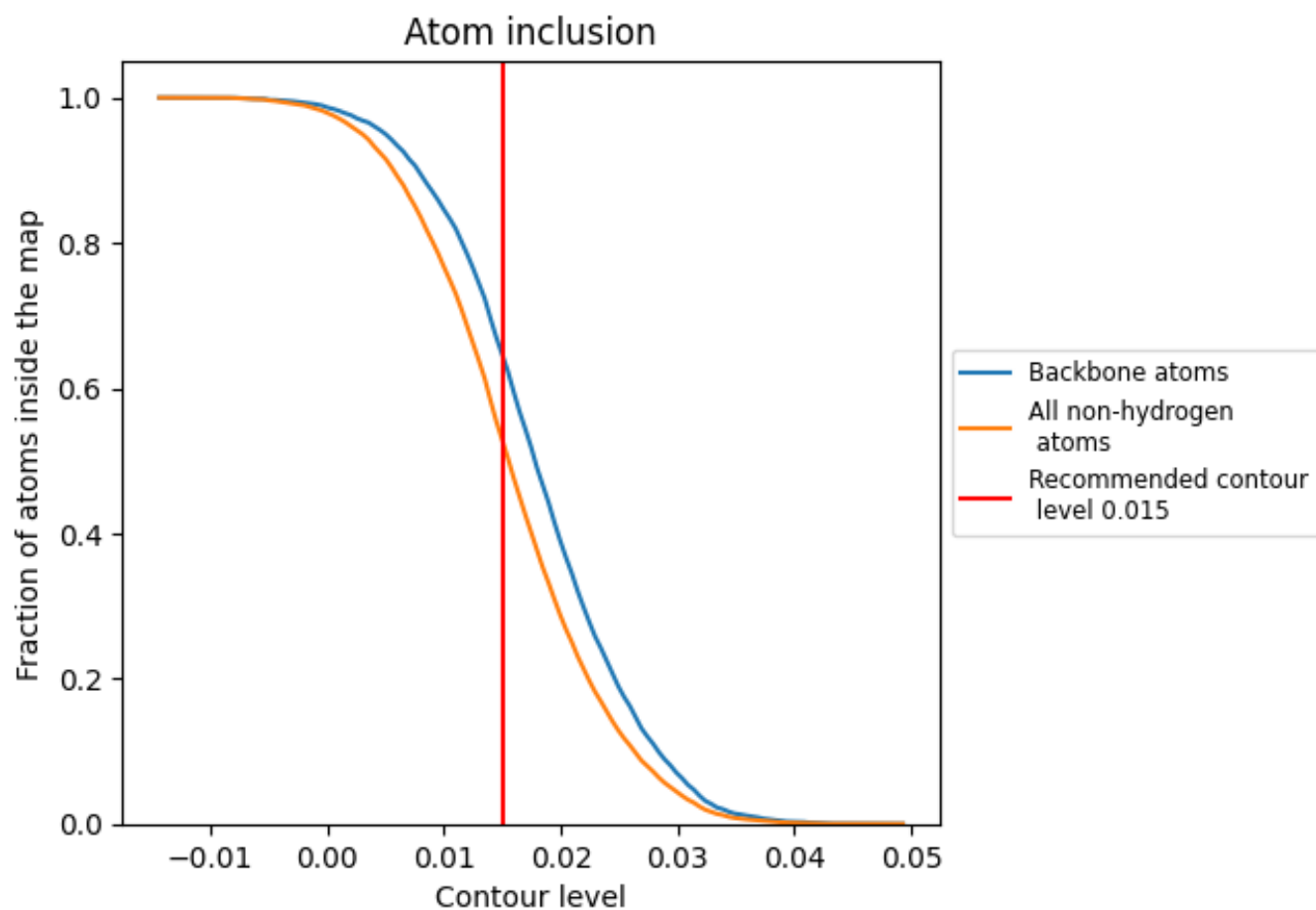
This section contains information regarding the fit between EMDB map EMD-13187 and PDB model 7P3X. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 53% of all non-hydrogen atoms, are inside the map.