



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Feb 6, 2017 – 05:09 PM EST

PDB ID : 5U8T
EMDB ID: : EMD-8519
Title : Structure of Eukaryotic CMG Helicase at a Replication Fork and Implications
Authors : Li, B.; Georgescu, R.; Yuan, Z.; Santos, R.; Sun, J.; Zhang, D.; Yurieva, O.;
Li, H.; O'Donnell, M.E.
Deposited on : 2016-12-15
Resolution : 4.90 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

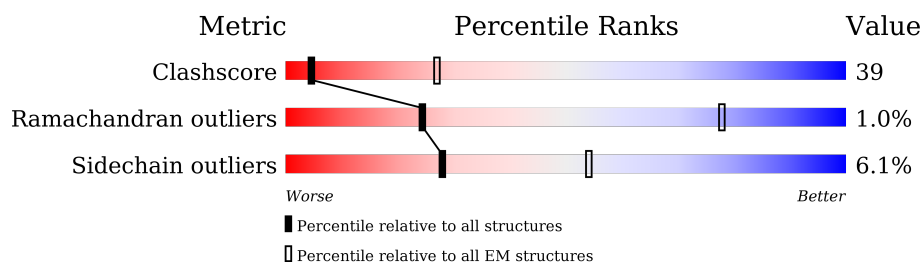
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.90 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 | 114402 | 924 |
| Ramachandran outliers | 111179 | 726 |
| Sidechain outliers | 111093 | 686 |

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | 2 | 868 | |
| 2 | 3 | 971 | |
| 3 | 4 | 933 | |
| 4 | 5 | 775 | |
| 5 | 6 | 1017 | |
| 6 | 7 | 845 | |
| 7 | A | 208 | |
| 8 | B | 213 | |
| 9 | C | 194 | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 10 | D | 294 | |
| 11 | E | 650 | |
| 12 | F | 14 | |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 13 | ANP | 2 | 901 | - | - | X | - |
| 13 | ANP | 3 | 1001 | - | - | X | - |
| 13 | ANP | 5 | 801 | - | - | X | - |

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 40788 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 DNA replication licensing factor MCM2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1 | 2 | 583 | Total | C | N | O | S | 0 | 0 |
| | | | 4591 | 2899 | 818 | 858 | 16 | | |

- Molecule 2 is a protein called DNA replication licensing factor MCM3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2 | 3 | 589 | Total | C | N | O | S | 0 | 0 |
| | | | 4624 | 2915 | 824 | 872 | 13 | | |

- Molecule 3 is a protein called DNA replication licensing factor MCM4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| 3 | 4 | 672 | Total | C | N | O | S | 0 | 0 |
| | | | 5318 | 3340 | 929 | 1021 | 28 | | |

- Molecule 4 is a protein called Minichromosome maintenance protein 5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4 | 5 | 602 | Total | C | N | O | S | 0 | 0 |
| | | | 4740 | 2980 | 815 | 921 | 24 | | |

- Molecule 5 is a protein called DNA replication licensing factor MCM6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5 | 6 | 661 | Total | C | N | O | S | 0 | 0 |
| | | | 5142 | 3247 | 905 | 967 | 23 | | |

- Molecule 6 is a protein called DNA replication licensing factor MCM7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 6 | 7 | 660 | Total | C | N | O | S | 0 | 0 |
| | | | 5201 | 3278 | 903 | 991 | 29 | | |

- Molecule 7 is a protein called DNA replication complex GINS protein PSF1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 7 | A | 208 | Total | C | N | O | S | 0 | 0 |
| | | | 1696 | 1065 | 290 | 331 | 10 | | |

- Molecule 8 is a protein called DNA replication complex GINS protein PSF2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8 | B | 181 | Total | C | N | O | S | 0 | 0 |
| | | | 1513 | 978 | 261 | 270 | 4 | | |

- Molecule 9 is a protein called DNA replication complex GINS protein PSF3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9 | C | 159 | Total | C | N | O | S | 0 | 0 |
| | | | 1288 | 843 | 207 | 232 | 6 | | |

- Molecule 10 is a protein called DNA replication complex GINS protein SLD5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 10 | D | 221 | Total | C | N | O | S | 0 | 0 |
| | | | 1820 | 1159 | 300 | 348 | 13 | | |

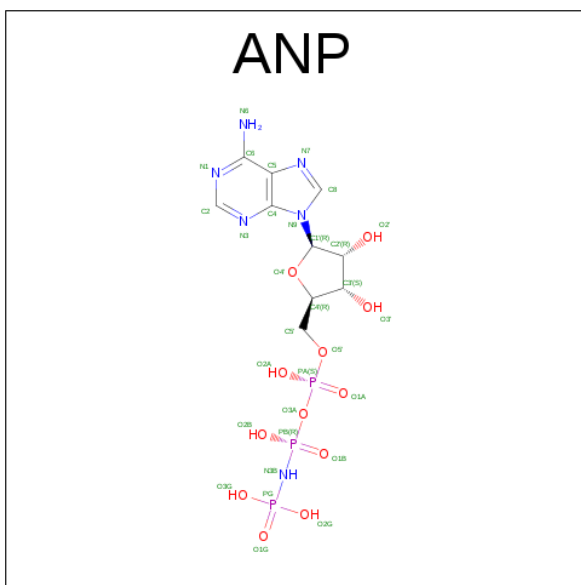
- Molecule 11 is a protein called Cell division control protein 45.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 11 | E | 553 | Total | C | N | O | S | 0 | 0 |
| | | | 4482 | 2862 | 763 | 844 | 13 | | |

- Molecule 12 is a DNA chain called DNA (5'-D(P*TP*TP*TP*TP*TP*TP*TP*TP*T
P*TP*TP*TP*T)-3').

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|-------|
| 12 | F | 14 | Total | C | N | O | P | 0 | 0 |
| | | | 280 | 140 | 28 | 98 | 14 | | |

- Molecule 13 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).

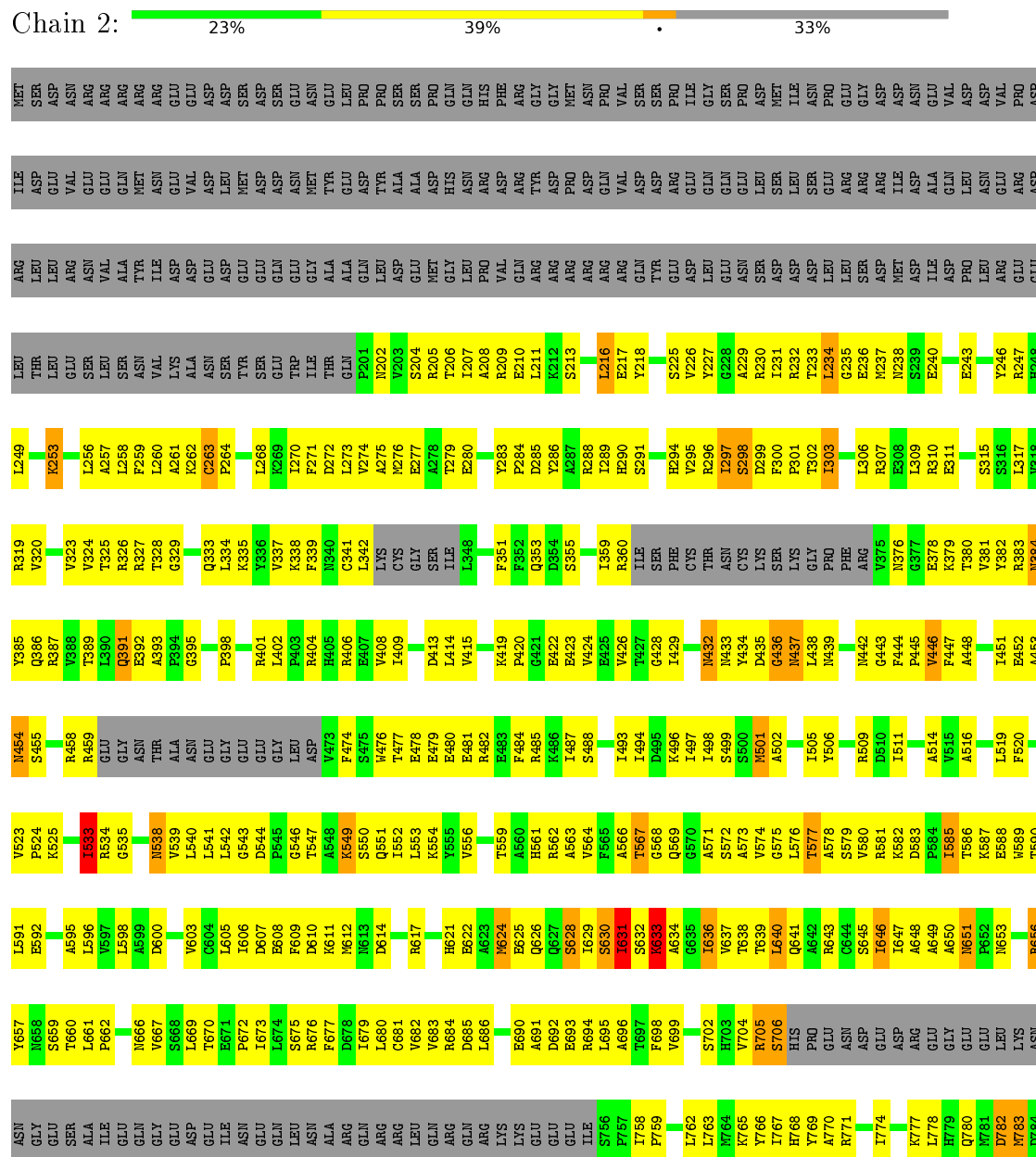


| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 13 | 2 | 1 | Total 31 | C 10 | N 6 | O 12 | P 3 | 0 |
| 13 | 3 | 1 | Total 31 | C 10 | N 6 | O 12 | P 3 | 0 |
| 13 | 5 | 1 | Total 31 | C 10 | N 6 | O 12 | P 3 | 0 |

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: DNA replication licensing factor MCM2



| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| ARG | ILE | ASN | GLU | GLU | LEU | PRO | GLU | GLU | GLU | LYS | PHE | SER | ALA | GLN | GLU | TYR | LEU | ALA | GLY | LEU | LYS | ILE | MET | SER | ASP | ARG | ASN | ASN | LEU | MET | VAL | ALA | ASP | ASP | LYS | VAL | TRP | ARG | VAL |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

- Molecule 3: DNA replication licensing factor MCM4

Chain 4: 27% 41% . 28%

| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | SER | SER | GLN | GLN | SER | SER | PRO | THR | LYS | GLU | ASP | ASN | ASN | SER | SER | SER | PRO | VAL | VAL | PRO | ASN | ASN | ASP | SER | SER | LEU | GLN | ALA | LEU | PHE | TYR | SER | SER | SER | SER | SER | GLN | GLY | ASP | ILE | TYR | GLY | ARG | ASN | ASN | SER | GLN | ASN | LEU | SER | GLN | GLY | GLY |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

ASN
TLE
ARG
ALA
ALA
TLE
GLY
SER
SER
PRO
LEU
ASN
PHE
PRO
SER
SER
SER
SER
GLN
GLN
ARG
GLN
ASN
SER
SER
ASP
VAL
PHE
GLN
SER
SER
GLN
GLY
ARG
GLN
GLN
ARG
TLE
TLE
SER
SER
SER
ALA
ALA
SER
GLY
ARG
SER
SER
ARG
TYR
HIS
SER
ASP
LEU
ARG
SER
ASP
ARG
ALA
ALA
PRO
THR
SER
SER

| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|
| SER | SER | LEU | GLY | ARG | ASN | GLY | GLN | ASN | ARG | VAL | HIS | MET | ARG | ARG | ASN | ASP | ASP | ASP | LEU | SER | SER | PRO | ARG | ARG | ARG | ILE | ILE | VAL | ASP | PHE | ASP | THR | THR | ARG | SER | GLY | VAL | ASN | LEU | LEU | THR | THR | ASP | THR | SER | SER | SER | SER | SER | ALA | PRO | PRO | PRO | GLU | SER | ALA | GLU | PRO | L177 | R178 | L179 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|

| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| T183 | T184 | T191 | T192 | T198 | T199 | S200 | F201 | K202 | Y203 | K204 | F205 | ARG | LVS | ILE | LEU | ASP | ASN | ASP | ASP | GLU | GLU | GLU | GLU | LEU | Y225 | Y226 | I227 | K228 | N231 | R234 | E235 | L236 | G237 | T238 | S239 | N240 | L241 | L242 | L243 | D244 | A245 | L248 | L249 | A250 | Y251 | T252 | K253 | Y254 | T255 |
|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|

| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| L257 | L258 | L259 | L260 | L261 | L264 | L265 | L266 | L267 | L268 | L269 | L270 | L271 | L272 | L275 | L276 | L277 | L278 | L279 | L280 | L281 | L282 | L283 | L284 | L285 | L289 | L290 | L291 | L292 | L293 | L296 | L297 | L301 | L302 | L303 | L304 | L305 | L306 | L307 | L308 | L309 | L311 | L312 | L313 | L314 | L315 | L316 | L317 | L318 | L319 | L320 | L321 | L322 | L323 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|

| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| K324 | K325 | K326 | K327 | K328 | K329 | K330 | K331 | K332 | K333 | K334 | K335 | K336 | K337 | K338 | K339 | K340 | K341 | K342 | K343 | K344 | K345 | K346 | K347 | K348 | K349 | K350 | K351 | K352 | K353 | K354 | K355 | K356 | K357 | K358 | K359 | K360 | K361 | K362 | K363 | K364 | K365 | K366 | K367 | K368 | K369 | K370 | K371 | K372 | K373 | K374 | K375 | K376 | K377 | K378 | K379 | K380 | K381 | K382 | K383 | K384 | K385 | K386 | K387 | K388 | K389 | K390 | K391 | K392 | K393 | K394 | K395 | K396 | K397 | K398 | K399 | K400 | K401 | K402 | K403 | K404 | K405 | K406 | K407 | K408 | K409 | K410 | K411 | K412 | K413 | K414 | K415 | K416 | K417 | K418 | K419 | K420 | K421 | K422 | K423 | K424 | K425 | K426 | K427 | K428 | K429 | K430 | K431 | K432 | K433 | K434 | K435 | K436 | K437 | K438 | K439 | K440 | K441 | K442 | K443 | K444 | K445 | K446 | K447 | K448 | K449 | K450 | K451 | K452 | K453 | K454 | K455 | K456 | K457 | K458 | K459 | K460 | K461 | K462 | K463 | K464 | K465 | K466 | K467 | K468 | K469 | K470 | K471 | K472 | K473 | K474 | K475 | K476 | K477 | K478 | K479 | K480 | K481 | K482 | K483 | K484 | K485 | K486 | K487 | K488 | K489 | K490 | K491 | K492 | K493 | K494 | K495 | K496 | K497 | K498 | K499 | K500 | K501 | K502 | K503 | K504 | K505 | K506 | K507 | K508 | K509 | K510 | K511 | K512 | K513 | K514 | K515 | K516 | K517 | K518 | K519 | K520 | K521 | K522 | K523 | K524 | K525 | K526 | K527 | K528 | K529 | K530 | K531 | K532 | K533 | K534 | K535 | K536 | K537 | K538 | K539 | K540 | K541 | K542 | K543 | K544 | K545 | K546 | K547 | K548 | K549 | K550 | K551 | K552 | K553 | K554 | K555 | K556 | K557 | K558 | K559 | K560 | K561 | K562 | K563 | K564 | K565 | K566 | K567 | K568 | K569 | K570 | K571 | K572 | K573 | K574 | K575 | K576 | K577 | K578 | K579 | K580 | K581 | K582 | K583 | K584 | K585 | K586 | K587 | K588 | K589 | K590 | K591 | K592 | K593 | K594 | K595 | K596 | K597 | K598 | K599 | K600 | K601 | K602 | K603 | K604 | K605 | K606 | K607 | K608 | K609 | K610 | K611 | K612 | K613 | K614 | K615 | K616 | K617 | K618 | K619 | K620 | K621 | K622 | K623 | K624 | K625 | K626 | K627 | K628 | K629 | K630 | K631 | K632 | K633 | K634 | K635 | K636 | K637 | K638 | K639 | K640 | K641 | K642 | K643 | K644 | K645 | K646 | K647 | K648 | K649 | K650 | K651 | K652 | K653 | K654 | K655 | K656 | K657 | K658 | K659 | K660 | K661 | K662 | K663 | K664 | K665 | K666 | K667 | K668 | K669 | K670 | K671 | K672 | K673 | K674 | K675 | K676 | K677 | K678 | K679 | K680 | K681 | K682 | K683 | K684 | K685 | K686 | K687 | K688 | K689 | K690 | K691 | K692 | K693 | K694 | K695 | K696 | K697 | K698 | K699 | K700 | K701 | K702 | K703 | K704 | K705 | K706 | K707 | K708 | K709 | K710 | K711 | K712 | K713 | K714 | K715 | K716 | K717 | K718 | K719 | K720 | K721 | K722 | K723 | K724 | K725 | K726 | K727 | K728 | K729 | K730 | K731 | K732 | K733 | K734 | K735 | K736 | K737 | K738 | K739 | K740 | K741 | K742 | K743 | K744 | K745 | K746 | K747 | K748 | K749 | K750 | K751 | K752 | K753 | K754 | K755 | K756 | K757 | K758 | K759 | K760 | K761 | K762 | K763 | K764 | K765 | K766 | K767 | K768 | K769 | K770 | K771 | K772 | K773 | K774 | K775 | K776 | K777 | K778 | K779 | K780 | K781 | K782 | K783 | K784 | K785 | K786 | K787 | K788 | K789 | K790 | K791 | K792 | K793 | K794 | K795 | K796 | K797 | K798 | K799 | K800 | K801 | K802 | K803 | K804 | K805 | K806 | K807 | K808 | K809 | K810 | K811 | K812 | K813 | K814 | K815 | K816 | K817 | K818 | K819 | K820 | K821 | K822 | K823 | K824 | K825 | K826 | K827 | K828 | K829 | K830 | K831 | K832 | K833 | K834 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|

| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| D393 | D394 | Q395 | Q396 | Q397 | Q398 | Q399 | Q400 | E401 | T402 | Q403 | D404 | F405 | D408 | G409 | Q410 | T411 | P412 | H413 | S414 | I415 | S416 | L417 | C418 | V419 | Y420 | E421 | E422 | L423 | V424 | R428 | A429 | G430 | D431 | R432 | I433 | E434 | V435 | T436 | G437 | T438 | F439 | R440 | S441 | L442 | Q443 | A446 | M447 | S448 | R449 | Q450 | R451 | V452 | L453 | K454 | S455 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|

| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|
| L456 | Y457 | K458 | T459 | Y460 | Y461 | Y462 | Y463 | Y464 | Y466 | Y467 | K468 | Y469 | Y470 | Y471 | Y472 | Y473 | Y474 | Y475 | Y476 | Y477 | Y478 | Y479 | Y480 | Y481 | Y482 | Y483 | Y484 | Y485 | Y486 | Y487 | Y488 | Y489 | Y490 | Y491 | Y492 | Y493 | Y494 | Y495 | Y496 | Y497 | Y498 | Y499 | Y500 | Y501 | Y502 | Y503 | Y504 | Y505 | Y506 | Y507 | Y508 | Y509 | Y510 | Y511 | Y512 | Y513 | Y514 | Y515 | Y516 | Y517 | Y518 | Y519 | Y520 | Y521 | Y522 | Y523 | Y524 | Y525 | Y526 | Y527 | Y528 | Y529 | Y530 | Y531 | Y532 | Y533 | Y534 | Y535 | Y536 | Y537 | Y538 | Y539 | Y540 | Y541 | Y542 | Y543 | Y544 | Y545 | Y546 | Y547 | Y548 | Y549 | Y550 | Y551 | Y552 | Y553 | Y554 | Y555 | Y556 | Y557 | Y558 | Y559 | Y560 | Y561 | Y562 | Y563 | Y564 | Y565 | Y566 | Y567 | Y568 | Y569 | Y570 | Y571 | Y572 | Y573 | Y574 | Y575 | Y576 | Y577 | Y578 | Y579 | Y580 | Y581 | Y582 | Y583 | Y584 | Y585 | Y586 | Y587 | Y588 | Y589 | Y590 | Y591 | Y592 | Y593 | Y594 | Y595 | Y596 | Y597 | Y598 | Y599 | Y600 | Y601 | Y602 | Y603 | Y604 | Y605 | Y606 | Y607 | Y608 | Y609 | Y610 | Y611 | Y612 | Y613 | Y614 | Y615 | Y616 | Y617 | Y618 | Y619 | Y620 | Y621 | Y622 | Y623 | Y624 | Y625 | Y626 | Y627 | Y628 | Y629 | Y630 | Y631 | Y632 | Y633 | Y634 | Y635 | Y636 | Y637 | Y638 | Y639 | Y640 | Y641 | Y642 | Y643 | Y644 | Y645 | Y646 | Y647 | Y648 | Y649 | Y650 | Y651 | Y652 | Y653 | Y654 | Y655 | Y656 | Y657 | Y658 | Y659 | Y660 | Y661 | Y662 | Y663 | Y664 | Y665 | Y666 | Y667 | Y668 | Y669 | Y670 | Y671 | Y672 | Y673 | Y674 | Y675 | Y676 | Y677 | Y678 | Y679 | Y680 | Y681 | Y682 | Y683 | Y684 | Y685 | Y686 | Y687 | Y688 | Y689 | Y690 | Y691 | Y692 | Y693 | Y694 | Y695 | Y696 | Y697 | Y698 | Y699 | Y700 | Y701 | Y702 | Y703 | Y704 | Y705 | Y706 | Y707 | Y708 | Y709 | Y710 | Y711 | Y712 | Y713 | Y714 | Y715 | Y716 | Y717 | Y718 | Y719 | Y720 | Y721 | Y722 | Y723 | Y724 | Y725 | Y726 | Y727 | Y728 | Y729 | Y730 | Y731 | Y732 | Y733 | Y734 | Y735 | Y736 | Y737 | Y738 | Y739 | Y740 | Y741 | Y742 | Y743 | Y744 | Y745 | Y746 | Y747 | Y748 | Y749 | Y750 | Y751 | Y752 | Y753 | Y754 | Y755 | Y756 | Y757 | Y758 | Y759 | Y760 | Y761 | Y762 | Y763 | Y764 | Y765 | Y766 | Y767 | Y768 | Y769 | Y770 | Y771 | Y772 | Y773 | Y774 | Y775 | Y776 | Y777 | Y778 | Y779 | Y780 | Y781 | Y782 | Y783 | Y784 | Y785 | Y786 | Y787 | Y788 | Y789 | Y790 | Y791 | Y792 | Y793 | Y794 | Y795 | Y796 | Y797 | Y798 | Y799 | Y800 | Y801 | Y802 | Y803 | Y804 | Y805 | Y806 | Y807 | Y808 | Y809 | Y810 | Y811 | Y812 | Y813 | Y814 | Y815 | Y816 | Y817 | Y818 | Y819 | Y820 | Y821 | Y822 | Y823 | Y824 | Y825 | Y826 | Y827 | Y828 | Y829 | Y830 | Y831 | Y832 | Y833 | Y834 | Y835 | Y836 | Y837 | Y838 | Y839 | Y840 | Y841 | Y842 | Y843 | Y844 | Y845 | Y846 | Y847 | Y848 | Y849 | Y850 | Y851 | Y852 | Y853 | Y854 | Y855 | Y856 | Y857 | Y858 | Y859 | Y860 | Y861 | Y862 | Y863 | Y864 | Y865 | Y866 | Y867 | Y868 | Y869 | Y870 | Y871 | Y872 | Y873 | Y874 | Y875 | Y876 | Y877 | Y878 | Y879 | Y880 | Y881 | Y882 | Y883 | Y884 | Y885 | Y886 | Y887 | Y888 | Y889 | Y890 | Y891 | Y892 | Y893 | Y894 | Y895 | Y896 | Y897 | Y898 | Y899 | Y900 | Y901 | Y902 | Y903 | Y904 | Y905 | Y906 | Y907 | Y908 | Y909 | Y910 | Y91 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|

| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| Y519 | Y520 | Y521 | Y522 | Y523 | Y524 | Y527 | Y530 | Y540 | Y541 | Y542 | Y543 | Y547 | Y557 | Y558 | Y559 | Y560 | Y561 | Y562 | Y563 | Y564 | Y565 | Y566 | Y567 | Y568 | Y569 | Y570 | Y571 | Y572 | Y573 | Y574 | Y575 | Y576 | Y577 | Y578 | Y579 | Y583 | Y587 | Y588 | Y589 | Y590 | Y591 | Y592 | Y593 | Y594 | Y595 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|

| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-------|
| S596 | S597 | S598 | S599 | S600 | S601 | S602 | S603 | S604 | S605 | S606 | S607 | S608 | S609 | S610 | S611 | S612 | S613 | S614 | S615 | S616 | S617 | S618 | S619 | S620 | S621 | S622 | S623 | S624 | S625 | S626 | S627 | S628 | S629 | S630 | S631 | S632 | S633 | S634 | S635 | S636 | S637 | S638 | S639 | S640 | S641 | S642 | S643 | S644 | S645 | S646 | S647 | S648 | S649 | S650 | S651 | S652 | S653 | S654 | S655 | S656 | S657 | S658 | S659 | S660 | S661 | S662 | S663 | S664 | S665 | S666 | S667 | S668 | S669 | S670 | S671 | S672 | S673 | S674 | S675 | S676 | S677 | S678 | S679 | S680 | S681 | S682 | S683 | S684 | S685 | S686 | S687 | S688 | S689 | S690 | S691 | S692 | S693 | S694 | S695 | S696 | S697 | S698 | S699 | S700 | S701 | S702 | S703 | S704 | S705 | S706 | S707 | S708 | S709 | S710 | S711 | S712 | S713 | S714 | S715 | S716 | S717 | S718 | S719 | S720 | S721 | S722 | S723 | S724 | S725 | S726 | S727 | S728 | S729 | S730 | S731 | S732 | S733 | S734 | S735 | S736 | S737 | S738 | S739 | S740 | S741 | S742 | S743 | S744 | S745 | S746 | S747 | S748 | S749 | S750 | S751 | S752 | S753 | S754 | S755 | S756 | S757 | S758 | S759 | S760 | S761 | S762 | S763 | S764 | S765 | S766 | S767 | S768 | S769 | S770 | S771 | S772 | S773 | S774 | S775 | S776 | S777 | S778 | S779 | S780 | S781 | S782 | S783 | S784 | S785 | S786 | S787 | S788 | S789 | S790 | S791 | S792 | S793 | S794 | S795 | S796 | S797 | S798 | S799 | S800 | S801 | S802 | S803 | S804 | S805 | S806 | S807 | S808 | S809 | S810 | S811 | S812 | S813 | S814 | S815 | S816 | S817 | S818 | S819 | S820 | S821 | S822 | S823 | S824 | S825 | S826 | S827 | S828 | S829 | S830 | S831 | S832 | S833 | S834 | S835 | S836 | S837 | S838 | S839 | S840 | S841 | S842 | S843 | S844 | S845 | S846 | S847 | S848 | S849 | S850 | S851 | S852 | S853 | S854 | S855 | S856 | S857 | S858 | S859 | S860 | S861 | S862 | S863 | S864 | S865 | S866 | S867 | S868 | S869 | S870 | S871 | S872 | S873 | S874 | S875 | S876 | S877 | S878 | S879 | S880 | S881 | S882 | S883 | S884 | S885 | S886 | S887 | S888 | S889 | S890 | S891 | S892 | S893 | S894 | S895 | S896 | S897 | S898 | S899 | S900 | S901 | S902 | S903 | S904 | S905 | S906 | S907 | S908 | S909 | S910 | S911 | S912 | S913 | S914 | S915 | S916 | S917 | S918 | S919 | S920 | S921 | S922 | S923 | S924 | S925 | S926 | S927 | S928 | S929 | S930 | S931 | S932 | S933 | S934 | S935 | S936 | S937 | S938 | S939 | S940 | S941 | S942 | S943 | S944 | S945 | S946 | S947 | S948 | S949 | S950 | S951 | S952 | S953 | S954 | S955 | S956 | S957 | S958 | S959 | S960 | S961 | S962 | S963 | S964 | S965 | S966 | S967 | S968 | S969 | S970 | S971 | S972 | S973 | S974 | S975 | S976 | S977 | S978 | S979 | S980 | S981 | S982 | S983 | S984 | S985 | S986 | S987 | S988 | S989 | S990 | S991 | S992 | S993 | S994 | S995 | S996 | S997 | S998 | S999 | S1000 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-------|

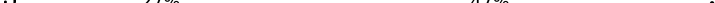
[illegible]

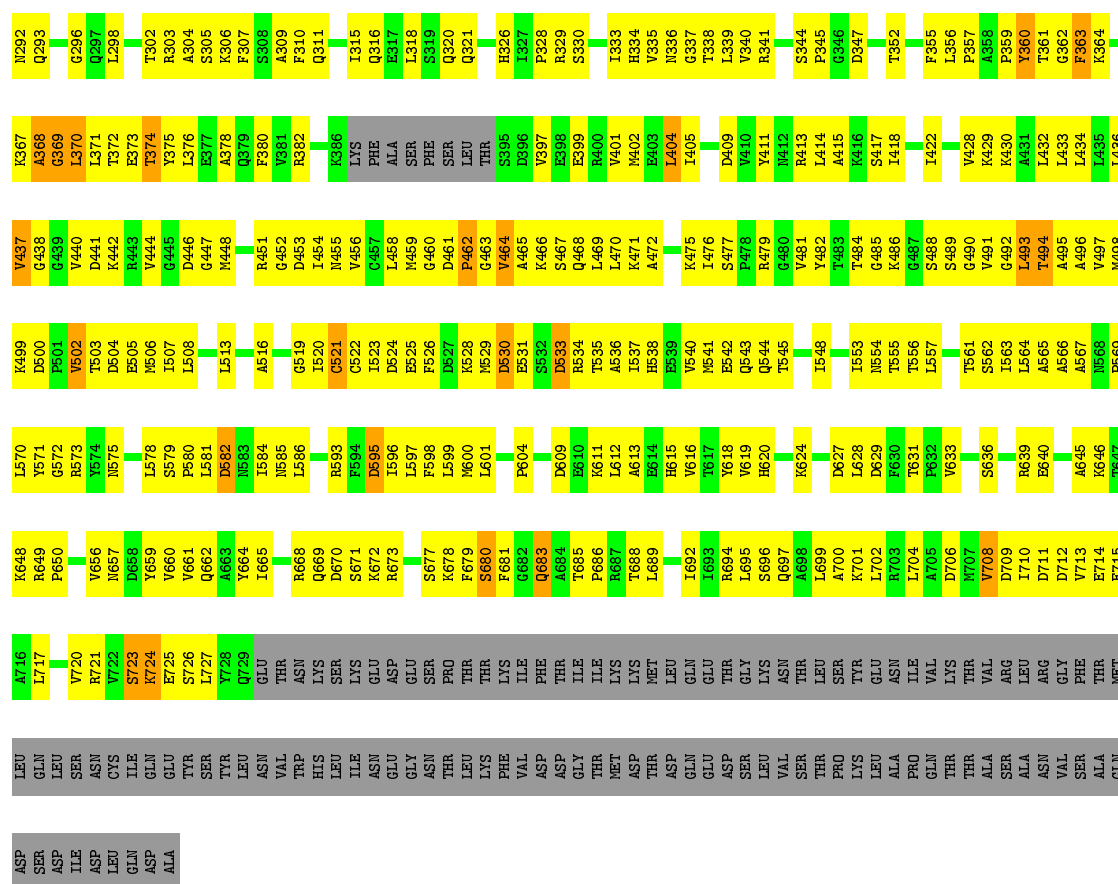
| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-------------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-------------|-------------|-------------|--|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|------------|
| E730 | ASP | LVS | PRQ | GLU | HIS | HLE | SER | GLN | ASP | E740 | E741 | E742 | | E747 | E748 | E749 | E750 | E751 | E752 | E753 | E754 | E755 | E756 | E757 | E758 | E759 | E760 | E761 | E762 | E763 | E764 | E765 | E766 | E767 | E768 | E769 | E770 | E771 | E772 | E773 | E774 | E775 | E776 | E777 | E778 | E779 | E780 | E781 | E782 | E783 | E784 | E785 | E786 | E787 | E788 | E789 | E790 | E791 | E792 | E793 | E794 | E795 | E796 | E797 | E798 | E799 | E800 | E801 | E802 | E803 | E804 | E805 | E806 | E807 | E808 | E809 | E810 | E811 | E812 | E813 | E814 | E815 | E816 | E817 | E818 | E819 | E820 | E821 | E822 | E823 | E824 | E825 | E826 | E827 | E828 | E829 | E830 | E831 | E832 | E833 | E834 | E835 | E836 | E837 | E838 | E839 | E840 | E841 | E842 | E843 | E844 | E845 | E846 | E847 | E848 | E849 | E850 | E851 | E852 | E853 | E854 | E855 | E856 | E857 | E858 | E859 | E860 | E861 | E862 | E863 | E864 | E865 | E866 | E867 | E868 | E869 | E870 | E871 | E872 | E873 | E874 | E875 | E876 | E877 | E878 | E879 | E880 | E881 | E882 | E883 | E884 | E885 | E886 | E887 | E888 | E889 | E890 | E891 | E892 | E893 | E894 | E895 | E896 | E897 | E898 | E899 | E900 | E901 | E902 | E903 | E904 | E905 | E906 | E907 | E908 | E909 | E910 | E911 | E912 | E913 | E914 | E915 | E916 | E917 | E918 | E919 | E920 | E921 | E922 | E923 | E924 | E925 | E926 | E927 | E928 | E929 | E930 | E931 | E932 | E933 | E934 | E935 | E936 | E937 | E938 | E939 | E940 | E941 | E942 | E943 | E944 | E945 | E946 | E947 | E948 | E949 | E950 | E951 | E952 | E953 | E954 | E955 | E956 | E957 | E958 | E959 | E960 | E961 | E962 | E963 | E964 | E965 | E966 | E967 | E968 | E969 | E970 | E971 | E972 | E973 | E974 | E975 | E976 | E977 | E978 | E979 | E980 | E981 | E982 | E983 | E984 | E985 | E986 | E987 | E988 | E989 | E990 | E991 | E992 | E993 | E994 | E995 | E996 | E997 | E998 | E999 | E1000 | E1001 | E1002 | E1003 | E1004 | E1005 | E1006 | E1007 | E1008 | E1009 | E1010 | E1011 | E1012 | E1013 | E1014 | E1015 | E1016 | E1017 | E1018 | E1019 | E1020 | E1021 | E1022 | E1023 | E1024 | E1025 | E1026 | E1027 | E1028 | E1029 | E1030 | E1031 | E1032 | E1033 | E1034 | E1035 | E1036 | E1037 | E1038 | E1039 | E1040 | E1041 | E1042 | E1043 | E1044 | E1045 | E1046 | E1047 | E1048 | E1049 | E1050 | E1051 | E1052 | E1053 | E1054 | E1055 | E1056 | E1057 | E1058 | E1059 | E1060 | E1061 | E1062 | E1063 | E1064 | E1065 | E1066 | E1067 | E1068 | E1069 | E1070 | E1071 | E10 |
|-------------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-------------|-------------|-------------|--|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|------------|

[illegible]

| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|
| Q856 | Q857 | Q858 | Q861 | Q862 | Q865 | Q872 | Q873 | Q876 | Q880 | Q886 | Q889 | Q890 | Q897 | Q898 | Q899 | Q900 | Q901 | Q902 | Q903 | Q904 | Q905 | Q906 | Q907 | Q908 | Q909 | Q910 | Q915 | Q919 | Q925 | Q928 | Q929 | ASW | ASW | ARG | VAL |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|

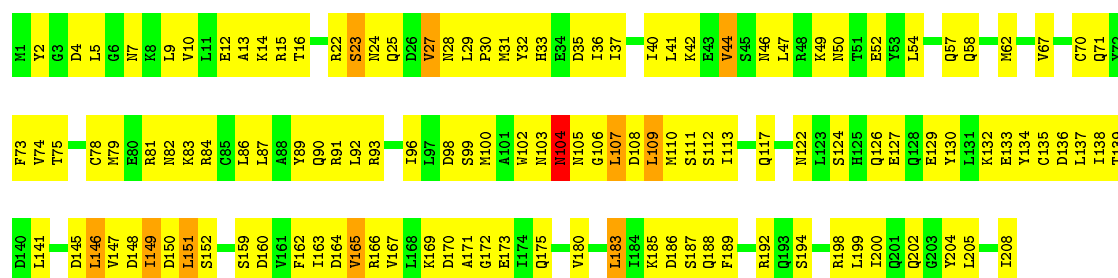
- Molecule 4: Minichromosome maintenance protein 5

Chain 5:  27% 47% .. 22%



• Molecule 7: DNA replication complex GINS protein PSF1

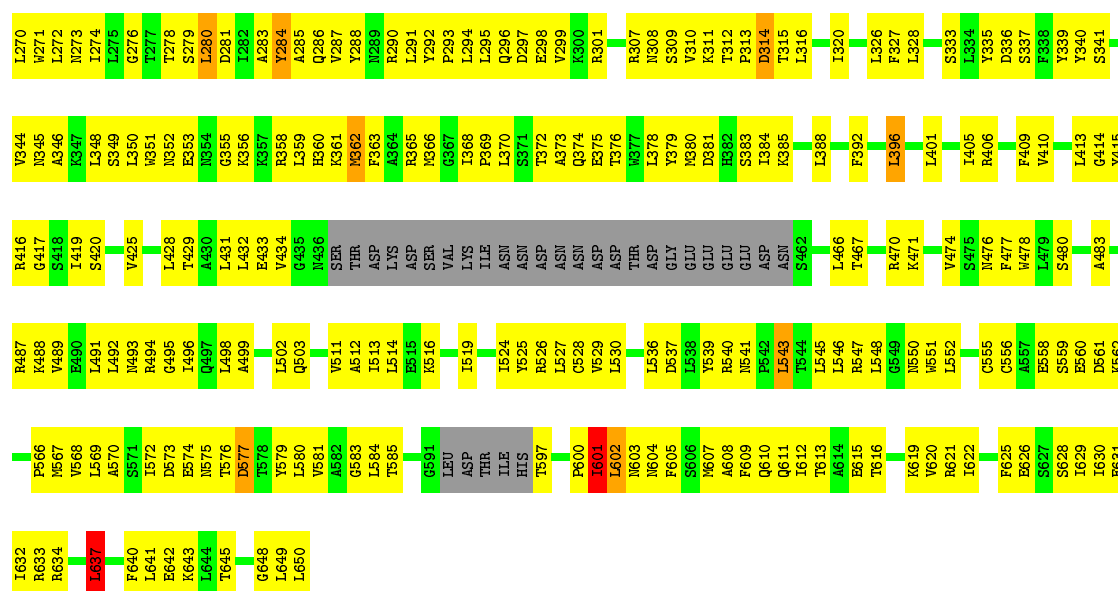
Chain A: 39% 56% 5%



• Molecule 8: DNA replication complex GINS protein PSF2

Chain B: 30% 52% 15%





- Molecule 12: DNA (5'-D(P*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*T)-3')



4 Experimental information

| Property | Value | Source |
|--------------------------------------|---------------------|-----------|
| Reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | Depositor |
| Number of particles used | 395443 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | Not provided | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | Not provided | Depositor |
| Minimum defocus (nm) | Not provided | Depositor |
| Maximum defocus (nm) | Not provided | Depositor |
| Magnification | Not provided | Depositor |
| Image detector | Not provided | Depositor |

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|-----------------|
| | | RMSZ | # $ Z > 2$ | RMSZ | # $ Z > 2$ |
| 1 | 2 | 0.37 | 1/4668 (0.0%) | 0.65 | 2/6306 (0.0%) |
| 10 | D | 0.34 | 0/1853 | 0.69 | 2/2500 (0.1%) |
| 11 | E | 0.33 | 0/4563 | 0.63 | 5/6173 (0.1%) |
| 12 | F | 0.88 | 1/307 (0.3%) | 1.42 | 3/472 (0.6%) |
| 2 | 3 | 0.32 | 0/4702 | 0.63 | 1/6374 (0.0%) |
| 3 | 4 | 0.31 | 0/5388 | 0.63 | 0/7273 |
| 4 | 5 | 0.34 | 0/4805 | 0.65 | 1/6489 (0.0%) |
| 5 | 6 | 0.36 | 0/5218 | 0.69 | 3/7039 (0.0%) |
| 6 | 7 | 0.33 | 0/5281 | 0.65 | 2/7136 (0.0%) |
| 7 | A | 0.36 | 0/1718 | 0.70 | 1/2314 (0.0%) |
| 8 | B | 0.33 | 0/1545 | 0.62 | 0/2092 |
| 9 | C | 0.32 | 0/1320 | 0.60 | 1/1784 (0.1%) |
| All | All | 0.34 | 2/41368 (0.0%) | 0.66 | 21/55952 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | 2 | 0 | 2 |
| 10 | D | 0 | 1 |
| 2 | 3 | 0 | 5 |
| 3 | 4 | 0 | 3 |
| 4 | 5 | 0 | 1 |
| 5 | 6 | 0 | 1 |
| 6 | 7 | 0 | 5 |
| 7 | A | 0 | 2 |
| All | All | 0 | 20 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | 2 | 633 | LYS | CE-NZ | 6.70 | 1.65 | 1.49 |
| 12 | F | 12 | DT | O5'-C5' | -5.01 | 1.29 | 1.42 |

All (21) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 6 | 7 | 369 | GLY | N-CA-C | 8.34 | 133.96 | 113.10 |
| 12 | F | 7 | DT | O4'-C4'-C3' | -7.76 | 101.35 | 106.00 |
| 12 | F | 12 | DT | OP1-P-OP2 | 7.47 | 130.81 | 119.60 |
| 10 | D | 269 | LEU | CA-CB-CG | 7.46 | 132.46 | 115.30 |
| 5 | 6 | 948 | LEU | CA-CB-CG | 7.37 | 132.25 | 115.30 |
| 5 | 6 | 839 | ASP | N-CA-C | 7.03 | 129.97 | 111.00 |
| 11 | E | 19 | SER | N-CA-C | 6.92 | 129.70 | 111.00 |
| 6 | 7 | 263 | ASP | N-CA-C | 6.33 | 128.09 | 111.00 |
| 11 | E | 34 | LEU | CA-CB-CG | 6.06 | 129.24 | 115.30 |
| 9 | C | 120 | LEU | CA-CB-CG | 5.80 | 128.65 | 115.30 |
| 2 | 3 | 428 | LEU | CA-CB-CG | 5.76 | 128.54 | 115.30 |
| 11 | E | 637 | LEU | CA-CB-CG | 5.66 | 128.31 | 115.30 |
| 4 | 5 | 179 | LEU | CA-CB-CG | 5.64 | 128.27 | 115.30 |
| 5 | 6 | 628 | LEU | CA-CB-CG | 5.50 | 127.96 | 115.30 |
| 1 | 2 | 436 | GLY | N-CA-C | 5.46 | 126.75 | 113.10 |
| 11 | E | 543 | LEU | CB-CG-CD1 | -5.42 | 101.78 | 111.00 |
| 7 | A | 146 | LEU | CA-CB-CG | 5.37 | 127.66 | 115.30 |
| 10 | D | 258 | VAL | N-CA-C | -5.23 | 96.88 | 111.00 |
| 11 | E | 27 | LEU | CA-CB-CG | 5.23 | 127.32 | 115.30 |
| 1 | 2 | 216 | LEU | CA-CB-CG | 5.20 | 127.27 | 115.30 |
| 12 | F | 12 | DT | O5'-P-OP2 | -5.17 | 101.04 | 105.70 |

There are no chirality outliers.

All (20) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 1 | 2 | 355 | SER | Peptide |
| 1 | 2 | 633 | LYS | Peptide |
| 2 | 3 | 163 | ALA | Peptide |
| 2 | 3 | 172 | THR | Peptide |
| 2 | 3 | 428 | LEU | Peptide |
| 2 | 3 | 437 | SER | Peptide |
| 2 | 3 | 498 | ALA | Peptide |
| 3 | 4 | 245 | ALA | Peptide |
| 3 | 4 | 374 | ILE | Peptide |
| 3 | 4 | 448 | SER | Peptide |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 4 | 5 | 348 | MET | Peptide |
| 5 | 6 | 560 | VAL | Peptide |
| 6 | 7 | 257 | VAL | Peptide |
| 6 | 7 | 360 | TYR | Peptide |
| 6 | 7 | 368 | ALA | Peptide |
| 6 | 7 | 680 | SER | Peptide |
| 6 | 7 | 683 | GLN | Peptide |
| 7 | A | 104 | ASN | Peptide |
| 7 | A | 159 | SER | Peptide |
| 10 | D | 200 | LYS | Peptide |

5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | 2 | 4591 | 0 | 4639 | 428 | 0 |
| 2 | 3 | 4624 | 0 | 4689 | 376 | 0 |
| 3 | 4 | 5318 | 0 | 5390 | 424 | 0 |
| 4 | 5 | 4740 | 0 | 4798 | 439 | 0 |
| 5 | 6 | 5142 | 0 | 5093 | 499 | 0 |
| 6 | 7 | 5201 | 0 | 5276 | 422 | 0 |
| 7 | A | 1696 | 0 | 1698 | 141 | 0 |
| 8 | B | 1513 | 0 | 1558 | 124 | 0 |
| 9 | C | 1288 | 0 | 1298 | 92 | 0 |
| 10 | D | 1820 | 0 | 1824 | 201 | 0 |
| 11 | E | 4482 | 0 | 4499 | 367 | 0 |
| 12 | F | 280 | 0 | 169 | 8 | 0 |
| 13 | 2 | 31 | 0 | 13 | 9 | 0 |
| 13 | 3 | 31 | 0 | 13 | 10 | 0 |
| 13 | 5 | 31 | 0 | 13 | 9 | 0 |
| All | All | 40788 | 0 | 40970 | 3219 | 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 39.

All (3219) 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) |
|-------------------|------------------|--------------------------|-------------------|
| 10:D:260:ILE:HG13 | 10:D:266:GLU:CG | 1.46 | 1.45 |
| 6:7:221:SER:CA | 6:7:222:SER:HB2 | 1.40 | 1.44 |
| 10:D:260:ILE:CG1 | 10:D:266:GLU:CD | 1.87 | 1.42 |
| 10:D:260:ILE:HG12 | 10:D:266:GLU:CD | 1.38 | 1.38 |
| 10:D:260:ILE:CG1 | 10:D:266:GLU:OE2 | 1.74 | 1.35 |
| 10:D:260:ILE:CD1 | 10:D:266:GLU:OE2 | 1.78 | 1.30 |
| 4:5:341:SER:O | 4:5:345:SER:HB2 | 1.28 | 1.30 |
| 4:5:623:SER:O | 4:5:627:VAL:HG13 | 1.27 | 1.30 |
| 6:7:221:SER:HA | 6:7:222:SER:CB | 1.58 | 1.29 |
| 6:7:490:GLY:O | 6:7:494:THR:HG22 | 1.33 | 1.20 |
| 10:D:260:ILE:CG2 | 10:D:265:GLU:HA | 1.71 | 1.18 |
| 7:A:108:ASP:HB3 | 7:A:109:LEU:CB | 1.74 | 1.17 |
| 1:2:632:SER:HB2 | 4:5:442:LYS:HB3 | 1.25 | 1.15 |
| 11:E:540:ARG:NH2 | 11:E:574:GLU:HB2 | 1.61 | 1.15 |
| 7:A:108:ASP:CB | 7:A:109:LEU:HB3 | 1.77 | 1.14 |
| 3:4:623:LEU:HD22 | 5:6:370:THR:HG21 | 1.23 | 1.13 |
| 3:4:623:LEU:HD22 | 5:6:370:THR:CG2 | 1.77 | 1.12 |
| 10:D:260:ILE:HD11 | 10:D:266:GLU:OE2 | 1.42 | 1.12 |
| 10:D:258:VAL:HB | 10:D:259:THR:HA | 1.24 | 1.11 |
| 1:2:846:VAL:O | 1:2:853:VAL:HG21 | 1.46 | 1.11 |
| 3:4:332:VAL:HB | 3:4:429:ALA:HA | 1.27 | 1.11 |
| 10:D:260:ILE:HG12 | 10:D:266:GLU:OE2 | 1.40 | 1.07 |
| 11:E:579:TYR:CE2 | 11:E:634:ARG:HB3 | 1.89 | 1.07 |
| 10:D:260:ILE:CG1 | 10:D:266:GLU:CG | 2.28 | 1.06 |
| 6:7:221:SER:N | 6:7:222:SER:HB2 | 1.69 | 1.05 |
| 6:7:221:SER:CA | 6:7:222:SER:CB | 2.25 | 1.05 |
| 3:4:624:SER:O | 3:4:626:GLY:O | 1.75 | 1.04 |
| 10:D:260:ILE:HG21 | 10:D:265:GLU:HA | 1.38 | 1.04 |
| 6:7:472:ALA:O | 6:7:476:ILE:HD13 | 1.57 | 1.04 |
| 5:6:418:SER:HG | 5:6:448:LEU:N | 1.58 | 1.01 |
| 11:E:576:THR:O | 11:E:577:ASP:CG | 1.99 | 1.01 |
| 10:D:260:ILE:HG23 | 10:D:265:GLU:C | 1.81 | 1.01 |
| 1:2:608:GLU:HB3 | 1:2:611:LYS:HD3 | 1.42 | 1.00 |
| 6:7:221:SER:HA | 6:7:222:SER:HB2 | 1.02 | 1.00 |
| 3:4:727:LEU:N | 3:4:728:TYR:HB3 | 1.77 | 1.00 |
| 4:5:143:ALA:HA | 11:E:379:TYR:HE2 | 1.23 | 1.00 |
| 3:4:449:ARG:HG3 | 3:4:450:GLN:H | 1.23 | 0.99 |
| 4:5:477:VAL:HB | 4:5:519:VAL:HA | 1.40 | 0.99 |
| 11:E:5:ILE:N | 11:E:142:CYS:HG | 1.61 | 0.98 |
| 3:4:432:ARG:NH2 | 6:7:557:LEU:HB3 | 1.77 | 0.98 |
| 3:4:589:VAL:HG21 | 3:4:624:SER:OG | 1.62 | 0.97 |
| 5:6:100:VAL:HG23 | 5:6:101:LYS:CG | 1.94 | 0.97 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:2:778:LEU:HG | 4:5:577:THR:CG2 | 1.94 | 0.97 |
| 4:5:196:ASN:HB3 | 4:5:197:PHE:HD1 | 1.30 | 0.97 |
| 3:4:202:LYS:HB3 | 3:4:203:TYR:HB3 | 1.47 | 0.97 |
| 4:5:448:GLY:HA2 | 4:5:486:ARG:HH12 | 1.27 | 0.96 |
| 1:2:540:LEU:HA | 1:2:648:ALA:HB3 | 1.48 | 0.95 |
| 5:6:790:ARG:NH2 | 5:6:839:ASP:O | 1.99 | 0.95 |
| 2:3:25:VAL:O | 2:3:29:GLN:HG2 | 1.66 | 0.95 |
| 11:E:15:ILE:O | 11:E:19:SER:OG | 1.83 | 0.95 |
| 5:6:653:HIS:HA | 5:6:656:MET:HG2 | 1.49 | 0.94 |
| 6:7:470:LEU:HD21 | 6:7:564:LEU:HD22 | 1.49 | 0.94 |
| 1:2:842:VAL:O | 1:2:846:VAL:HG23 | 1.67 | 0.93 |
| 6:7:489:SER:O | 6:7:493:LEU:HG | 1.68 | 0.93 |
| 10:D:260:ILE:HG13 | 10:D:266:GLU:HG3 | 0.96 | 0.93 |
| 10:D:260:ILE:CG1 | 10:D:266:GLU:HG3 | 1.92 | 0.93 |
| 3:4:689:THR:HG1 | 3:4:851:GLN:N | 1.68 | 0.92 |
| 5:6:558:SER:HB3 | 5:6:559:THR:HA | 1.51 | 0.92 |
| 6:7:94:LEU:HB2 | 6:7:95:GLN:HB2 | 1.52 | 0.92 |
| 4:5:482:PHE:HB3 | 4:5:523:ALA:HB2 | 1.51 | 0.91 |
| 3:4:623:LEU:CD2 | 5:6:370:THR:HG21 | 2.00 | 0.91 |
| 1:2:502:ALA:HB1 | 1:2:505:ILE:HB | 1.51 | 0.91 |
| 5:6:304:LEU:HD11 | 5:6:307:ALA:HB2 | 1.52 | 0.91 |
| 6:7:489:SER:O | 6:7:493:LEU:CD2 | 2.18 | 0.91 |
| 6:7:459:MET:HB2 | 6:7:597:LEU:HD21 | 1.53 | 0.91 |
| 2:3:533:ILE:HG22 | 2:3:535:LEU:H | 1.35 | 0.91 |
| 6:7:220:ILE:C | 6:7:222:SER:HB2 | 1.92 | 0.90 |
| 2:3:192:VAL:HB | 6:7:329:ARG:HH12 | 1.36 | 0.90 |
| 5:6:167:ALA:O | 5:6:171:SER:OG | 1.89 | 0.89 |
| 10:D:260:ILE:CG2 | 10:D:265:GLU:CA | 2.50 | 0.89 |
| 10:D:260:ILE:HG23 | 10:D:265:GLU:CA | 2.02 | 0.89 |
| 6:7:118:CYS:SG | 6:7:198:ARG:NH2 | 2.45 | 0.89 |
| 4:5:664:ALA:HA | 4:5:676:HIS:HE1 | 1.36 | 0.89 |
| 8:B:7:LEU:N | 8:B:8:GLN:HA | 1.85 | 0.89 |
| 6:7:490:GLY:O | 6:7:494:THR:CG2 | 2.21 | 0.88 |
| 6:7:472:ALA:O | 6:7:476:ILE:CD1 | 2.22 | 0.88 |
| 4:5:369:ILE:HG23 | 4:5:594:ILE:HD11 | 1.56 | 0.88 |
| 1:2:634:ALA:O | 4:5:448:GLY:N | 2.07 | 0.87 |
| 1:2:384:ASN:HB2 | 1:2:415:VAL:HG21 | 1.57 | 0.87 |
| 11:E:540:ARG:HH21 | 11:E:574:GLU:HB2 | 1.37 | 0.87 |
| 1:2:580:VAL:HG22 | 1:2:591:LEU:HG | 1.57 | 0.86 |
| 6:7:459:MET:HB3 | 6:7:599:LEU:HA | 1.55 | 0.86 |
| 4:5:276:MET:HG2 | 4:5:328:ILE:HB | 1.56 | 0.86 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:6:646:ILE:HA | 5:6:649:GLN:HG2 | 1.54 | 0.86 |
| 6:7:256:GLU:HA | 6:7:273:VAL:HG21 | 1.57 | 0.86 |
| 10:D:260:ILE:HG23 | 10:D:265:GLU:HA | 1.57 | 0.86 |
| 3:4:804:LEU:HD21 | 3:4:828:LEU:HD12 | 1.57 | 0.86 |
| 11:E:579:TYR:O | 11:E:581:VAL:HG23 | 1.76 | 0.86 |
| 10:D:260:ILE:HG13 | 10:D:266:GLU:CD | 1.73 | 0.86 |
| 2:3:104:ARG:NH1 | 9:C:90:THR:HG23 | 1.90 | 0.86 |
| 6:7:466:LYS:HA | 6:7:469:LEU:HD13 | 1.57 | 0.85 |
| 6:7:520:ILE:HA | 6:7:562:SER:HB2 | 1.57 | 0.85 |
| 10:D:67:TRP:HE1 | 10:D:142:SER:HB3 | 1.41 | 0.85 |
| 10:D:123:LYS:HE3 | 11:E:20:SER:HB3 | 1.56 | 0.85 |
| 3:4:629:CYS:HB3 | 3:4:671:ILE:HG12 | 1.57 | 0.85 |
| 4:5:413:LEU:HD13 | 4:5:553:ILE:HG13 | 1.58 | 0.85 |
| 1:2:574:VAL:HG22 | 1:2:595:ALA:HB2 | 1.57 | 0.85 |
| 3:4:243:LEU:HD22 | 3:4:305:PRO:HA | 1.59 | 0.85 |
| 5:6:689:TYR:HA | 5:6:690:ASN:HB2 | 1.58 | 0.85 |
| 5:6:720:ASN:O | 5:6:724:ASP:N | 2.10 | 0.85 |
| 6:7:315:ILE:HD13 | 6:7:333:ILE:HD12 | 1.59 | 0.85 |
| 11:E:83:LEU:HD21 | 11:E:86:PHE:HB2 | 1.58 | 0.84 |
| 5:6:693:LEU:HD13 | 5:6:698:ASN:HA | 1.58 | 0.84 |
| 10:D:79:TYR:HA | 10:D:147:ARG:HH12 | 1.43 | 0.84 |
| 3:4:713:ASP:HB2 | 3:4:716:ASN:HB2 | 1.56 | 0.84 |
| 10:D:250:GLU:HA | 10:D:256:TYR:HB3 | 1.59 | 0.84 |
| 2:3:176:LEU:HD23 | 2:3:177:ASN:HB2 | 1.60 | 0.84 |
| 1:2:325:THR:HG21 | 1:2:391:GLN:HB3 | 1.60 | 0.84 |
| 1:2:611:LYS:HE2 | 5:6:650:VAL:HG21 | 1.59 | 0.84 |
| 4:5:649:THR:H | 4:5:652:GLN:HG3 | 1.43 | 0.83 |
| 8:B:11:PHE:HB2 | 8:B:179:ASN:HD21 | 1.41 | 0.83 |
| 1:2:262:LYS:HE2 | 1:2:263:CYS:SG | 2.17 | 0.83 |
| 5:6:802:SER:HA | 5:6:805:ARG:HG2 | 1.58 | 0.83 |
| 5:6:570:ASN:HD21 | 5:6:678:ILE:H | 1.24 | 0.83 |
| 3:4:332:VAL:CB | 3:4:429:ALA:HA | 2.07 | 0.83 |
| 1:2:428:GLY:HA3 | 1:2:453:ALA:HA | 1.60 | 0.83 |
| 11:E:33:CYS:SG | 11:E:34:LEU:N | 2.50 | 0.83 |
| 3:4:563:ASN:ND2 | 3:4:649:MET:SD | 2.52 | 0.83 |
| 6:7:440:VAL:HG11 | 6:7:649:ARG:HA | 1.58 | 0.83 |
| 2:3:389:VAL:HG12 | 2:3:390:GLU:H | 1.44 | 0.83 |
| 4:5:39:ARG:HG2 | 4:5:41:ASP:H | 1.42 | 0.83 |
| 3:4:248:LEU:HB2 | 3:4:258:TYR:HB2 | 1.60 | 0.82 |
| 5:6:795:ILE:HG22 | 5:6:799:GLN:HG3 | 1.61 | 0.82 |
| 5:6:533:ILE:HG21 | 5:6:548:LEU:HD11 | 1.60 | 0.82 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:7:461:ASP:HB3 | 6:7:569:PRO:HD2 | 1.61 | 0.82 |
| 8:B:71:VAL:HB | 8:B:75:ILE:HD11 | 1.59 | 0.82 |
| 11:E:502:LEU:HD13 | 11:E:547:ARG:HH22 | 1.44 | 0.82 |
| 3:4:771:VAL:HG13 | 5:6:728:ALA:HB1 | 1.59 | 0.82 |
| 1:2:591:LEU:HB3 | 4:5:270:MET:HE1 | 1.60 | 0.82 |
| 10:D:220:ASP:HB3 | 10:D:221:GLU:HG2 | 1.60 | 0.82 |
| 6:7:489:SER:O | 6:7:493:LEU:CG | 2.28 | 0.82 |
| 2:3:172:THR:O | 2:3:175:HIS:ND1 | 2.13 | 0.82 |
| 3:4:587:ARG:HD3 | 3:4:623:LEU:O | 1.80 | 0.82 |
| 1:2:571:ALA:HB3 | 5:6:664:ALA:HB3 | 1.61 | 0.82 |
| 6:7:504:ASP:HB3 | 6:7:505:GLU:HB3 | 1.62 | 0.82 |
| 5:6:326:LYS:H | 5:6:327:TYR:HA | 1.45 | 0.81 |
| 3:4:448:SER:HB3 | 3:4:449:ARG:HB3 | 1.60 | 0.81 |
| 3:4:342:MET:HB3 | 3:4:360:ILE:HD13 | 1.63 | 0.81 |
| 6:7:670:ASP:HA | 6:7:673:ARG:HG2 | 1.60 | 0.81 |
| 11:E:344:VAL:HG13 | 11:E:348:LEU:HD12 | 1.59 | 0.81 |
| 2:3:519:VAL:HG22 | 2:3:534:ALA:HB2 | 1.62 | 0.81 |
| 4:5:143:ALA:HA | 11:E:379:TYR:CE2 | 2.11 | 0.81 |
| 5:6:791:SER:HB3 | 5:6:835:ILE:HG22 | 1.63 | 0.81 |
| 5:6:100:VAL:HG23 | 5:6:101:LYS:HG2 | 1.61 | 0.81 |
| 1:2:294:HIS:O | 1:2:296:ARG:NH1 | 2.14 | 0.81 |
| 3:4:589:VAL:CG2 | 3:4:624:SER:OG | 2.28 | 0.81 |
| 5:6:525:ILE:HA | 5:6:528:LYS:HB2 | 1.62 | 0.81 |
| 11:E:604:ASN:HB2 | 11:E:650:LEU:HD23 | 1.63 | 0.80 |
| 3:4:338:VAL:HB | 5:6:452:ILE:HD11 | 1.62 | 0.80 |
| 4:5:261:ILE:HD11 | 4:5:264:LEU:HG | 1.61 | 0.80 |
| 10:D:132:GLU:HG2 | 10:D:135:ARG:HH12 | 1.46 | 0.80 |
| 11:E:26:GLN:HB3 | 11:E:78:ILE:HA | 1.63 | 0.80 |
| 1:2:610:ASP:OD2 | 1:2:651:ASN:ND2 | 2.15 | 0.80 |
| 1:2:684:ARG:HB3 | 1:2:685:ASP:HB3 | 1.63 | 0.80 |
| 4:5:184:ARG:HH11 | 4:5:240:PRO:HA | 1.46 | 0.80 |
| 5:6:796:THR:HG22 | 5:6:798:ARG:H | 1.46 | 0.80 |
| 7:A:145:ASP:HA | 7:A:146:LEU:HB3 | 1.64 | 0.80 |
| 10:D:230:ILE:HD12 | 10:D:291:VAL:HG21 | 1.62 | 0.80 |
| 6:7:490:GLY:HA2 | 6:7:493:LEU:HD11 | 1.63 | 0.80 |
| 6:7:228:ARG:HH12 | 6:7:326:HIS:HB3 | 1.45 | 0.80 |
| 1:2:675:SER:HG | 1:2:806:THR:HG1 | 1.25 | 0.80 |
| 1:2:641:GLN:HB3 | 1:2:643:ARG:HH12 | 1.46 | 0.79 |
| 5:6:603:SER:H | 5:6:604:SER:HA | 1.48 | 0.79 |
| 1:2:792:ASP:O | 1:2:859:ARG:NH1 | 2.16 | 0.79 |
| 2:3:437:SER:HA | 2:3:440:VAL:H | 1.45 | 0.79 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:D:216:VAL:HG13 | 10:D:217:ASN:HA | 1.65 | 0.79 |
| 11:E:29:ILE:HD13 | 11:E:31:VAL:HG23 | 1.65 | 0.79 |
| 4:5:138:ILE:HG12 | 4:5:282:LEU:HD21 | 1.63 | 0.79 |
| 11:E:363:PHE:HA | 11:E:366:MET:HB2 | 1.63 | 0.79 |
| 1:2:338:LYS:HD2 | 1:2:379:LYS:HB3 | 1.63 | 0.79 |
| 2:3:405:ILE:HG23 | 2:3:545:LEU:HB2 | 1.64 | 0.79 |
| 3:4:449:ARG:HG3 | 3:4:450:GLN:N | 1.97 | 0.79 |
| 3:4:726:ASN:C | 3:4:727:LEU:HG | 2.03 | 0.79 |
| 6:7:143:LEU:HD21 | 6:7:197:THR:HG22 | 1.65 | 0.79 |
| 10:D:256:TYR:HB2 | 10:D:257:THR:HG23 | 1.65 | 0.79 |
| 2:3:665:GLU:HG2 | 2:3:666:ARG:HG3 | 1.64 | 0.78 |
| 11:E:572:ILE:HG12 | 11:E:577:ASP:HA | 1.64 | 0.78 |
| 6:7:289:CYS:HB3 | 6:7:296:GLY:HA3 | 1.63 | 0.78 |
| 11:E:540:ARG:HH22 | 11:E:574:GLU:HB2 | 1.49 | 0.78 |
| 10:D:216:VAL:HG22 | 10:D:219:ILE:HG13 | 1.66 | 0.78 |
| 11:E:337:SER:O | 11:E:341:SER:OG | 2.01 | 0.78 |
| 11:E:61:ILE:HD12 | 11:E:61:ILE:H | 1.48 | 0.78 |
| 2:3:177:ASN:ND2 | 4:5:246:GLU:O | 2.17 | 0.78 |
| 6:7:677:SER:O | 6:7:680:SER:HB3 | 1.83 | 0.78 |
| 11:E:288:TYR:OH | 11:E:406:ARG:NH1 | 2.16 | 0.78 |
| 1:2:846:VAL:O | 1:2:853:VAL:CG2 | 2.29 | 0.78 |
| 2:3:382:LEU:HD12 | 2:3:385:LEU:HD12 | 1.66 | 0.78 |
| 11:E:26:GLN:HG3 | 11:E:78:ILE:HG13 | 1.66 | 0.78 |
| 3:4:798:LEU:HA | 3:4:801:MET:HB2 | 1.63 | 0.78 |
| 7:A:79:MET:HB3 | 10:D:206:LEU:HD11 | 1.66 | 0.78 |
| 5:6:112:ARG:HH22 | 5:6:183:LYS:HG3 | 1.47 | 0.78 |
| 11:E:572:ILE:HD13 | 11:E:579:TYR:H | 1.48 | 0.78 |
| 3:4:512:VAL:HG12 | 3:4:518:LEU:HD12 | 1.66 | 0.78 |
| 5:6:151:ILE:O | 5:6:266:SER:OG | 2.00 | 0.78 |
| 1:2:538:ASN:HB2 | 1:2:677:PHE:HA | 1.64 | 0.77 |
| 3:4:721:ALA:O | 3:4:725:THR:N | 2.17 | 0.77 |
| 11:E:335:TYR:HB2 | 11:E:373:ALA:HB1 | 1.66 | 0.77 |
| 4:5:656:ILE:HA | 4:5:659:ILE:HD12 | 1.64 | 0.77 |
| 5:6:765:LEU:HD12 | 5:6:819:ILE:HB | 1.66 | 0.77 |
| 3:4:432:ARG:HH22 | 6:7:557:LEU:HB3 | 1.49 | 0.77 |
| 10:D:232:VAL:HB | 10:D:271:ILE:HA | 1.67 | 0.77 |
| 1:2:501:MET:HG2 | 1:2:516:ALA:HB2 | 1.67 | 0.77 |
| 3:4:433:ILE:HD13 | 3:4:469:VAL:HA | 1.67 | 0.77 |
| 5:6:100:VAL:HG23 | 5:6:101:LYS:HG3 | 1.66 | 0.77 |
| 8:B:168:LEU:HB2 | 10:D:276:VAL:HB | 1.67 | 0.77 |
| 2:3:275:ASP:OD1 | 2:3:275:ASP:N | 2.16 | 0.77 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:2:632:SER:HB2 | 4:5:442:LYS:CB | 2.12 | 0.77 |
| 3:4:303:VAL:HG12 | 3:4:305:PRO:HD3 | 1.65 | 0.77 |
| 3:4:623:LEU:HD22 | 5:6:370:THR:HG23 | 1.67 | 0.77 |
| 5:6:533:ILE:O | 5:6:587:TYR:CZ | 2.38 | 0.77 |
| 5:6:794:ARG:H | 5:6:795:ILE:HA | 1.48 | 0.77 |
| 6:7:68:GLN:O | 6:7:72:ASN:N | 2.18 | 0.77 |
| 2:3:261:MET:HB2 | 2:3:264:MET:HG2 | 1.66 | 0.77 |
| 4:5:579:ASN:HB2 | 4:5:582:ALA:HB3 | 1.65 | 0.77 |
| 11:E:315:THR:N | 11:E:316:LEU:HB3 | 2.00 | 0.77 |
| 1:2:813:ILE:HD12 | 1:2:841:VAL:HG21 | 1.65 | 0.77 |
| 1:2:231:ILE:HG23 | 1:2:279:THR:HG23 | 1.66 | 0.76 |
| 6:7:368:ALA:H | 6:7:370:LEU:HD22 | 1.48 | 0.76 |
| 1:2:338:LYS:H | 1:2:380:THR:HG22 | 1.49 | 0.76 |
| 1:2:569:GLN:HB2 | 1:2:612:MET:HA | 1.66 | 0.76 |
| 3:4:315:ARG:NH1 | 6:7:250:ASP:OD1 | 2.18 | 0.76 |
| 4:5:414:LEU:HD13 | 4:5:422:LYS:HB2 | 1.66 | 0.76 |
| 10:D:260:ILE:HG22 | 10:D:264:LYS:O | 1.85 | 0.76 |
| 1:2:777:LYS:H | 1:2:828:PHE:HA | 1.51 | 0.76 |
| 1:2:523:VAL:HG12 | 1:2:525:LYS:HB3 | 1.67 | 0.76 |
| 1:2:672:PRO:HA | 4:5:418:PRO:HG3 | 1.66 | 0.76 |
| 5:6:117:GLN:O | 5:6:121:ASP:N | 2.19 | 0.76 |
| 5:6:530:VAL:HA | 5:6:533:ILE:HD11 | 1.67 | 0.76 |
| 11:E:150:ASP:HB3 | 11:E:152:LEU:HB2 | 1.67 | 0.76 |
| 2:3:272:ARG:HD2 | 4:5:171:VAL:HG13 | 1.67 | 0.76 |
| 4:5:287:ILE:HD11 | 4:5:342:ILE:HG23 | 1.68 | 0.76 |
| 2:3:437:SER:HB3 | 2:3:438:SER:HA | 1.67 | 0.76 |
| 2:3:435:ARG:NH1 | 2:3:477:LYS:O | 2.18 | 0.76 |
| 5:6:773:LEU:HD12 | 5:6:824:ILE:HG21 | 1.66 | 0.76 |
| 1:2:422:GLU:OE2 | 1:2:562:ARG:NH1 | 2.19 | 0.75 |
| 2:3:189:THR:HA | 2:3:256:ILE:HD12 | 1.68 | 0.75 |
| 2:3:428:LEU:HB3 | 2:3:429:ALA:HA | 1.68 | 0.75 |
| 3:4:928:ARG:HB2 | 5:6:946:ASN:HB2 | 1.68 | 0.75 |
| 8:B:21:GLU:HA | 8:B:73:LEU:HD23 | 1.66 | 0.75 |
| 11:E:92:LEU:HA | 11:E:95:PHE:HB3 | 1.68 | 0.75 |
| 3:4:830:ARG:O | 3:4:834:LYS:N | 2.19 | 0.75 |
| 1:2:790:TYR:OH | 1:2:794:ARG:NH2 | 2.19 | 0.75 |
| 3:4:726:ASN:O | 3:4:727:LEU:HG | 1.86 | 0.74 |
| 6:7:493:LEU:HD21 | 6:7:533:ASP:CG | 2.07 | 0.74 |
| 2:3:195:LYS:HE3 | 6:7:369:GLY:HA3 | 1.69 | 0.74 |
| 1:2:448:ALA:HA | 5:6:301:ARG:HD3 | 1.69 | 0.74 |
| 5:6:828:TYR:OH | 5:6:832:ARG:NH2 | 2.21 | 0.74 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:4:252:LYS:HG2 | 3:4:253:GLN:HA | 1.67 | 0.74 |
| 5:6:162:GLU:HG3 | 5:6:165:ALA:HB3 | 1.69 | 0.74 |
| 2:3:113:GLY:HA2 | 2:3:116:VAL:HB | 1.68 | 0.74 |
| 5:6:819:ILE:HG22 | 5:6:820:THR:H | 1.53 | 0.74 |
| 10:D:76:LEU:HD11 | 10:D:147:ARG:HE | 1.52 | 0.74 |
| 3:4:598:ALA:HA | 3:4:644:VAL:HG22 | 1.68 | 0.74 |
| 5:6:533:ILE:O | 5:6:587:TYR:CE1 | 2.40 | 0.74 |
| 8:B:25:ILE:HD12 | 8:B:87:ILE:HD13 | 1.70 | 0.74 |
| 7:A:84:ARG:HH22 | 10:D:217:ASN:HB3 | 1.53 | 0.74 |
| 1:2:692:ASP:OD2 | 5:6:781:ARG:NH2 | 2.20 | 0.74 |
| 11:E:576:THR:O | 11:E:577:ASP:CB | 2.34 | 0.74 |
| 1:2:286:TYR:HA | 1:2:289:ILE:HB | 1.70 | 0.74 |
| 5:6:792:SER:HA | 5:6:793:TYR:HB2 | 1.69 | 0.74 |
| 1:2:268:LEU:HA | 1:2:271:PHE:HB3 | 1.70 | 0.74 |
| 1:2:398:PRO:HG2 | 1:2:401:ARG:HD2 | 1.69 | 0.74 |
| 5:6:628:LEU:HG | 5:6:631:ALA:HB3 | 1.69 | 0.74 |
| 5:6:720:ASN:HB3 | 5:6:723:ILE:HB | 1.68 | 0.74 |
| 6:7:220:ILE:HB | 6:7:222:SER:OG | 1.87 | 0.73 |
| 6:7:255:VAL:HG23 | 6:7:258:ILE:HG13 | 1.69 | 0.73 |
| 3:4:725:THR:HG23 | 6:7:657:ASN:HD21 | 1.51 | 0.73 |
| 11:E:576:THR:O | 11:E:577:ASP:OD2 | 2.04 | 0.73 |
| 2:3:156:SER:HB2 | 2:3:325:THR:HG22 | 1.69 | 0.73 |
| 4:5:66:GLU:HA | 4:5:69:ILE:HG22 | 1.69 | 0.73 |
| 5:6:570:ASN:HD21 | 5:6:678:ILE:N | 1.85 | 0.73 |
| 6:7:256:GLU:HG3 | 6:7:257:VAL:HG22 | 1.69 | 0.73 |
| 6:7:645:ALA:HB1 | 6:7:701:LYS:HB3 | 1.70 | 0.73 |
| 1:2:659:SER:HA | 3:4:928:ARG:HH22 | 1.53 | 0.73 |
| 2:3:138:ASP:CG | 2:3:140:PRO:HD2 | 2.08 | 0.73 |
| 6:7:476:ILE:N | 6:7:476:ILE:HD12 | 2.03 | 0.73 |
| 10:D:258:VAL:CB | 10:D:259:THR:HA | 2.06 | 0.73 |
| 1:2:384:ASN:OD1 | 1:2:384:ASN:N | 2.14 | 0.73 |
| 2:3:276:VAL:HG22 | 2:3:321:ILE:HB | 1.69 | 0.73 |
| 11:E:81:LEU:HB3 | 11:E:120:ILE:HG13 | 1.71 | 0.73 |
| 3:4:862:GLN:HA | 3:4:865:LEU:HB2 | 1.71 | 0.73 |
| 11:E:159:TYR:O | 11:E:163:LEU:N | 2.15 | 0.73 |
| 11:E:579:TYR:HB2 | 11:E:632:ILE:O | 1.87 | 0.73 |
| 2:3:214:TYR:HA | 2:3:227:THR:HG21 | 1.70 | 0.73 |
| 2:3:298:PHE:HD1 | 2:3:321:ILE:HG12 | 1.52 | 0.73 |
| 1:2:488:SER:HA | 1:2:493:ILE:HD13 | 1.71 | 0.73 |
| 3:4:254:THR:HB | 3:4:257:LEU:HB3 | 1.70 | 0.73 |
| 5:6:288:LEU:H | 5:6:399:GLY:H | 1.37 | 0.73 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:3:394:GLU:O | 2:3:395:ASN:ND2 | 2.14 | 0.72 |
| 6:7:258:ILE:H | 6:7:305:SER:HA | 1.51 | 0.72 |
| 8:B:17:GLN:OE1 | 9:C:190:TRP:NE1 | 2.19 | 0.72 |
| 9:C:112:ILE:HG23 | 9:C:113:MET:HE2 | 1.71 | 0.72 |
| 3:4:557:ARG:HH22 | 3:4:652:GLN:HB3 | 1.53 | 0.72 |
| 5:6:137:ARG:NH2 | 5:6:192:TYR:OH | 2.22 | 0.72 |
| 4:5:43:GLN:HB3 | 9:C:192:PHE:CZ | 2.23 | 0.72 |
| 1:2:780:GLN:HE22 | 4:5:573:ILE:HG22 | 1.53 | 0.72 |
| 3:4:557:ARG:HE | 3:4:668:ARG:HH21 | 1.37 | 0.72 |
| 4:5:379:PHE:HB3 | 4:5:568:ILE:HD13 | 1.70 | 0.72 |
| 7:A:149:ILE:HA | 7:A:150:ASP:HB2 | 1.71 | 0.72 |
| 1:2:533:ILE:HD13 | 4:5:576:HIS:CE1 | 2.25 | 0.72 |
| 11:E:25:CYS:HB3 | 11:E:26:GLN:HA | 1.69 | 0.72 |
| 11:E:392:PHE:HA | 11:E:396:LEU:HD23 | 1.72 | 0.72 |
| 3:4:543:GLN:HA | 3:4:562:ILE:HD11 | 1.71 | 0.72 |
| 8:B:184:PHE:O | 8:B:188:ILE:HD12 | 1.90 | 0.72 |
| 8:B:5:ALA:O | 8:B:8:GLN:HB3 | 1.88 | 0.72 |
| 5:6:511:ASP:OD1 | 5:6:514:ASN:ND2 | 2.22 | 0.72 |
| 5:6:810:ILE:HD11 | 5:6:827:ALA:HB2 | 1.69 | 0.72 |
| 2:3:554:ASN:HB2 | 2:3:557:ARG:HB2 | 1.71 | 0.72 |
| 3:4:572:THR:HG21 | 3:4:708:VAL:HG21 | 1.71 | 0.72 |
| 1:2:778:LEU:HG | 4:5:577:THR:HG21 | 1.71 | 0.72 |
| 8:B:119:TRP:HE1 | 8:B:174:SER:HB2 | 1.53 | 0.72 |
| 3:4:234:ARG:HB2 | 3:4:291:TYR:HE2 | 1.55 | 0.71 |
| 5:6:294:VAL:HB | 5:6:391:PRO:HA | 1.72 | 0.71 |
| 5:6:695:LEU:H | 5:6:838:VAL:HG13 | 1.54 | 0.71 |
| 11:E:19:SER:O | 11:E:25:CYS:SG | 2.48 | 0.71 |
| 3:4:428:ARG:O | 3:4:429:ALA:HB2 | 1.87 | 0.71 |
| 3:4:765:ALA:HB1 | 3:4:819:LEU:HD12 | 1.71 | 0.71 |
| 5:6:944:LYS:HD2 | 5:6:957:GLU:HB3 | 1.70 | 0.71 |
| 1:2:422:GLU:HG3 | 1:2:598:LEU:HD11 | 1.71 | 0.71 |
| 1:2:856:GLN:HE22 | 1:2:859:ARG:HH21 | 1.37 | 0.71 |
| 2:3:190:SER:O | 2:3:254:GLN:NE2 | 2.21 | 0.71 |
| 3:4:601:LEU:HG | 3:4:620:ALA:HB3 | 1.72 | 0.71 |
| 4:5:138:ILE:HG23 | 4:5:332:GLY:HA3 | 1.72 | 0.71 |
| 1:2:546:GLY:HA3 | 5:6:796:THR:HG23 | 1.73 | 0.71 |
| 4:5:588:GLU:O | 4:5:593:GLU:N | 2.23 | 0.71 |
| 1:2:614:ASP:OD1 | 1:2:617:ARG:NH1 | 2.24 | 0.71 |
| 6:7:490:GLY:C | 6:7:494:THR:HG22 | 2.11 | 0.71 |
| 11:E:29:ILE:HA | 11:E:82:LEU:HB3 | 1.72 | 0.71 |
| 4:5:578:GLY:O | 4:5:579:ASN:C | 2.28 | 0.71 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:7:334:HIS:N | 6:7:376:LEU:O | 2.22 | 0.71 |
| 1:2:656:ARG:NH1 | 5:6:793:TYR:O | 2.23 | 0.71 |
| 2:3:193:ARG:HD2 | 6:7:371:LEU:HG | 1.73 | 0.71 |
| 3:4:364:VAL:HB | 3:4:366:GLN:HE22 | 1.56 | 0.71 |
| 4:5:196:ASN:HB3 | 4:5:197:PHE:CD1 | 2.21 | 0.71 |
| 4:5:412:VAL:HG22 | 4:5:552:MET:HB2 | 1.72 | 0.71 |
| 9:C:118:LYS:HD2 | 9:C:118:LYS:O | 1.91 | 0.71 |
| 5:6:603:SER:HB3 | 5:6:607:GLY:HA2 | 1.72 | 0.70 |
| 11:E:498:LEU:O | 11:E:502:LEU:HG | 1.90 | 0.70 |
| 2:3:292:VAL:HG11 | 2:3:326:VAL:HG13 | 1.72 | 0.70 |
| 3:4:758:ILE:HD13 | 3:4:813:LEU:HA | 1.73 | 0.70 |
| 5:6:609:THR:HG23 | 5:6:663:ILE:HG12 | 1.73 | 0.70 |
| 2:3:39:ARG:HH22 | 2:3:132:LEU:HD11 | 1.56 | 0.70 |
| 4:5:298:TYR:HA | 4:5:328:ILE:HG12 | 1.73 | 0.70 |
| 11:E:269:ASN:O | 11:E:273:ASN:ND2 | 2.23 | 0.70 |
| 1:2:542:LEU:HD23 | 1:2:682:VAL:HG13 | 1.73 | 0.70 |
| 3:4:524:ARG:HG3 | 3:4:742:LEU:HD23 | 1.73 | 0.70 |
| 5:6:653:HIS:CD2 | 5:6:705:ILE:HA | 2.27 | 0.70 |
| 3:4:646:HIS:HA | 3:4:701:ARG:HH22 | 1.56 | 0.70 |
| 5:6:695:LEU:HA | 5:6:698:ASN:HB2 | 1.73 | 0.70 |
| 5:6:937:VAL:HG12 | 5:6:941:LEU:HD21 | 1.72 | 0.70 |
| 11:E:637:LEU:HA | 11:E:640:PHE:HB3 | 1.72 | 0.70 |
| 4:5:384:ILE:HG13 | 4:5:554:PHE:HD2 | 1.55 | 0.70 |
| 1:2:780:GLN:NE2 | 4:5:573:ILE:O | 2.25 | 0.70 |
| 7:A:134:TYR:HE1 | 10:D:186:HIS:HD1 | 1.38 | 0.70 |
| 2:3:450:ARG:O | 2:3:456:ARG:NH1 | 2.25 | 0.70 |
| 6:7:220:ILE:C | 6:7:222:SER:CB | 2.60 | 0.70 |
| 9:C:55:ALA:HB2 | 9:C:74:LEU:HD11 | 1.72 | 0.70 |
| 4:5:422:LYS:NZ | 13:5:801:ANP:O2B | 2.25 | 0.70 |
| 6:7:221:SER:HA | 6:7:222:SER:HB3 | 1.70 | 0.70 |
| 4:5:455:ARG:HA | 4:5:462:PHE:HA | 1.72 | 0.69 |
| 2:3:440:VAL:HG12 | 2:3:461:ALA:HB3 | 1.74 | 0.69 |
| 3:4:634:PHE:HA | 3:4:637:MET:HG2 | 1.74 | 0.69 |
| 5:6:533:ILE:CG2 | 5:6:548:LEU:HD11 | 2.22 | 0.69 |
| 6:7:432:LEU:HD11 | 6:7:469:LEU:HD23 | 1.75 | 0.69 |
| 7:A:199:LEU:HB2 | 7:A:205:LEU:HG | 1.72 | 0.69 |
| 2:3:193:ARG:NH2 | 2:3:452:THR:OG1 | 2.21 | 0.69 |
| 5:6:566:ARG:NH2 | 5:6:655:ALA:O | 2.21 | 0.69 |
| 2:3:259:GLN:HG3 | 2:3:273:SER:HB3 | 1.74 | 0.69 |
| 6:7:357:PRO:HA | 6:7:374:THR:HA | 1.74 | 0.69 |
| 6:7:82:LEU:HA | 6:7:85:ILE:HD12 | 1.75 | 0.69 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:A:108:ASP:HB3 | 7:A:109:LEU:HB3 | 0.83 | 0.69 |
| 8:B:52:LEU:HD13 | 10:D:125:PRO:HB2 | 1.72 | 0.69 |
| 10:D:266:GLU:HB3 | 10:D:268:GLU:HG3 | 1.74 | 0.69 |
| 4:5:434:PRO:HA | 4:5:600:LYS:HE2 | 1.74 | 0.69 |
| 4:5:414:LEU:HB2 | 4:5:522:ALA:HA | 1.73 | 0.69 |
| 5:6:297:THR:HA | 5:6:359:VAL:HG12 | 1.75 | 0.69 |
| 6:7:271:GLN:NE2 | 6:7:279:THR:O | 2.24 | 0.69 |
| 1:2:218:TYR:HB3 | 1:2:227:TYR:HE2 | 1.57 | 0.69 |
| 1:2:442:ASN:OD1 | 1:2:443:GLY:N | 2.24 | 0.69 |
| 5:6:953:GLU:O | 5:6:957:GLU:HG2 | 1.93 | 0.69 |
| 11:E:45:LEU:HD21 | 11:E:82:LEU:HD11 | 1.74 | 0.69 |
| 2:3:33:ASP:HB2 | 2:3:39:ARG:HH11 | 1.58 | 0.69 |
| 3:4:876:GLN:NE2 | 3:4:880:SER:O | 2.26 | 0.69 |
| 4:5:83:PRO:O | 4:5:87:ILE:HG13 | 1.92 | 0.69 |
| 6:7:662:GLN:HA | 6:7:665:ILE:HD12 | 1.74 | 0.69 |
| 10:D:143:TYR:OH | 10:D:147:ARG:NH1 | 2.25 | 0.69 |
| 10:D:260:ILE:HG23 | 10:D:266:GLU:N | 2.08 | 0.69 |
| 11:E:270:LEU:O | 11:E:274:ILE:HG13 | 1.92 | 0.69 |
| 2:3:413:THR:HB | 2:3:415:LYS:HE2 | 1.75 | 0.69 |
| 5:6:625:ALA:HB3 | 5:6:626:GLY:HA2 | 1.75 | 0.69 |
| 6:7:680:SER:HB2 | 6:7:681:PHE:HA | 1.74 | 0.69 |
| 1:2:404:ARG:NH2 | 5:6:297:THR:OG1 | 2.25 | 0.69 |
| 2:3:209:PHE:O | 6:7:7:SER:OG | 2.08 | 0.69 |
| 6:7:139:LEU:HA | 6:7:142:ILE:HB | 1.74 | 0.69 |
| 1:2:550:SER:N | 13:2:901:ANP:O1A | 2.25 | 0.69 |
| 2:3:223:THR:HG21 | 4:5:245:HIS:H | 1.58 | 0.69 |
| 7:A:188:GLN:HG3 | 11:E:58:ILE:HD12 | 1.74 | 0.69 |
| 1:2:571:ALA:CB | 5:6:664:ALA:HB3 | 2.23 | 0.69 |
| 3:4:824:GLU:HA | 3:4:827:ARG:HB3 | 1.75 | 0.69 |
| 4:5:55:LEU:HB3 | 9:C:137:HIS:HB3 | 1.73 | 0.69 |
| 5:6:612:VAL:HG23 | 5:6:623:ILE:HA | 1.75 | 0.69 |
| 1:2:547:THR:O | 13:2:901:ANP:O2A | 2.11 | 0.68 |
| 1:2:706:SER:OG | 1:2:706:SER:O | 2.11 | 0.68 |
| 2:3:229:ALA:CB | 6:7:370:LEU:HD21 | 2.24 | 0.68 |
| 4:5:547:LEU:HD22 | 4:5:553:ILE:HG12 | 1.73 | 0.68 |
| 5:6:284:ILE:HA | 5:6:401:GLU:HB3 | 1.75 | 0.68 |
| 5:6:361:ILE:HD12 | 5:6:397:PHE:HE2 | 1.57 | 0.68 |
| 11:E:577:ASP:HB2 | 11:E:633:ARG:HE | 1.58 | 0.68 |
| 1:2:638:THR:H | 4:5:445:SER:H | 1.40 | 0.68 |
| 1:2:806:THR:H | 1:2:809:HIS:HB2 | 1.57 | 0.68 |
| 2:3:23:ASP:OD1 | 2:3:26:ARG:NH2 | 2.26 | 0.68 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:3:257:THR:HA | 2:3:275:ASP:HA | 1.75 | 0.68 |
| 4:5:282:LEU:HD22 | 4:5:333:ILE:HG22 | 1.75 | 0.68 |
| 7:A:200:ILE:HD11 | 7:A:208:ILE:HD11 | 1.75 | 0.68 |
| 1:2:541:LEU:N | 1:2:648:ALA:O | 2.22 | 0.68 |
| 2:3:48:TYR:HB3 | 2:3:92:LEU:HD11 | 1.76 | 0.68 |
| 3:4:607:ARG:HG2 | 3:4:609:VAL:H | 1.57 | 0.68 |
| 3:4:692:ILE:HD11 | 3:4:705:VAL:HG11 | 1.75 | 0.68 |
| 4:5:341:SER:O | 4:5:345:SER:CB | 2.24 | 0.68 |
| 4:5:623:SER:O | 4:5:627:VAL:CG1 | 2.23 | 0.68 |
| 2:3:347:ILE:O | 2:3:351:ASN:ND2 | 2.27 | 0.68 |
| 5:6:738:ARG:HD3 | 5:6:740:GLU:H | 1.59 | 0.68 |
| 7:A:147:VAL:H | 7:A:148:ASP:HA | 1.59 | 0.68 |
| 3:4:623:LEU:HB3 | 5:6:370:THR:HG21 | 1.76 | 0.68 |
| 5:6:522:ASP:HB2 | 5:6:525:ILE:HG23 | 1.74 | 0.68 |
| 11:E:316:LEU:HD11 | 11:E:414:GLY:N | 2.09 | 0.68 |
| 1:2:339:PHE:HA | 1:2:378:GLU:HB3 | 1.75 | 0.68 |
| 2:3:163:ALA:H | 2:3:164:HIS:HB2 | 1.58 | 0.68 |
| 2:3:406:LEU:HD12 | 2:3:514:ALA:HB3 | 1.75 | 0.68 |
| 10:D:258:VAL:HB | 10:D:259:THR:CA | 2.14 | 0.68 |
| 10:D:232:VAL:HG21 | 10:D:269:LEU:HD12 | 1.76 | 0.68 |
| 6:7:466:LYS:HD2 | 6:7:566:ALA:HB1 | 1.75 | 0.68 |
| 3:4:718:ARG:HG3 | 6:7:661:VAL:HG11 | 1.74 | 0.68 |
| 11:E:85:GLY:N | 11:E:123:LEU:O | 2.26 | 0.68 |
| 2:3:687:ARG:HB3 | 6:7:604:PRO:HB3 | 1.76 | 0.68 |
| 7:A:46:ASN:O | 7:A:50:ASN:ND2 | 2.27 | 0.68 |
| 11:E:381:ASP:HB2 | 11:E:384:ILE:HG13 | 1.76 | 0.68 |
| 1:2:824:ARG:NH2 | 1:2:833:ASP:OD1 | 2.27 | 0.67 |
| 2:3:101:ASP:HA | 2:3:104:ARG:HH21 | 1.59 | 0.67 |
| 3:4:683:ASN:HD21 | 3:4:686:LEU:HD22 | 1.59 | 0.67 |
| 11:E:140:ILE:HA | 11:E:141:GLN:HB3 | 1.75 | 0.67 |
| 1:2:328:THR:O | 1:2:386:GLN:NE2 | 2.26 | 0.67 |
| 6:7:434:LEU:HD13 | 6:7:695:LEU:HD22 | 1.76 | 0.67 |
| 7:A:71:GLN:HA | 7:A:74:VAL:HB | 1.76 | 0.67 |
| 11:E:31:VAL:HG22 | 11:E:42:THR:HG21 | 1.74 | 0.67 |
| 3:4:524:ARG:HG3 | 3:4:742:LEU:CD2 | 2.24 | 0.67 |
| 6:7:104:SER:OG | 6:7:216:ARG:NE | 2.27 | 0.67 |
| 6:7:256:GLU:N | 6:7:306:LYS:O | 2.22 | 0.67 |
| 2:3:25:VAL:CG2 | 2:3:124:PRO:HB2 | 2.25 | 0.67 |
| 6:7:461:ASP:HB2 | 6:7:462:PRO:HA | 1.77 | 0.67 |
| 3:4:873:LEU:HD22 | 5:6:942:LEU:HG | 1.76 | 0.67 |
| 4:5:255:PHE:HA | 4:5:277:THR:HG22 | 1.76 | 0.67 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:5:413:LEU:HD11 | 4:5:550:PHE:CD2 | 2.29 | 0.67 |
| 6:7:208:SER:HB2 | 6:7:209:GLN:HA | 1.76 | 0.67 |
| 5:6:143:MET:HE3 | 5:6:148:LEU:H | 1.60 | 0.67 |
| 11:E:540:ARG:NH2 | 11:E:574:GLU:CB | 2.50 | 0.67 |
| 2:3:429:ALA:H | 2:3:469:VAL:H | 1.43 | 0.67 |
| 5:6:396:LYS:HB3 | 5:6:460:ILE:HG22 | 1.76 | 0.67 |
| 8:B:10:THR:HA | 8:B:182:ARG:HH11 | 1.60 | 0.67 |
| 8:B:112:PHE:O | 8:B:152:ARG:NH1 | 2.26 | 0.67 |
| 2:3:199:SER:HB3 | 2:3:212:ARG:HB3 | 1.76 | 0.67 |
| 3:4:589:VAL:HG21 | 3:4:624:SER:CB | 2.25 | 0.67 |
| 5:6:400:VAL:HG23 | 5:6:455:LEU:O | 1.94 | 0.67 |
| 10:D:83:LEU:O | 10:D:87:LEU:HG | 1.95 | 0.67 |
| 1:2:423:GLU:HB2 | 1:2:459:ARG:HD3 | 1.77 | 0.67 |
| 2:3:183:GLU:N | 2:3:183:GLU:OE1 | 2.23 | 0.67 |
| 3:4:714:GLU:H | 3:4:715:LYS:HB3 | 1.58 | 0.67 |
| 5:6:381:LEU:HB3 | 5:6:386:VAL:HA | 1.77 | 0.67 |
| 5:6:533:ILE:O | 5:6:587:TYR:OH | 2.13 | 0.67 |
| 6:7:26:VAL:H | 6:7:63:TYR:HB2 | 1.59 | 0.67 |
| 3:4:647:GLU:O | 3:4:651:GLN:HB2 | 1.95 | 0.67 |
| 6:7:458:LEU:HB2 | 6:7:566:ALA:HA | 1.77 | 0.67 |
| 2:3:30:GLU:O | 2:3:34:THR:OG1 | 2.13 | 0.66 |
| 3:4:521:LEU:HD11 | 3:4:741:VAL:O | 1.96 | 0.66 |
| 3:4:607:ARG:HA | 3:4:614:LEU:HA | 1.75 | 0.66 |
| 5:6:122:PHE:HB2 | 5:6:124:VAL:HB | 1.78 | 0.66 |
| 8:B:10:THR:OG1 | 8:B:179:ASN:OD1 | 2.13 | 0.66 |
| 2:3:701:THR:O | 2:3:704:THR:OG1 | 2.13 | 0.66 |
| 2:3:192:VAL:HB | 6:7:329:ARG:NH1 | 2.07 | 0.66 |
| 7:A:149:ILE:HD11 | 10:D:141:ARG:HG2 | 1.76 | 0.66 |
| 1:2:653:ASN:ND2 | 1:2:666:ASN:O | 2.28 | 0.66 |
| 3:4:302:LYS:NZ | 3:4:421:ASP:OD2 | 2.28 | 0.66 |
| 3:4:527:ALA:HB1 | 3:4:530:ILE:HD13 | 1.77 | 0.66 |
| 1:2:660:THR:OG1 | 3:4:928:ARG:NH1 | 2.28 | 0.66 |
| 4:5:453:VAL:HG21 | 4:5:509:ILE:HD11 | 1.77 | 0.66 |
| 6:7:318:LEU:HD23 | 6:7:321:GLN:HG3 | 1.77 | 0.66 |
| 2:3:339:ARG:HB2 | 2:3:340:GLN:HA | 1.77 | 0.66 |
| 2:3:706:ILE:O | 2:3:710:THR:OG1 | 2.13 | 0.66 |
| 3:4:354:HIS:CD2 | 3:4:356:MET:HG2 | 2.31 | 0.66 |
| 4:5:426:LEU:HD21 | 4:5:520:LEU:HD22 | 1.78 | 0.66 |
| 6:7:656:VAL:O | 6:7:660:VAL:HG23 | 1.96 | 0.66 |
| 8:B:7:LEU:H | 8:B:8:GLN:HA | 1.61 | 0.66 |
| 10:D:218:MET:HA | 10:D:220:ASP:N | 2.10 | 0.66 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:2:325:THR:OG1 | 1:2:389:THR:O | 2.12 | 0.66 |
| 2:3:451:GLU:HG3 | 2:3:452:THR:HG23 | 1.76 | 0.66 |
| 3:4:701:ARG:HA | 3:4:796:ARG:HH21 | 1.61 | 0.66 |
| 4:5:562:GLU:HB3 | 4:5:563:GLU:HG3 | 1.76 | 0.66 |
| 7:A:7:ASN:HA | 7:A:10:VAL:HG12 | 1.78 | 0.66 |
| 8:B:12:SER:HB3 | 8:B:15:GLU:HG3 | 1.76 | 0.66 |
| 1:2:234:LEU:HB3 | 1:2:237:MET:HB3 | 1.78 | 0.66 |
| 2:3:116:VAL:HG12 | 2:3:117:GLU:HG3 | 1.77 | 0.66 |
| 5:6:355:ASP:HB3 | 5:6:356:TRP:HA | 1.77 | 0.66 |
| 11:E:360:HIS:HA | 11:E:363:PHE:HD2 | 1.61 | 0.66 |
| 4:5:571:HIS:O | 4:5:581:ASN:ND2 | 2.29 | 0.66 |
| 6:7:668:ARG:HD2 | 6:7:672:LYS:HZ1 | 1.59 | 0.66 |
| 1:2:484:PHE:CE1 | 1:2:766:TYR:HA | 2.30 | 0.66 |
| 2:3:439:GLY:HA3 | 2:3:442:LEU:HD22 | 1.78 | 0.66 |
| 3:4:714:GLU:N | 3:4:715:LYS:HB3 | 2.11 | 0.66 |
| 4:5:321:VAL:N | 4:5:323:ILE:HG13 | 2.11 | 0.66 |
| 4:5:649:THR:N | 4:5:652:GLN:HG3 | 2.09 | 0.66 |
| 5:6:533:ILE:HG12 | 5:6:548:LEU:HD11 | 1.77 | 0.66 |
| 1:2:572:SER:C | 5:6:664:ALA:HB2 | 2.16 | 0.66 |
| 1:2:567:THR:HG23 | 1:2:568:GLY:N | 2.10 | 0.66 |
| 2:3:156:SER:O | 2:3:324:ASN:ND2 | 2.28 | 0.66 |
| 8:B:52:LEU:HD11 | 10:D:129:MET:HB2 | 1.78 | 0.66 |
| 11:E:621:ARG:HB2 | 11:E:631:GLU:HB2 | 1.78 | 0.66 |
| 2:3:367:LEU:HD12 | 2:3:378:LYS:HB3 | 1.78 | 0.65 |
| 6:7:69:LYS:HA | 6:7:72:ASN:HB2 | 1.78 | 0.65 |
| 10:D:94:GLN:HA | 10:D:97:LEU:HB3 | 1.78 | 0.65 |
| 1:2:539:VAL:HB | 1:2:647:ILE:HA | 1.79 | 0.65 |
| 4:5:377:SER:OG | 4:5:424:GLN:NE2 | 2.27 | 0.65 |
| 4:5:451:ALA:HB2 | 4:5:470:VAL:HG21 | 1.78 | 0.65 |
| 5:6:171:SER:O | 5:6:286:SER:HB2 | 1.96 | 0.65 |
| 5:6:561:GLU:N | 5:6:562:GLY:HA3 | 2.10 | 0.65 |
| 6:7:496:ALA:O | 6:7:508:LEU:HG | 1.95 | 0.65 |
| 1:2:789:VAL:HG13 | 1:2:863:ILE:HD12 | 1.78 | 0.65 |
| 1:2:632:SER:CB | 4:5:442:LYS:HB3 | 2.16 | 0.65 |
| 7:A:138:ILE:HD12 | 7:A:141:LEU:HD23 | 1.77 | 0.65 |
| 11:E:131:LEU:O | 11:E:155:GLN:NE2 | 2.29 | 0.65 |
| 3:4:589:VAL:HB | 3:4:629:CYS:HA | 1.78 | 0.65 |
| 5:6:662:SER:HB3 | 5:6:671:THR:HG22 | 1.78 | 0.65 |
| 10:D:200:LYS:H | 10:D:201:TYR:HB2 | 1.61 | 0.65 |
| 11:E:73:GLN:HG2 | 11:E:74:LEU:HG | 1.77 | 0.65 |
| 1:2:803:PHE:HB3 | 1:2:805:ILE:H | 1.61 | 0.65 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:7:21:ILE:HG21 | 6:7:117:PHE:HA | 1.77 | 0.65 |
| 5:6:122:PHE:HA | 5:6:123:SER:HB2 | 1.78 | 0.65 |
| 1:2:436:GLY:N | 1:2:437:ASN:HA | 2.11 | 0.65 |
| 1:2:481:GLU:HA | 1:2:484:PHE:HB3 | 1.79 | 0.65 |
| 3:4:572:THR:HB | 3:4:574:LYS:HE3 | 1.79 | 0.65 |
| 2:3:314:LEU:HD23 | 4:5:253:GLN:HE22 | 1.62 | 0.65 |
| 6:7:368:ALA:N | 6:7:370:LEU:HD22 | 2.11 | 0.65 |
| 10:D:159:ARG:HA | 10:D:162:ASN:HB3 | 1.78 | 0.65 |
| 1:2:334:LEU:HA | 1:2:382:TYR:CD1 | 2.32 | 0.65 |
| 1:2:317:LEU:HA | 1:2:429:ILE:HG22 | 1.79 | 0.65 |
| 3:4:613:GLN:HG3 | 5:6:360:ARG:HH22 | 1.62 | 0.65 |
| 4:5:481:GLU:HG2 | 4:5:484:LYS:HB2 | 1.79 | 0.65 |
| 4:5:53:ASN:HB3 | 4:5:58:ASN:HB3 | 1.79 | 0.65 |
| 4:5:62:THR:HA | 4:5:138:ILE:O | 1.97 | 0.65 |
| 5:6:348:VAL:O | 5:6:351:SER:OG | 2.14 | 0.65 |
| 11:E:526:ARG:HB2 | 11:E:567:MET:SD | 2.37 | 0.65 |
| 1:2:685:ASP:O | 5:6:794:ARG:NE | 2.25 | 0.65 |
| 3:4:907:LEU:HD23 | 3:4:910:LEU:HD12 | 1.78 | 0.65 |
| 4:5:664:ALA:HA | 4:5:676:HIS:CE1 | 2.26 | 0.65 |
| 5:6:783:ASP:OD1 | 5:6:783:ASP:N | 2.27 | 0.65 |
| 6:7:513:LEU:HA | 6:7:561:THR:HG21 | 1.79 | 0.65 |
| 2:3:471:CYS:HA | 2:3:513:ILE:O | 1.97 | 0.64 |
| 2:3:47:VAL:HG12 | 2:3:51:ASN:HD21 | 1.63 | 0.64 |
| 3:4:201:PHE:HB2 | 3:4:202:LYS:HA | 1.79 | 0.64 |
| 4:5:181:ILE:HG21 | 4:5:241:TYR:HB3 | 1.78 | 0.64 |
| 11:E:489:VAL:O | 11:E:493:ASN:ND2 | 2.29 | 0.64 |
| 5:6:174:TYR:CE2 | 5:6:178:LEU:HD11 | 2.33 | 0.64 |
| 5:6:605:ALA:O | 5:6:607:GLY:HA3 | 1.96 | 0.64 |
| 6:7:531:GLU:HA | 6:7:534:ARG:HB2 | 1.78 | 0.64 |
| 6:7:575:ASN:HB3 | 6:7:578:LEU:HD22 | 1.79 | 0.64 |
| 9:C:104:PHE:O | 9:C:108:ALA:N | 2.28 | 0.64 |
| 9:C:105:PHE:HZ | 9:C:127:LEU:HD22 | 1.62 | 0.64 |
| 11:E:285:ALA:HB1 | 11:E:288:TYR:HB3 | 1.79 | 0.64 |
| 11:E:611:GLN:HG3 | 11:E:649:LEU:HD21 | 1.78 | 0.64 |
| 6:7:311:GLN:O | 6:7:335:VAL:HB | 1.96 | 0.64 |
| 4:5:165:ILE:HG12 | 4:5:291:ARG:HA | 1.79 | 0.64 |
| 4:5:356:GLU:O | 4:5:360:LEU:HG | 1.98 | 0.64 |
| 5:6:964:VAL:HA | 5:6:967:ARG:HB3 | 1.79 | 0.64 |
| 7:A:167:VAL:HG21 | 7:A:183:LEU:HD12 | 1.79 | 0.64 |
| 11:E:292:TYR:O | 11:E:296:GLN:N | 2.28 | 0.64 |
| 2:3:139:VAL:N | 2:3:140:PRO:HD2 | 2.12 | 0.64 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:4:332:VAL:HB | 3:4:429:ALA:CA | 2.18 | 0.64 |
| 3:4:461:VAL:HG12 | 3:4:463:VAL:H | 1.63 | 0.64 |
| 3:4:649:MET:HG3 | 3:4:701:ARG:HD3 | 1.78 | 0.64 |
| 4:5:366:LEU:HA | 4:5:369:ILE:HG22 | 1.79 | 0.64 |
| 4:5:464:LEU:HD23 | 4:5:466:GLY:H | 1.61 | 0.64 |
| 2:3:139:VAL:N | 2:3:140:PRO:CD | 2.58 | 0.64 |
| 3:4:271:ILE:O | 3:4:275:THR:HG23 | 1.97 | 0.64 |
| 4:5:343:TRP:O | 4:5:344:ASN:HB3 | 1.96 | 0.64 |
| 4:5:378:ILE:HA | 13:5:801:ANP:HN61 | 1.62 | 0.64 |
| 10:D:59:ASP:OD2 | 10:D:90:ARG:NH1 | 2.30 | 0.64 |
| 3:4:183:THR:HG21 | 3:4:267:GLU:HG3 | 1.80 | 0.64 |
| 4:5:375:ALA:HB3 | 4:5:385:LYS:HE3 | 1.80 | 0.64 |
| 6:7:23:ASP:O | 6:7:27:THR:OG1 | 2.16 | 0.64 |
| 2:3:292:VAL:HG11 | 2:3:326:VAL:CG1 | 2.27 | 0.64 |
| 10:D:123:LYS:HD3 | 11:E:22:HIS:NE2 | 2.13 | 0.64 |
| 3:4:241:LEU:HD22 | 3:4:303:VAL:HG22 | 1.79 | 0.64 |
| 3:4:574:LYS:NZ | 3:4:675:ALA:O | 2.23 | 0.64 |
| 3:4:682:TYR:O | 3:4:691:ASN:ND2 | 2.31 | 0.64 |
| 4:5:368:GLU:O | 4:5:371:THR:OG1 | 2.12 | 0.64 |
| 4:5:254:GLN:HB3 | 4:5:278:CYS:HB2 | 1.80 | 0.63 |
| 11:E:24:SER:HB2 | 11:E:25:CYS:HB2 | 1.80 | 0.63 |
| 2:3:433:THR:HG23 | 4:5:503:SER:HB3 | 1.81 | 0.63 |
| 2:3:524:ASP:HA | 2:3:532:ASN:HD21 | 1.63 | 0.63 |
| 3:4:289:LEU:HB3 | 3:4:293:LEU:HD21 | 1.80 | 0.63 |
| 3:4:443:PRO:HB2 | 3:4:453:LEU:HD22 | 1.80 | 0.63 |
| 4:5:606:CYS:O | 4:5:665:LYS:NZ | 2.29 | 0.63 |
| 5:6:304:LEU:HA | 5:6:353:PHE:CE1 | 2.32 | 0.63 |
| 1:2:575:GLY:N | 5:6:664:ALA:HB1 | 2.13 | 0.63 |
| 2:3:49:ASN:OD1 | 2:3:50:SER:N | 2.32 | 0.63 |
| 3:4:727:LEU:N | 3:4:728:TYR:CB | 2.58 | 0.63 |
| 5:6:119:LEU:HD11 | 5:6:188:VAL:HG21 | 1.81 | 0.63 |
| 5:6:355:ASP:OD2 | 5:6:383:GLY:N | 2.31 | 0.63 |
| 6:7:147:ARG:HH21 | 6:7:197:THR:HG23 | 1.63 | 0.63 |
| 6:7:108:GLN:OE1 | 6:7:237:GLN:NE2 | 2.31 | 0.63 |
| 6:7:489:SER:O | 6:7:493:LEU:HD23 | 1.97 | 0.63 |
| 4:5:440:SER:HA | 4:5:480:ASP:HB2 | 1.80 | 0.63 |
| 11:E:575:ASN:O | 11:E:576:THR:OG1 | 2.07 | 0.63 |
| 3:4:419:VAL:HB | 3:4:423:LEU:HB2 | 1.81 | 0.63 |
| 4:5:144:ASN:HD22 | 11:E:375:GLU:HA | 1.63 | 0.63 |
| 1:2:229:ALA:O | 1:2:233:THR:OG1 | 2.14 | 0.63 |
| 2:3:53:ALA:HA | 6:7:218:LYS:HD2 | 1.80 | 0.63 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:4:830:ARG:HA | 3:4:833:ILE:HB | 1.81 | 0.63 |
| 4:5:343:TRP:O | 4:5:344:ASN:CB | 2.47 | 0.63 |
| 4:5:639:GLU:HB2 | 4:5:641:THR:HG23 | 1.81 | 0.63 |
| 5:6:523:GLU:OE1 | 5:6:524:HIS:ND1 | 2.31 | 0.63 |
| 5:6:708:ARG:HD3 | 5:6:798:ARG:HD3 | 1.80 | 0.63 |
| 6:7:411:TYR:CD1 | 6:7:433:LEU:HD23 | 2.34 | 0.63 |
| 6:7:417:SER:HB3 | 6:7:633:VAL:HB | 1.81 | 0.63 |
| 1:2:309:LEU:O | 1:2:310:ARG:NH1 | 2.31 | 0.63 |
| 2:3:564:HIS:HA | 2:3:567:ARG:HG2 | 1.81 | 0.63 |
| 3:4:771:VAL:HG22 | 5:6:732:VAL:HG21 | 1.80 | 0.63 |
| 7:A:109:LEU:HG | 7:A:111:SER:HB3 | 1.80 | 0.63 |
| 10:D:224:TRP:O | 10:D:280:GLU:N | 2.31 | 0.63 |
| 1:2:612:MET:O | 1:2:617:ARG:NH2 | 2.32 | 0.63 |
| 1:2:630:SER:HA | 4:5:445:SER:HB2 | 1.81 | 0.63 |
| 10:D:269:LEU:HD13 | 10:D:275:TYR:CD2 | 2.34 | 0.63 |
| 1:2:320:VAL:HB | 1:2:426:VAL:HG23 | 1.79 | 0.63 |
| 2:3:434:GLY:N | 2:3:473:ASP:O | 2.32 | 0.63 |
| 5:6:533:ILE:HG21 | 5:6:548:LEU:CD1 | 2.28 | 0.63 |
| 5:6:560:VAL:HB | 5:6:561:GLU:HA | 1.81 | 0.63 |
| 1:2:573:ALA:HB2 | 5:6:663:ILE:O | 1.99 | 0.63 |
| 6:7:541:MET:HB2 | 6:7:593:ARG:HH11 | 1.64 | 0.63 |
| 8:B:11:PHE:HB2 | 8:B:179:ASN:ND2 | 2.12 | 0.63 |
| 2:3:171:LEU:HD23 | 2:3:172:THR:H | 1.64 | 0.62 |
| 3:4:324:LYS:O | 3:4:438:THR:HA | 1.99 | 0.62 |
| 5:6:581:LYS:NZ | 5:6:682:ALA:O | 2.32 | 0.62 |
| 1:2:704:VAL:HG13 | 5:6:766:THR:HG23 | 1.81 | 0.62 |
| 7:A:31:MET:O | 7:A:93:ARG:NH2 | 2.31 | 0.62 |
| 1:2:581:ARG:NH1 | 1:2:592:GLU:OE2 | 2.32 | 0.62 |
| 2:3:706:ILE:HG21 | 6:7:620:HIS:HE2 | 1.64 | 0.62 |
| 6:7:265:CYS:N | 6:7:289:CYS:SG | 2.66 | 0.62 |
| 6:7:543:GLN:HG3 | 6:7:544:GLN:H | 1.65 | 0.62 |
| 8:B:165:GLU:N | 8:B:165:GLU:OE1 | 2.30 | 0.62 |
| 10:D:73:SER:OG | 10:D:150:LYS:NZ | 2.31 | 0.62 |
| 1:2:335:LYS:HB2 | 1:2:381:VAL:O | 2.00 | 0.62 |
| 2:3:360:PHE:HD1 | 2:3:715:VAL:HG11 | 1.64 | 0.62 |
| 5:6:653:HIS:CD2 | 5:6:656:MET:HB2 | 2.34 | 0.62 |
| 5:6:805:ARG:HA | 5:6:808:GLU:CD | 2.20 | 0.62 |
| 11:E:351:TRP:HB2 | 11:E:511:VAL:HG13 | 1.81 | 0.62 |
| 1:2:641:GLN:HB3 | 1:2:643:ARG:NH1 | 2.14 | 0.62 |
| 2:3:100:LEU:HB3 | 2:3:111:TRP:HZ3 | 1.65 | 0.62 |
| 5:6:625:ALA:HB2 | 5:6:629:MET:HE2 | 1.80 | 0.62 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 6:7:513:LEU:HD13 | 6:7:540:VAL:HG21 | 1.80 | 0.62 |
| 11:E:30:PHE:CE2 | 11:E:81:LEU:HD21 | 2.35 | 0.62 |
| 3:4:628:VAL:HA | 3:4:670:SER:O | 1.99 | 0.62 |
| 5:6:610:ALA:HB3 | 5:6:663:ILE:HG21 | 1.80 | 0.62 |
| 10:D:143:TYR:O | 10:D:147:ARG:HG3 | 1.99 | 0.62 |
| 3:4:234:ARG:HB3 | 3:4:280:MET:HE1 | 1.80 | 0.62 |
| 3:4:236:LEU:HB3 | 3:4:238:THR:HG23 | 1.80 | 0.62 |
| 4:5:349:PHE:CD2 | 4:5:351:GLU:HA | 2.34 | 0.62 |
| 1:2:438:LEU:HD13 | 5:6:301:ARG:HH12 | 1.63 | 0.62 |
| 5:6:614:ARG:NH2 | 12:F:12:DT:O4' | 2.32 | 0.62 |
| 10:D:200:LYS:HB2 | 10:D:201:TYR:CG | 2.35 | 0.62 |
| 2:3:168:PRO:HG2 | 2:3:260:GLU:HB3 | 1.82 | 0.62 |
| 3:4:695:PRO:HB2 | 3:4:697:PRO:HG2 | 1.82 | 0.62 |
| 5:6:831:LEU:O | 5:6:835:ILE:HG13 | 1.99 | 0.62 |
| 11:E:285:ALA:HB3 | 11:E:286:GLN:HA | 1.82 | 0.62 |
| 11:E:292:TYR:HB2 | 11:E:293:PRO:HD3 | 1.82 | 0.62 |
| 2:3:138:ASP:CB | 2:3:140:PRO:HD2 | 2.30 | 0.62 |
| 3:4:400:GLN:HG3 | 6:7:508:LEU:HB2 | 1.81 | 0.62 |
| 3:4:428:ARG:O | 3:4:429:ALA:CB | 2.47 | 0.62 |
| 3:4:758:ILE:HD11 | 3:4:813:LEU:HD23 | 1.81 | 0.62 |
| 4:5:136:GLN:HB2 | 4:5:280:ARG:HE | 1.65 | 0.62 |
| 5:6:576:ASP:O | 5:6:579:THR:OG1 | 2.09 | 0.62 |
| 5:6:703:ALA:HA | 5:6:706:MET:HB3 | 1.81 | 0.62 |
| 7:A:100:MET:HG2 | 7:A:117:GLN:HE21 | 1.64 | 0.62 |
| 9:C:170:GLU:O | 9:C:174:LYS:N | 2.33 | 0.62 |
| 11:E:312:THR:OG1 | 11:E:314:ASP:O | 2.18 | 0.62 |
| 1:2:414:LEU:HD22 | 1:2:455:SER:HA | 1.81 | 0.62 |
| 3:4:418:CYS:O | 3:4:419:VAL:HG22 | 2.00 | 0.62 |
| 5:6:941:LEU:HD22 | 5:6:958:ARG:HH21 | 1.65 | 0.62 |
| 1:2:622:GLU:HG3 | 1:2:626:GLN:NE2 | 2.15 | 0.62 |
| 2:3:100:LEU:HB3 | 2:3:111:TRP:CZ3 | 2.35 | 0.62 |
| 3:4:547:GLY:HA3 | 3:4:560:GLY:HA2 | 1.81 | 0.62 |
| 4:5:410:ILE:O | 4:5:411:ASN:ND2 | 2.31 | 0.62 |
| 5:6:796:THR:HG22 | 5:6:798:ARG:N | 2.14 | 0.62 |
| 7:A:37:ILE:O | 7:A:41:LEU:HG | 2.00 | 0.62 |
| 8:B:195:ILE:HG22 | 9:C:109:ILE:HD13 | 1.81 | 0.62 |
| 9:C:180:SER:O | 9:C:183:SER:OG | 2.15 | 0.62 |
| 2:3:414:ALA:HA | 13:3:1001:ANP:H5'1 | 1.82 | 0.61 |
| 5:6:399:GLY:HA2 | 5:6:454:PHE:CZ | 2.35 | 0.61 |
| 5:6:662:SER:HA | 5:6:671:THR:HA | 1.82 | 0.61 |
| 3:4:549:ASN:OD1 | 3:4:559:ARG:NH2 | 2.33 | 0.61 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:A:138:ILE:HA | 7:A:141:LEU:HD23 | 1.82 | 0.61 |
| 11:E:530:LEU:HD22 | 11:E:536:LEU:HD11 | 1.81 | 0.61 |
| 3:4:722:LYS:HA | 3:4:725:THR:HB | 1.80 | 0.61 |
| 3:4:727:LEU:H | 3:4:728:TYR:HB3 | 1.65 | 0.61 |
| 4:5:347:THR:HB | 4:5:349:PHE:HA | 1.81 | 0.61 |
| 6:7:459:MET:HG3 | 6:7:460:GLY:H | 1.64 | 0.61 |
| 8:B:13:PRO:HA | 8:B:16:ILE:HG12 | 1.81 | 0.61 |
| 8:B:192:LEU:O | 8:B:195:ILE:HG13 | 2.00 | 0.61 |
| 1:2:300:PHE:O | 1:2:302:THR:OG1 | 2.15 | 0.61 |
| 6:7:415:ALA:HA | 6:7:418:ILE:HD12 | 1.81 | 0.61 |
| 7:A:150:ASP:OD1 | 7:A:198:ARG:NH2 | 2.34 | 0.61 |
| 10:D:74:PRO:HG3 | 10:D:279:TYR:CG | 2.36 | 0.61 |
| 11:E:413:LEU:HD23 | 11:E:416:ARG:HD2 | 1.81 | 0.61 |
| 4:5:64:ASN:HD21 | 4:5:66:GLU:HB2 | 1.65 | 0.61 |
| 5:6:540:HIS:HD2 | 5:6:715:ILE:HG21 | 1.66 | 0.61 |
| 11:E:336:ASP:HA | 11:E:339:TYR:HB3 | 1.82 | 0.61 |
| 11:E:551:TRP:HE3 | 11:E:552:LEU:HD12 | 1.65 | 0.61 |
| 1:2:853:VAL:HA | 1:2:856:GLN:HB3 | 1.82 | 0.61 |
| 3:4:396:VAL:HA | 3:4:418:CYS:HA | 1.82 | 0.61 |
| 10:D:260:ILE:HG12 | 10:D:266:GLU:OE1 | 1.96 | 0.61 |
| 2:3:254:GLN:HE21 | 2:3:256:ILE:HD11 | 1.64 | 0.61 |
| 4:5:51:ARG:HA | 4:5:54:ILE:HG12 | 1.83 | 0.61 |
| 4:5:553:ILE:HD12 | 4:5:553:ILE:H | 1.66 | 0.61 |
| 5:6:919:LYS:HD2 | 5:6:936:ILE:HB | 1.82 | 0.61 |
| 11:E:12:TYR:CE1 | 11:E:48:LEU:HD21 | 2.36 | 0.61 |
| 11:E:316:LEU:HD21 | 11:E:413:LEU:O | 2.00 | 0.61 |
| 1:2:479:GLU:O | 1:2:482:ARG:HG2 | 2.01 | 0.61 |
| 1:2:543:GLY:N | 1:2:650:ALA:O | 2.33 | 0.61 |
| 2:3:301:LEU:H | 2:3:319:THR:HG22 | 1.66 | 0.61 |
| 2:3:356:LYS:HB2 | 2:3:359:ILE:HG23 | 1.83 | 0.61 |
| 5:6:189:VAL:O | 5:6:193:ALA:N | 2.33 | 0.61 |
| 5:6:940:TYR:OH | 5:6:957:GLU:OE1 | 2.19 | 0.61 |
| 9:C:82:THR:HA | 9:C:85:MET:HG2 | 1.81 | 0.61 |
| 11:E:33:CYS:SG | 11:E:62:PHE:HA | 2.40 | 0.61 |
| 11:E:68:ARG:HB2 | 11:E:95:PHE:CE2 | 2.35 | 0.61 |
| 1:2:296:ARG:O | 1:2:455:SER:OG | 2.08 | 0.61 |
| 3:4:822:VAL:HA | 3:4:825:ALA:HB3 | 1.83 | 0.61 |
| 6:7:82:LEU:HB3 | 6:7:207:LEU:HD23 | 1.83 | 0.61 |
| 11:E:243:GLN:N | 11:E:607:MET:SD | 2.74 | 0.61 |
| 11:E:577:ASP:HB2 | 11:E:633:ARG:NE | 2.15 | 0.61 |
| 1:2:299:ASP:HB3 | 1:2:319:ARG:NH1 | 2.16 | 0.61 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:3:244:GLU:O | 2:3:248:SER:OG | 2.16 | 0.61 |
| 2:3:409:GLY:O | 2:3:415:LYS:NZ | 2.34 | 0.61 |
| 3:4:518:LEU:HG | 3:4:522:LEU:HG | 1.83 | 0.61 |
| 4:5:349:PHE:HD2 | 4:5:351:GLU:HA | 1.65 | 0.61 |
| 7:A:198:ARG:O | 7:A:202:GLN:HB2 | 2.01 | 0.61 |
| 9:C:162:THR:N | 9:C:163:SER:HA | 2.14 | 0.61 |
| 2:3:193:ARG:HH22 | 2:3:452:THR:HG1 | 1.49 | 0.60 |
| 4:5:339:THR:O | 4:5:341:SER:OG | 2.17 | 0.60 |
| 5:6:690:ASN:HB3 | 5:6:693:LEU:HD12 | 1.83 | 0.60 |
| 2:3:554:ASN:O | 2:3:558:ASP:N | 2.34 | 0.60 |
| 3:4:826:VAL:HA | 3:4:829:ILE:HD12 | 1.81 | 0.60 |
| 5:6:943:GLN:HA | 5:6:946:ASN:HD21 | 1.66 | 0.60 |
| 6:7:228:ARG:NH1 | 6:7:326:HIS:HB3 | 2.15 | 0.60 |
| 6:7:369:GLY:H | 6:7:371:LEU:HB2 | 1.66 | 0.60 |
| 2:3:210:HIS:HB3 | 6:7:5:LEU:HD21 | 1.83 | 0.60 |
| 6:7:440:VAL:HG23 | 6:7:697:GLN:HB3 | 1.81 | 0.60 |
| 11:E:311:LYS:N | 11:E:312:THR:HA | 2.16 | 0.60 |
| 1:2:564:VAL:HG11 | 1:2:595:ALA:HB1 | 1.83 | 0.60 |
| 1:2:793:LEU:HD11 | 1:2:863:ILE:HG21 | 1.83 | 0.60 |
| 13:3:1001:ANP:O2B | 13:3:1001:ANP:O3G | 2.20 | 0.60 |
| 2:3:105:GLU:OE1 | 2:3:105:GLU:N | 2.34 | 0.60 |
| 2:3:402:ASP:N | 2:3:402:ASP:OD1 | 2.29 | 0.60 |
| 7:A:22:ARG:HB3 | 7:A:23:SER:HA | 1.83 | 0.60 |
| 7:A:67:VAL:HG21 | 9:C:25:PRO:HD2 | 1.83 | 0.60 |
| 11:E:431:LEU:O | 11:E:476:ASN:ND2 | 2.33 | 0.60 |
| 2:3:53:ALA:O | 6:7:217:LYS:NZ | 2.32 | 0.60 |
| 3:4:608:ASP:OD2 | 3:4:611:THR:OG1 | 2.18 | 0.60 |
| 3:4:725:THR:O | 3:4:728:TYR:HB2 | 2.01 | 0.60 |
| 9:C:107:LEU:O | 9:C:110:LYS:N | 2.32 | 0.60 |
| 4:5:144:ASN:ND2 | 11:E:374:GLN:O | 2.35 | 0.60 |
| 1:2:783:MET:HB3 | 4:5:573:ILE:HG21 | 1.81 | 0.60 |
| 3:4:517:ASP:O | 3:4:521:LEU:N | 2.26 | 0.60 |
| 4:5:485:MET:HE3 | 4:5:490:ARG:HA | 1.84 | 0.60 |
| 4:5:675:ARG:HA | 4:5:678:ASP:HB2 | 1.84 | 0.60 |
| 5:6:725:THR:HA | 5:6:728:ALA:HB3 | 1.84 | 0.60 |
| 6:7:664:TYR:CG | 6:7:689:LEU:HD13 | 2.36 | 0.60 |
| 11:E:346:ALA:HB2 | 11:E:555:CYS:HA | 1.84 | 0.60 |
| 11:E:583:GLY:N | 11:E:628:SER:O | 2.27 | 0.60 |
| 1:2:275:ALA:O | 1:2:279:THR:N | 2.33 | 0.60 |
| 1:2:611:LYS:N | 1:2:611:LYS:HD2 | 2.17 | 0.60 |
| 2:3:303:ALA:HB1 | 2:3:307:ASN:HB2 | 1.83 | 0.60 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:5:137:LEU:HD11 | 4:5:139:LEU:HD23 | 1.82 | 0.60 |
| 11:E:567:MET:HB2 | 11:E:584:LEU:HB2 | 1.83 | 0.60 |
| 11:E:92:LEU:O | 11:E:96:LEU:N | 2.34 | 0.60 |
| 2:3:161:PHE:HB3 | 2:3:162:GLY:HA3 | 1.84 | 0.60 |
| 2:3:229:ALA:O | 2:3:230:ILE:HG23 | 2.01 | 0.60 |
| 11:E:512:ALA:O | 11:E:516:LYS:HG3 | 2.02 | 0.60 |
| 4:5:338:GLU:HG2 | 4:5:340:SER:OG | 2.01 | 0.60 |
| 3:4:260:GLN:HG2 | 6:7:135:LYS:HZ1 | 1.66 | 0.60 |
| 1:2:283:TYR:O | 1:2:285:ASP:N | 2.33 | 0.60 |
| 3:4:755:LYS:HA | 3:4:810:LYS:HD3 | 1.82 | 0.60 |
| 4:5:66:GLU:N | 4:5:66:GLU:OE1 | 2.35 | 0.60 |
| 5:6:304:LEU:HD12 | 5:6:353:PHE:HE1 | 1.67 | 0.60 |
| 11:E:346:ALA:HB1 | 11:E:558:GLU:HG3 | 1.83 | 0.60 |
| 1:2:778:LEU:HG | 4:5:577:THR:HG22 | 1.83 | 0.59 |
| 2:3:553:ILE:HG22 | 4:5:630:ARG:HH11 | 1.67 | 0.59 |
| 5:6:357:GLN:HE21 | 5:6:381:LEU:HD12 | 1.66 | 0.59 |
| 6:7:113:PHE:O | 6:7:117:PHE:HB3 | 2.00 | 0.59 |
| 11:E:227:LYS:O | 11:E:231:HIS:ND1 | 2.30 | 0.59 |
| 1:2:306:LEU:HD11 | 1:2:406:ARG:HG2 | 1.84 | 0.59 |
| 1:2:803:PHE:HB3 | 1:2:805:ILE:HD12 | 1.83 | 0.59 |
| 3:4:642:ARG:HA | 3:4:645:LEU:HB2 | 1.85 | 0.59 |
| 3:4:758:ILE:CD1 | 3:4:813:LEU:HA | 2.31 | 0.59 |
| 5:6:910:VAL:O | 5:6:914:ASN:HB2 | 2.02 | 0.59 |
| 6:7:490:GLY:HA2 | 6:7:493:LEU:CD1 | 2.32 | 0.59 |
| 8:B:25:ILE:HD11 | 8:B:73:LEU:HA | 1.84 | 0.59 |
| 2:3:200:VAL:HB | 2:3:244:GLU:HB2 | 1.83 | 0.59 |
| 2:3:372:TYR:OH | 2:3:564:HIS:HB3 | 2.02 | 0.59 |
| 6:7:495:ALA:HB3 | 6:7:557:LEU:HD21 | 1.84 | 0.59 |
| 6:7:521:CYS:N | 6:7:562:SER:O | 2.27 | 0.59 |
| 7:A:47:LEU:HD22 | 7:A:79:MET:SD | 2.42 | 0.59 |
| 8:B:132:ASP:N | 8:B:132:ASP:OD1 | 2.31 | 0.59 |
| 11:E:574:GLU:O | 11:E:575:ASN:HB2 | 2.01 | 0.59 |
| 2:3:25:VAL:HG22 | 2:3:124:PRO:HB2 | 1.85 | 0.59 |
| 2:3:228:PRO:HB2 | 2:3:229:ALA:HB2 | 1.85 | 0.59 |
| 4:5:136:GLN:HA | 4:5:280:ARG:HH21 | 1.66 | 0.59 |
| 5:6:616:GLU:N | 5:6:617:GLU:HA | 2.17 | 0.59 |
| 6:7:364:LYS:O | 6:7:367:LYS:N | 2.36 | 0.59 |
| 11:E:148:VAL:HG13 | 11:E:150:ASP:HB2 | 1.84 | 0.59 |
| 1:2:328:THR:HG22 | 1:2:387:ARG:O | 2.02 | 0.59 |
| 2:3:368:ALA:HB1 | 2:3:371:ILE:HB | 1.84 | 0.59 |
| 3:4:686:LEU:HD12 | 3:4:687:PRO:HD2 | 1.84 | 0.59 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2:659:SER:HA | 3:4:928:ARG:NH2 | 2.18 | 0.59 |
| 5:6:400:VAL:CG2 | 5:6:455:LEU:O | 2.49 | 0.59 |
| 6:7:444:VAL:HG22 | 6:7:448:MET:H | 1.68 | 0.59 |
| 7:A:150:ASP:HB2 | 10:D:141:ARG:HH21 | 1.68 | 0.59 |
| 10:D:231:HIS:O | 10:D:292:ALA:N | 2.35 | 0.59 |
| 11:E:434:VAL:O | 11:E:476:ASN:ND2 | 2.34 | 0.59 |
| 2:3:229:ALA:CB | 6:7:370:LEU:CD2 | 2.81 | 0.59 |
| 3:4:234:ARG:HB2 | 3:4:291:TYR:CE2 | 2.36 | 0.59 |
| 4:5:298:TYR:HD1 | 4:5:328:ILE:HD11 | 1.67 | 0.59 |
| 4:5:633:LEU:HD12 | 4:5:648:ILE:HG13 | 1.85 | 0.59 |
| 10:D:70:GLU:O | 10:D:150:LYS:NZ | 2.35 | 0.59 |
| 11:E:541:ASN:HD21 | 11:E:543:LEU:HB2 | 1.66 | 0.59 |
| 2:3:408:VAL:HA | 2:3:516:ALA:O | 2.03 | 0.59 |
| 3:4:605:ILE:HG13 | 3:4:616:LEU:HD12 | 1.84 | 0.59 |
| 3:4:886:LEU:O | 3:4:890:ILE:HG12 | 2.03 | 0.59 |
| 6:7:128:PRO:HD2 | 6:7:129:THR:HA | 1.84 | 0.59 |
| 10:D:77:LEU:O | 10:D:147:ARG:NH2 | 2.36 | 0.59 |
| 8:B:122:LEU:O | 8:B:126:LEU:HG | 2.03 | 0.59 |
| 10:D:59:ASP:HB3 | 10:D:87:LEU:HD21 | 1.85 | 0.59 |
| 11:E:576:THR:C | 11:E:577:ASP:CG | 2.59 | 0.59 |
| 1:2:633:LYS:HD2 | 12:F:12:DT:P | 2.43 | 0.59 |
| 1:2:605:LEU:HD23 | 1:2:647:ILE:HB | 1.83 | 0.59 |
| 3:4:435:VAL:HA | 3:4:466:VAL:HG22 | 1.84 | 0.59 |
| 5:6:307:ALA:HA | 5:6:351:SER:HB3 | 1.84 | 0.59 |
| 5:6:795:ILE:CG2 | 5:6:799:GLN:HG3 | 2.30 | 0.59 |
| 5:6:806:LEU:HD13 | 5:6:827:ALA:HB1 | 1.85 | 0.59 |
| 2:3:326:VAL:HG12 | 2:3:326:VAL:O | 2.02 | 0.59 |
| 6:7:380:PHE:HE2 | 6:7:382:ARG:HB2 | 1.68 | 0.59 |
| 11:E:327:PHE:N | 11:E:341:SER:OG | 2.32 | 0.59 |
| 2:3:186:VAL:O | 2:3:289:GLY:N | 2.28 | 0.58 |
| 2:3:679:ILE:HB | 2:3:705:LEU:HD13 | 1.85 | 0.58 |
| 5:6:182:GLN:HG2 | 5:6:265:ILE:HD13 | 1.85 | 0.58 |
| 5:6:723:ILE:O | 5:6:727:LEU:HG | 2.03 | 0.58 |
| 6:7:284:CYS:SG | 6:7:289:CYS:HB2 | 2.42 | 0.58 |
| 6:7:650:PRO:HA | 6:7:706:ASP:HA | 1.85 | 0.58 |
| 8:B:59:ALA:HB1 | 8:B:60:LEU:HB2 | 1.84 | 0.58 |
| 11:E:540:ARG:HH22 | 11:E:574:GLU:CB | 2.13 | 0.58 |
| 5:6:689:TYR:HD2 | 5:6:716:LEU:HD12 | 1.68 | 0.58 |
| 6:7:282:SER:HA | 6:7:298:LEU:HD11 | 1.85 | 0.58 |
| 7:A:5:LEU:HD11 | 7:A:36:ILE:HD11 | 1.86 | 0.58 |
| 2:3:428:LEU:HB3 | 2:3:429:ALA:CA | 2.33 | 0.58 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:5:301:TYR:CE1 | 4:5:303:SER:HB3 | 2.39 | 0.58 |
| 4:5:374:ILE:HA | 4:5:428:PHE:CE2 | 2.38 | 0.58 |
| 5:6:765:LEU:HB2 | 5:6:819:ILE:HD13 | 1.85 | 0.58 |
| 5:6:714:VAL:HB | 5:6:837:ARG:HD3 | 1.84 | 0.58 |
| 6:7:465:ALA:HB1 | 6:7:468:GLN:HG2 | 1.83 | 0.58 |
| 1:2:499:SER:HB2 | 1:2:509:ARG:HH22 | 1.68 | 0.58 |
| 1:2:661:LEU:HB3 | 1:2:662:PRO:HD2 | 1.84 | 0.58 |
| 2:3:196:LEU:HD23 | 6:7:370:LEU:HB2 | 1.85 | 0.58 |
| 2:3:43:ARG:O | 2:3:47:VAL:HG23 | 2.02 | 0.58 |
| 4:5:176:ALA:HA | 4:5:250:PHE:CD1 | 2.39 | 0.58 |
| 4:5:342:ILE:HG13 | 4:5:342:ILE:O | 2.03 | 0.58 |
| 5:6:610:ALA:HA | 5:6:624:GLU:HG2 | 1.85 | 0.58 |
| 6:7:71:ALA:HB1 | 6:7:129:THR:HG21 | 1.86 | 0.58 |
| 8:B:113:SER:O | 8:B:172:ASN:ND2 | 2.27 | 0.58 |
| 1:2:506:TYR:HB2 | 1:2:698:PHE:CE2 | 2.39 | 0.58 |
| 1:2:549:LYS:HA | 1:2:552:ILE:HD12 | 1.84 | 0.58 |
| 2:3:200:VAL:HG21 | 2:3:247:TYR:CD2 | 2.39 | 0.58 |
| 3:4:348:LYS:O | 3:4:383:SER:N | 2.24 | 0.58 |
| 3:4:705:VAL:H | 3:4:832:ALA:HB2 | 1.68 | 0.58 |
| 5:6:143:MET:HE3 | 5:6:148:LEU:N | 2.18 | 0.58 |
| 5:6:914:ASN:O | 5:6:918:ARG:HB2 | 2.04 | 0.58 |
| 6:7:142:ILE:O | 6:7:146:ARG:HG2 | 2.04 | 0.58 |
| 2:3:228:PRO:CB | 2:3:229:ALA:HB2 | 2.33 | 0.58 |
| 3:4:601:LEU:HB3 | 3:4:621:LEU:HG | 1.86 | 0.58 |
| 6:7:203:TYR:OH | 6:7:338:THR:N | 2.37 | 0.58 |
| 9:C:178:LYS:O | 9:C:182:GLU:HG2 | 2.04 | 0.58 |
| 11:E:579:TYR:CD1 | 11:E:637:LEU:HD21 | 2.39 | 0.58 |
| 2:3:32:LEU:HG | 2:3:132:LEU:HD22 | 1.85 | 0.58 |
| 3:4:280:MET:O | 3:4:284:ILE:HG12 | 2.04 | 0.58 |
| 3:4:348:LYS:N | 3:4:383:SER:O | 2.35 | 0.58 |
| 4:5:136:GLN:NE2 | 4:5:279:ASP:O | 2.33 | 0.58 |
| 4:5:321:VAL:CA | 4:5:323:ILE:HG13 | 2.34 | 0.58 |
| 6:7:68:GLN:HG2 | 6:7:72:ASN:HD21 | 1.69 | 0.58 |
| 8:B:120:LEU:HB2 | 8:B:176:LEU:HD13 | 1.85 | 0.58 |
| 10:D:138:PHE:HA | 10:D:141:ARG:HH11 | 1.68 | 0.58 |
| 1:2:534:ARG:HH11 | 1:2:815:ARG:HH22 | 1.52 | 0.58 |
| 7:A:136:ASP:O | 7:A:139:THR:OG1 | 2.20 | 0.58 |
| 10:D:62:ASP:HA | 10:D:65:LYS:HB3 | 1.86 | 0.58 |
| 4:5:673:GLN:HB2 | 4:5:676:HIS:HB2 | 1.85 | 0.58 |
| 4:5:76:TYR:HA | 4:5:79:LEU:HB3 | 1.85 | 0.58 |
| 5:6:545:LYS:O | 5:6:549:LEU:HG | 2.03 | 0.58 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:6:533:ILE:CG1 | 5:6:548:LEU:HD11 | 2.32 | 0.58 |
| 5:6:558:SER:HB3 | 5:6:559:THR:CA | 2.31 | 0.58 |
| 6:7:259:ALA:HB3 | 6:7:304:ALA:HB1 | 1.86 | 0.58 |
| 6:7:664:TYR:CD1 | 6:7:689:LEU:HD13 | 2.38 | 0.58 |
| 9:C:3:TYR:HE1 | 10:D:218:MET:HG3 | 1.69 | 0.58 |
| 10:D:60:PHE:HA | 10:D:63:LEU:HB3 | 1.84 | 0.58 |
| 11:E:24:SER:HB3 | 11:E:55:GLN:OE1 | 2.03 | 0.58 |
| 1:2:524:PRO:HB2 | 1:2:525:LYS:HA | 1.85 | 0.58 |
| 3:4:777:MET:SD | 3:4:830:ARG:NE | 2.77 | 0.58 |
| 13:3:1001:ANP:O5' | 4:5:651:ARG:NH1 | 2.36 | 0.58 |
| 5:6:326:LYS:N | 5:6:327:TYR:HA | 2.12 | 0.58 |
| 10:D:144:ILE:HG13 | 10:D:145:ARG:N | 2.19 | 0.58 |
| 10:D:211:ASP:HB2 | 10:D:219:ILE:HD11 | 1.86 | 0.58 |
| 2:3:371:ILE:HA | 13:3:1001:ANP:N6 | 2.18 | 0.57 |
| 3:4:568:GLY:HA3 | 3:4:708:VAL:HB | 1.86 | 0.57 |
| 4:5:571:HIS:O | 4:5:575:ILE:HG13 | 2.04 | 0.57 |
| 3:4:554:LYS:NZ | 5:6:752:ARG:HH22 | 2.02 | 0.57 |
| 5:6:550:GLN:HG2 | 5:6:569:ILE:HG23 | 1.86 | 0.57 |
| 6:7:534:ARG:HH21 | 6:7:586:LEU:HD23 | 1.67 | 0.57 |
| 9:C:132:ALA:HA | 9:C:135:LEU:HB2 | 1.86 | 0.57 |
| 11:E:30:PHE:HE2 | 11:E:81:LEU:HD21 | 1.69 | 0.57 |
| 11:E:30:PHE:HD1 | 11:E:61:ILE:HD11 | 1.69 | 0.57 |
| 11:E:642:GLU:O | 11:E:645:THR:OG1 | 2.22 | 0.57 |
| 1:2:546:GLY:CA | 5:6:796:THR:HG23 | 2.34 | 0.57 |
| 2:3:378:LYS:HA | 2:3:381:ILE:HD12 | 1.85 | 0.57 |
| 3:4:402:THR:O | 3:4:405:PHE:N | 2.34 | 0.57 |
| 4:5:654:GLU:O | 4:5:657:ILE:HB | 2.05 | 0.57 |
| 5:6:168:MET:O | 5:6:171:SER:HB2 | 2.03 | 0.57 |
| 1:2:656:ARG:NH1 | 5:6:792:SER:HB2 | 2.19 | 0.57 |
| 7:A:106:GLY:H | 7:A:107:LEU:HD22 | 1.69 | 0.57 |
| 10:D:257:THR:H | 10:D:269:LEU:HB2 | 1.68 | 0.57 |
| 11:E:5:ILE:N | 11:E:142:CYS:SG | 2.74 | 0.57 |
| 2:3:291:ARG:HB2 | 2:3:329:LEU:HG | 1.85 | 0.57 |
| 3:4:447:ASN:O | 3:4:450:GLN:HB2 | 2.04 | 0.57 |
| 5:6:966:LYS:HA | 5:6:969:VAL:HG12 | 1.85 | 0.57 |
| 1:2:573:ALA:HB3 | 5:6:670:ALA:H | 1.67 | 0.57 |
| 3:4:367:GLU:N | 3:4:367:GLU:OE1 | 2.36 | 0.57 |
| 4:5:148:LEU:HD23 | 4:5:260:GLU:HB3 | 1.85 | 0.57 |
| 4:5:375:ALA:HB1 | 4:5:378:ILE:H | 1.70 | 0.57 |
| 4:5:486:ARG:NH2 | 4:5:489:ASP:OD2 | 2.34 | 0.57 |
| 4:5:407:ARG:CZ | 4:5:658:ARG:HH12 | 2.18 | 0.57 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:6:124:VAL:HG11 | 5:6:132:VAL:HG23 | 1.86 | 0.57 |
| 6:7:612:LEU:O | 6:7:616:VAL:HG23 | 2.04 | 0.57 |
| 9:C:50:LEU:O | 9:C:54:LEU:HG | 2.05 | 0.57 |
| 11:E:81:LEU:N | 11:E:119:ASP:O | 2.38 | 0.57 |
| 11:E:29:ILE:HG22 | 11:E:82:LEU:HD13 | 1.85 | 0.57 |
| 1:2:302:THR:O | 1:2:303:ILE:HG22 | 2.04 | 0.57 |
| 5:6:765:LEU:HD22 | 5:6:770:ARG:HB3 | 1.87 | 0.57 |
| 6:7:374:THR:OG1 | 6:7:375:TYR:N | 2.36 | 0.57 |
| 8:B:92:TRP:CD2 | 8:B:116:PRO:HG2 | 2.40 | 0.57 |
| 1:2:763:LEU:O | 1:2:766:TYR:HB3 | 2.04 | 0.57 |
| 2:3:40:ASP:OD1 | 2:3:41:SER:N | 2.33 | 0.57 |
| 3:4:900:SER:HA | 3:4:903:ILE:HD12 | 1.87 | 0.57 |
| 4:5:66:GLU:OE1 | 4:5:141:SER:OG | 2.21 | 0.57 |
| 4:5:22:ASP:O | 4:5:26:GLU:HG2 | 2.05 | 0.57 |
| 4:5:323:ILE:O | 4:5:323:ILE:HG22 | 2.04 | 0.57 |
| 5:6:365:ALA:HA | 5:6:368:ILE:HG12 | 1.85 | 0.57 |
| 6:7:689:LEU:O | 6:7:692:ILE:HG22 | 2.04 | 0.57 |
| 7:A:170:ASP:HB3 | 7:A:204:TYR:CD1 | 2.40 | 0.57 |
| 9:C:86:ASN:HA | 9:C:89:LYS:HD3 | 1.85 | 0.57 |
| 10:D:132:GLU:HA | 10:D:135:ARG:HH22 | 1.70 | 0.57 |
| 10:D:132:GLU:HA | 10:D:135:ARG:NH2 | 2.18 | 0.57 |
| 10:D:57:GLN:N | 10:D:57:GLN:OE1 | 2.38 | 0.57 |
| 11:E:556:CYS:O | 11:E:560:GLU:HG2 | 2.03 | 0.57 |
| 3:4:418:CYS:SG | 3:4:419:VAL:N | 2.78 | 0.57 |
| 6:7:411:TYR:HD1 | 6:7:702:LEU:CD1 | 2.18 | 0.57 |
| 11:E:249:ASN:HB2 | 11:E:254:GLN:HE22 | 1.70 | 0.57 |
| 11:E:287:VAL:HG13 | 11:E:290:ARG:HH11 | 1.69 | 0.57 |
| 1:2:686:LEU:HG | 5:6:788:PHE:CE1 | 2.40 | 0.57 |
| 3:4:748:THR:HA | 3:4:751:ILE:HD12 | 1.86 | 0.57 |
| 3:4:688:VAL:HG11 | 3:4:836:TYR:HD1 | 1.69 | 0.57 |
| 3:4:388:ARG:HH22 | 5:6:176:ARG:HD2 | 1.69 | 0.57 |
| 3:4:623:LEU:CD2 | 5:6:370:THR:CG2 | 2.66 | 0.57 |
| 5:6:696:ARG:HD2 | 5:6:706:MET:SD | 2.43 | 0.57 |
| 6:7:302:THR:O | 6:7:305:SER:OG | 2.22 | 0.57 |
| 6:7:479:ARG:HG3 | 6:7:516:ALA:HB1 | 1.86 | 0.57 |
| 1:2:422:GLU:OE1 | 1:2:458:ARG:NE | 2.37 | 0.57 |
| 5:6:268:PHE:HB3 | 5:6:458:HIS:CE1 | 2.40 | 0.57 |
| 5:6:636:CYS:HB3 | 5:6:678:ILE:HD13 | 1.87 | 0.57 |
| 6:7:720:VAL:O | 6:7:723:SER:OG | 2.23 | 0.57 |
| 11:E:149:ASP:N | 11:E:150:ASP:HA | 2.19 | 0.57 |
| 1:2:238:ASN:HD21 | 11:E:370:LEU:HB2 | 1.70 | 0.57 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 11:E:64:TYR:HB2 | 11:E:625:PHE:HA | 1.87 | 0.57 |
| 1:2:578:ALA:O | 1:2:631:ILE:HG21 | 2.04 | 0.56 |
| 1:2:569:GLN:HB2 | 1:2:612:MET:HG2 | 1.87 | 0.56 |
| 2:3:491:GLU:HB2 | 2:3:542:ARG:NE | 2.20 | 0.56 |
| 2:3:716:ARG:HH12 | 2:3:722:ASN:HB3 | 1.70 | 0.56 |
| 3:4:349:CYS:SG | 3:4:382:MET:HA | 2.45 | 0.56 |
| 3:4:365:ILE:O | 5:6:420:THR:OG1 | 2.22 | 0.56 |
| 3:4:395:GLN:HB2 | 3:4:424:VAL:HG13 | 1.87 | 0.56 |
| 4:5:439:THR:HA | 4:5:444:SER:CB | 2.34 | 0.56 |
| 5:6:418:SER:HA | 5:6:448:LEU:HG | 1.87 | 0.56 |
| 5:6:908:LYS:HB3 | 5:6:960:LEU:HD21 | 1.86 | 0.56 |
| 6:7:481:VAL:HG22 | 6:7:516:ALA:HB3 | 1.85 | 0.56 |
| 10:D:92:SER:HA | 10:D:95:SER:HB3 | 1.87 | 0.56 |
| 11:E:244:GLY:HA3 | 11:E:602:LEU:HB3 | 1.87 | 0.56 |
| 1:2:568:GLY:HA2 | 1:2:606:ILE:HG23 | 1.86 | 0.56 |
| 3:4:557:ARG:NH2 | 3:4:652:GLN:HB3 | 2.18 | 0.56 |
| 3:4:798:LEU:HG | 5:6:735:HIS:CE1 | 2.40 | 0.56 |
| 5:6:801:GLU:OE2 | 5:6:805:ARG:NE | 2.36 | 0.56 |
| 1:2:233:THR:O | 1:2:237:MET:N | 2.31 | 0.56 |
| 1:2:637:VAL:HA | 4:5:447:ALA:HB2 | 1.86 | 0.56 |
| 5:6:403:VAL:CG1 | 5:6:450:TYR:HB3 | 2.35 | 0.56 |
| 11:E:12:TYR:HE1 | 11:E:48:LEU:HD21 | 1.68 | 0.56 |
| 11:E:425:VAL:HA | 11:E:428:LEU:HD12 | 1.87 | 0.56 |
| 1:2:334:LEU:HA | 1:2:382:TYR:HD1 | 1.68 | 0.56 |
| 1:2:295:VAL:O | 1:2:454:ASN:ND2 | 2.39 | 0.56 |
| 1:2:805:ILE:HA | 1:2:809:HIS:ND1 | 2.21 | 0.56 |
| 1:2:837:ALA:O | 1:2:841:VAL:HG23 | 2.04 | 0.56 |
| 2:3:669:PRO:O | 2:3:720:THR:HA | 2.05 | 0.56 |
| 4:5:47:ARG:HD3 | 8:B:146:GLN:HG2 | 1.85 | 0.56 |
| 4:5:559:ASP:HB2 | 4:5:561:ASN:ND2 | 2.20 | 0.56 |
| 4:5:571:HIS:ND1 | 4:5:575:ILE:HD11 | 2.21 | 0.56 |
| 5:6:261:ARG:HD2 | 5:6:263:PHE:HE1 | 1.70 | 0.56 |
| 5:6:517:LYS:HA | 5:6:520:VAL:HG22 | 1.86 | 0.56 |
| 6:7:646:LYS:HA | 6:7:701:LYS:HE3 | 1.86 | 0.56 |
| 7:A:27:VAL:HG13 | 7:A:28:ASN:H | 1.70 | 0.56 |
| 1:2:240:GLU:HB3 | 1:2:290:HIS:ND1 | 2.20 | 0.56 |
| 5:6:364:ASN:HB3 | 5:6:394:ARG:HD3 | 1.86 | 0.56 |
| 3:4:929:LEU:HB2 | 5:6:947:ASP:HB3 | 1.88 | 0.56 |
| 11:E:536:LEU:HB3 | 11:E:573:ASP:HB2 | 1.88 | 0.56 |
| 11:E:559:SER:HA | 11:E:560:GLU:HB3 | 1.87 | 0.56 |
| 1:2:856:GLN:HE22 | 1:2:859:ARG:NH2 | 2.01 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:3:156:SER:CB | 2:3:325:THR:HG22 | 2.35 | 0.56 |
| 4:5:156:VAL:HG22 | 4:5:298:TYR:HD2 | 1.71 | 0.56 |
| 4:5:371:THR:O | 4:5:385:LYS:HE2 | 2.06 | 0.56 |
| 5:6:944:LYS:O | 5:6:948:LEU:HD13 | 2.06 | 0.56 |
| 7:A:96:ILE:O | 7:A:99:SER:OG | 2.22 | 0.56 |
| 10:D:269:LEU:HA | 10:D:275:TYR:CE2 | 2.41 | 0.56 |
| 10:D:286:LEU:HD11 | 10:D:293:LEU:HD11 | 1.86 | 0.56 |
| 11:E:12:TYR:O | 11:E:15:ILE:HG22 | 2.05 | 0.56 |
| 11:E:81:LEU:O | 11:E:121:TYR:N | 2.36 | 0.56 |
| 2:3:197:ILE:HD11 | 2:3:251:ILE:HB | 1.87 | 0.56 |
| 4:5:264:LEU:HB2 | 4:5:265:VAL:HG22 | 1.88 | 0.56 |
| 6:7:215:TYR:HE1 | 6:7:217:LYS:HD3 | 1.71 | 0.56 |
| 9:C:165:PHE:O | 9:C:168:LYS:HG2 | 2.06 | 0.56 |
| 3:4:578:LEU:HD21 | 3:4:672:LEU:HD22 | 1.87 | 0.56 |
| 4:5:417:ASP:O | 4:5:420:THR:OG1 | 2.21 | 0.56 |
| 6:7:147:ARG:HA | 6:7:150:ASN:HB3 | 1.88 | 0.56 |
| 6:7:545:THR:HG23 | 6:7:556:THR:HB | 1.88 | 0.56 |
| 11:E:161:LYS:HB3 | 11:E:233:TYR:CE2 | 2.40 | 0.56 |
| 11:E:86:PHE:CE1 | 11:E:625:PHE:HB2 | 2.40 | 0.56 |
| 1:2:573:ALA:HB3 | 5:6:670:ALA:N | 2.21 | 0.56 |
| 2:3:296:GLY:HA2 | 2:3:324:ASN:HB2 | 1.88 | 0.56 |
| 2:3:294:VAL:HG22 | 2:3:326:VAL:HG22 | 1.87 | 0.56 |
| 2:3:712:HIS:ND1 | 2:3:725:ASP:OD1 | 2.39 | 0.56 |
| 3:4:590:TYR:HA | 3:4:630:CYS:O | 2.06 | 0.56 |
| 6:7:436:LEU:HD23 | 6:7:477:SER:HB2 | 1.87 | 0.56 |
| 11:E:474:VAL:O | 11:E:477:PHE:HB3 | 2.06 | 0.56 |
| 11:E:566:PRO:HB2 | 11:E:605:PHE:CE2 | 2.41 | 0.56 |
| 2:3:216:ASP:OD1 | 2:3:217:ALA:N | 2.39 | 0.56 |
| 2:3:389:VAL:HG22 | 2:3:714:LYS:HE3 | 1.88 | 0.56 |
| 4:5:256:LEU:HD12 | 4:5:256:LEU:H | 1.71 | 0.56 |
| 3:4:613:GLN:HB3 | 5:6:360:ARG:HH12 | 1.71 | 0.56 |
| 5:6:829:ASP:HA | 5:6:832:ARG:HB3 | 1.88 | 0.56 |
| 6:7:456:VAL:O | 6:7:564:LEU:HG | 2.05 | 0.56 |
| 10:D:260:ILE:CG2 | 10:D:261:PRO:HD2 | 2.36 | 0.56 |
| 10:D:74:PRO:HG3 | 10:D:279:TYR:CD2 | 2.41 | 0.56 |
| 11:E:231:HIS:HA | 11:E:234:GLU:HB2 | 1.88 | 0.56 |
| 11:E:254:GLN:OE1 | 11:E:254:GLN:N | 2.39 | 0.56 |
| 11:E:315:THR:H | 11:E:316:LEU:HB3 | 1.67 | 0.56 |
| 11:E:546:LEU:O | 11:E:550:ASN:HB2 | 2.05 | 0.56 |
| 1:2:285:ASP:O | 1:2:286:TYR:HB2 | 2.06 | 0.56 |
| 1:2:296:ARG:HH21 | 1:2:413:ASP:HB2 | 1.71 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:3:474:GLU:HG3 | 4:5:491:VAL:CG1 | 2.35 | 0.56 |
| 3:4:758:ILE:HG22 | 3:4:760:PRO:HD3 | 1.88 | 0.56 |
| 4:5:375:ALA:HB1 | 4:5:378:ILE:HB | 1.88 | 0.56 |
| 7:A:50:ASN:O | 7:A:54:LEU:HG | 2.05 | 0.56 |
| 8:B:11:PHE:HE1 | 10:D:71:ARG:HB2 | 1.69 | 0.56 |
| 8:B:137:PRO:HA | 8:B:141:LEU:HD13 | 1.88 | 0.56 |
| 8:B:193:ARG:CZ | 10:D:225:ASN:HB3 | 2.36 | 0.56 |
| 9:C:135:LEU:HD13 | 9:C:176:ILE:HD11 | 1.88 | 0.56 |
| 4:5:40:LEU:O | 11:E:416:ARG:NH2 | 2.39 | 0.56 |
| 1:2:625:GLU:CD | 13:5:801:ANP:HNB1 | 2.09 | 0.55 |
| 2:3:176:LEU:HD12 | 2:3:298:PHE:HE2 | 1.71 | 0.55 |
| 2:3:200:VAL:HG23 | 2:3:248:SER:HB3 | 1.88 | 0.55 |
| 3:4:506:LEU:HD23 | 3:4:509:ILE:HD12 | 1.89 | 0.55 |
| 6:7:367:LYS:HA | 6:7:368:ALA:HB3 | 1.86 | 0.55 |
| 8:B:140:GLU:O | 8:B:144:LYS:HG2 | 2.05 | 0.55 |
| 11:E:543:LEU:HA | 11:E:546:LEU:HB3 | 1.87 | 0.55 |
| 2:3:438:SER:OG | 12:F:9:DT:OP2 | 2.09 | 0.55 |
| 1:2:435:ASP:N | 1:2:436:GLY:HA3 | 2.21 | 0.55 |
| 2:3:491:GLU:HB2 | 2:3:542:ARG:CZ | 2.37 | 0.55 |
| 3:4:304:ARG:NH2 | 3:4:422:GLU:OE1 | 2.39 | 0.55 |
| 4:5:321:VAL:HA | 4:5:323:ILE:HG13 | 1.88 | 0.55 |
| 7:A:104:ASN:O | 7:A:104:ASN:ND2 | 2.35 | 0.55 |
| 11:E:308:ASN:HA | 11:E:309:SER:HB2 | 1.87 | 0.55 |
| 2:3:108:ARG:HA | 2:3:111:TRP:HB3 | 1.89 | 0.55 |
| 2:3:227:THR:N | 2:3:228:PRO:HD2 | 2.21 | 0.55 |
| 2:3:379:LYS:O | 2:3:383:LEU:HG | 2.07 | 0.55 |
| 3:4:321:ASP:N | 3:4:321:ASP:OD1 | 2.35 | 0.55 |
| 4:5:407:ARG:HD2 | 4:5:497:MET:O | 2.06 | 0.55 |
| 7:A:2:TYR:OH | 7:A:75:THR:HA | 2.04 | 0.55 |
| 10:D:216:VAL:CG1 | 10:D:217:ASN:HA | 2.37 | 0.55 |
| 11:E:151:THR:HB | 11:E:153:GLY:N | 2.22 | 0.55 |
| 1:2:567:THR:HG23 | 1:2:568:GLY:H | 1.72 | 0.55 |
| 2:3:163:ALA:N | 2:3:164:HIS:HB2 | 2.21 | 0.55 |
| 2:3:195:LYS:NZ | 2:3:218:THR:OG1 | 2.39 | 0.55 |
| 2:3:46:GLN:HA | 2:3:49:ASN:HD21 | 1.70 | 0.55 |
| 3:4:574:LYS:HD3 | 3:4:674:SER:HB2 | 1.87 | 0.55 |
| 4:5:287:ILE:HD11 | 4:5:342:ILE:CG2 | 2.34 | 0.55 |
| 5:6:124:VAL:CG2 | 5:6:132:VAL:HA | 2.36 | 0.55 |
| 5:6:134:LYS:HB3 | 5:6:137:ARG:H | 1.70 | 0.55 |
| 5:6:155:TYR:CE1 | 5:6:167:ALA:HB1 | 2.42 | 0.55 |
| 3:4:385:ILE:HG22 | 3:4:388:ARG:H | 1.71 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:4:710:ASP:OD1 | 6:7:672:LYS:NZ | 2.35 | 0.55 |
| 4:5:25:THR:HA | 4:5:28:ILE:HD12 | 1.87 | 0.55 |
| 4:5:555:ILE:HG22 | 4:5:557:LYS:HD3 | 1.88 | 0.55 |
| 4:5:28:ILE:HG23 | 4:5:93:ALA:HB2 | 1.87 | 0.55 |
| 6:7:143:LEU:HA | 6:7:146:ARG:HB2 | 1.89 | 0.55 |
| 6:7:461:ASP:OD2 | 6:7:573:ARG:HA | 2.07 | 0.55 |
| 6:7:24:PHE:HE1 | 6:7:85:ILE:HA | 1.71 | 0.55 |
| 7:A:42:LYS:O | 7:A:46:ASN:HB2 | 2.07 | 0.55 |
| 10:D:69:ASN:HA | 10:D:293:LEU:HD22 | 1.89 | 0.55 |
| 1:2:432:ASN:HB2 | 1:2:447:PHE:HB3 | 1.89 | 0.55 |
| 1:2:581:ARG:NH2 | 5:6:621:TYR:HB3 | 2.22 | 0.55 |
| 4:5:428:PHE:O | 4:5:432:VAL:HG23 | 2.07 | 0.55 |
| 5:6:290:ILE:HD13 | 5:6:454:PHE:CZ | 2.42 | 0.55 |
| 6:7:470:LEU:HD13 | 6:7:522:CYS:HB3 | 1.88 | 0.55 |
| 8:B:124:ARG:HD3 | 9:C:190:TRP:CH2 | 2.41 | 0.55 |
| 10:D:200:LYS:N | 10:D:201:TYR:HB2 | 2.22 | 0.55 |
| 11:E:574:GLU:O | 11:E:575:ASN:CB | 2.54 | 0.55 |
| 2:3:483:ARG:HD3 | 2:3:539:LEU:HD11 | 1.87 | 0.55 |
| 3:4:332:VAL:HG13 | 3:4:397:ILE:HG21 | 1.89 | 0.55 |
| 3:4:919:LEU:HD13 | 3:4:925:ARG:HD2 | 1.89 | 0.55 |
| 5:6:105:ASP:O | 5:6:108:GLY:N | 2.40 | 0.55 |
| 5:6:288:LEU:H | 5:6:399:GLY:N | 2.05 | 0.55 |
| 5:6:551:MET:HA | 5:6:635:ILE:HD11 | 1.89 | 0.55 |
| 5:6:768:GLU:OE1 | 5:6:768:GLU:N | 2.35 | 0.55 |
| 5:6:777:TYR:CZ | 5:6:781:ARG:HD2 | 2.42 | 0.55 |
| 10:D:84:MET:O | 10:D:87:LEU:HB2 | 2.07 | 0.55 |
| 1:2:207:ILE:HG22 | 1:2:211:LEU:HD23 | 1.88 | 0.55 |
| 1:2:256:LEU:HD23 | 1:2:259:PHE:HD2 | 1.72 | 0.55 |
| 1:2:567:THR:O | 1:2:606:ILE:HG23 | 2.07 | 0.55 |
| 2:3:176:LEU:HD22 | 4:5:250:PHE:HD2 | 1.72 | 0.55 |
| 3:4:245:ALA:HB3 | 3:4:306:TYR:O | 2.05 | 0.55 |
| 6:7:134:TYR:HB2 | 6:7:141:VAL:HG12 | 1.89 | 0.55 |
| 7:A:170:ASP:HB3 | 7:A:204:TYR:HD1 | 1.70 | 0.55 |
| 11:E:360:HIS:HA | 11:E:363:PHE:CD2 | 2.40 | 0.55 |
| 1:2:276:MET:O | 1:2:280:GLU:N | 2.40 | 0.55 |
| 1:2:702:SER:O | 5:6:559:THR:HG21 | 2.06 | 0.55 |
| 2:3:372:TYR:CZ | 2:3:564:HIS:HB3 | 2.41 | 0.55 |
| 3:4:417:LEU:HB2 | 3:4:463:VAL:HG11 | 1.88 | 0.55 |
| 3:4:550:LYS:HE2 | 3:4:558:TYR:HD2 | 1.71 | 0.55 |
| 5:6:274:HIS:CG | 5:6:288:LEU:HD11 | 2.42 | 0.55 |
| 1:2:571:ALA:O | 5:6:663:ILE:HA | 2.07 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:6:610:ALA:H | 5:6:663:ILE:HD13 | 1.72 | 0.55 |
| 6:7:482:TYR:HA | 6:7:522:CYS:HB2 | 1.89 | 0.55 |
| 6:7:499:LYS:NZ | 6:7:500:ASP:O | 2.36 | 0.55 |
| 8:B:120:LEU:HD11 | 8:B:177:GLU:HG3 | 1.89 | 0.55 |
| 11:E:433:GLU:OE1 | 11:E:433:GLU:N | 2.34 | 0.55 |
| 1:2:766:TYR:OH | 1:2:823:MET:O | 2.25 | 0.55 |
| 3:4:453:LEU:H | 6:7:280:PRO:HD3 | 1.71 | 0.55 |
| 3:4:596:SER:O | 3:4:641:THR:OG1 | 2.25 | 0.55 |
| 3:4:638:SER:OG | 3:4:641:THR:OG1 | 2.15 | 0.55 |
| 3:4:646:HIS:HA | 3:4:701:ARG:NH2 | 2.21 | 0.55 |
| 3:4:547:GLY:O | 3:4:810:LYS:NZ | 2.40 | 0.55 |
| 5:6:923:VAL:HA | 5:6:926:GLU:HG2 | 1.88 | 0.55 |
| 6:7:422:ILE:HD13 | 6:7:469:LEU:HD11 | 1.88 | 0.55 |
| 6:7:533:ASP:OD1 | 6:7:533:ASP:N | 2.39 | 0.55 |
| 6:7:68:GLN:HG2 | 6:7:72:ASN:ND2 | 2.21 | 0.55 |
| 7:A:90:GLN:HA | 7:A:93:ARG:HB3 | 1.88 | 0.55 |
| 10:D:83:LEU:HD23 | 10:D:83:LEU:O | 2.07 | 0.55 |
| 1:2:553:LEU:HD12 | 1:2:554:LYS:N | 2.22 | 0.54 |
| 2:3:517:ASN:ND2 | 13:3:1001:ANP:O1G | 2.31 | 0.54 |
| 2:3:254:GLN:NE2 | 2:3:256:ILE:HD11 | 2.21 | 0.54 |
| 6:7:318:LEU:HG | 6:7:320:GLN:HG2 | 1.88 | 0.54 |
| 10:D:137:LYS:HG2 | 10:D:141:ARG:NH1 | 2.21 | 0.54 |
| 11:E:81:LEU:HD22 | 11:E:82:LEU:H | 1.73 | 0.54 |
| 2:3:201:HIS:HB3 | 2:3:241:LEU:HB3 | 1.89 | 0.54 |
| 2:3:25:VAL:HG23 | 2:3:124:PRO:HB2 | 1.89 | 0.54 |
| 2:3:667:VAL:HG11 | 2:3:719:LYS:NZ | 2.21 | 0.54 |
| 5:6:803:MET:HA | 5:6:806:LEU:HD12 | 1.87 | 0.54 |
| 1:2:631:ILE:HG13 | 4:5:445:SER:O | 2.07 | 0.54 |
| 13:3:1001:ANP:O2A | 13:3:1001:ANP:O2B | 2.25 | 0.54 |
| 3:4:183:THR:OG1 | 6:7:303:ARG:NH2 | 2.41 | 0.54 |
| 3:4:330:GLY:HA2 | 3:4:403:PRO:HD2 | 1.89 | 0.54 |
| 4:5:390:CYS:O | 4:5:662:SER:HB2 | 2.07 | 0.54 |
| 4:5:64:ASN:ND2 | 4:5:66:GLU:HB2 | 2.21 | 0.54 |
| 7:A:13:ALA:HA | 7:A:16:THR:HG22 | 1.89 | 0.54 |
| 1:2:519:LEU:HD13 | 1:2:556:VAL:HG13 | 1.88 | 0.54 |
| 3:4:889:GLN:O | 3:4:897:ARG:NH1 | 2.41 | 0.54 |
| 4:5:685:GLN:O | 4:5:688:THR:OG1 | 2.25 | 0.54 |
| 5:6:796:THR:O | 5:6:799:GLN:HG2 | 2.07 | 0.54 |
| 6:7:245:ILE:HG12 | 6:7:347:ASP:O | 2.07 | 0.54 |
| 6:7:260:TYR:CD1 | 6:7:298:LEU:HD13 | 2.43 | 0.54 |
| 7:A:109:LEU:HD23 | 7:A:109:LEU:O | 2.07 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 7:A:162:PHE:HD1 | 7:A:192:ARG:HA | 1.73 | 0.54 |
| 7:A:33:HIS:HB3 | 7:A:36:ILE:HG22 | 1.88 | 0.54 |
| 11:E:355:GLY:HA2 | 11:E:358:ARG:HB3 | 1.88 | 0.54 |
| 1:2:324:VAL:HG23 | 1:2:422:GLU:O | 2.07 | 0.54 |
| 1:2:696:ALA:HA | 1:2:699:VAL:HB | 1.89 | 0.54 |
| 3:4:773:ALA:O | 3:4:777:MET:HG2 | 2.07 | 0.54 |
| 5:6:637:CYS:HA | 5:6:679:LEU:O | 2.06 | 0.54 |
| 6:7:595:ASP:HB3 | 6:7:694:ARG:NH1 | 2.23 | 0.54 |
| 8:B:121:VAL:HG22 | 8:B:176:LEU:HD12 | 1.89 | 0.54 |
| 9:C:97:LEU:O | 9:C:100:ILE:HG12 | 2.07 | 0.54 |
| 10:D:212:THR:N | 10:D:213:GLU:HA | 2.21 | 0.54 |
| 1:2:639:THR:HA | 4:5:445:SER:HB3 | 1.89 | 0.54 |
| 4:5:382:GLU:N | 4:5:382:GLU:OE1 | 2.38 | 0.54 |
| 13:5:801:ANP:O2B | 13:5:801:ANP:O3G | 2.26 | 0.54 |
| 5:6:152:TYR:HB3 | 5:6:268:PHE:HE2 | 1.71 | 0.54 |
| 5:6:574:VAL:HG12 | 5:6:684:PRO:HG3 | 1.89 | 0.54 |
| 5:6:796:THR:HG22 | 5:6:798:ARG:HB3 | 1.89 | 0.54 |
| 6:7:147:ARG:NH2 | 6:7:192:PHE:HB2 | 2.23 | 0.54 |
| 8:B:163:LEU:HD22 | 8:B:189:MET:HE2 | 1.90 | 0.54 |
| 12:F:7:DT:H5' | 12:F:7:DT:C6 | 2.43 | 0.54 |
| 2:3:371:ILE:HA | 13:3:1001:ANP:HN61 | 1.71 | 0.54 |
| 2:3:433:THR:O | 2:3:433:THR:OG1 | 2.26 | 0.54 |
| 6:7:103:VAL:HG11 | 6:7:207:LEU:HD21 | 1.89 | 0.54 |
| 7:A:29:LEU:HD23 | 7:A:93:ARG:HD3 | 1.88 | 0.54 |
| 10:D:144:ILE:O | 10:D:148:LEU:HG | 2.08 | 0.54 |
| 11:E:83:LEU:HB3 | 11:E:122:VAL:HG22 | 1.90 | 0.54 |
| 11:E:327:PHE:CE2 | 11:E:503:GLN:HG3 | 2.43 | 0.54 |
| 1:2:289:ILE:HG22 | 1:2:290:HIS:CE1 | 2.43 | 0.54 |
| 1:2:419:LYS:NZ | 1:2:598:LEU:HD12 | 2.23 | 0.54 |
| 4:5:488:GLU:HG2 | 4:5:489:ASP:N | 2.23 | 0.54 |
| 4:5:554:PHE:HZ | 4:5:683:LEU:O | 1.90 | 0.54 |
| 5:6:283:LYS:HD2 | 5:6:288:LEU:HD22 | 1.90 | 0.54 |
| 5:6:796:THR:CG2 | 5:6:798:ARG:HB3 | 2.38 | 0.54 |
| 6:7:203:TYR:OH | 6:7:339:LEU:N | 2.33 | 0.54 |
| 7:A:102:TRP:HB3 | 10:D:145:ARG:NH2 | 2.22 | 0.54 |
| 10:D:132:GLU:HG2 | 10:D:135:ARG:NH1 | 2.18 | 0.54 |
| 10:D:176:SER:HB3 | 10:D:179:GLU:HG3 | 1.89 | 0.54 |
| 10:D:257:THR:O | 10:D:268:GLU:HB3 | 2.08 | 0.54 |
| 10:D:264:LYS:HG2 | 10:D:265:GLU:H | 1.72 | 0.54 |
| 11:E:5:ILE:HG12 | 11:E:142:CYS:SG | 2.48 | 0.54 |
| 1:2:333:GLN:HB2 | 1:2:385:TYR:HB2 | 1.90 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:4:432:ARG:HH12 | 6:7:555:THR:HB | 1.73 | 0.54 |
| 3:4:521:LEU:O | 3:4:524:ARG:HG2 | 2.08 | 0.54 |
| 4:5:479:ILE:CG2 | 4:5:482:PHE:HB2 | 2.38 | 0.54 |
| 5:6:648:ASP:N | 5:6:648:ASP:OD1 | 2.29 | 0.54 |
| 5:6:727:LEU:O | 5:6:731:ILE:HB | 2.08 | 0.54 |
| 5:6:834:SER:HA | 5:6:837:ARG:HB2 | 1.90 | 0.54 |
| 5:6:833:GLN:O | 5:6:837:ARG:N | 2.41 | 0.54 |
| 6:7:460:GLY:HA3 | 6:7:600:MET:O | 2.08 | 0.54 |
| 10:D:171:LEU:HB2 | 10:D:173:ASP:H | 1.71 | 0.54 |
| 11:E:499:ALA:HA | 11:E:502:LEU:HD12 | 1.90 | 0.54 |
| 1:2:493:ILE:HG13 | 1:2:494:ILE:N | 2.23 | 0.54 |
| 3:4:333:LEU:HD21 | 3:4:400:GLN:HG2 | 1.89 | 0.54 |
| 4:5:414:LEU:HD11 | 4:5:425:LEU:HD22 | 1.90 | 0.54 |
| 4:5:482:PHE:HB3 | 4:5:523:ALA:CB | 2.32 | 0.54 |
| 5:6:538:PHE:HB2 | 5:6:730:HIS:ND1 | 2.22 | 0.54 |
| 5:6:773:LEU:HD21 | 5:6:800:LEU:HD11 | 1.91 | 0.54 |
| 6:7:668:ARG:HH22 | 6:7:686:PRO:HD3 | 1.73 | 0.54 |
| 8:B:103:GLN:O | 8:B:107:THR:HG22 | 2.07 | 0.54 |
| 8:B:54:THR:HG22 | 10:D:132:GLU:HG3 | 1.88 | 0.54 |
| 11:E:613:THR:HG22 | 11:E:620:VAL:HG11 | 1.90 | 0.54 |
| 1:2:328:THR:HG23 | 1:2:329:GLY:O | 2.08 | 0.53 |
| 3:4:225:TYR:N | 3:4:228:LYS:HB2 | 2.23 | 0.53 |
| 3:4:393:ASP:OD1 | 5:6:281:SER:N | 2.40 | 0.53 |
| 1:2:631:ILE:N | 4:5:445:SER:O | 2.41 | 0.53 |
| 4:5:59:TYR:HD1 | 4:5:135:PHE:HE1 | 1.57 | 0.53 |
| 5:6:147:ASP:OD2 | 5:6:261:ARG:NH2 | 2.41 | 0.53 |
| 5:6:941:LEU:HA | 5:6:944:LYS:HD3 | 1.90 | 0.53 |
| 6:7:498:MET:HG3 | 6:7:498:MET:O | 2.08 | 0.53 |
| 7:A:47:LEU:HD21 | 7:A:75:THR:HB | 1.90 | 0.53 |
| 7:A:189:PHE:CE1 | 11:E:57:GLN:HB2 | 2.43 | 0.53 |
| 2:3:292:VAL:HG12 | 2:3:294:VAL:HG23 | 1.90 | 0.53 |
| 4:5:349:PHE:CZ | 4:5:354:GLU:HG3 | 2.43 | 0.53 |
| 4:5:55:LEU:HD22 | 9:C:137:HIS:CG | 2.43 | 0.53 |
| 1:2:778:LEU:CG | 4:5:577:THR:CG2 | 2.78 | 0.53 |
| 5:6:276:ILE:HD13 | 5:6:375:ARG:O | 2.08 | 0.53 |
| 7:A:89:TYR:OH | 7:A:93:ARG:NH2 | 2.42 | 0.53 |
| 9:C:15:GLU:HB3 | 9:C:45:SER:HB2 | 1.90 | 0.53 |
| 10:D:257:THR:H | 10:D:269:LEU:CB | 2.20 | 0.53 |
| 1:2:549:LYS:NZ | 13:2:901:ANP:O3G | 2.35 | 0.53 |
| 2:3:199:SER:HB2 | 2:3:214:TYR:CE2 | 2.44 | 0.53 |
| 2:3:225:ILE:H | 2:3:225:ILE:HD12 | 1.73 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:6:402:ILE:HG13 | 5:6:453:SER:OG | 2.09 | 0.53 |
| 5:6:551:MET:O | 5:6:759:ARG:NH1 | 2.41 | 0.53 |
| 5:6:810:ILE:O | 5:6:814:ASN:ND2 | 2.40 | 0.53 |
| 7:A:145:ASP:HA | 7:A:146:LEU:CB | 2.38 | 0.53 |
| 8:B:165:GLU:HG3 | 8:B:193:ARG:HA | 1.88 | 0.53 |
| 8:B:50:TRP:N | 8:B:51:GLN:OE1 | 2.41 | 0.53 |
| 9:C:165:PHE:CE2 | 9:C:169:LEU:HD11 | 2.43 | 0.53 |
| 9:C:26:GLY:H | 9:C:36:ARG:HG3 | 1.74 | 0.53 |
| 11:E:126:HIS:CD2 | 11:E:247:VAL:HG22 | 2.44 | 0.53 |
| 2:3:527:ARG:HD3 | 2:3:531:GLN:HB2 | 1.91 | 0.53 |
| 3:4:179:ILE:HD11 | 3:4:184:ASN:HB2 | 1.89 | 0.53 |
| 4:5:439:THR:HA | 4:5:444:SER:OG | 2.09 | 0.53 |
| 5:6:168:MET:HA | 5:6:171:SER:HB2 | 1.91 | 0.53 |
| 6:7:111:ASN:HB2 | 6:7:356:LEU:HD11 | 1.91 | 0.53 |
| 11:E:259:LEU:HG | 11:E:264:GLU:HB2 | 1.90 | 0.53 |
| 4:5:77:LYS:HZ3 | 11:E:383:SER:H | 1.57 | 0.53 |
| 11:E:607:MET:O | 11:E:611:GLN:HG2 | 2.08 | 0.53 |
| 13:2:901:ANP:HNB1 | 5:6:653:HIS:HE1 | 1.56 | 0.53 |
| 2:3:403:ILE:HG22 | 2:3:405:ILE:HD11 | 1.91 | 0.53 |
| 3:4:202:LYS:CB | 3:4:203:TYR:HB3 | 2.30 | 0.53 |
| 3:4:277:LYS:O | 3:4:281:VAL:HG23 | 2.07 | 0.53 |
| 4:5:209:ARG:HA | 4:5:241:TYR:CE2 | 2.42 | 0.53 |
| 4:5:496:ALA:HB1 | 4:5:515:SER:OG | 2.08 | 0.53 |
| 4:5:568:ILE:O | 4:5:572:VAL:HG23 | 2.09 | 0.53 |
| 2:3:412:SER:OG | 4:5:649:THR:HB | 2.08 | 0.53 |
| 13:2:901:ANP:O3G | 5:6:704:PRO:HB3 | 2.08 | 0.53 |
| 5:6:794:ARG:N | 5:6:795:ILE:HA | 2.22 | 0.53 |
| 10:D:228:VAL:O | 10:D:276:VAL:HG13 | 2.08 | 0.53 |
| 11:E:433:GLU:HB3 | 11:E:541:ASN:ND2 | 2.24 | 0.53 |
| 11:E:605:PHE:HA | 11:E:608:ALA:HB3 | 1.89 | 0.53 |
| 4:5:392:LEU:HB3 | 4:5:603:ILE:HD13 | 1.91 | 0.53 |
| 1:2:533:ILE:CD1 | 4:5:576:HIS:CE1 | 2.92 | 0.53 |
| 5:6:552:LEU:HD23 | 5:6:812:ARG:HB2 | 1.90 | 0.53 |
| 5:6:729:SER:OG | 5:6:730:HIS:N | 2.42 | 0.53 |
| 11:E:579:TYR:HE2 | 11:E:634:ARG:HB3 | 1.66 | 0.53 |
| 11:E:76:ASP:H | 11:E:78:ILE:HD13 | 1.72 | 0.53 |
| 11:E:97:GLU:HA | 11:E:98:ILE:O | 2.09 | 0.53 |
| 1:2:428:GLY:HA3 | 1:2:452:GLU:O | 2.08 | 0.53 |
| 2:3:303:ALA:CB | 2:3:307:ASN:HB2 | 2.39 | 0.53 |
| 2:3:682:ASN:O | 2:3:686:LEU:HG | 2.09 | 0.53 |
| 3:4:335:SER:HB3 | 3:4:395:GLN:HE22 | 1.74 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:5:411:ASN:HA | 4:5:519:VAL:O | 2.09 | 0.53 |
| 5:6:140:ILE:HA | 5:6:143:MET:HB3 | 1.89 | 0.53 |
| 5:6:355:ASP:HB3 | 5:6:356:TRP:CA | 2.38 | 0.53 |
| 11:E:349:SER:HA | 11:E:351:TRP:CZ3 | 2.44 | 0.53 |
| 1:2:839:LYS:HD3 | 1:2:864:TYR:HA | 1.91 | 0.53 |
| 2:3:314:LEU:HD23 | 4:5:253:GLN:NE2 | 2.24 | 0.53 |
| 2:3:156:SER:CA | 2:3:325:THR:HG22 | 2.39 | 0.53 |
| 2:3:518:PRO:HG3 | 2:3:524:ASP:HB2 | 1.90 | 0.53 |
| 3:4:802:ILE:O | 3:4:806:GLU:N | 2.31 | 0.53 |
| 2:3:223:THR:CG2 | 4:5:245:HIS:H | 2.20 | 0.53 |
| 4:5:548:SER:HB2 | 4:5:649:THR:HG21 | 1.90 | 0.53 |
| 5:6:362:GLN:HG3 | 5:6:376:THR:HG21 | 1.91 | 0.53 |
| 5:6:529:LEU:O | 5:6:533:ILE:HG13 | 2.09 | 0.53 |
| 6:7:88:TYR:O | 6:7:92:LYS:HG2 | 2.09 | 0.53 |
| 7:A:129:GLU:HA | 7:A:132:LYS:HE3 | 1.91 | 0.53 |
| 8:B:97:GLU:O | 8:B:100:ARG:HG2 | 2.08 | 0.53 |
| 11:E:93:GLU:HG3 | 11:E:98:ILE:HG22 | 1.90 | 0.53 |
| 1:2:585:ILE:HG12 | 1:2:586:THR:HG23 | 1.91 | 0.53 |
| 2:3:176:LEU:HA | 2:3:298:PHE:HD2 | 1.73 | 0.53 |
| 2:3:386:MET:HB3 | 2:3:714:LYS:HD2 | 1.90 | 0.53 |
| 4:5:235:ASN:HA | 4:5:236:CYS:C | 2.29 | 0.53 |
| 4:5:170:SER:HB3 | 4:5:254:GLN:O | 2.08 | 0.53 |
| 4:5:365:LYS:O | 4:5:369:ILE:N | 2.37 | 0.53 |
| 4:5:626:PHE:CD2 | 4:5:653:LEU:HD12 | 2.43 | 0.53 |
| 5:6:625:ALA:HB1 | 5:6:629:MET:HB2 | 1.90 | 0.53 |
| 5:6:640:GLU:HA | 5:6:682:ALA:HA | 1.91 | 0.53 |
| 5:6:784:ASP:OD2 | 5:6:795:ILE:HG12 | 2.08 | 0.53 |
| 6:7:660:VAL:HG12 | 6:7:689:LEU:HD11 | 1.91 | 0.53 |
| 8:B:51:GLN:H | 8:B:53:ILE:HD12 | 1.74 | 0.53 |
| 11:E:34:LEU:HD21 | 11:E:543:LEU:HD11 | 1.90 | 0.53 |
| 1:2:519:LEU:HG | 1:2:767:ILE:HD13 | 1.91 | 0.53 |
| 3:4:448:SER:CB | 3:4:449:ARG:HB3 | 2.35 | 0.53 |
| 4:5:439:THR:O | 4:5:479:ILE:HA | 2.09 | 0.53 |
| 4:5:545:THR:O | 4:5:548:SER:OG | 2.19 | 0.53 |
| 5:6:654:GLU:HB2 | 5:6:661:ILE:HG12 | 1.91 | 0.53 |
| 8:B:16:ILE:O | 8:B:20:VAL:HG12 | 2.08 | 0.53 |
| 8:B:198:ALA:HB1 | 9:C:113:MET:HE3 | 1.90 | 0.53 |
| 7:A:81:ARG:HD3 | 9:C:49:TRP:CD2 | 2.44 | 0.53 |
| 11:E:11:ALA:HB1 | 11:E:121:TYR:HE1 | 1.72 | 0.53 |
| 11:E:257:SER:HA | 11:E:260:SER:HB3 | 1.91 | 0.53 |
| 11:E:271:TRP:HA | 11:E:274:ILE:HD12 | 1.91 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2:484:PHE:HA | 1:2:487:ILE:HD12 | 1.91 | 0.52 |
| 1:2:541:LEU:HA | 1:2:681:CYS:HB2 | 1.91 | 0.52 |
| 1:2:578:ALA:O | 1:2:631:ILE:HD13 | 2.09 | 0.52 |
| 2:3:306:MET:HB3 | 4:5:206:SER:HA | 1.91 | 0.52 |
| 3:4:794:THR:HG22 | 3:4:797:GLN:HG2 | 1.90 | 0.52 |
| 4:5:209:ARG:HA | 4:5:241:TYR:HE2 | 1.74 | 0.52 |
| 4:5:321:VAL:HG23 | 4:5:322:ALA:HA | 1.91 | 0.52 |
| 6:7:116:LEU:O | 6:7:119:ARG:HG2 | 2.09 | 0.52 |
| 6:7:257:VAL:HA | 6:7:258:ILE:HB | 1.90 | 0.52 |
| 8:B:195:ILE:HD11 | 9:C:125:SER:HB2 | 1.91 | 0.52 |
| 9:C:20:PHE:CD1 | 9:C:72:VAL:HG22 | 2.44 | 0.52 |
| 11:E:298:GLU:HA | 11:E:301:ARG:HB2 | 1.91 | 0.52 |
| 1:2:553:LEU:CD2 | 1:2:607:ASP:HB3 | 2.39 | 0.52 |
| 3:4:679:GLY:HA3 | 3:4:681:ARG:O | 2.08 | 0.52 |
| 3:4:823:GLN:OE1 | 3:4:823:GLN:N | 2.39 | 0.52 |
| 4:5:448:GLY:HA2 | 4:5:486:ARG:NH1 | 2.11 | 0.52 |
| 6:7:333:ILE:HG12 | 6:7:376:LEU:HB3 | 1.91 | 0.52 |
| 11:E:494:ARG:O | 11:E:498:LEU:HG | 2.08 | 0.52 |
| 11:E:98:ILE:N | 11:E:99:ASP:HB3 | 2.24 | 0.52 |
| 1:2:778:LEU:HD13 | 1:2:783:MET:HG2 | 1.91 | 0.52 |
| 2:3:475:PHE:HE1 | 2:3:486:ILE:HD13 | 1.74 | 0.52 |
| 3:4:928:ARG:CB | 5:6:946:ASN:HB2 | 2.38 | 0.52 |
| 5:6:126:SER:H | 5:6:131:GLU:HG3 | 1.74 | 0.52 |
| 3:4:411:THR:OG1 | 6:7:507:ILE:HD13 | 2.09 | 0.52 |
| 6:7:721:ARG:O | 6:7:725:GLU:HG2 | 2.10 | 0.52 |
| 8:B:185:ILE:H | 8:B:185:ILE:HD12 | 1.73 | 0.52 |
| 9:C:47:PRO:HD2 | 9:C:50:LEU:HD21 | 1.92 | 0.52 |
| 10:D:144:ILE:HG13 | 10:D:145:ARG:H | 1.73 | 0.52 |
| 10:D:195:ASN:HA | 10:D:199:LEU:HD12 | 1.91 | 0.52 |
| 1:2:216:LEU:HD12 | 1:2:217:GLU:HB3 | 1.91 | 0.52 |
| 2:3:201:HIS:HA | 2:3:242:THR:O | 2.08 | 0.52 |
| 3:4:239:SER:OG | 3:4:240:ASN:N | 2.41 | 0.52 |
| 3:4:315:ARG:N | 3:4:401:GLU:OE1 | 2.43 | 0.52 |
| 3:4:726:ASN:C | 3:4:728:TYR:HB3 | 2.29 | 0.52 |
| 4:5:482:PHE:CB | 4:5:523:ALA:HB2 | 2.32 | 0.52 |
| 5:6:284:ILE:N | 5:6:401:GLU:OE1 | 2.42 | 0.52 |
| 5:6:308:SER:CB | 5:6:350:ARG:HB2 | 2.40 | 0.52 |
| 5:6:530:VAL:O | 5:6:533:ILE:HD12 | 2.09 | 0.52 |
| 5:6:634:GLY:H | 5:6:676:THR:HG22 | 1.74 | 0.52 |
| 1:2:271:PHE:CE2 | 1:2:295:VAL:HG11 | 2.45 | 0.52 |
| 1:2:335:LYS:HE3 | 1:2:383:ARG:HD2 | 1.92 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:2:538:ASN:HB3 | 1:2:677:PHE:HD1 | 1.74 | 0.52 |
| 3:4:826:VAL:O | 3:4:830:ARG:HG2 | 2.09 | 0.52 |
| 4:5:409:ASP:O | 4:5:410:ILE:HG12 | 2.10 | 0.52 |
| 5:6:118:PHE:HB2 | 5:6:161:ARG:HD3 | 1.91 | 0.52 |
| 5:6:556:HIS:H | 5:6:567:GLY:HA2 | 1.75 | 0.52 |
| 5:6:608:LEU:HD23 | 5:6:628:LEU:HD13 | 1.89 | 0.52 |
| 5:6:936:ILE:HA | 5:6:939:TRP:HE1 | 1.74 | 0.52 |
| 6:7:249:SER:O | 6:7:311:GLN:HG3 | 2.10 | 0.52 |
| 6:7:437:VAL:HG21 | 6:7:702:LEU:HD21 | 1.91 | 0.52 |
| 6:7:495:ALA:CB | 6:7:557:LEU:HD21 | 2.40 | 0.52 |
| 6:7:680:SER:CB | 6:7:681:PHE:HA | 2.38 | 0.52 |
| 1:2:424:VAL:HG23 | 1:2:458:ARG:HA | 1.91 | 0.52 |
| 1:2:516:ALA:HA | 1:2:519:LEU:HB3 | 1.91 | 0.52 |
| 1:2:596:LEU:HD12 | 1:2:629:ILE:HD11 | 1.90 | 0.52 |
| 2:3:223:THR:HG21 | 4:5:244:ILE:HA | 1.90 | 0.52 |
| 2:3:176:LEU:HD12 | 2:3:298:PHE:CE2 | 2.45 | 0.52 |
| 2:3:661:GLN:HA | 2:3:664:LYS:HD3 | 1.90 | 0.52 |
| 3:4:399:LEU:HB3 | 3:4:415:ILE:HB | 1.91 | 0.52 |
| 3:4:332:VAL:CG1 | 3:4:429:ALA:HA | 2.39 | 0.52 |
| 3:4:578:LEU:HD13 | 3:4:630:CYS:HB3 | 1.92 | 0.52 |
| 3:4:925:ARG:HH21 | 3:4:928:ARG:HD3 | 1.74 | 0.52 |
| 6:7:609:ASP:HA | 6:7:612:LEU:HB3 | 1.92 | 0.52 |
| 7:A:175:GLN:HB3 | 7:A:180:VAL:HA | 1.91 | 0.52 |
| 8:B:120:LEU:HD13 | 8:B:176:LEU:HD22 | 1.91 | 0.52 |
| 9:C:186:ASP:OD1 | 9:C:189:ARG:NH2 | 2.42 | 0.52 |
| 10:D:169:ILE:HG22 | 10:D:170:SER:H | 1.73 | 0.52 |
| 1:2:624:MET:HE3 | 1:2:676:ARG:HD2 | 1.92 | 0.52 |
| 2:3:685:ASP:O | 2:3:689:ASP:HB2 | 2.10 | 0.52 |
| 3:4:336:THR:O | 3:4:395:GLN:NE2 | 2.36 | 0.52 |
| 3:4:347:PHE:CE1 | 3:4:384:LEU:HD12 | 2.43 | 0.52 |
| 1:2:641:GLN:NE2 | 4:5:263:GLU:HA | 2.24 | 0.52 |
| 4:5:629:ILE:HG22 | 4:5:648:ILE:HD11 | 1.91 | 0.52 |
| 5:6:118:PHE:O | 5:6:123:SER:OG | 2.26 | 0.52 |
| 5:6:540:HIS:CD2 | 5:6:715:ILE:HG21 | 2.44 | 0.52 |
| 5:6:560:VAL:HB | 5:6:561:GLU:CA | 2.40 | 0.52 |
| 6:7:235:LEU:HD22 | 6:7:357:PRO:HD3 | 1.91 | 0.52 |
| 6:7:404:LEU:HD11 | 6:7:414:LEU:HD21 | 1.92 | 0.52 |
| 8:B:115:LEU:HD11 | 8:B:152:ARG:CZ | 2.39 | 0.52 |
| 11:E:405:ILE:HD12 | 11:E:405:ILE:H | 1.75 | 0.52 |
| 1:2:306:LEU:HD22 | 1:2:392:GLU:HB2 | 1.90 | 0.52 |
| 2:3:278:LEU:HB3 | 2:3:282:LEU:HB2 | 1.92 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:3:559:ARG:O | 2:3:562:SER:OG | 2.20 | 0.52 |
| 1:2:780:GLN:NE2 | 4:5:573:ILE:HG22 | 2.24 | 0.52 |
| 4:5:572:VAL:HA | 4:5:575:ILE:HD12 | 1.92 | 0.52 |
| 5:6:103:VAL:HB | 5:6:104:ASP:HB2 | 1.91 | 0.52 |
| 3:4:387:ASN:HD21 | 5:6:402:ILE:HG22 | 1.75 | 0.52 |
| 7:A:2:TYR:CE2 | 7:A:78:CYS:HB2 | 2.44 | 0.52 |
| 9:C:3:TYR:CG | 9:C:4:TYR:N | 2.78 | 0.52 |
| 11:E:67:LEU:HD12 | 11:E:86:PHE:HD2 | 1.75 | 0.52 |
| 1:2:243:GLU:OE2 | 1:2:298:SER:HB3 | 2.10 | 0.52 |
| 3:4:446:ALA:O | 3:4:447:ASN:OD1 | 2.27 | 0.52 |
| 3:4:633:GLU:OE2 | 3:4:676:ASN:HB2 | 2.10 | 0.52 |
| 5:6:755:ILE:O | 5:6:759:ARG:N | 2.42 | 0.52 |
| 6:7:316:GLN:HG2 | 6:7:330:SER:HB3 | 1.92 | 0.52 |
| 10:D:168:LEU:HD21 | 10:D:173:ASP:OD2 | 2.09 | 0.52 |
| 11:E:327:PHE:CE2 | 11:E:328:LEU:HG | 2.45 | 0.52 |
| 2:3:491:GLU:OE2 | 2:3:700:ARG:NH1 | 2.43 | 0.52 |
| 4:5:252:ASP:OD1 | 4:5:253:GLN:N | 2.42 | 0.52 |
| 4:5:560:HIS:N | 4:5:560:HIS:ND1 | 2.56 | 0.52 |
| 4:5:398:LYS:HZ1 | 4:5:613:ARG:HD2 | 1.72 | 0.52 |
| 2:3:566:LEU:HD13 | 4:5:619:ALA:HB1 | 1.92 | 0.52 |
| 4:5:662:SER:OG | 4:5:663:LEU:N | 2.44 | 0.52 |
| 8:B:119:TRP:HZ2 | 8:B:177:GLU:OE2 | 1.93 | 0.52 |
| 8:B:18:PHE:CE1 | 10:D:135:ARG:HG2 | 2.45 | 0.52 |
| 10:D:161:LEU:HD21 | 10:D:169:ILE:HA | 1.92 | 0.52 |
| 1:2:433:ASN:HB2 | 1:2:434:TYR:HB3 | 1.91 | 0.51 |
| 4:5:632:GLN:O | 4:5:636:ASN:HB2 | 2.09 | 0.51 |
| 5:6:519:MET:O | 5:6:525:ILE:HG21 | 2.10 | 0.51 |
| 6:7:428:VAL:HA | 6:7:598:PHE:CE2 | 2.45 | 0.51 |
| 11:E:38:ALA:O | 11:E:42:THR:N | 2.31 | 0.51 |
| 3:4:461:VAL:O | 3:4:463:VAL:HG22 | 2.10 | 0.51 |
| 4:5:347:THR:OG1 | 4:5:348:MET:HA | 2.10 | 0.51 |
| 1:2:632:SER:HA | 4:5:443:GLY:H | 1.74 | 0.51 |
| 6:7:248:VAL:HG11 | 6:7:345:PRO:HD3 | 1.92 | 0.51 |
| 3:4:410:GLN:HE21 | 6:7:345:PRO:HG3 | 1.76 | 0.51 |
| 8:B:112:PHE:HB3 | 8:B:152:ARG:NH1 | 2.25 | 0.51 |
| 8:B:197:THR:HG22 | 10:D:263:LEU:HD23 | 1.91 | 0.51 |
| 11:E:155:GLN:HA | 11:E:158:ALA:HB3 | 1.93 | 0.51 |
| 11:E:157:GLU:O | 11:E:161:LYS:HB2 | 2.10 | 0.51 |
| 11:E:561:ASP:HB3 | 11:E:562:LYS:HG2 | 1.92 | 0.51 |
| 2:3:20:VAL:O | 2:3:24:ARG:HG2 | 2.11 | 0.51 |
| 6:7:362:GLY:HA2 | 6:7:363:PHE:CD2 | 2.46 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:7:516:ALA:O | 6:7:561:THR:HG22 | 2.10 | 0.51 |
| 11:E:619:LYS:HD2 | 11:E:633:ARG:HG3 | 1.93 | 0.51 |
| 1:2:454:ASN:O | 1:2:454:ASN:ND2 | 2.40 | 0.51 |
| 1:2:686:LEU:HG | 5:6:788:PHE:CZ | 2.45 | 0.51 |
| 1:2:484:PHE:CZ | 1:2:766:TYR:HA | 2.44 | 0.51 |
| 1:2:794:ARG:HH11 | 4:5:560:HIS:HA | 1.76 | 0.51 |
| 3:4:277:LYS:HA | 3:4:301:TYR:HD2 | 1.76 | 0.51 |
| 5:6:570:ASN:ND2 | 5:6:678:ILE:H | 2.02 | 0.51 |
| 1:2:660:THR:HG21 | 5:6:947:ASP:HB2 | 1.93 | 0.51 |
| 9:C:16:PHE:HZ | 9:C:107:LEU:HD21 | 1.75 | 0.51 |
| 1:2:474:PHE:HZ | 1:2:561:HIS:HA | 1.76 | 0.51 |
| 1:2:477:THR:HG22 | 1:2:478:GLU:H | 1.74 | 0.51 |
| 1:2:550:SER:HB2 | 13:2:901:ANP:O1A | 2.10 | 0.51 |
| 2:3:686:LEU:O | 2:3:690:ASP:N | 2.40 | 0.51 |
| 3:4:203:TYR:CG | 3:4:204:LYS:N | 2.77 | 0.51 |
| 3:4:329:LYS:HB2 | 3:4:402:THR:HG22 | 1.93 | 0.51 |
| 4:5:253:GLN:HE21 | 4:5:277:THR:HB | 1.75 | 0.51 |
| 4:5:338:GLU:N | 4:5:339:THR:HA | 2.26 | 0.51 |
| 4:5:343:TRP:C | 4:5:345:SER:HA | 2.31 | 0.51 |
| 6:7:579:SER:O | 6:7:582:ASP:HB2 | 2.10 | 0.51 |
| 6:7:659:TYR:CG | 6:7:710:ILE:HD11 | 2.45 | 0.51 |
| 7:A:166:ARG:HG3 | 7:A:188:GLN:HB3 | 1.92 | 0.51 |
| 11:E:125:ALA:HB1 | 11:E:248:VAL:H | 1.75 | 0.51 |
| 1:2:253:LYS:HE2 | 1:2:253:LYS:HA | 1.92 | 0.51 |
| 1:2:544:ASP:OD2 | 1:2:547:THR:OG1 | 2.27 | 0.51 |
| 1:2:816:ILE:O | 1:2:819:SER:OG | 2.28 | 0.51 |
| 3:4:319:PRO:HB3 | 6:7:307:PHE:HB2 | 1.91 | 0.51 |
| 4:5:136:GLN:CB | 4:5:280:ARG:HE | 2.24 | 0.51 |
| 4:5:441:GLY:HA3 | 4:5:443:GLY:N | 2.25 | 0.51 |
| 4:5:631:LYS:HE3 | 4:5:635:ILE:HD11 | 1.91 | 0.51 |
| 6:7:490:GLY:O | 6:7:494:THR:N | 2.41 | 0.51 |
| 8:B:61:ASN:OD1 | 8:B:62:ASN:N | 2.44 | 0.51 |
| 9:C:20:PHE:HE1 | 9:C:46:LEU:HD11 | 1.75 | 0.51 |
| 1:2:628:SER:HB2 | 1:2:640:LEU:O | 2.10 | 0.51 |
| 1:2:496:LYS:HG2 | 1:2:758:ILE:HG13 | 1.93 | 0.51 |
| 1:2:796:GLU:HB2 | 1:2:859:ARG:HE | 1.76 | 0.51 |
| 2:3:472:ILE:HD13 | 2:3:475:PHE:CD1 | 2.46 | 0.51 |
| 2:3:556:ILE:H | 2:3:556:ILE:HD12 | 1.75 | 0.51 |
| 3:4:547:GLY:HA2 | 3:4:806:GLU:HG3 | 1.93 | 0.51 |
| 3:4:720:LEU:O | 3:4:724:LEU:HG | 2.10 | 0.51 |
| 4:5:407:ARG:HD3 | 4:5:498:GLU:HA | 1.92 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:6:656:MET:HG3 | 5:6:709:PHE:CE1 | 2.46 | 0.51 |
| 6:7:619:VAL:HG12 | 6:7:620:HIS:ND1 | 2.26 | 0.51 |
| 7:A:58:GLN:HA | 7:A:62:MET:HB2 | 1.92 | 0.51 |
| 11:E:30:PHE:CD1 | 11:E:61:ILE:HD11 | 2.45 | 0.51 |
| 1:2:260:LEU:HA | 1:2:264:PRO:HB3 | 1.92 | 0.51 |
| 1:2:690:GLU:HA | 1:2:693:GLU:CD | 2.31 | 0.51 |
| 1:2:695:LEU:O | 1:2:699:VAL:HG23 | 2.09 | 0.51 |
| 1:2:838:ILE:O | 1:2:842:VAL:HG23 | 2.11 | 0.51 |
| 3:4:330:GLY:O | 3:4:432:ARG:HA | 2.10 | 0.51 |
| 4:5:239:ASP:OD1 | 4:5:239:ASP:N | 2.43 | 0.51 |
| 4:5:377:SER:HB3 | 4:5:378:ILE:HD12 | 1.93 | 0.51 |
| 6:7:584:ILE:HG22 | 6:7:586:LEU:H | 1.76 | 0.51 |
| 7:A:173:GLU:HB3 | 7:A:183:LEU:H | 1.74 | 0.51 |
| 7:A:35:ASP:N | 7:A:35:ASP:OD1 | 2.43 | 0.51 |
| 1:2:566:ALA:O | 1:2:572:SER:HB2 | 2.10 | 0.51 |
| 1:2:579:SER:HA | 1:2:633:LYS:HE3 | 1.93 | 0.51 |
| 1:2:778:LEU:CD1 | 4:5:577:THR:HG23 | 2.41 | 0.51 |
| 2:3:216:ASP:O | 2:3:219:THR:HG22 | 2.11 | 0.51 |
| 2:3:483:ARG:HA | 2:3:486:ILE:HD12 | 1.92 | 0.51 |
| 2:3:533:ILE:CG2 | 2:3:540:LEU:HD11 | 2.40 | 0.51 |
| 3:4:861:LEU:O | 3:4:865:LEU:HG | 2.10 | 0.51 |
| 3:4:919:LEU:HB2 | 3:4:925:ARG:HB2 | 1.93 | 0.51 |
| 5:6:920:ILE:HB | 5:6:924:ASP:HB3 | 1.92 | 0.51 |
| 6:7:255:VAL:CG2 | 6:7:258:ILE:HG13 | 2.40 | 0.51 |
| 7:A:49:LYS:O | 7:A:52:GLU:HG2 | 2.10 | 0.51 |
| 10:D:78:PRO:HA | 10:D:174:LEU:HD12 | 1.93 | 0.51 |
| 8:B:11:PHE:CE1 | 10:D:71:ARG:HB2 | 2.45 | 0.51 |
| 3:4:692:ILE:HG21 | 3:4:699:LEU:HD13 | 1.91 | 0.51 |
| 4:5:184:ARG:HD2 | 4:5:240:PRO:HA | 1.91 | 0.51 |
| 4:5:439:THR:HA | 4:5:444:SER:HB2 | 1.92 | 0.51 |
| 5:6:179:PRO:O | 5:6:183:LYS:HG2 | 2.11 | 0.51 |
| 5:6:303:GLU:HB2 | 5:6:354:LEU:HG | 1.92 | 0.51 |
| 6:7:340:VAL:HG13 | 6:7:341:ARG:HG3 | 1.92 | 0.51 |
| 6:7:536:ALA:O | 6:7:540:VAL:HG23 | 2.10 | 0.51 |
| 10:D:260:ILE:CG2 | 10:D:264:LYS:O | 2.56 | 0.51 |
| 11:E:339:TYR:O | 11:E:350:LEU:HD13 | 2.11 | 0.51 |
| 11:E:600:PRO:O | 11:E:601:ILE:HG13 | 2.11 | 0.51 |
| 2:3:104:ARG:NH2 | 9:C:86:ASN:HB2 | 2.25 | 0.50 |
| 2:3:198:ARG:O | 2:3:248:SER:HB2 | 2.11 | 0.50 |
| 2:3:671:LEU:HD11 | 2:3:676:ILE:HD11 | 1.93 | 0.50 |
| 3:4:200:SER:HB3 | 3:4:202:LYS:HB2 | 1.92 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:4:682:TYR:CZ | 3:4:707:LEU:HD21 | 2.46 | 0.50 |
| 4:5:104:LEU:HD22 | 4:5:105:SER:H | 1.76 | 0.50 |
| 6:7:256:GLU:O | 6:7:306:LYS:HB3 | 2.11 | 0.50 |
| 7:A:170:ASP:OD2 | 7:A:204:TYR:HA | 2.10 | 0.50 |
| 11:E:514:LEU:HD11 | 11:E:555:CYS:SG | 2.51 | 0.50 |
| 1:2:264:PRO:HG3 | 1:2:317:LEU:N | 2.26 | 0.50 |
| 1:2:767:ILE:HG13 | 1:2:768:HIS:N | 2.26 | 0.50 |
| 3:4:261:LEU:HB2 | 3:4:268:VAL:HG11 | 1.93 | 0.50 |
| 4:5:101:ILE:HG23 | 8:B:150:GLU:OE2 | 2.11 | 0.50 |
| 4:5:153:SER:OG | 4:5:154:GLU:N | 2.44 | 0.50 |
| 4:5:287:ILE:HG12 | 4:5:342:ILE:HD13 | 1.92 | 0.50 |
| 5:6:149:ASN:HB3 | 5:6:262:VAL:O | 2.11 | 0.50 |
| 6:7:428:VAL:HA | 6:7:598:PHE:CD2 | 2.46 | 0.50 |
| 6:7:440:VAL:HG21 | 6:7:650:PRO:HD2 | 1.93 | 0.50 |
| 6:7:685:THR:HB | 6:7:686:PRO:HD2 | 1.93 | 0.50 |
| 8:B:107:THR:HG23 | 8:B:108:HIS:ND1 | 2.26 | 0.50 |
| 8:B:134:PHE:HB2 | 8:B:137:PRO:HG3 | 1.91 | 0.50 |
| 11:E:345:ASN:ND2 | 11:E:555:CYS:HB2 | 2.27 | 0.50 |
| 2:3:495:VAL:HG23 | 2:3:508:ALA:HB2 | 1.94 | 0.50 |
| 3:4:750:TYR:CE1 | 3:4:754:ALA:HB2 | 2.47 | 0.50 |
| 3:4:766:ALA:O | 3:4:770:LEU:HB3 | 2.11 | 0.50 |
| 4:5:679:GLU:O | 4:5:683:LEU:HB2 | 2.11 | 0.50 |
| 5:6:653:HIS:HA | 5:6:656:MET:CG | 2.31 | 0.50 |
| 6:7:227:VAL:HG13 | 6:7:230:ILE:HD12 | 1.93 | 0.50 |
| 6:7:89:GLN:HA | 6:7:92:LYS:HB2 | 1.94 | 0.50 |
| 8:B:193:ARG:HD2 | 10:D:278:ARG:NE | 2.25 | 0.50 |
| 11:E:612:ILE:HG21 | 11:E:640:PHE:CD1 | 2.46 | 0.50 |
| 1:2:301:PRO:HA | 1:2:302:THR:OG1 | 2.10 | 0.50 |
| 1:2:586:THR:HA | 4:5:457:PRO:HB2 | 1.93 | 0.50 |
| 2:3:258:VAL:O | 2:3:273:SER:HA | 2.11 | 0.50 |
| 2:3:347:ILE:HA | 2:3:350:ILE:HD13 | 1.93 | 0.50 |
| 3:4:204:LYS:HA | 3:4:205:PHE:C | 2.31 | 0.50 |
| 3:4:346:PHE:H | 3:4:389:CYS:HB3 | 1.77 | 0.50 |
| 3:4:449:ARG:C | 3:4:451:ARG:H | 2.15 | 0.50 |
| 3:4:566:LEU:HA | 3:4:706:TYR:HB2 | 1.92 | 0.50 |
| 5:6:109:GLU:O | 5:6:112:ARG:HB3 | 2.10 | 0.50 |
| 5:6:533:ILE:HG22 | 5:6:587:TYR:CE2 | 2.47 | 0.50 |
| 5:6:819:ILE:HA | 5:6:823:PHE:HD2 | 1.76 | 0.50 |
| 5:6:834:SER:HA | 5:6:837:ARG:HD2 | 1.92 | 0.50 |
| 5:6:945:GLU:O | 5:6:948:LEU:HD22 | 2.11 | 0.50 |
| 6:7:493:LEU:HD22 | 6:7:533:ASP:HB3 | 1.92 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:7:481:VAL:CG2 | 6:7:516:ALA:HB3 | 2.41 | 0.50 |
| 11:E:5:ILE:N | 11:E:142:CYS:O | 2.44 | 0.50 |
| 11:E:22:HIS:HA | 11:E:23:SER:C | 2.30 | 0.50 |
| 11:E:315:THR:N | 11:E:316:LEU:CB | 2.73 | 0.50 |
| 1:2:256:LEU:HD23 | 1:2:259:PHE:CD2 | 2.47 | 0.50 |
| 2:3:562:SER:O | 2:3:566:LEU:HG | 2.11 | 0.50 |
| 4:5:412:VAL:C | 4:5:413:LEU:HD12 | 2.32 | 0.50 |
| 6:7:440:VAL:HG22 | 6:7:701:LYS:HD2 | 1.93 | 0.50 |
| 7:A:32:TYR:CA | 7:A:93:ARG:HH12 | 2.24 | 0.50 |
| 8:B:124:ARG:HD3 | 9:C:190:TRP:CZ3 | 2.47 | 0.50 |
| 10:D:269:LEU:HD13 | 10:D:275:TYR:HD2 | 1.75 | 0.50 |
| 11:E:18:ASN:O | 11:E:79:ASN:ND2 | 2.34 | 0.50 |
| 11:E:158:ALA:HB1 | 11:E:237:LEU:HD22 | 1.93 | 0.50 |
| 11:E:128:PRO:HB2 | 11:E:240:TYR:CZ | 2.47 | 0.50 |
| 1:2:302:THR:OG1 | 1:2:319:ARG:HB3 | 2.12 | 0.50 |
| 1:2:706:SER:O | 5:6:762:LYS:NZ | 2.45 | 0.50 |
| 2:3:400:ARG:O | 2:3:707:ARG:NE | 2.39 | 0.50 |
| 3:4:291:TYR:HB2 | 3:4:296:ILE:HG12 | 1.93 | 0.50 |
| 5:6:170:ILE:O | 5:6:174:TYR:HB2 | 2.11 | 0.50 |
| 5:6:377:LEU:HD11 | 5:6:454:PHE:HB2 | 1.93 | 0.50 |
| 5:6:776:LYS:HA | 5:6:779:GLU:HG2 | 1.94 | 0.50 |
| 7:A:113:ILE:H | 7:A:113:ILE:HD12 | 1.77 | 0.50 |
| 7:A:124:SER:OG | 7:A:127:GLU:HG2 | 2.12 | 0.50 |
| 7:A:4:ASP:OD1 | 7:A:4:ASP:N | 2.43 | 0.50 |
| 8:B:173:LEU:HD23 | 8:B:178:ILE:HG12 | 1.94 | 0.50 |
| 11:E:42:THR:O | 11:E:46:SER:N | 2.32 | 0.50 |
| 3:4:330:GLY:HA3 | 3:4:400:GLN:O | 2.12 | 0.50 |
| 3:4:812:LYS:HE3 | 3:4:814:LYS:HG3 | 1.93 | 0.50 |
| 4:5:181:ILE:HG12 | 4:5:243:ILE:HA | 1.93 | 0.50 |
| 4:5:384:ILE:HD13 | 4:5:414:LEU:HD23 | 1.93 | 0.50 |
| 1:2:632:SER:HA | 4:5:443:GLY:N | 2.27 | 0.50 |
| 6:7:581:LEU:HB2 | 6:7:681:PHE:CZ | 2.47 | 0.50 |
| 8:B:54:THR:CG2 | 10:D:132:GLU:HG3 | 2.42 | 0.50 |
| 11:E:144:ASP:OD2 | 11:E:148:VAL:HB | 2.12 | 0.50 |
| 11:E:603:ASN:OD1 | 11:E:605:PHE:N | 2.36 | 0.50 |
| 11:E:609:PHE:O | 11:E:613:THR:HG23 | 2.12 | 0.50 |
| 1:2:782:ASP:N | 1:2:782:ASP:OD1 | 2.38 | 0.50 |
| 2:3:237:GLU:O | 2:3:239:ASN:N | 2.44 | 0.50 |
| 2:3:41:SER:HA | 2:3:44:SER:HB3 | 1.93 | 0.50 |
| 1:2:778:LEU:HD12 | 4:5:577:THR:HG23 | 1.93 | 0.50 |
| 6:7:724:LYS:C | 6:7:726:SER:H | 2.15 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 11:E:615:GLU:HG2 | 11:E:616:THR:H | 1.77 | 0.50 |
| 2:3:111:TRP:CZ2 | 9:C:90:THR:HG22 | 2.47 | 0.50 |
| 2:3:196:LEU:HA | 2:3:250:PHE:CD1 | 2.47 | 0.50 |
| 3:4:330:GLY:C | 3:4:432:ARG:HA | 2.32 | 0.50 |
| 3:4:314:MET:SD | 3:4:415:ILE:HA | 2.52 | 0.50 |
| 3:4:592:SER:OG | 3:4:593:GLY:N | 2.45 | 0.50 |
| 2:3:313:THR:HA | 4:5:301:TYR:CD1 | 2.47 | 0.50 |
| 4:5:659:ILE:O | 4:5:662:SER:OG | 2.18 | 0.50 |
| 4:5:71:TYR:HD1 | 11:E:415:TYR:HE1 | 1.59 | 0.50 |
| 5:6:839:ASP:O | 5:6:840:VAL:C | 2.51 | 0.50 |
| 6:7:352:THR:OG1 | 6:7:380:PHE:HB3 | 2.11 | 0.50 |
| 10:D:191:LEU:HA | 10:D:194:VAL:HG12 | 1.94 | 0.50 |
| 10:D:254:PRO:HG2 | 10:D:270:THR:HG21 | 1.94 | 0.50 |
| 11:E:537:ASP:HA | 11:E:540:ARG:HG3 | 1.94 | 0.50 |
| 1:2:246:TYR:CE2 | 1:2:300:PHE:HD1 | 2.30 | 0.49 |
| 1:2:256:LEU:HA | 1:2:259:PHE:CD2 | 2.46 | 0.49 |
| 1:2:641:GLN:HE22 | 4:5:263:GLU:HA | 1.76 | 0.49 |
| 2:3:374:HIS:HB2 | 2:3:378:LYS:NZ | 2.26 | 0.49 |
| 3:4:613:GLN:CG | 5:6:360:ARG:HH22 | 2.25 | 0.49 |
| 4:5:166:ILE:HD11 | 4:5:256:LEU:HD23 | 1.94 | 0.49 |
| 5:6:134:LYS:N | 5:6:135:VAL:HA | 2.27 | 0.49 |
| 5:6:641:PHE:CD1 | 5:6:682:ALA:HB2 | 2.47 | 0.49 |
| 3:4:264:TYR:HE2 | 6:7:135:LYS:HE2 | 1.76 | 0.49 |
| 6:7:475:LYS:C | 6:7:476:ILE:HD12 | 2.32 | 0.49 |
| 6:7:493:LEU:HD21 | 6:7:533:ASP:CB | 2.42 | 0.49 |
| 7:A:82:ASN:O | 7:A:86:LEU:HG | 2.12 | 0.49 |
| 11:E:83:LEU:N | 11:E:121:TYR:O | 2.45 | 0.49 |
| 11:E:67:LEU:HD11 | 11:E:83:LEU:HD11 | 1.94 | 0.49 |
| 2:3:113:GLY:HA3 | 2:3:121:PHE:CE2 | 2.47 | 0.49 |
| 2:3:300:SER:HB2 | 4:5:250:PHE:CE2 | 2.46 | 0.49 |
| 2:3:409:GLY:O | 2:3:518:PRO:HD3 | 2.12 | 0.49 |
| 2:3:47:VAL:HG12 | 2:3:51:ASN:ND2 | 2.26 | 0.49 |
| 3:4:506:LEU:O | 3:4:509:ILE:HB | 2.12 | 0.49 |
| 3:4:747:LEU:O | 3:4:751:ILE:HG13 | 2.12 | 0.49 |
| 3:4:872:VAL:O | 3:4:876:GLN:N | 2.35 | 0.49 |
| 4:5:628:THR:O | 4:5:632:GLN:HB2 | 2.10 | 0.49 |
| 6:7:446:ASP:HB2 | 6:7:447:GLY:HA2 | 1.92 | 0.49 |
| 10:D:151:ILE:O | 10:D:155:SER:N | 2.45 | 0.49 |
| 11:E:124:ASP:OD1 | 11:E:125:ALA:N | 2.45 | 0.49 |
| 2:3:359:ILE:O | 2:3:363:LEU:HG | 2.12 | 0.49 |
| 3:4:198:LEU:HG | 3:4:227:ILE:HD11 | 1.94 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:6:527:ASP:OD2 | 5:6:531:ARG:NH1 | 2.45 | 0.49 |
| 6:7:523:ILE:HG21 | 6:7:526:PHE:HD1 | 1.77 | 0.49 |
| 6:7:581:LEU:HB2 | 6:7:681:PHE:HZ | 1.77 | 0.49 |
| 6:7:711:ASP:HA | 6:7:714:GLU:HB3 | 1.93 | 0.49 |
| 9:C:165:PHE:CZ | 9:C:169:LEU:HD11 | 2.47 | 0.49 |
| 10:D:60:PHE:HE1 | 10:D:139:VAL:HG21 | 1.78 | 0.49 |
| 11:E:258:LEU:O | 11:E:262:ILE:HG13 | 2.11 | 0.49 |
| 1:2:226:VAL:O | 1:2:230:ARG:HG2 | 2.11 | 0.49 |
| 1:2:272:ASP:OD1 | 1:2:273:LEU:N | 2.46 | 0.49 |
| 2:3:130:THR:HG22 | 2:3:153:TRP:CD1 | 2.47 | 0.49 |
| 4:5:491:VAL:HA | 4:5:494:HIS:HB2 | 1.93 | 0.49 |
| 5:6:765:LEU:CD2 | 5:6:770:ARG:HB3 | 2.42 | 0.49 |
| 10:D:103:MET:HA | 10:D:106:LEU:HD13 | 1.93 | 0.49 |
| 10:D:56:PRO:HA | 10:D:90:ARG:HH12 | 1.78 | 0.49 |
| 11:E:67:LEU:HD12 | 11:E:86:PHE:CD2 | 2.47 | 0.49 |
| 1:2:626:GLN:HA | 4:5:427:LYS:HZ1 | 1.78 | 0.49 |
| 1:2:810:LEU:O | 1:2:813:ILE:HG12 | 2.11 | 0.49 |
| 1:2:858:ARG:HA | 1:2:861:PHE:CE2 | 2.47 | 0.49 |
| 2:3:300:SER:HB2 | 4:5:250:PHE:HE2 | 1.78 | 0.49 |
| 2:3:702:LEU:O | 2:3:705:LEU:N | 2.43 | 0.49 |
| 3:4:362:ARG:O | 3:4:364:VAL:HG22 | 2.12 | 0.49 |
| 3:4:365:ILE:HB | 5:6:419:SER:HA | 1.94 | 0.49 |
| 4:5:413:LEU:HD11 | 4:5:550:PHE:CG | 2.47 | 0.49 |
| 1:2:636:ILE:HG23 | 4:5:446:ALA:HB3 | 1.94 | 0.49 |
| 5:6:560:VAL:HB | 5:6:561:GLU:HG3 | 1.93 | 0.49 |
| 5:6:695:LEU:O | 5:6:695:LEU:HD23 | 2.12 | 0.49 |
| 5:6:793:TYR:CD2 | 5:6:795:ILE:HG23 | 2.48 | 0.49 |
| 6:7:112:HIS:CE1 | 6:7:116:LEU:HD13 | 2.47 | 0.49 |
| 7:A:130:TYR:CD2 | 10:D:193:LEU:HD22 | 2.47 | 0.49 |
| 8:B:142:ARG:NH1 | 11:E:314:ASP:OD2 | 2.45 | 0.49 |
| 11:E:69:ARG:O | 11:E:73:GLN:HB2 | 2.12 | 0.49 |
| 1:2:603:VAL:HG22 | 1:2:645:SER:HB2 | 1.93 | 0.49 |
| 3:4:666:ASN:HD22 | 3:4:668:ARG:NH2 | 2.10 | 0.49 |
| 6:7:128:PRO:CD | 6:7:129:THR:HA | 2.42 | 0.49 |
| 6:7:73:ARG:HA | 6:7:199:ARG:HH22 | 1.78 | 0.49 |
| 7:A:192:ARG:H | 11:E:55:GLN:HE21 | 1.61 | 0.49 |
| 11:E:256:TYR:OH | 11:E:298:GLU:OE1 | 2.22 | 0.49 |
| 1:2:232:ARG:HA | 1:2:283:TYR:CE2 | 2.47 | 0.49 |
| 1:2:582:LYS:HA | 1:2:589:TRP:HA | 1.93 | 0.49 |
| 2:3:252:ASP:OD1 | 2:3:253:HIS:N | 2.46 | 0.49 |
| 2:3:41:SER:O | 2:3:45:ILE:HG12 | 2.12 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:3:50:SER:HA | 2:3:53:ALA:HB3 | 1.95 | 0.49 |
| 3:4:416:SER:OG | 3:4:459:THR:O | 2.26 | 0.49 |
| 3:4:644:VAL:O | 3:4:648:VAL:HG23 | 2.12 | 0.49 |
| 4:5:625:ASN:O | 4:5:629:ILE:HG13 | 2.12 | 0.49 |
| 5:6:126:SER:O | 5:6:132:VAL:HB | 2.12 | 0.49 |
| 5:6:290:ILE:HD13 | 5:6:454:PHE:CE1 | 2.48 | 0.49 |
| 5:6:385:SER:HA | 5:6:388:ARG:HE | 1.78 | 0.49 |
| 5:6:939:TRP:O | 5:6:942:LEU:HB3 | 2.13 | 0.49 |
| 5:6:965:ILE:O | 5:6:969:VAL:HB | 2.13 | 0.49 |
| 2:3:53:ALA:HA | 6:7:218:LYS:CD | 2.42 | 0.49 |
| 3:4:456:LEU:HG | 6:7:254:ALA:HA | 1.94 | 0.49 |
| 6:7:269:VAL:HG21 | 6:7:285:THR:HB | 1.93 | 0.49 |
| 6:7:669:GLN:O | 6:7:673:ARG:N | 2.36 | 0.49 |
| 7:A:100:MET:HE2 | 7:A:117:GLN:HG2 | 1.94 | 0.49 |
| 10:D:67:TRP:HD1 | 10:D:143:TYR:HB2 | 1.78 | 0.49 |
| 11:E:467:THR:O | 11:E:471:LYS:HB2 | 2.12 | 0.49 |
| 11:E:620:VAL:HG13 | 11:E:630:ILE:HD12 | 1.94 | 0.49 |
| 1:2:842:VAL:C | 1:2:846:VAL:HG23 | 2.32 | 0.49 |
| 3:4:331:LEU:HB2 | 3:4:430:GLY:HA2 | 1.94 | 0.49 |
| 4:5:91:GLU:OE2 | 4:5:137:LEU:N | 2.46 | 0.49 |
| 4:5:600:LYS:O | 4:5:604:THR:HG23 | 2.13 | 0.49 |
| 5:6:641:PHE:HD1 | 5:6:682:ALA:HB2 | 1.77 | 0.49 |
| 6:7:21:ILE:HD13 | 6:7:117:PHE:HA | 1.95 | 0.49 |
| 6:7:262:CYS:HA | 6:7:298:LEU:HB3 | 1.93 | 0.49 |
| 6:7:488:SER:OG | 6:7:492:GLY:O | 2.30 | 0.49 |
| 9:C:162:THR:HG21 | 9:C:166:LEU:HD13 | 1.93 | 0.49 |
| 11:E:291:LEU:HD23 | 11:E:294:LEU:HD12 | 1.95 | 0.49 |
| 1:2:326:ARG:NH2 | 1:2:389:THR:HG21 | 2.28 | 0.49 |
| 1:2:442:ASN:OD1 | 1:2:444:PHE:N | 2.41 | 0.49 |
| 1:2:770:ALA:O | 1:2:774:ILE:HG22 | 2.13 | 0.49 |
| 2:3:260:GLU:CD | 2:3:272:ARG:H | 2.16 | 0.49 |
| 2:3:277:ILE:HD12 | 2:3:320:LEU:HD11 | 1.95 | 0.49 |
| 4:5:379:PHE:HD2 | 4:5:568:ILE:HB | 1.77 | 0.49 |
| 4:5:450:THR:HG21 | 4:5:492:ALA:HB3 | 1.95 | 0.49 |
| 5:6:696:ARG:HA | 5:6:706:MET:HE3 | 1.94 | 0.49 |
| 6:7:146:ARG:HH22 | 6:7:304:ALA:HA | 1.78 | 0.49 |
| 6:7:220:ILE:O | 6:7:222:SER:CB | 2.60 | 0.49 |
| 7:A:130:TYR:CG | 10:D:193:LEU:HD22 | 2.48 | 0.49 |
| 8:B:157:LEU:HD21 | 9:C:137:HIS:NE2 | 2.28 | 0.49 |
| 7:A:192:ARG:H | 11:E:55:GLN:NE2 | 2.10 | 0.49 |
| 1:2:636:ILE:HG12 | 1:2:638:THR:HG23 | 1.94 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:3:476:ASP:OD2 | 2:3:517:ASN:N | 2.46 | 0.49 |
| 3:4:754:ALA:O | 3:4:758:ILE:HD12 | 2.13 | 0.49 |
| 1:2:705:ARG:HB2 | 5:6:559:THR:HB | 1.94 | 0.49 |
| 5:6:831:LEU:HB3 | 5:6:835:ILE:HD11 | 1.95 | 0.49 |
| 6:7:228:ARG:HH12 | 6:7:326:HIS:CB | 2.22 | 0.49 |
| 6:7:648:LYS:HE2 | 6:7:704:LEU:HD22 | 1.95 | 0.49 |
| 7:A:126:GLN:OE1 | 10:D:197:SER:OG | 2.22 | 0.49 |
| 8:B:193:ARG:NH1 | 10:D:225:ASN:HB3 | 2.28 | 0.49 |
| 1:2:402:LEU:HD11 | 3:4:660:GLY:HA2 | 1.95 | 0.48 |
| 1:2:850:LYS:HG3 | 1:2:852:SER:H | 1.78 | 0.48 |
| 4:5:578:GLY:O | 4:5:580:ALA:N | 2.45 | 0.48 |
| 5:6:269:ASN:H | 5:6:396:LYS:HE2 | 1.78 | 0.48 |
| 5:6:649:GLN:HB3 | 5:6:705:ILE:HD13 | 1.95 | 0.48 |
| 5:6:777:TYR:HD1 | 5:6:780:LEU:HD13 | 1.78 | 0.48 |
| 6:7:151:GLU:O | 6:7:155:SER:N | 2.45 | 0.48 |
| 6:7:677:SER:O | 6:7:678:LYS:C | 2.49 | 0.48 |
| 7:A:9:LEU:HD21 | 7:A:89:TYR:HB2 | 1.94 | 0.48 |
| 11:E:12:TYR:O | 11:E:16:LEU:HG | 2.13 | 0.48 |
| 11:E:351:TRP:HB3 | 11:E:511:VAL:HG22 | 1.95 | 0.48 |
| 2:3:480:ASP:N | 2:3:480:ASP:OD1 | 2.45 | 0.48 |
| 3:4:341:ASP:HB3 | 3:4:343:LYS:HZ1 | 1.78 | 0.48 |
| 4:5:627:VAL:O | 4:5:631:LYS:HB2 | 2.12 | 0.48 |
| 6:7:217:LYS:O | 6:7:220:ILE:HG12 | 2.12 | 0.48 |
| 6:7:204:PHE:O | 6:7:380:PHE:HB2 | 2.12 | 0.48 |
| 6:7:484:THR:HA | 6:7:524:ASP:H | 1.77 | 0.48 |
| 8:B:14:GLU:O | 8:B:17:GLN:HG2 | 2.12 | 0.48 |
| 10:D:60:PHE:HD1 | 10:D:63:LEU:HD23 | 1.77 | 0.48 |
| 11:E:31:VAL:HG11 | 11:E:477:PHE:CZ | 2.47 | 0.48 |
| 11:E:34:LEU:HD21 | 11:E:432:LEU:HB3 | 1.95 | 0.48 |
| 1:2:607:ASP:HA | 1:2:649:ALA:O | 2.14 | 0.48 |
| 2:3:176:LEU:HD22 | 4:5:250:PHE:CD2 | 2.48 | 0.48 |
| 4:5:652:GLN:O | 4:5:656:ILE:HG13 | 2.14 | 0.48 |
| 6:7:213:ARG:C | 6:7:215:TYR:HB3 | 2.34 | 0.48 |
| 6:7:255:VAL:HG23 | 6:7:258:ILE:CG1 | 2.40 | 0.48 |
| 6:7:618:TYR:HE2 | 6:7:624:LYS:O | 1.96 | 0.48 |
| 6:7:628:LEU:N | 6:7:629:ASP:HA | 2.28 | 0.48 |
| 8:B:198:ALA:CB | 9:C:113:MET:HE3 | 2.43 | 0.48 |
| 10:D:54:VAL:HA | 10:D:86:ARG:HH12 | 1.78 | 0.48 |
| 1:2:572:SER:HB3 | 5:6:662:SER:HB2 | 1.95 | 0.48 |
| 1:2:595:ALA:O | 1:2:598:LEU:HB3 | 2.12 | 0.48 |
| 3:4:258:TYR:CZ | 3:4:308:VAL:HG12 | 2.48 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:4:308:VAL:HG21 | 3:4:325:LEU:HD12 | 1.94 | 0.48 |
| 4:5:21:ASP:O | 4:5:25:THR:N | 2.47 | 0.48 |
| 4:5:568:ILE:HD12 | 4:5:571:HIS:HB3 | 1.96 | 0.48 |
| 5:6:727:LEU:HA | 5:6:731:ILE:HG13 | 1.95 | 0.48 |
| 5:6:732:VAL:O | 5:6:736:MET:HG2 | 2.13 | 0.48 |
| 6:7:135:LYS:HA | 6:7:136:ASP:C | 2.33 | 0.48 |
| 9:C:88:ILE:HD12 | 9:C:127:LEU:HD12 | 1.95 | 0.48 |
| 11:E:545:LEU:HA | 11:E:548:LEU:HB3 | 1.95 | 0.48 |
| 1:2:444:PHE:HB3 | 1:2:445:PRO:HD2 | 1.95 | 0.48 |
| 2:3:360:PHE:CD1 | 2:3:715:VAL:HG11 | 2.46 | 0.48 |
| 2:3:671:LEU:HA | 2:3:721:VAL:HB | 1.94 | 0.48 |
| 4:5:91:GLU:HA | 4:5:94:ILE:HG13 | 1.95 | 0.48 |
| 6:7:380:PHE:CE2 | 6:7:382:ARG:HB2 | 2.47 | 0.48 |
| 6:7:520:ILE:HG13 | 6:7:562:SER:HB2 | 1.95 | 0.48 |
| 6:7:596:ILE:HG23 | 6:7:723:SER:HB3 | 1.94 | 0.48 |
| 8:B:92:TRP:CE2 | 8:B:116:PRO:HG2 | 2.48 | 0.48 |
| 1:2:409:ILE:HB | 1:2:452:GLU:HG2 | 1.96 | 0.48 |
| 2:3:487:HIS:HB3 | 2:3:542:ARG:HH21 | 1.79 | 0.48 |
| 2:3:494:THR:HA | 2:3:508:ALA:H | 1.78 | 0.48 |
| 2:3:95:ARG:NH2 | 2:3:281:ASP:OD1 | 2.47 | 0.48 |
| 4:5:349:PHE:CE2 | 4:5:353:GLU:HB2 | 2.48 | 0.48 |
| 5:6:807:SER:HB2 | 5:6:819:ILE:HG21 | 1.96 | 0.48 |
| 6:7:226:SER:HB2 | 6:7:321:GLN:HB3 | 1.95 | 0.48 |
| 6:7:228:ARG:HH22 | 6:7:326:HIS:HB3 | 1.78 | 0.48 |
| 6:7:463:GLY:C | 6:7:465:ALA:H | 2.17 | 0.48 |
| 8:B:167:HIS:NE2 | 10:D:267:VAL:HG11 | 2.28 | 0.48 |
| 8:B:30:ARG:HD3 | 8:B:66:MET:HE1 | 1.95 | 0.48 |
| 11:E:25:CYS:H | 11:E:26:GLN:CA | 2.26 | 0.48 |
| 11:E:327:PHE:CZ | 11:E:328:LEU:HG | 2.48 | 0.48 |
| 7:A:188:GLN:HG2 | 11:E:478:TRP:CH2 | 2.48 | 0.48 |
| 1:2:829:VAL:HG13 | 1:2:833:ASP:HB2 | 1.96 | 0.48 |
| 3:4:713:ASP:HB2 | 3:4:716:ASN:CB | 2.38 | 0.48 |
| 4:5:407:ARG:CD | 4:5:498:GLU:HA | 2.44 | 0.48 |
| 5:6:516:LEU:O | 5:6:520:VAL:HG13 | 2.14 | 0.48 |
| 5:6:546:GLY:O | 5:6:550:GLN:N | 2.46 | 0.48 |
| 5:6:560:VAL:CB | 5:6:561:GLU:HA | 2.43 | 0.48 |
| 6:7:359:PRO:HA | 6:7:360:TYR:HA | 1.66 | 0.48 |
| 6:7:530:ASP:O | 6:7:534:ARG:NH1 | 2.43 | 0.48 |
| 6:7:535:THR:HA | 6:7:538:HIS:HB3 | 1.95 | 0.48 |
| 10:D:231:HIS:HA | 10:D:274:ILE:HG22 | 1.95 | 0.48 |
| 10:D:70:GLU:O | 10:D:73:SER:OG | 2.22 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 11:E:307:ARG:HD3 | 11:E:308:ASN:H | 1.78 | 0.48 |
| 2:3:340:GLN:HB3 | 2:3:661:GLN:HE22 | 1.78 | 0.48 |
| 2:3:340:GLN:HG2 | 2:3:341:MET:H | 1.78 | 0.48 |
| 2:3:712:HIS:CD2 | 2:3:728:VAL:HG21 | 2.48 | 0.48 |
| 3:4:803:ARG:HA | 3:4:806:GLU:HG2 | 1.94 | 0.48 |
| 4:5:165:ILE:N | 4:5:259:GLN:O | 2.29 | 0.48 |
| 4:5:374:ILE:HG21 | 4:5:388:ILE:HD13 | 1.96 | 0.48 |
| 5:6:289:SER:HA | 5:6:397:PHE:O | 2.14 | 0.48 |
| 6:7:696:SER:HA | 6:7:699:LEU:HB2 | 1.96 | 0.48 |
| 7:A:14:LYS:HA | 9:C:6:ILE:HD13 | 1.96 | 0.48 |
| 9:C:18:CYS:HB3 | 9:C:72:VAL:CG1 | 2.44 | 0.48 |
| 11:E:24:SER:O | 11:E:26:GLN:NE2 | 2.47 | 0.48 |
| 11:E:57:GLN:OE1 | 11:E:58:ILE:N | 2.47 | 0.48 |
| 1:2:640:LEU:HD23 | 1:2:640:LEU:HA | 1.51 | 0.48 |
| 3:4:443:PRO:HD3 | 3:4:457:TYR:CE2 | 2.49 | 0.48 |
| 3:4:572:THR:HG23 | 3:4:708:VAL:HG11 | 1.95 | 0.48 |
| 4:5:413:LEU:HG | 4:5:521:ALA:HB3 | 1.96 | 0.48 |
| 5:6:777:TYR:CG | 5:6:800:LEU:HD13 | 2.49 | 0.48 |
| 10:D:133:LEU:O | 10:D:136:LEU:N | 2.46 | 0.48 |
| 10:D:54:VAL:HA | 10:D:86:ARG:NH1 | 2.28 | 0.48 |
| 11:E:558:GLU:HB2 | 11:E:559:SER:C | 2.33 | 0.48 |
| 11:E:613:THR:HG21 | 11:E:622:ILE:HD11 | 1.94 | 0.48 |
| 2:3:246:GLY:N | 6:7:236:GLY:HA3 | 2.29 | 0.48 |
| 2:3:347:ILE:HD11 | 2:3:662:TYR:CZ | 2.49 | 0.48 |
| 2:3:372:TYR:H | 13:3:1001:ANP:HN62 | 1.62 | 0.48 |
| 2:3:470:VAL:HB | 2:3:512:VAL:HG13 | 1.95 | 0.48 |
| 3:4:324:LYS:NZ | 6:7:138:VAL:HG11 | 2.29 | 0.48 |
| 3:4:354:HIS:HD2 | 3:4:356:MET:HG2 | 1.76 | 0.48 |
| 3:4:592:SER:HA | 3:4:632:ASP:HB2 | 1.96 | 0.48 |
| 5:6:596:VAL:HG21 | 5:6:631:ALA:HB2 | 1.95 | 0.48 |
| 5:6:616:GLU:CB | 5:6:620:ASP:HA | 2.43 | 0.48 |
| 5:6:918:ARG:HD3 | 5:6:918:ARG:HA | 1.71 | 0.48 |
| 6:7:21:ILE:HG12 | 6:7:117:PHE:HD1 | 1.78 | 0.48 |
| 6:7:227:VAL:HA | 6:7:230:ILE:HG13 | 1.95 | 0.48 |
| 8:B:50:TRP:N | 8:B:51:GLN:HA | 2.28 | 0.48 |
| 1:2:580:VAL:HG12 | 1:2:589:TRP:HB3 | 1.96 | 0.47 |
| 1:2:696:ALA:HB1 | 5:6:800:LEU:HD22 | 1.95 | 0.47 |
| 2:3:200:VAL:HG21 | 2:3:247:TYR:CE2 | 2.49 | 0.47 |
| 2:3:255:ARG:O | 2:3:256:ILE:HD13 | 2.14 | 0.47 |
| 3:4:249:LEU:HA | 3:4:250:ALA:HA | 1.61 | 0.47 |
| 5:6:819:ILE:O | 5:6:820:THR:HG23 | 2.14 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:7:257:VAL:H | 6:7:273:VAL:CG2 | 2.25 | 0.47 |
| 8:B:118:ASN:N | 8:B:118:ASN:OD1 | 2.47 | 0.47 |
| 8:B:60:LEU:HB3 | 8:B:63:MET:HG2 | 1.95 | 0.47 |
| 11:E:480:SER:HA | 11:E:483:ALA:HB3 | 1.96 | 0.47 |
| 1:2:408:VAL:HA | 1:2:451:ILE:O | 2.14 | 0.47 |
| 1:2:660:THR:OG1 | 5:6:947:ASP:HA | 2.14 | 0.47 |
| 1:2:785:LYS:HG3 | 1:2:788:ARG:HH21 | 1.78 | 0.47 |
| 2:3:101:ASP:OD2 | 9:C:86:ASN:ND2 | 2.48 | 0.47 |
| 2:3:533:ILE:HG21 | 2:3:540:LEU:HD11 | 1.96 | 0.47 |
| 3:4:633:GLU:N | 3:4:674:SER:O | 2.38 | 0.47 |
| 4:5:294:ILE:HG12 | 4:5:333:ILE:HG13 | 1.96 | 0.47 |
| 4:5:371:THR:HG21 | 4:5:386:LYS:HG2 | 1.96 | 0.47 |
| 4:5:441:GLY:HA3 | 4:5:442:LYS:C | 2.35 | 0.47 |
| 4:5:540:ILE:HG22 | 4:5:546:ILE:HD13 | 1.96 | 0.47 |
| 5:6:591:PHE:CE1 | 5:6:752:ARG:HG3 | 2.49 | 0.47 |
| 5:6:731:ILE:HG22 | 5:6:735:HIS:CD2 | 2.49 | 0.47 |
| 10:D:269:LEU:HA | 10:D:275:TYR:HE2 | 1.76 | 0.47 |
| 11:E:268:SER:O | 11:E:271:TRP:N | 2.48 | 0.47 |
| 11:E:60:PRO:HG3 | 11:E:478:TRP:NE1 | 2.29 | 0.47 |
| 11:E:29:ILE:HD11 | 11:E:58:ILE:HG23 | 1.96 | 0.47 |
| 1:2:264:PRO:HD2 | 1:2:315:SER:O | 2.14 | 0.47 |
| 1:2:566:ALA:C | 1:2:572:SER:HB2 | 2.35 | 0.47 |
| 1:2:585:ILE:HG23 | 1:2:586:THR:H | 1.78 | 0.47 |
| 2:3:25:VAL:CG2 | 2:3:124:PRO:CB | 2.92 | 0.47 |
| 2:3:172:THR:OG1 | 2:3:173:ALA:HA | 2.14 | 0.47 |
| 2:3:21:PHE:O | 2:3:25:VAL:HG23 | 2.13 | 0.47 |
| 3:4:228:LYS:HA | 3:4:231:ASN:HB2 | 1.95 | 0.47 |
| 3:4:330:GLY:HA2 | 3:4:403:PRO:CD | 2.43 | 0.47 |
| 3:4:386:HIS:CE1 | 5:6:405:PRO:HD3 | 2.48 | 0.47 |
| 6:7:567:ALA:O | 6:7:569:PRO:HD3 | 2.14 | 0.47 |
| 8:B:56:ASP:N | 8:B:56:ASP:OD1 | 2.35 | 0.47 |
| 10:D:79:TYR:CE2 | 10:D:81:HIS:HB3 | 2.49 | 0.47 |
| 1:2:338:LYS:O | 1:2:378:GLU:N | 2.26 | 0.47 |
| 1:2:379:LYS:NZ | 4:5:82:GLU:OE2 | 2.46 | 0.47 |
| 1:2:525:LYS:HE2 | 4:5:576:HIS:ND1 | 2.30 | 0.47 |
| 1:2:525:LYS:HE3 | 4:5:576:HIS:O | 2.13 | 0.47 |
| 2:3:234:GLU:OE1 | 2:3:240:LYS:HD2 | 2.14 | 0.47 |
| 2:3:405:ILE:HB | 2:3:513:ILE:HG12 | 1.96 | 0.47 |
| 3:4:631:ILE:O | 3:4:674:SER:N | 2.48 | 0.47 |
| 3:4:775:VAL:O | 3:4:779:LYS:N | 2.45 | 0.47 |
| 3:4:821:ASP:N | 3:4:821:ASP:OD1 | 2.47 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:5:21:ASP:OD1 | 4:5:21:ASP:N | 2.47 | 0.47 |
| 4:5:253:GLN:HE21 | 4:5:277:THR:CB | 2.27 | 0.47 |
| 5:6:659:GLN:HG3 | 5:6:675:ARG:HA | 1.96 | 0.47 |
| 6:7:650:PRO:HG3 | 6:7:700:ALA:HB3 | 1.95 | 0.47 |
| 7:A:110:MET:N | 7:A:111:SER:HA | 2.27 | 0.47 |
| 7:A:175:GLN:CB | 7:A:180:VAL:HA | 2.44 | 0.47 |
| 9:C:172:MET:O | 9:C:176:ILE:HG23 | 2.14 | 0.47 |
| 10:D:260:ILE:HG23 | 10:D:261:PRO:HD2 | 1.97 | 0.47 |
| 11:E:370:LEU:O | 11:E:374:GLN:HG2 | 2.15 | 0.47 |
| 1:2:550:SER:OG | 13:2:901:ANP:O1G | 2.26 | 0.47 |
| 3:4:854:LYS:HE2 | 3:4:857:ILE:HD11 | 1.97 | 0.47 |
| 4:5:382:GLU:HA | 4:5:385:LYS:HB3 | 1.97 | 0.47 |
| 4:5:422:LYS:HA | 4:5:425:LEU:HB3 | 1.95 | 0.47 |
| 5:6:614:ARG:CZ | 5:6:614:ARG:HB3 | 2.44 | 0.47 |
| 5:6:665:LYS:HD3 | 5:6:665:LYS:HA | 1.72 | 0.47 |
| 5:6:776:LYS:O | 5:6:780:LEU:N | 2.47 | 0.47 |
| 5:6:761:PHE:HB2 | 5:6:812:ARG:HE | 1.79 | 0.47 |
| 6:7:107:GLN:HA | 6:7:238:LEU:HB3 | 1.96 | 0.47 |
| 6:7:114:THR:HG23 | 6:7:204:PHE:HE2 | 1.79 | 0.47 |
| 6:7:437:VAL:HG12 | 6:7:701:LYS:HZ1 | 1.80 | 0.47 |
| 6:7:87:GLN:O | 6:7:90:ASN:HB2 | 2.15 | 0.47 |
| 7:A:185:LYS:HD2 | 7:A:186:ASP:N | 2.29 | 0.47 |
| 2:3:260:GLU:OE1 | 2:3:260:GLU:N | 2.40 | 0.47 |
| 2:3:389:VAL:HG21 | 2:3:669:PRO:HD2 | 1.95 | 0.47 |
| 3:4:796:ARG:O | 3:4:799:GLU:HB3 | 2.15 | 0.47 |
| 2:3:317:PHE:HE2 | 4:5:176:ALA:HB2 | 1.80 | 0.47 |
| 4:5:566:ILE:O | 4:5:570:ASN:HB2 | 2.15 | 0.47 |
| 4:5:635:ILE:HA | 4:5:638:LEU:HG | 1.96 | 0.47 |
| 5:6:126:SER:HB3 | 5:6:131:GLU:HB3 | 1.96 | 0.47 |
| 5:6:298:SER:O | 5:6:357:GLN:HB2 | 2.15 | 0.47 |
| 6:7:18:PHE:CE1 | 6:7:120:ALA:HB2 | 2.50 | 0.47 |
| 6:7:455:ASN:HA | 6:7:563:ILE:O | 2.13 | 0.47 |
| 9:C:7:ASP:HA | 9:C:10:LEU:HB3 | 1.95 | 0.47 |
| 9:C:58:GLY:HA3 | 9:C:69:VAL:O | 2.15 | 0.47 |
| 11:E:280:LEU:O | 11:E:283:ALA:N | 2.42 | 0.47 |
| 11:E:359:LEU:O | 11:E:362:MET:HB2 | 2.15 | 0.47 |
| 1:2:828:PHE:CE2 | 11:E:516:LYS:HG2 | 2.49 | 0.47 |
| 11:E:519:ILE:HA | 11:E:528:CYS:SG | 2.55 | 0.47 |
| 1:2:432:ASN:N | 1:2:432:ASN:OD1 | 2.48 | 0.47 |
| 1:2:435:ASP:HB3 | 1:2:447:PHE:HE1 | 1.79 | 0.47 |
| 1:2:796:GLU:O | 1:2:799:SER:HB2 | 2.14 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:3:201:HIS:NE2 | 2:3:232:PRO:HD2 | 2.29 | 0.47 |
| 4:5:22:ASP:HA | 4:5:25:THR:HB | 1.95 | 0.47 |
| 4:5:149:ARG:NH2 | 4:5:269:GLU:OE1 | 2.48 | 0.47 |
| 4:5:382:GLU:O | 4:5:386:LYS:HG3 | 2.15 | 0.47 |
| 5:6:313:MET:HA | 5:6:314:CYS:HA | 1.62 | 0.47 |
| 5:6:368:ILE:HG21 | 5:6:374:PRO:HB3 | 1.97 | 0.47 |
| 5:6:603:SER:N | 5:6:604:SER:HA | 2.17 | 0.47 |
| 7:A:23:SER:N | 7:A:24:ASN:HA | 2.29 | 0.47 |
| 10:D:137:LYS:HG2 | 10:D:141:ARG:HH12 | 1.80 | 0.47 |
| 11:E:222:LYS:HA | 11:E:225:GLN:HB3 | 1.97 | 0.47 |
| 11:E:41:ALA:HB1 | 11:E:255:ILE:HD12 | 1.95 | 0.47 |
| 11:E:284:TYR:HB2 | 11:E:285:ALA:H | 1.56 | 0.47 |
| 11:E:32:SER:HA | 11:E:33:CYS:HA | 1.41 | 0.47 |
| 11:E:372:THR:HG23 | 11:E:375:GLU:OE1 | 2.15 | 0.47 |
| 1:2:232:ARG:HG3 | 1:2:283:TYR:OH | 2.14 | 0.47 |
| 2:3:200:VAL:HG21 | 2:3:247:TYR:HD2 | 1.80 | 0.47 |
| 2:3:662:TYR:HE1 | 2:3:666:ARG:HD2 | 1.79 | 0.47 |
| 3:4:330:GLY:O | 3:4:399:LEU:HD11 | 2.15 | 0.47 |
| 4:5:299:SER:OG | 4:5:300:ILE:N | 2.48 | 0.47 |
| 1:2:676:ARG:HH12 | 4:5:418:PRO:HB2 | 1.79 | 0.47 |
| 5:6:753:ARG:HA | 5:6:756:LYS:HE2 | 1.96 | 0.47 |
| 5:6:945:GLU:HA | 5:6:948:LEU:HD13 | 1.97 | 0.47 |
| 5:6:943:GLN:HA | 5:6:946:ASN:ND2 | 2.29 | 0.47 |
| 6:7:519:GLY:O | 6:7:562:SER:N | 2.39 | 0.47 |
| 6:7:645:ALA:HB1 | 6:7:701:LYS:CB | 2.44 | 0.47 |
| 11:E:89:VAL:O | 11:E:130:ASN:ND2 | 2.48 | 0.47 |
| 11:E:264:GLU:N | 11:E:264:GLU:OE1 | 2.44 | 0.47 |
| 11:E:28:VAL:HG12 | 11:E:29:ILE:O | 2.15 | 0.47 |
| 11:E:566:PRO:HB2 | 11:E:605:PHE:HE2 | 1.76 | 0.47 |
| 1:2:567:THR:HG22 | 1:2:572:SER:HB2 | 1.96 | 0.47 |
| 3:4:629:CYS:SG | 3:4:630:CYS:N | 2.87 | 0.47 |
| 3:4:689:THR:OG1 | 3:4:851:GLN:N | 2.40 | 0.47 |
| 4:5:473:ASP:HA | 4:5:517:THR:HG22 | 1.95 | 0.47 |
| 4:5:379:PHE:CD2 | 4:5:568:ILE:HB | 2.49 | 0.47 |
| 4:5:575:ILE:HG13 | 4:5:581:ASN:HD22 | 1.78 | 0.47 |
| 4:5:98:ALA:O | 4:5:102:SER:N | 2.42 | 0.47 |
| 5:6:371:GLY:HA3 | 6:7:554:ASN:OD1 | 2.15 | 0.47 |
| 5:6:608:LEU:HA | 5:6:627:ALA:HB3 | 1.96 | 0.47 |
| 5:6:711:LEU:HB3 | 5:6:713:PHE:CE1 | 2.50 | 0.47 |
| 6:7:441:ASP:H | 6:7:452:GLY:HA2 | 1.78 | 0.47 |
| 6:7:485:GLY:H | 6:7:525:GLU:HB2 | 1.80 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:B:94:THR:O | 8:B:98:LEU:HG | 2.15 | 0.47 |
| 9:C:101:ASN:HD22 | 9:C:104:PHE:HB2 | 1.79 | 0.47 |
| 11:E:419:ILE:HG22 | 11:E:420:SER:O | 2.14 | 0.47 |
| 11:E:489:VAL:HG12 | 11:E:493:ASN:HD21 | 1.79 | 0.47 |
| 4:5:344:ASN:N | 4:5:345:SER:HA | 2.29 | 0.47 |
| 4:5:353:GLU:O | 4:5:357:PHE:N | 2.43 | 0.47 |
| 1:2:580:VAL:HG21 | 4:5:446:ALA:HB1 | 1.95 | 0.47 |
| 4:5:514:ASN:OD1 | 4:5:516:ARG:NH2 | 2.48 | 0.47 |
| 5:6:122:PHE:HA | 5:6:123:SER:CB | 2.45 | 0.47 |
| 5:6:529:LEU:O | 5:6:533:ILE:CG1 | 2.62 | 0.47 |
| 5:6:656:MET:SD | 5:6:678:ILE:HG13 | 2.55 | 0.47 |
| 5:6:964:VAL:HG13 | 5:6:967:ARG:NE | 2.30 | 0.47 |
| 6:7:476:ILE:N | 6:7:476:ILE:CD1 | 2.73 | 0.47 |
| 6:7:489:SER:O | 6:7:493:LEU:HD21 | 2.13 | 0.47 |
| 7:A:103:ASN:OD1 | 7:A:104:ASN:N | 2.44 | 0.47 |
| 8:B:184:PHE:O | 8:B:188:ILE:CD1 | 2.63 | 0.47 |
| 1:2:323:VAL:HG23 | 1:2:393:ALA:HB2 | 1.97 | 0.47 |
| 2:3:101:ASP:OD1 | 2:3:104:ARG:NH2 | 2.48 | 0.47 |
| 2:3:389:VAL:HG12 | 2:3:390:GLU:N | 2.23 | 0.47 |
| 3:4:258:TYR:OH | 3:4:308:VAL:HG12 | 2.15 | 0.47 |
| 3:4:618:SER:HB3 | 3:4:622:VAL:HB | 1.95 | 0.47 |
| 4:5:166:ILE:HG12 | 4:5:258:LEU:HB3 | 1.97 | 0.47 |
| 4:5:384:ILE:HG13 | 4:5:554:PHE:CD2 | 2.43 | 0.47 |
| 4:5:565:ASP:O | 4:5:568:ILE:N | 2.48 | 0.47 |
| 5:6:174:TYR:O | 5:6:178:LEU:HD12 | 2.15 | 0.47 |
| 5:6:363:GLU:HB3 | 5:6:374:PRO:HB2 | 1.96 | 0.47 |
| 5:6:660:THR:HG22 | 5:6:673:ASN:HA | 1.96 | 0.47 |
| 5:6:758:ALA:HA | 5:6:761:PHE:CE2 | 2.49 | 0.47 |
| 6:7:454:ILE:HG22 | 6:7:456:VAL:HG23 | 1.96 | 0.47 |
| 8:B:151:ILE:O | 8:B:154:ILE:HG13 | 2.14 | 0.47 |
| 10:D:159:ARG:NH2 | 10:D:187:SER:OG | 2.48 | 0.47 |
| 11:E:158:ALA:HB2 | 11:E:237:LEU:HD13 | 1.97 | 0.47 |
| 11:E:641:LEU:O | 11:E:645:THR:HG23 | 2.15 | 0.47 |
| 1:2:270:ILE:O | 1:2:274:VAL:HG23 | 2.15 | 0.46 |
| 1:2:337:VAL:HB | 1:2:351:PHE:H | 1.79 | 0.46 |
| 2:3:104:ARG:HH22 | 9:C:86:ASN:HB2 | 1.79 | 0.46 |
| 3:4:794:THR:HG23 | 3:4:796:ARG:H | 1.79 | 0.46 |
| 3:4:910:LEU:O | 3:4:915:LYS:N | 2.32 | 0.46 |
| 4:5:184:ARG:HH21 | 4:5:242:ILE:HD11 | 1.80 | 0.46 |
| 5:6:288:LEU:O | 5:6:399:GLY:N | 2.48 | 0.46 |
| 5:6:713:PHE:HA | 5:6:834:SER:OG | 2.16 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:6:777:TYR:O | 5:6:780:LEU:HB3 | 2.14 | 0.46 |
| 6:7:459:MET:HG3 | 6:7:460:GLY:N | 2.30 | 0.46 |
| 7:A:27:VAL:HG11 | 7:A:100:MET:CE | 2.45 | 0.46 |
| 7:A:151:LEU:O | 10:D:145:ARG:NH1 | 2.48 | 0.46 |
| 10:D:260:ILE:HD12 | 10:D:260:ILE:H | 1.80 | 0.46 |
| 11:E:164:GLU:OE1 | 11:E:164:GLU:N | 2.46 | 0.46 |
| 1:2:549:LYS:HG3 | 1:2:550:SER:H | 1.81 | 0.46 |
| 3:4:666:ASN:HD22 | 3:4:668:ARG:HH22 | 1.61 | 0.46 |
| 5:6:130:GLY:CA | 5:6:131:GLU:HB3 | 2.45 | 0.46 |
| 5:6:361:ILE:HD12 | 5:6:397:PHE:CE2 | 2.45 | 0.46 |
| 8:B:7:LEU:HD22 | 8:B:10:THR:HG23 | 1.98 | 0.46 |
| 10:D:212:THR:H | 10:D:213:GLU:HA | 1.79 | 0.46 |
| 10:D:237:ASP:OD2 | 10:D:248:GLU:N | 2.48 | 0.46 |
| 2:3:151:HIS:CG | 2:3:152:PRO:HD2 | 2.50 | 0.46 |
| 3:4:573:SER:HA | 3:4:576:GLN:HG2 | 1.96 | 0.46 |
| 3:4:646:HIS:HE1 | 3:4:698:LEU:HD13 | 1.79 | 0.46 |
| 3:4:613:GLN:OE1 | 5:6:360:ARG:NH1 | 2.49 | 0.46 |
| 5:6:689:TYR:CD2 | 5:6:716:LEU:HD12 | 2.50 | 0.46 |
| 5:6:727:LEU:HB3 | 5:6:731:ILE:HD12 | 1.97 | 0.46 |
| 7:A:98:ASP:O | 7:A:102:TRP:HD1 | 1.98 | 0.46 |
| 8:B:92:TRP:CH2 | 8:B:93:LEU:HD12 | 2.50 | 0.46 |
| 9:C:16:PHE:CZ | 9:C:107:LEU:HD21 | 2.50 | 0.46 |
| 10:D:268:GLU:O | 10:D:269:LEU:HD22 | 2.16 | 0.46 |
| 11:E:320:ILE:HG22 | 11:E:409:PHE:HD1 | 1.80 | 0.46 |
| 1:2:296:ARG:HD2 | 1:2:414:LEU:HD21 | 1.97 | 0.46 |
| 1:2:487:ILE:O | 1:2:493:ILE:HG21 | 2.15 | 0.46 |
| 2:3:490:MET:HB2 | 2:3:542:ARG:HD2 | 1.97 | 0.46 |
| 2:3:680:VAL:HG13 | 6:7:613:ALA:HB3 | 1.96 | 0.46 |
| 3:4:572:THR:CG2 | 3:4:708:VAL:HG11 | 2.45 | 0.46 |
| 4:5:176:ALA:HA | 4:5:250:PHE:CE1 | 2.51 | 0.46 |
| 4:5:360:LEU:HB3 | 4:5:366:LEU:HD22 | 1.97 | 0.46 |
| 4:5:50:LEU:HD11 | 4:5:135:PHE:CZ | 2.51 | 0.46 |
| 4:5:660:THR:HG22 | 4:5:677:VAL:HG13 | 1.98 | 0.46 |
| 5:6:186:ARG:O | 5:6:190:ARG:HB2 | 2.16 | 0.46 |
| 5:6:689:TYR:HB3 | 5:6:691:ARG:HD3 | 1.97 | 0.46 |
| 5:6:950:SER:HB2 | 5:6:953:GLU:HG2 | 1.98 | 0.46 |
| 6:7:467:SER:O | 6:7:471:LYS:HB2 | 2.14 | 0.46 |
| 6:7:669:GLN:O | 6:7:673:ARG:HG2 | 2.16 | 0.46 |
| 6:7:714:GLU:HA | 6:7:717:LEU:HB2 | 1.96 | 0.46 |
| 7:A:105:ASN:ND2 | 7:A:110:MET:SD | 2.88 | 0.46 |
| 7:A:171:ALA:HA | 7:A:172:GLY:HA3 | 1.68 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:E:155:GLN:HA | 11:E:158:ALA:CB | 2.46 | 0.46 |
| 11:E:234:GLU:O | 11:E:238:GLU:HB2 | 2.16 | 0.46 |
| 11:E:376:THR:HG22 | 11:E:378:LEU:H | 1.80 | 0.46 |
| 11:E:316:LEU:HD21 | 11:E:413:LEU:C | 2.34 | 0.46 |
| 1:2:428:GLY:CA | 1:2:453:ALA:HA | 2.37 | 0.46 |
| 2:3:384:MET:HA | 2:3:403:ILE:HD13 | 1.98 | 0.46 |
| 3:4:447:ASN:N | 3:4:448:SER:HA | 2.29 | 0.46 |
| 3:4:570:PRO:HD3 | 3:4:680:SER:HB2 | 1.97 | 0.46 |
| 4:5:375:ALA:CB | 4:5:378:ILE:HB | 2.45 | 0.46 |
| 4:5:425:LEU:O | 4:5:429:VAL:HG23 | 2.16 | 0.46 |
| 4:5:493:ILE:O | 4:5:497:MET:HG3 | 2.16 | 0.46 |
| 5:6:122:PHE:CB | 5:6:124:VAL:HB | 2.45 | 0.46 |
| 5:6:357:GLN:HG2 | 5:6:386:VAL:HG23 | 1.96 | 0.46 |
| 8:B:184:PHE:CZ | 9:C:132:ALA:HB1 | 2.50 | 0.46 |
| 8:B:18:PHE:HE1 | 10:D:135:ARG:HG2 | 1.80 | 0.46 |
| 10:D:195:ASN:HA | 10:D:199:LEU:HB2 | 1.97 | 0.46 |
| 10:D:255:CYS:HB2 | 10:D:270:THR:HG22 | 1.98 | 0.46 |
| 11:E:120:ILE:HB | 11:E:139:ILE:O | 2.15 | 0.46 |
| 3:4:566:LEU:HG | 3:4:672:LEU:HD21 | 1.97 | 0.46 |
| 5:6:397:PHE:HD1 | 5:6:459:VAL:HG22 | 1.80 | 0.46 |
| 7:A:187:SER:OG | 11:E:57:GLN:NE2 | 2.43 | 0.46 |
| 7:A:67:VAL:O | 7:A:70:CYS:HB2 | 2.15 | 0.46 |
| 8:B:184:PHE:CE1 | 8:B:188:ILE:HD11 | 2.51 | 0.46 |
| 8:B:187:GLU:CD | 9:C:176:ILE:HG22 | 2.36 | 0.46 |
| 10:D:135:ARG:CZ | 10:D:135:ARG:HB3 | 2.46 | 0.46 |
| 10:D:257:THR:O | 10:D:269:LEU:HB2 | 2.15 | 0.46 |
| 11:E:353:GLU:O | 11:E:356:LYS:HB3 | 2.16 | 0.46 |
| 11:E:466:LEU:O | 11:E:470:ARG:HG3 | 2.16 | 0.46 |
| 1:2:210:GLU:O | 1:2:213:SER:HB3 | 2.15 | 0.46 |
| 1:2:813:ILE:HD12 | 1:2:841:VAL:CG2 | 2.42 | 0.46 |
| 1:2:812:SER:O | 1:2:816:ILE:HG13 | 2.16 | 0.46 |
| 2:3:195:LYS:HZ1 | 2:3:218:THR:HG1 | 1.61 | 0.46 |
| 5:6:801:GLU:OE1 | 5:6:805:ARG:NH2 | 2.44 | 0.46 |
| 5:6:909:TYR:HA | 5:6:912:MET:HB2 | 1.98 | 0.46 |
| 7:A:133:GLU:O | 7:A:136:ASP:HB2 | 2.15 | 0.46 |
| 7:A:102:TRP:CZ3 | 7:A:151:LEU:HD23 | 2.51 | 0.46 |
| 9:C:53:ILE:HG12 | 9:C:54:LEU:N | 2.31 | 0.46 |
| 10:D:162:ASN:HA | 10:D:169:ILE:HG23 | 1.98 | 0.46 |
| 11:E:140:ILE:HA | 11:E:141:GLN:CB | 2.43 | 0.46 |
| 1:2:624:MET:HB2 | 1:2:624:MET:HE3 | 1.83 | 0.46 |
| 3:4:428:ARG:HE | 5:6:369:PRO:CG | 2.29 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:4:563:ASN:OD1 | 3:4:563:ASN:N | 2.47 | 0.46 |
| 4:5:353:GLU:O | 4:5:356:GLU:HG2 | 2.15 | 0.46 |
| 4:5:439:THR:H | 4:5:478:CYS:HB2 | 1.80 | 0.46 |
| 4:5:409:ASP:O | 4:5:518:SER:HB2 | 2.16 | 0.46 |
| 5:6:302:PRO:HB2 | 5:6:353:PHE:CD2 | 2.50 | 0.46 |
| 5:6:356:TRP:CZ3 | 5:6:380:ILE:HB | 2.51 | 0.46 |
| 5:6:730:HIS:CE1 | 5:6:734:LEU:HD21 | 2.51 | 0.46 |
| 5:6:767:LYS:HG2 | 5:6:769:ALA:H | 1.81 | 0.46 |
| 5:6:811:ALA:O | 5:6:815:CYS:N | 2.49 | 0.46 |
| 11:E:358:ARG:O | 11:E:361:LYS:HB3 | 2.15 | 0.46 |
| 11:E:625:PHE:CE1 | 11:E:626:GLU:HB2 | 2.51 | 0.46 |
| 1:2:533:ILE:HD13 | 4:5:576:HIS:NE2 | 2.30 | 0.46 |
| 1:2:856:GLN:NE2 | 1:2:859:ARG:HH21 | 2.09 | 0.46 |
| 2:3:29:GLN:O | 2:3:32:LEU:HB2 | 2.16 | 0.46 |
| 2:3:566:LEU:HB3 | 4:5:619:ALA:HB1 | 1.98 | 0.46 |
| 3:4:397:ILE:HB | 3:4:417:LEU:HD11 | 1.98 | 0.46 |
| 3:4:821:ASP:OD1 | 3:4:822:VAL:HG23 | 2.16 | 0.46 |
| 4:5:396:SER:HB3 | 4:5:661:GLU:CD | 2.36 | 0.46 |
| 4:5:412:VAL:HB | 4:5:520:LEU:HG | 1.97 | 0.46 |
| 4:5:411:ASN:ND2 | 4:5:519:VAL:HB | 2.30 | 0.46 |
| 5:6:566:ARG:HA | 5:6:567:GLY:HA3 | 1.73 | 0.46 |
| 6:7:143:LEU:O | 6:7:146:ARG:HB2 | 2.16 | 0.46 |
| 6:7:493:LEU:HD11 | 6:7:533:ASP:HA | 1.98 | 0.46 |
| 6:7:656:VAL:HG11 | 6:7:708:VAL:O | 2.16 | 0.46 |
| 7:A:107:LEU:HD21 | 7:A:152:SER:C | 2.36 | 0.46 |
| 8:B:198:ALA:HB1 | 9:C:113:MET:SD | 2.56 | 0.46 |
| 9:C:46:LEU:HB3 | 9:C:50:LEU:HD11 | 1.98 | 0.46 |
| 11:E:130:ASN:OD1 | 11:E:131:LEU:N | 2.48 | 0.46 |
| 11:E:133:ASN:O | 11:E:140:ILE:CD1 | 2.64 | 0.46 |
| 11:E:256:TYR:HB2 | 11:E:273:ASN:OD1 | 2.16 | 0.46 |
| 11:E:524:ILE:HB | 11:E:525:TYR:HD2 | 1.80 | 0.46 |
| 1:2:519:LEU:HD21 | 1:2:559:THR:HG21 | 1.98 | 0.46 |
| 2:3:520:PHE:HB3 | 2:3:527:ARG:HH22 | 1.80 | 0.46 |
| 3:4:419:VAL:HG23 | 3:4:420:TYR:N | 2.31 | 0.46 |
| 3:4:550:LYS:HE2 | 3:4:558:TYR:CD2 | 2.49 | 0.46 |
| 3:4:603:ALA:HA | 3:4:617:GLU:O | 2.16 | 0.46 |
| 3:4:501:ILE:HG23 | 3:4:749:MET:HE3 | 1.97 | 0.46 |
| 4:5:41:ASP:HA | 4:5:42:SER:HA | 1.66 | 0.46 |
| 4:5:496:ALA:HB2 | 4:5:502:ILE:HG12 | 1.98 | 0.46 |
| 4:5:578:GLY:O | 4:5:579:ASN:OD1 | 2.35 | 0.46 |
| 4:5:420:THR:N | 13:5:801:ANP:O2A | 2.49 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:6:714:VAL:HB | 5:6:837:ARG:HB3 | 1.98 | 0.46 |
| 6:7:26:VAL:H | 6:7:63:TYR:CB | 2.28 | 0.46 |
| 8:B:97:GLU:OE2 | 8:B:101:LYS:NZ | 2.39 | 0.46 |
| 10:D:75:GLU:OE1 | 10:D:222:PRO:HA | 2.16 | 0.46 |
| 11:E:133:ASN:O | 11:E:142:CYS:HB3 | 2.16 | 0.46 |
| 11:E:150:ASP:N | 11:E:151:THR:HA | 2.31 | 0.46 |
| 11:E:28:VAL:HG13 | 11:E:57:GLN:O | 2.15 | 0.46 |
| 11:E:26:GLN:CB | 11:E:78:ILE:HA | 2.39 | 0.46 |
| 1:2:494:ILE:O | 1:2:498:ILE:HG13 | 2.16 | 0.45 |
| 1:2:657:TYR:HE2 | 1:2:660:THR:HG22 | 1.81 | 0.45 |
| 1:2:520:PHE:CE2 | 1:2:822:LYS:HB3 | 2.50 | 0.45 |
| 2:3:435:ARG:HA | 2:3:436:GLY:HA3 | 1.54 | 0.45 |
| 2:3:565:VAL:O | 2:3:568:THR:HB | 2.16 | 0.45 |
| 3:4:199:MET:H | 3:4:227:ILE:HG12 | 1.80 | 0.45 |
| 3:4:467:LYS:HG3 | 3:4:468:LYS:HB2 | 1.97 | 0.45 |
| 4:5:300:ILE:HD13 | 4:5:326:PRO:HA | 1.97 | 0.45 |
| 4:5:68:LEU:HD21 | 4:5:76:TYR:HB2 | 1.98 | 0.45 |
| 5:6:270:LEU:H | 5:6:396:LYS:NZ | 2.14 | 0.45 |
| 5:6:532:SER:HB2 | 5:6:746:PHE:HB2 | 1.96 | 0.45 |
| 5:6:555:VAL:HG13 | 5:6:808:GLU:HG2 | 1.97 | 0.45 |
| 6:7:422:ILE:HD13 | 6:7:469:LEU:CD1 | 2.46 | 0.45 |
| 6:7:411:TYR:HD1 | 6:7:702:LEU:HD13 | 1.82 | 0.45 |
| 7:A:163:ILE:HG22 | 7:A:164:ASP:H | 1.80 | 0.45 |
| 7:A:185:LYS:HD2 | 7:A:186:ASP:H | 1.80 | 0.45 |
| 7:A:130:TYR:HB2 | 10:D:193:LEU:HD13 | 1.98 | 0.45 |
| 11:E:81:LEU:HB3 | 11:E:120:ILE:HA | 1.98 | 0.45 |
| 11:E:349:SER:HB3 | 11:E:352:ASN:ND2 | 2.31 | 0.45 |
| 11:E:483:ALA:HA | 11:E:491:LEU:HD11 | 1.97 | 0.45 |
| 11:E:637:LEU:O | 11:E:641:LEU:HG | 2.16 | 0.45 |
| 1:2:432:ASN:HA | 1:2:448:ALA:O | 2.16 | 0.45 |
| 1:2:479:GLU:H | 1:2:479:GLU:CD | 2.17 | 0.45 |
| 1:2:520:PHE:CD1 | 1:2:823:MET:HG2 | 2.52 | 0.45 |
| 2:3:28:PHE:O | 2:3:31:PHE:HB3 | 2.16 | 0.45 |
| 3:4:257:LEU:HD12 | 3:4:260:GLN:HB2 | 1.97 | 0.45 |
| 3:4:410:GLN:OE1 | 3:4:411:THR:HG22 | 2.16 | 0.45 |
| 4:5:479:ILE:O | 4:5:522:ALA:HB3 | 2.16 | 0.45 |
| 1:2:778:LEU:H | 4:5:577:THR:HG21 | 1.81 | 0.45 |
| 3:4:336:THR:O | 5:6:375:ARG:NH1 | 2.49 | 0.45 |
| 5:6:558:SER:CB | 5:6:559:THR:HA | 2.28 | 0.45 |
| 5:6:941:LEU:HD13 | 5:6:958:ARG:NH2 | 2.31 | 0.45 |
| 8:B:24:PRO:HB2 | 8:B:70:GLU:OE2 | 2.15 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:C:105:PHE:CZ | 9:C:127:LEU:HD22 | 2.48 | 0.45 |
| 1:2:624:MET:HG2 | 1:2:646:ILE:CD1 | 2.47 | 0.45 |
| 3:4:779:LYS:HD2 | 3:4:779:LYS:HA | 1.71 | 0.45 |
| 4:5:146:ILE:HD12 | 4:5:160:VAL:HG13 | 1.99 | 0.45 |
| 4:5:143:ALA:HB3 | 4:5:161:ARG:CD | 2.46 | 0.45 |
| 5:6:777:TYR:CD1 | 5:6:780:LEU:HD13 | 2.51 | 0.45 |
| 5:6:956:GLU:O | 5:6:960:LEU:HB2 | 2.16 | 0.45 |
| 6:7:203:TYR:HE2 | 6:7:338:THR:HB | 1.81 | 0.45 |
| 6:7:273:VAL:O | 6:7:273:VAL:HG12 | 2.16 | 0.45 |
| 6:7:334:HIS:O | 6:7:378:ALA:N | 2.46 | 0.45 |
| 6:7:451:ARG:HA | 6:7:452:GLY:HA3 | 1.64 | 0.45 |
| 7:A:199:LEU:CB | 7:A:205:LEU:HG | 2.45 | 0.45 |
| 10:D:230:ILE:HA | 10:D:293:LEU:HA | 1.97 | 0.45 |
| 8:B:167:HIS:NE2 | 10:D:267:VAL:CG1 | 2.79 | 0.45 |
| 11:E:25:CYS:H | 11:E:26:GLN:CB | 2.30 | 0.45 |
| 11:E:288:TYR:HA | 11:E:291:LEU:HB2 | 1.98 | 0.45 |
| 11:E:493:ASN:HA | 11:E:496:ILE:HD12 | 1.99 | 0.45 |
| 1:2:828:PHE:CZ | 11:E:516:LYS:HG2 | 2.52 | 0.45 |
| 11:E:536:LEU:HD13 | 11:E:536:LEU:HA | 1.78 | 0.45 |
| 12:F:12:DT:H1' | 12:F:13:DT:OP2 | 2.15 | 0.45 |
| 1:2:788:ARG:O | 1:2:791:ALA:HB3 | 2.16 | 0.45 |
| 1:2:839:LYS:HD2 | 1:2:839:LYS:HA | 1.61 | 0.45 |
| 2:3:533:ILE:O | 2:3:534:ALA:HB3 | 2.16 | 0.45 |
| 3:4:373:ARG:HD3 | 3:4:373:ARG:HA | 1.54 | 0.45 |
| 4:5:149:ARG:NH1 | 4:5:272:ARG:HG3 | 2.32 | 0.45 |
| 4:5:398:LYS:NZ | 4:5:613:ARG:HD2 | 2.31 | 0.45 |
| 4:5:442:LYS:O | 4:5:449:LEU:HD12 | 2.17 | 0.45 |
| 4:5:497:MET:HG2 | 4:5:519:VAL:HG21 | 1.99 | 0.45 |
| 4:5:537:GLY:C | 4:5:539:ASN:H | 2.19 | 0.45 |
| 5:6:791:SER:CB | 5:6:835:ILE:HG22 | 2.41 | 0.45 |
| 6:7:677:SER:O | 6:7:680:SER:N | 2.49 | 0.45 |
| 6:7:87:GLN:OE1 | 6:7:214:ARG:NH1 | 2.49 | 0.45 |
| 7:A:135:CYS:O | 7:A:139:THR:HG23 | 2.17 | 0.45 |
| 8:B:30:ARG:NH1 | 8:B:66:MET:HE1 | 2.30 | 0.45 |
| 9:C:6:ILE:HG13 | 9:C:7:ASP:N | 2.32 | 0.45 |
| 10:D:215:SER:HA | 10:D:216:VAL:HA | 1.55 | 0.45 |
| 10:D:83:LEU:O | 10:D:86:ARG:HG2 | 2.16 | 0.45 |
| 1:2:216:LEU:HD12 | 1:2:217:GLU:N | 2.31 | 0.45 |
| 1:2:288:ARG:HH21 | 11:E:384:ILE:HG12 | 1.82 | 0.45 |
| 1:2:419:LYS:HG3 | 1:2:420:PRO:HD2 | 1.99 | 0.45 |
| 2:3:96:ILE:HD13 | 2:3:129:LEU:HD11 | 1.99 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:3:363:LEU:HD22 | 2:3:656:LEU:HD12 | 1.97 | 0.45 |
| 2:3:436:GLY:O | 4:5:506:LYS:HG2 | 2.17 | 0.45 |
| 3:4:397:ILE:O | 3:4:417:LEU:HG | 2.17 | 0.45 |
| 3:4:434:GLU:HB3 | 3:4:467:LYS:O | 2.16 | 0.45 |
| 4:5:413:LEU:HB2 | 4:5:553:ILE:HA | 1.99 | 0.45 |
| 4:5:629:ILE:HG22 | 4:5:648:ILE:CD1 | 2.47 | 0.45 |
| 5:6:547:ILE:O | 5:6:550:GLN:HB2 | 2.17 | 0.45 |
| 5:6:941:LEU:HA | 5:6:944:LYS:CD | 2.47 | 0.45 |
| 6:7:67:LEU:HD11 | 6:7:121:ILE:HG23 | 1.99 | 0.45 |
| 7:A:84:ARG:HH12 | 10:D:217:ASN:CB | 2.30 | 0.45 |
| 11:E:259:LEU:HD21 | 11:E:269:ASN:HD22 | 1.81 | 0.45 |
| 11:E:561:ASP:HB3 | 11:E:562:LYS:CG | 2.47 | 0.45 |
| 11:E:607:MET:O | 11:E:610:GLN:HB2 | 2.17 | 0.45 |
| 1:2:206:THR:HA | 1:2:209:ARG:HD3 | 1.99 | 0.45 |
| 1:2:253:LYS:CE | 1:2:253:LYS:HA | 2.44 | 0.45 |
| 1:2:614:ASP:HA | 1:2:617:ARG:NH1 | 2.31 | 0.45 |
| 1:2:803:PHE:HB2 | 1:2:804:PRO:HA | 1.98 | 0.45 |
| 2:3:377:ILE:O | 2:3:381:ILE:HG13 | 2.16 | 0.45 |
| 2:3:466:ASP:HA | 2:3:510:CYS:SG | 2.57 | 0.45 |
| 2:3:706:ILE:HD13 | 6:7:620:HIS:CE1 | 2.52 | 0.45 |
| 3:4:634:PHE:CZ | 3:4:642:ARG:HG2 | 2.52 | 0.45 |
| 3:4:567:CYS:HB3 | 3:4:675:ALA:HB3 | 1.99 | 0.45 |
| 3:4:749:MET:O | 3:4:752:SER:OG | 2.28 | 0.45 |
| 4:5:44:PHE:HB2 | 4:5:47:ARG:HB3 | 1.98 | 0.45 |
| 4:5:411:ASN:HB3 | 4:5:550:PHE:CD1 | 2.52 | 0.45 |
| 4:5:585:ASN:O | 4:5:589:GLU:HG2 | 2.16 | 0.45 |
| 5:6:112:ARG:HH22 | 5:6:183:LYS:CG | 2.25 | 0.45 |
| 5:6:611:ALA:N | 5:6:624:GLU:HG2 | 2.32 | 0.45 |
| 5:6:823:PHE:O | 5:6:826:GLU:HB2 | 2.17 | 0.45 |
| 10:D:274:ILE:O | 10:D:274:ILE:HG13 | 2.16 | 0.45 |
| 11:E:125:ALA:HB2 | 11:E:249:ASN:O | 2.16 | 0.45 |
| 11:E:147:THR:OG1 | 11:E:148:VAL:N | 2.50 | 0.45 |
| 11:E:29:ILE:CD1 | 11:E:31:VAL:HG23 | 2.42 | 0.45 |
| 11:E:414:GLY:O | 11:E:417:GLY:N | 2.37 | 0.45 |
| 1:2:571:ALA:HB3 | 5:6:664:ALA:O | 2.16 | 0.45 |
| 1:2:667:VAL:HG22 | 1:2:669:LEU:H | 1.82 | 0.45 |
| 2:3:226:PRO:C | 2:3:228:PRO:HD2 | 2.37 | 0.45 |
| 2:3:405:ILE:HD13 | 2:3:513:ILE:HD11 | 1.99 | 0.45 |
| 3:4:202:LYS:HB3 | 3:4:203:TYR:CB | 2.32 | 0.45 |
| 3:4:348:LYS:HG2 | 3:4:354:HIS:O | 2.17 | 0.45 |
| 4:5:568:ILE:O | 4:5:571:HIS:HB3 | 2.17 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:5:68:LEU:CD2 | 4:5:76:TYR:HB2 | 2.47 | 0.45 |
| 1:2:581:ARG:HH22 | 5:6:621:TYR:HB3 | 1.79 | 0.45 |
| 5:6:721:GLU:N | 5:6:721:GLU:OE1 | 2.42 | 0.45 |
| 7:A:135:CYS:O | 7:A:138:ILE:HG22 | 2.17 | 0.45 |
| 7:A:165:VAL:HG11 | 7:A:205:LEU:HD22 | 1.99 | 0.45 |
| 7:A:194:SER:OG | 10:D:134:GLU:OE2 | 2.29 | 0.45 |
| 11:E:286:GLN:NE2 | 11:E:597:THR:HG21 | 2.31 | 0.45 |
| 11:E:310:VAL:HG13 | 11:E:311:LYS:HD2 | 1.98 | 0.45 |
| 11:E:559:SER:HB2 | 11:E:560:GLU:C | 2.37 | 0.45 |
| 1:2:339:PHE:HD1 | 1:2:341:CYS:H | 1.65 | 0.45 |
| 1:2:693:GLU:H | 1:2:693:GLU:HG3 | 1.65 | 0.45 |
| 2:3:410:ASP:OD1 | 2:3:522:GLN:HA | 2.17 | 0.45 |
| 4:5:91:GLU:HA | 4:5:94:ILE:CG1 | 2.46 | 0.45 |
| 5:6:559:THR:O | 5:6:559:THR:OG1 | 2.32 | 0.45 |
| 5:6:610:ALA:H | 5:6:663:ILE:HG21 | 1.81 | 0.45 |
| 7:A:84:ARG:HD3 | 7:A:84:ARG:HA | 1.75 | 0.45 |
| 8:B:107:THR:HG23 | 8:B:108:HIS:CE1 | 2.52 | 0.45 |
| 9:C:20:PHE:HA | 9:C:72:VAL:HA | 1.98 | 0.45 |
| 10:D:262:ASP:OD1 | 10:D:263:LEU:N | 2.49 | 0.45 |
| 11:E:585:THR:HB | 11:E:601:ILE:HD11 | 1.99 | 0.45 |
| 1:2:481:GLU:O | 1:2:485:ARG:HG2 | 2.17 | 0.45 |
| 2:3:39:ARG:NH2 | 2:3:132:LEU:HD11 | 2.29 | 0.45 |
| 3:4:191:THR:HG23 | 3:4:192:THR:HG23 | 1.98 | 0.45 |
| 3:4:688:VAL:HG22 | 3:4:838:THR:HG22 | 1.99 | 0.45 |
| 4:5:353:GLU:HB3 | 4:5:357:PHE:CE2 | 2.52 | 0.45 |
| 4:5:455:ARG:HH11 | 4:5:460:ARG:HD2 | 1.81 | 0.45 |
| 5:6:786:GLN:HG3 | 5:6:787:GLY:HA2 | 1.99 | 0.45 |
| 5:6:801:GLU:CD | 5:6:805:ARG:HH21 | 2.21 | 0.45 |
| 6:7:404:LEU:HD21 | 6:7:414:LEU:HD11 | 1.98 | 0.45 |
| 8:B:169:GLN:HG2 | 10:D:275:TYR:CE1 | 2.52 | 0.45 |
| 9:C:76:PRO:HA | 9:C:77:PRO:HD3 | 1.81 | 0.45 |
| 10:D:220:ASP:HA | 10:D:222:PRO:HD2 | 1.98 | 0.45 |
| 11:E:15:ILE:HD13 | 11:E:121:TYR:HE2 | 1.82 | 0.45 |
| 11:E:495:GLY:HA2 | 11:E:498:LEU:HB2 | 1.99 | 0.45 |
| 1:2:234:LEU:HA | 1:2:235:GLY:C | 2.37 | 0.45 |
| 1:2:588:GLU:H | 1:2:588:GLU:CD | 2.19 | 0.45 |
| 1:2:609:PHE:CZ | 1:2:648:ALA:HB1 | 2.52 | 0.45 |
| 2:3:674:GLU:HB3 | 2:3:723:LYS:HB2 | 1.99 | 0.45 |
| 3:4:631:ILE:H | 3:4:673:ALA:HA | 1.82 | 0.45 |
| 3:4:761:ILE:O | 3:4:817:VAL:HG12 | 2.17 | 0.45 |
| 3:4:769:GLU:OE1 | 3:4:823:GLN:NE2 | 2.50 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:5:179:LEU:HD22 | 4:5:243:ILE:HG12 | 1.99 | 0.45 |
| 5:6:650:VAL:HA | 5:6:653:HIS:HB3 | 1.99 | 0.45 |
| 11:E:622:ILE:O | 11:E:622:ILE:HG22 | 2.17 | 0.45 |
| 11:E:615:GLU:OE1 | 11:E:643:LYS:HB3 | 2.16 | 0.45 |
| 5:6:665:LYS:NZ | 12:F:14:DT:OP1 | 2.36 | 0.45 |
| 2:3:373:GLY:O | 2:3:378:LYS:NZ | 2.36 | 0.44 |
| 2:3:474:GLU:HG3 | 4:5:491:VAL:HG11 | 1.98 | 0.44 |
| 2:3:497:ILE:O | 2:3:503:HIS:HA | 2.17 | 0.44 |
| 3:4:264:TYR:CE2 | 6:7:135:LYS:HE2 | 2.52 | 0.44 |
| 3:4:267:GLU:O | 3:4:270:SER:OG | 2.23 | 0.44 |
| 4:5:420:THR:HG23 | 4:5:556:VAL:HG11 | 2.00 | 0.44 |
| 5:6:168:MET:O | 5:6:171:SER:N | 2.48 | 0.44 |
| 5:6:293:THR:HG23 | 5:6:392:GLY:HA2 | 1.98 | 0.44 |
| 5:6:362:GLN:HA | 5:6:376:THR:HG21 | 1.98 | 0.44 |
| 1:2:656:ARG:HB2 | 5:6:794:ARG:HH22 | 1.81 | 0.44 |
| 2:3:229:ALA:HB1 | 6:7:370:LEU:CD2 | 2.46 | 0.44 |
| 6:7:411:TYR:HD1 | 6:7:702:LEU:HD12 | 1.83 | 0.44 |
| 7:A:105:ASN:HB3 | 7:A:110:MET:SD | 2.56 | 0.44 |
| 7:A:134:TYR:O | 7:A:137:LEU:HB3 | 2.18 | 0.44 |
| 8:B:51:GLN:N | 8:B:52:LEU:HA | 2.32 | 0.44 |
| 10:D:161:LEU:HD21 | 10:D:168:LEU:O | 2.17 | 0.44 |
| 11:E:163:LEU:HA | 11:E:164:GLU:HA | 1.70 | 0.44 |
| 11:E:34:LEU:HD11 | 11:E:543:LEU:HG | 1.99 | 0.44 |
| 1:2:208:ALA:HA | 1:2:211:LEU:HG | 1.99 | 0.44 |
| 1:2:327:ARG:HE | 1:2:420:PRO:HD3 | 1.83 | 0.44 |
| 1:2:480:GLU:HB3 | 1:2:765:LYS:HE2 | 1.98 | 0.44 |
| 1:2:685:ASP:N | 1:2:685:ASP:OD1 | 2.50 | 0.44 |
| 1:2:850:LYS:HG3 | 1:2:851:VAL:N | 2.31 | 0.44 |
| 2:3:24:ARG:CZ | 2:3:121:PHE:HE1 | 2.30 | 0.44 |
| 2:3:245:TYR:CZ | 6:7:357:PRO:HG2 | 2.53 | 0.44 |
| 2:3:524:ASP:OD1 | 2:3:532:ASN:ND2 | 2.50 | 0.44 |
| 3:4:677:PRO:HB3 | 3:4:682:TYR:HB3 | 1.99 | 0.44 |
| 3:4:767:LYS:O | 3:4:771:VAL:HB | 2.17 | 0.44 |
| 3:4:854:LYS:HB3 | 3:4:857:ILE:HD11 | 1.99 | 0.44 |
| 4:5:156:VAL:HG22 | 4:5:298:TYR:CD2 | 2.50 | 0.44 |
| 4:5:374:ILE:HD13 | 4:5:388:ILE:HB | 1.99 | 0.44 |
| 5:6:169:ALA:O | 5:6:173:GLN:HB2 | 2.18 | 0.44 |
| 5:6:919:LYS:NZ | 5:6:929:GLU:OE2 | 2.33 | 0.44 |
| 6:7:18:PHE:CZ | 6:7:120:ALA:HB2 | 2.52 | 0.44 |
| 6:7:355:PHE:CZ | 6:7:374:THR:HG21 | 2.52 | 0.44 |
| 6:7:451:ARG:HB2 | 6:7:453:ASP:N | 2.32 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:7:529:MET:HE2 | 6:7:533:ASP:HB2 | 1.98 | 0.44 |
| 11:E:131:LEU:HD22 | 11:E:237:LEU:HD11 | 1.98 | 0.44 |
| 11:E:290:ARG:C | 11:E:293:PRO:HD2 | 2.37 | 0.44 |
| 11:E:577:ASP:O | 11:E:633:ARG:HA | 2.17 | 0.44 |
| 1:2:286:TYR:HA | 1:2:289:ILE:CB | 2.45 | 0.44 |
| 2:3:169:ARG:NH2 | 2:3:272:ARG:HH12 | 2.15 | 0.44 |
| 3:4:718:ARG:O | 3:4:722:LYS:HG2 | 2.17 | 0.44 |
| 4:5:184:ARG:NH1 | 4:5:239:ASP:O | 2.51 | 0.44 |
| 4:5:286:VAL:HG11 | 4:5:292:VAL:HG11 | 1.99 | 0.44 |
| 4:5:345:SER:OG | 4:5:346:VAL:N | 2.51 | 0.44 |
| 4:5:402:ASP:O | 4:5:404:MET:N | 2.51 | 0.44 |
| 4:5:477:VAL:HG11 | 4:5:519:VAL:HG22 | 2.00 | 0.44 |
| 5:6:134:LYS:CB | 5:6:137:ARG:H | 2.29 | 0.44 |
| 5:6:142:PHE:HA | 5:6:145:ILE:HG12 | 1.99 | 0.44 |
| 3:4:388:ARG:NH2 | 5:6:176:ARG:HD2 | 2.32 | 0.44 |
| 5:6:794:ARG:HA | 5:6:794:ARG:HD3 | 1.78 | 0.44 |
| 6:7:228:ARG:HA | 6:7:228:ARG:HD3 | 1.77 | 0.44 |
| 6:7:362:GLY:HA2 | 6:7:363:PHE:CG | 2.52 | 0.44 |
| 6:7:472:ALA:O | 6:7:476:ILE:HD12 | 2.13 | 0.44 |
| 6:7:247:ARG:CZ | 6:7:502:VAL:HG21 | 2.47 | 0.44 |
| 6:7:543:GLN:CG | 6:7:544:GLN:H | 2.28 | 0.44 |
| 6:7:571:TYR:HA | 6:7:572:GLY:HA2 | 1.70 | 0.44 |
| 8:B:102:ILE:HG22 | 8:B:148:LEU:HG | 1.99 | 0.44 |
| 9:C:33:ASN:HB3 | 9:C:34:PRO:HD3 | 1.99 | 0.44 |
| 10:D:200:LYS:HB2 | 10:D:201:TYR:CD2 | 2.53 | 0.44 |
| 10:D:286:LEU:HD21 | 10:D:293:LEU:HD11 | 1.98 | 0.44 |
| 10:D:66:SER:O | 10:D:70:GLU:HB2 | 2.18 | 0.44 |
| 11:E:27:LEU:HA | 11:E:80:SER:O | 2.17 | 0.44 |
| 2:3:115:LEU:HA | 2:3:179:LEU:HB3 | 1.99 | 0.44 |
| 2:3:138:ASP:OD2 | 2:3:140:PRO:HD2 | 2.17 | 0.44 |
| 2:3:33:ASP:HB2 | 2:3:39:ARG:NH1 | 2.31 | 0.44 |
| 3:4:627:GLY:O | 3:4:669:SER:HB2 | 2.18 | 0.44 |
| 3:4:728:TYR:CG | 3:4:729:LEU:N | 2.83 | 0.44 |
| 4:5:296:GLY:HA2 | 4:5:331:LEU:H | 1.81 | 0.44 |
| 5:6:575:GLY:HA3 | 5:6:715:ILE:O | 2.18 | 0.44 |
| 5:6:662:SER:HB3 | 5:6:670:ALA:O | 2.18 | 0.44 |
| 5:6:787:GLY:O | 5:6:790:ARG:HB2 | 2.17 | 0.44 |
| 5:6:948:LEU:CD1 | 5:6:954:TYR:HA | 2.48 | 0.44 |
| 6:7:260:TYR:HD1 | 6:7:298:LEU:HD13 | 1.81 | 0.44 |
| 6:7:374:THR:O | 6:7:375:TYR:HB3 | 2.17 | 0.44 |
| 6:7:493:LEU:CD2 | 6:7:533:ASP:HB3 | 2.48 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:7:595:ASP:N | 6:7:595:ASP:OD1 | 2.44 | 0.44 |
| 7:A:167:VAL:HG13 | 7:A:170:ASP:HB2 | 2.00 | 0.44 |
| 11:E:278:THR:HA | 11:E:281:ASP:CG | 2.38 | 0.44 |
| 1:2:342:LEU:HD11 | 1:2:376:ASN:HD21 | 1.82 | 0.44 |
| 1:2:567:THR:O | 1:2:606:ILE:HA | 2.18 | 0.44 |
| 1:2:547:THR:HG21 | 1:2:683:VAL:HB | 1.99 | 0.44 |
| 2:3:21:PHE:CE1 | 2:3:124:PRO:HD3 | 2.52 | 0.44 |
| 3:4:431:ASP:HB3 | 3:4:433:ILE:CD1 | 2.48 | 0.44 |
| 4:5:331:LEU:HA | 4:5:332:GLY:HA2 | 1.61 | 0.44 |
| 4:5:636:ASN:CG | 4:5:643:ARG:HH22 | 2.21 | 0.44 |
| 4:5:34:PHE:HA | 4:5:71:TYR:CZ | 2.53 | 0.44 |
| 5:6:124:VAL:HG21 | 5:6:133:GLU:H | 1.82 | 0.44 |
| 5:6:512:GLU:O | 5:6:516:LEU:HG | 2.18 | 0.44 |
| 5:6:561:GLU:N | 5:6:562:GLY:CA | 2.79 | 0.44 |
| 1:2:551:GLN:OE1 | 5:6:563:ILE:HG21 | 2.18 | 0.44 |
| 5:6:585:LEU:HD23 | 5:6:585:LEU:HA | 1.55 | 0.44 |
| 5:6:655:ALA:O | 5:6:659:GLN:HA | 2.18 | 0.44 |
| 5:6:758:ALA:HA | 5:6:761:PHE:CD2 | 2.53 | 0.44 |
| 5:6:806:LEU:HB3 | 5:6:827:ALA:HB1 | 1.99 | 0.44 |
| 6:7:372:THR:O | 6:7:373:GLU:HB3 | 2.17 | 0.44 |
| 6:7:476:ILE:O | 6:7:639:ARG:HD3 | 2.17 | 0.44 |
| 6:7:486:LYS:NZ | 6:7:530:ASP:OD2 | 2.33 | 0.44 |
| 7:A:36:ILE:O | 7:A:40:ILE:HG13 | 2.17 | 0.44 |
| 7:A:92:LEU:O | 7:A:96:ILE:HG22 | 2.17 | 0.44 |
| 10:D:151:ILE:HA | 10:D:158:LEU:HD11 | 1.99 | 0.44 |
| 1:2:218:TYR:O | 1:2:225:SER:OG | 2.24 | 0.44 |
| 1:2:437:ASN:ND2 | 1:2:437:ASN:O | 2.35 | 0.44 |
| 1:2:625:GLU:OE1 | 13:5:801:ANP:N3B | 2.50 | 0.44 |
| 2:3:154:LYS:HA | 2:3:154:LYS:HD3 | 1.61 | 0.44 |
| 3:4:833:ILE:HA | 3:4:836:TYR:CD2 | 2.52 | 0.44 |
| 4:5:264:LEU:HA | 4:5:265:VAL:HA | 1.79 | 0.44 |
| 4:5:385:LYS:HA | 4:5:388:ILE:HD12 | 1.98 | 0.44 |
| 4:5:498:GLU:N | 4:5:498:GLU:OE1 | 2.51 | 0.44 |
| 5:6:581:LYS:HD3 | 5:6:681:ALA:HB1 | 1.99 | 0.44 |
| 5:6:807:SER:HA | 5:6:810:ILE:HB | 1.99 | 0.44 |
| 6:7:235:LEU:HD23 | 6:7:235:LEU:HA | 1.68 | 0.44 |
| 6:7:309:ALA:O | 6:7:336:ASN:HA | 2.18 | 0.44 |
| 6:7:240:THR:HA | 6:7:352:THR:HG22 | 1.99 | 0.44 |
| 7:A:12:GLU:O | 7:A:15:ARG:HG2 | 2.18 | 0.44 |
| 9:C:52:ARG:HG3 | 9:C:114:LEU:HD13 | 2.00 | 0.44 |
| 11:E:541:ASN:ND2 | 11:E:543:LEU:HB2 | 2.32 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:2:271:PHE:CE2 | 1:2:295:VAL:HG21 | 2.52 | 0.44 |
| 1:2:856:GLN:NE2 | 1:2:856:GLN:O | 2.50 | 0.44 |
| 2:3:414:ALA:H | 13:3:1001:ANP:H5'2 | 1.83 | 0.44 |
| 3:4:331:LEU:CD1 | 6:7:553:ILE:HG12 | 2.48 | 0.44 |
| 3:4:455:SER:HB3 | 6:7:276:ARG:O | 2.18 | 0.44 |
| 3:4:597:SER:HB2 | 3:4:640:SER:OG | 2.17 | 0.44 |
| 3:4:862:GLN:NE2 | 3:4:909:ARG:HB3 | 2.33 | 0.44 |
| 4:5:412:VAL:O | 4:5:521:ALA:N | 2.35 | 0.44 |
| 4:5:439:THR:OG1 | 4:5:478:CYS:O | 2.24 | 0.44 |
| 2:3:558:ASP:OD2 | 4:5:627:VAL:HA | 2.18 | 0.44 |
| 5:6:175:TYR:HA | 5:6:178:LEU:HD13 | 2.00 | 0.44 |
| 1:2:395:GLY:HA2 | 5:6:672:LEU:HA | 1.99 | 0.44 |
| 5:6:793:TYR:HB3 | 5:6:795:ILE:HA | 1.99 | 0.44 |
| 6:7:362:GLY:HA2 | 6:7:363:PHE:CB | 2.47 | 0.44 |
| 6:7:422:ILE:HG13 | 6:7:422:ILE:O | 2.18 | 0.44 |
| 7:A:83:LYS:HE2 | 10:D:206:LEU:HB3 | 2.00 | 0.44 |
| 8:B:108:HIS:O | 8:B:155:LYS:NZ | 2.29 | 0.44 |
| 8:B:182:ARG:N | 8:B:183:PRO:HD2 | 2.33 | 0.44 |
| 8:B:7:LEU:HD11 | 8:B:12:SER:HB2 | 1.98 | 0.44 |
| 9:C:75:LEU:HG | 9:C:76:PRO:HD2 | 2.00 | 0.44 |
| 10:D:220:ASP:HA | 10:D:221:GLU:HA | 1.56 | 0.44 |
| 1:2:341:CYS:N | 1:2:342:LEU:HA | 2.32 | 0.44 |
| 2:3:127:LYS:O | 2:3:131:ASP:HB2 | 2.18 | 0.44 |
| 2:3:139:VAL:HB | 2:3:140:PRO:HD3 | 1.98 | 0.44 |
| 3:4:331:LEU:HD13 | 6:7:553:ILE:HG12 | 2.00 | 0.44 |
| 3:4:512:VAL:HG13 | 3:4:515:ARG:NH1 | 2.32 | 0.44 |
| 3:4:682:TYR:HB2 | 3:4:691:ASN:ND2 | 2.32 | 0.44 |
| 3:4:688:VAL:HG11 | 3:4:836:TYR:HA | 1.99 | 0.44 |
| 4:5:677:VAL:HG12 | 4:5:681:ILE:CD1 | 2.48 | 0.44 |
| 5:6:178:LEU:N | 5:6:179:PRO:HD2 | 2.33 | 0.44 |
| 5:6:584:PHE:O | 5:6:587:TYR:HB3 | 2.17 | 0.44 |
| 5:6:937:VAL:O | 5:6:941:LEU:HG | 2.17 | 0.44 |
| 10:D:63:LEU:HD11 | 10:D:140:ILE:HG22 | 2.00 | 0.44 |
| 1:2:485:ARG:NH1 | 1:2:825:LEU:HD23 | 2.33 | 0.44 |
| 1:2:538:ASN:CB | 1:2:677:PHE:HA | 2.41 | 0.44 |
| 1:2:767:ILE:O | 1:2:771:ARG:HG3 | 2.18 | 0.44 |
| 2:3:411:PRO:HB3 | 13:3:1001:ANP:O2G | 2.18 | 0.44 |
| 2:3:48:TYR:HD2 | 2:3:92:LEU:HG | 1.83 | 0.44 |
| 3:4:395:GLN:HG2 | 3:4:396:VAL:H | 1.83 | 0.44 |
| 3:4:568:GLY:O | 3:4:677:PRO:HD2 | 2.18 | 0.44 |
| 4:5:86:ILE:O | 4:5:89:LEU:N | 2.50 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:6:710:ASP:HA | 5:6:711:LEU:HA | 1.39 | 0.44 |
| 6:7:24:PHE:HD1 | 6:7:88:TYR:CD2 | 2.36 | 0.44 |
| 6:7:335:VAL:HG11 | 6:7:340:VAL:HA | 2.00 | 0.44 |
| 7:A:149:ILE:HG23 | 7:A:151:LEU:N | 2.33 | 0.44 |
| 7:A:33:HIS:O | 7:A:37:ILE:HG12 | 2.18 | 0.44 |
| 8:B:185:ILE:HG22 | 8:B:189:MET:HG2 | 1.98 | 0.44 |
| 8:B:18:PHE:O | 8:B:22:ASN:ND2 | 2.51 | 0.44 |
| 8:B:57:ASP:OD1 | 8:B:58:LYS:N | 2.51 | 0.44 |
| 9:C:27:LEU:CD2 | 9:C:29:TYR:H | 2.31 | 0.44 |
| 10:D:125:PRO:HA | 10:D:128:CYS:HB3 | 2.00 | 0.44 |
| 10:D:229:PHE:HD1 | 10:D:276:VAL:HG21 | 1.82 | 0.44 |
| 11:E:124:ASP:CG | 11:E:126:HIS:HD1 | 2.21 | 0.44 |
| 11:E:34:LEU:HD11 | 11:E:543:LEU:CG | 2.48 | 0.44 |
| 11:E:540:ARG:HH22 | 11:E:574:GLU:CA | 2.31 | 0.44 |
| 11:E:26:GLN:O | 11:E:79:ASN:N | 2.51 | 0.44 |
| 1:2:246:TYR:OH | 1:2:257:ALA:HB1 | 2.18 | 0.43 |
| 1:2:246:TYR:CE2 | 1:2:300:PHE:CD1 | 3.06 | 0.43 |
| 1:2:563:ALA:HA | 1:2:603:VAL:O | 2.17 | 0.43 |
| 2:3:420:ARG:O | 2:3:423:LEU:HB3 | 2.17 | 0.43 |
| 2:3:475:PHE:CE1 | 2:3:486:ILE:HD13 | 2.53 | 0.43 |
| 2:3:372:TYR:OH | 2:3:560:SER:O | 2.24 | 0.43 |
| 3:4:349:CYS:HB2 | 3:4:351:VAL:O | 2.17 | 0.43 |
| 3:4:345:ALA:HA | 3:4:389:CYS:HB3 | 1.98 | 0.43 |
| 3:4:824:GLU:HA | 3:4:827:ARG:CB | 2.44 | 0.43 |
| 4:5:342:ILE:HA | 4:5:343:TRP:HA | 1.57 | 0.43 |
| 4:5:438:TYR:HA | 4:5:478:CYS:HB2 | 1.99 | 0.43 |
| 4:5:531:ASP:OD2 | 4:5:539:ASN:ND2 | 2.51 | 0.43 |
| 4:5:640:SER:OG | 4:5:640:SER:O | 2.30 | 0.43 |
| 5:6:417:PRO:O | 5:6:448:LEU:N | 2.50 | 0.43 |
| 5:6:819:ILE:HG22 | 5:6:820:THR:N | 2.26 | 0.43 |
| 5:6:830:LEU:HA | 5:6:833:GLN:OE1 | 2.18 | 0.43 |
| 6:7:203:TYR:CE2 | 6:7:339:LEU:HG | 2.53 | 0.43 |
| 6:7:292:ASN:OD1 | 6:7:293:GLN:HB2 | 2.18 | 0.43 |
| 9:C:139:ALA:HB1 | 9:C:184:TYR:CZ | 2.53 | 0.43 |
| 11:E:25:CYS:N | 11:E:26:GLN:HA | 2.33 | 0.43 |
| 1:2:774:ILE:HG12 | 1:2:825:LEU:HA | 1.99 | 0.43 |
| 2:3:167:SER:HB3 | 2:3:168:PRO:HD2 | 2.00 | 0.43 |
| 2:3:244:GLU:HB3 | 2:3:247:TYR:HB3 | 2.01 | 0.43 |
| 2:3:667:VAL:HG11 | 2:3:719:LYS:HZ1 | 1.83 | 0.43 |
| 2:3:98:ILE:HB | 2:3:157:PHE:HD1 | 1.83 | 0.43 |
| 3:4:437:GLY:CA | 3:4:464:VAL:H | 2.31 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:4:909:ARG:CZ | 5:6:685:VAL:HB | 2.48 | 0.43 |
| 4:5:329:LYS:HD2 | 4:5:329:LYS:HA | 1.79 | 0.43 |
| 4:5:617:GLN:O | 4:5:620:GLU:HG2 | 2.18 | 0.43 |
| 5:6:594:ARG:HD2 | 5:6:633:ASN:O | 2.17 | 0.43 |
| 5:6:695:LEU:HA | 5:6:698:ASN:CB | 2.44 | 0.43 |
| 5:6:941:LEU:HD22 | 5:6:944:LYS:HZ3 | 1.83 | 0.43 |
| 6:7:370:LEU:HD22 | 6:7:370:LEU:HA | 1.69 | 0.43 |
| 7:A:110:MET:SD | 7:A:113:ILE:HG13 | 2.58 | 0.43 |
| 10:D:70:GLU:OE2 | 10:D:147:ARG:HG2 | 2.18 | 0.43 |
| 11:E:384:ILE:O | 11:E:388:LEU:HB2 | 2.18 | 0.43 |
| 11:E:38:ALA:HA | 11:E:251:ILE:HD11 | 1.99 | 0.43 |
| 11:E:429:THR:HA | 11:E:432:LEU:CD1 | 2.48 | 0.43 |
| 11:E:340:TYR:HB3 | 11:E:503:GLN:HE21 | 1.83 | 0.43 |
| 1:2:506:TYR:OH | 1:2:694:ARG:HD3 | 2.18 | 0.43 |
| 2:3:279:ASP:H | 2:3:282:LEU:HD12 | 1.83 | 0.43 |
| 2:3:368:ALA:CB | 2:3:378:LYS:HE3 | 2.48 | 0.43 |
| 2:3:449:ASP:HA | 2:3:454:GLU:O | 2.18 | 0.43 |
| 3:4:521:LEU:HD11 | 3:4:741:VAL:HB | 2.00 | 0.43 |
| 3:4:774:TYR:CG | 3:4:798:LEU:HD22 | 2.54 | 0.43 |
| 4:5:176:ALA:CB | 4:5:194:ILE:HG21 | 2.48 | 0.43 |
| 4:5:577:THR:O | 4:5:577:THR:HG23 | 2.18 | 0.43 |
| 4:5:652:GLN:HB3 | 4:5:652:GLN:HE21 | 1.67 | 0.43 |
| 5:6:266:SER:HB2 | 5:6:458:HIS:CD2 | 2.53 | 0.43 |
| 5:6:399:GLY:C | 5:6:400:VAL:CG2 | 2.85 | 0.43 |
| 5:6:399:GLY:O | 5:6:400:VAL:HG23 | 2.18 | 0.43 |
| 6:7:201:PHE:CZ | 6:7:337:GLY:HA2 | 2.53 | 0.43 |
| 10:D:154:PHE:O | 10:D:158:LEU:HG | 2.18 | 0.43 |
| 10:D:69:ASN:O | 10:D:73:SER:HB3 | 2.18 | 0.43 |
| 11:E:131:LEU:HD21 | 11:E:240:TYR:HD2 | 1.83 | 0.43 |
| 11:E:251:ILE:O | 11:E:255:ILE:HG13 | 2.18 | 0.43 |
| 11:E:513:ILE:HG12 | 11:E:516:LYS:HZ1 | 1.82 | 0.43 |
| 11:E:558:GLU:N | 11:E:559:SER:HA | 2.32 | 0.43 |
| 11:E:79:ASN:OD1 | 11:E:80:SER:OG | 2.23 | 0.43 |
| 1:2:204:SER:O | 1:2:207:ILE:HB | 2.18 | 0.43 |
| 1:2:339:PHE:CD2 | 1:2:376:ASN:HB3 | 2.53 | 0.43 |
| 2:3:122:ILE:O | 2:3:126:GLU:HB2 | 2.19 | 0.43 |
| 2:3:695:SER:HB3 | 2:3:696:PRO:HA | 2.00 | 0.43 |
| 3:4:351:VAL:HA | 3:4:352:CYS:HA | 1.55 | 0.43 |
| 5:6:194:PRO:O | 5:6:261:ARG:NE | 2.51 | 0.43 |
| 5:6:533:ILE:HG12 | 5:6:548:LEU:HD21 | 1.99 | 0.43 |
| 5:6:689:TYR:HB2 | 5:6:716:LEU:HD12 | 2.00 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 6:7:146:ARG:HH12 | 6:7:304:ALA:HA | 1.84 | 0.43 |
| 6:7:484:THR:OG1 | 6:7:485:GLY:N | 2.50 | 0.43 |
| 10:D:205:GLU:N | 10:D:205:GLU:OE1 | 2.46 | 0.43 |
| 11:E:25:CYS:H | 11:E:26:GLN:HA | 1.83 | 0.43 |
| 11:E:285:ALA:HB3 | 11:E:286:GLN:CA | 2.47 | 0.43 |
| 2:3:138:ASP:HB3 | 2:3:140:PRO:HD2 | 2.00 | 0.43 |
| 2:3:227:THR:N | 2:3:228:PRO:CD | 2.81 | 0.43 |
| 2:3:374:HIS:O | 2:3:378:LYS:HG2 | 2.19 | 0.43 |
| 2:3:520:PHE:HB3 | 2:3:527:ARG:NH2 | 2.32 | 0.43 |
| 4:5:409:ASP:C | 4:5:410:ILE:HG12 | 2.39 | 0.43 |
| 5:6:122:PHE:CG | 5:6:124:VAL:HB | 2.54 | 0.43 |
| 5:6:122:PHE:CD1 | 5:6:124:VAL:HB | 2.54 | 0.43 |
| 5:6:532:SER:HB3 | 5:6:745:PRO:HG2 | 1.99 | 0.43 |
| 1:2:577:THR:OG1 | 5:6:666:ALA:HB2 | 2.18 | 0.43 |
| 6:7:101:ASP:OD2 | 6:7:105:ALA:N | 2.51 | 0.43 |
| 6:7:541:MET:HB2 | 6:7:593:ARG:HD3 | 2.00 | 0.43 |
| 7:A:108:ASP:CB | 7:A:109:LEU:CB | 2.62 | 0.43 |
| 7:A:29:LEU:HD23 | 7:A:93:ARG:CD | 2.49 | 0.43 |
| 7:A:73:PHE:CE2 | 9:C:53:ILE:HG13 | 2.54 | 0.43 |
| 9:C:109:ILE:HA | 9:C:112:ILE:HG22 | 2.00 | 0.43 |
| 9:C:131:ARG:HA | 9:C:131:ARG:HD3 | 1.71 | 0.43 |
| 11:E:276:GLY:O | 11:E:279:SER:HB3 | 2.19 | 0.43 |
| 11:E:286:GLN:HA | 11:E:286:GLN:OE1 | 2.18 | 0.43 |
| 11:E:328:LEU:HD11 | 11:E:499:ALA:HB3 | 2.01 | 0.43 |
| 11:E:388:LEU:HG | 11:E:392:PHE:CZ | 2.53 | 0.43 |
| 1:2:213:SER:HA | 1:2:217:GLU:OE1 | 2.17 | 0.43 |
| 1:2:334:LEU:HA | 1:2:382:TYR:CE1 | 2.53 | 0.43 |
| 1:2:520:PHE:CE1 | 1:2:823:MET:HG2 | 2.53 | 0.43 |
| 2:3:518:PRO:CG | 2:3:524:ASP:HB2 | 2.49 | 0.43 |
| 2:3:317:PHE:CE2 | 4:5:176:ALA:HB2 | 2.54 | 0.43 |
| 4:5:207:LEU:HA | 4:5:208:PRO:HD2 | 1.81 | 0.43 |
| 4:5:413:LEU:HD12 | 4:5:413:LEU:N | 2.34 | 0.43 |
| 5:6:173:GLN:O | 5:6:176:ARG:HB3 | 2.19 | 0.43 |
| 6:7:147:ARG:HH22 | 6:7:192:PHE:HB2 | 1.83 | 0.43 |
| 11:E:579:TYR:CD1 | 11:E:637:LEU:CD2 | 3.02 | 0.43 |
| 1:2:271:PHE:HE2 | 1:2:295:VAL:HG11 | 1.82 | 0.43 |
| 1:2:628:SER:OG | 1:2:629:ILE:N | 2.51 | 0.43 |
| 2:3:400:ARG:HE | 2:3:707:ARG:NH2 | 2.17 | 0.43 |
| 3:4:443:PRO:HD3 | 3:4:457:TYR:CZ | 2.54 | 0.43 |
| 4:5:130:ASN:HA | 4:5:131:SER:HA | 1.79 | 0.43 |
| 4:5:375:ALA:HA | 4:5:376:PRO:HD2 | 1.89 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:5:397:LYS:NZ | 4:5:399:ILE:HD11 | 2.34 | 0.43 |
| 5:6:541:GLU:O | 5:6:544:LYS:HG2 | 2.19 | 0.43 |
| 5:6:915:MET:HA | 5:6:918:ARG:HB2 | 2.01 | 0.43 |
| 6:7:441:ASP:OD1 | 6:7:442:LYS:N | 2.51 | 0.43 |
| 6:7:470:LEU:HA | 6:7:470:LEU:HD23 | 1.62 | 0.43 |
| 6:7:689:LEU:HD12 | 6:7:692:ILE:HG21 | 2.00 | 0.43 |
| 7:A:105:ASN:HA | 7:A:106:GLY:HA3 | 1.71 | 0.43 |
| 7:A:109:LEU:O | 7:A:110:MET:C | 2.56 | 0.43 |
| 7:A:7:ASN:HA | 7:A:10:VAL:CG1 | 2.48 | 0.43 |
| 8:B:77:LEU:HD21 | 8:B:129:LYS:HE3 | 1.99 | 0.43 |
| 7:A:87:LEU:HD23 | 10:D:198:ILE:HD11 | 2.00 | 0.43 |
| 11:E:126:HIS:O | 11:E:127:ARG:NH1 | 2.46 | 0.43 |
| 11:E:487:ARG:HG3 | 11:E:488:LYS:N | 2.33 | 0.43 |
| 1:2:621:HIS:HA | 1:2:624:MET:HE1 | 2.00 | 0.43 |
| 2:3:195:LYS:HA | 6:7:371:LEU:HA | 2.00 | 0.43 |
| 2:3:439:GLY:HA3 | 2:3:442:LEU:HB2 | 2.00 | 0.43 |
| 2:3:342:LEU:HD21 | 2:3:661:GLN:HE21 | 1.84 | 0.43 |
| 3:4:239:SER:OG | 3:4:301:TYR:HA | 2.18 | 0.43 |
| 3:4:714:GLU:HG3 | 3:4:718:ARG:HH12 | 1.84 | 0.43 |
| 3:4:858:GLN:OE1 | 3:4:906:ALA:HB2 | 2.19 | 0.43 |
| 4:5:149:ARG:HG3 | 4:5:265:VAL:O | 2.18 | 0.43 |
| 4:5:430:GLU:OE1 | 4:5:431:LYS:HG2 | 2.18 | 0.43 |
| 4:5:386:LYS:NZ | 4:5:679:GLU:OE2 | 2.52 | 0.43 |
| 5:6:658:GLN:C | 5:6:660:THR:H | 2.22 | 0.43 |
| 5:6:912:MET:HB3 | 5:6:964:VAL:HG21 | 2.00 | 0.43 |
| 6:7:269:VAL:HG21 | 6:7:285:THR:CB | 2.49 | 0.43 |
| 6:7:411:TYR:OH | 6:7:430:LYS:HG3 | 2.18 | 0.43 |
| 6:7:442:LYS:HA | 6:7:442:LYS:HD2 | 1.80 | 0.43 |
| 3:4:579:GLN:HG3 | 6:7:542:GLU:HG3 | 2.01 | 0.43 |
| 7:A:102:TRP:CE3 | 7:A:151:LEU:HD23 | 2.54 | 0.43 |
| 7:A:199:LEU:HA | 7:A:202:GLN:CB | 2.48 | 0.43 |
| 7:A:41:LEU:HA | 7:A:44:VAL:HG12 | 2.01 | 0.43 |
| 8:B:165:GLU:HA | 8:B:166:SER:HA | 1.49 | 0.43 |
| 8:B:181:LEU:HD13 | 8:B:185:ILE:HD11 | 2.00 | 0.43 |
| 11:E:268:SER:O | 11:E:272:LEU:HG | 2.18 | 0.43 |
| 11:E:316:LEU:HD11 | 11:E:414:GLY:CA | 2.49 | 0.43 |
| 1:2:307:ARG:NH1 | 1:2:398:PRO:HG3 | 2.33 | 0.43 |
| 1:2:778:LEU:HA | 1:2:829:VAL:HB | 2.01 | 0.43 |
| 2:3:276:VAL:HG21 | 2:3:294:VAL:HG11 | 2.00 | 0.43 |
| 2:3:298:PHE:CD1 | 2:3:321:ILE:HG12 | 2.43 | 0.43 |
| 4:5:166:ILE:HA | 4:5:258:LEU:HA | 2.01 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:2:600:ASP:HB3 | 4:5:268:GLY:HA2 | 1.99 | 0.43 |
| 4:5:300:ILE:HG22 | 4:5:324:ARG:HB2 | 2.00 | 0.43 |
| 4:5:347:THR:CB | 4:5:349:PHE:HA | 2.47 | 0.43 |
| 5:6:261:ARG:HD2 | 5:6:263:PHE:CE1 | 2.50 | 0.43 |
| 5:6:284:ILE:HG13 | 5:6:402:ILE:HA | 2.01 | 0.43 |
| 5:6:403:VAL:HG11 | 5:6:450:TYR:HB3 | 2.01 | 0.43 |
| 6:7:192:PHE:HB3 | 6:7:196:LEU:HD13 | 2.00 | 0.43 |
| 9:C:181:HIS:ND1 | 9:C:185:LYS:HD2 | 2.34 | 0.43 |
| 11:E:291:LEU:O | 11:E:295:LEU:HG | 2.18 | 0.43 |
| 1:2:202:ASN:O | 1:2:205:ARG:HB3 | 2.18 | 0.43 |
| 1:2:670:THR:OG1 | 1:2:672:PRO:HD2 | 2.19 | 0.43 |
| 1:2:783:MET:SD | 1:2:834:LEU:HD11 | 2.58 | 0.43 |
| 2:3:464:LEU:HD12 | 2:3:464:LEU:HA | 1.89 | 0.43 |
| 3:4:282:SER:O | 3:4:285:VAL:HG22 | 2.18 | 0.43 |
| 3:4:363:GLY:O | 3:4:364:VAL:HG13 | 2.18 | 0.43 |
| 3:4:332:VAL:O | 3:4:429:ALA:HB1 | 2.18 | 0.43 |
| 3:4:501:ILE:HG21 | 3:4:506:LEU:HD21 | 2.01 | 0.43 |
| 3:4:559:ARG:HB3 | 3:4:560:GLY:H | 1.58 | 0.43 |
| 3:4:683:ASN:ND2 | 3:4:686:LEU:HD22 | 2.31 | 0.43 |
| 4:5:36:LEU:HD22 | 4:5:47:ARG:CZ | 2.49 | 0.43 |
| 4:5:559:ASP:HB2 | 4:5:561:ASN:HD21 | 1.83 | 0.43 |
| 4:5:571:HIS:HA | 4:5:581:ASN:HD21 | 1.84 | 0.43 |
| 5:6:599:SER:HA | 5:6:639:ASP:H | 1.83 | 0.43 |
| 6:7:528:LYS:N | 6:7:528:LYS:HD2 | 2.34 | 0.43 |
| 6:7:24:PHE:CE1 | 6:7:85:ILE:HA | 2.53 | 0.43 |
| 8:B:147:ASP:O | 8:B:150:GLU:HB3 | 2.19 | 0.43 |
| 9:C:29:TYR:HE2 | 9:C:44:LEU:HD13 | 1.83 | 0.43 |
| 10:D:256:TYR:HD1 | 10:D:257:THR:OG1 | 2.02 | 0.43 |
| 11:E:536:LEU:HA | 11:E:539:TYR:HD2 | 1.84 | 0.43 |
| 1:2:311:GLU:N | 1:2:311:GLU:OE1 | 2.42 | 0.42 |
| 1:2:497:ILE:HG13 | 1:2:497:ILE:H | 1.63 | 0.42 |
| 2:3:347:ILE:HG12 | 2:3:351:ASN:HD21 | 1.84 | 0.42 |
| 2:3:487:HIS:NE2 | 2:3:539:LEU:HG | 2.34 | 0.42 |
| 2:3:504:THR:HG21 | 6:7:328:PRO:HB2 | 2.01 | 0.42 |
| 2:3:555:GLU:HA | 2:3:558:ASP:HB3 | 2.00 | 0.42 |
| 3:4:257:LEU:HA | 3:4:260:GLN:HB2 | 2.00 | 0.42 |
| 3:4:508:LYS:O | 3:4:512:VAL:HG23 | 2.19 | 0.42 |
| 3:4:579:GLN:O | 3:4:583:LYS:NZ | 2.29 | 0.42 |
| 4:5:151:LEU:HA | 4:5:155:HIS:NE2 | 2.33 | 0.42 |
| 4:5:179:LEU:HD12 | 4:5:192:ILE:HB | 2.00 | 0.42 |
| 4:5:421:ALA:HA | 13:5:801:ANP:C5' | 2.49 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:5:486:ARG:O | 4:5:490:ARG:HB2 | 2.19 | 0.42 |
| 4:5:50:LEU:HD12 | 4:5:50:LEU:HA | 1.73 | 0.42 |
| 5:6:287:LEU:HG | 5:6:398:THR:CG2 | 2.49 | 0.42 |
| 5:6:764:ILE:O | 5:6:818:GLU:HA | 2.19 | 0.42 |
| 6:7:209:GLN:HB3 | 6:7:212:ALA:HB2 | 2.01 | 0.42 |
| 3:4:714:GLU:OE2 | 6:7:665:ILE:HG21 | 2.18 | 0.42 |
| 7:A:91:ARG:HA | 10:D:190:TRP:HH2 | 1.83 | 0.42 |
| 8:B:112:PHE:HD1 | 8:B:152:ARG:HG3 | 1.84 | 0.42 |
| 8:B:149:ARG:NH1 | 8:B:153:GLN:OE1 | 2.52 | 0.42 |
| 10:D:273:SER:HB3 | 10:D:275:TYR:CE1 | 2.53 | 0.42 |
| 11:E:266:ASN:HB2 | 11:E:269:ASN:ND2 | 2.33 | 0.42 |
| 11:E:285:ALA:CB | 11:E:288:TYR:HB3 | 2.47 | 0.42 |
| 1:2:631:ILE:HB | 1:2:633:LYS:HE2 | 2.02 | 0.42 |
| 1:2:638:THR:H | 4:5:445:SER:N | 2.13 | 0.42 |
| 2:3:553:ILE:O | 2:3:553:ILE:HG13 | 2.19 | 0.42 |
| 2:3:662:TYR:CE1 | 2:3:666:ARG:HD2 | 2.54 | 0.42 |
| 2:3:94:HIS:HB3 | 2:3:153:TRP:CE3 | 2.54 | 0.42 |
| 3:4:276:ILE:HA | 3:4:279:CYS:HB2 | 2.01 | 0.42 |
| 3:4:311:CYS:HB3 | 3:4:326:ILE:HG23 | 2.01 | 0.42 |
| 3:4:630:CYS:HA | 3:4:672:LEU:O | 2.19 | 0.42 |
| 4:5:176:ALA:HA | 4:5:250:PHE:HD1 | 1.82 | 0.42 |
| 5:6:144:LYS:HE2 | 5:6:194:PRO:HD2 | 2.01 | 0.42 |
| 5:6:328:THR:HA | 5:6:329:GLU:HA | 1.80 | 0.42 |
| 5:6:948:LEU:HD11 | 5:6:954:TYR:HA | 2.01 | 0.42 |
| 6:7:333:ILE:HD13 | 6:7:376:LEU:HD23 | 2.01 | 0.42 |
| 6:7:493:LEU:CD2 | 6:7:533:ASP:CB | 2.97 | 0.42 |
| 9:C:84:VAL:O | 9:C:88:ILE:HG23 | 2.19 | 0.42 |
| 10:D:136:LEU:O | 10:D:139:VAL:HB | 2.19 | 0.42 |
| 10:D:285:LEU:HD22 | 10:D:290:LYS:HD2 | 2.00 | 0.42 |
| 11:E:288:TYR:HA | 11:E:291:LEU:CG | 2.49 | 0.42 |
| 11:E:295:LEU:O | 11:E:299:VAL:HG23 | 2.19 | 0.42 |
| 11:E:580:LEU:HD11 | 11:E:629:ILE:HD11 | 2.01 | 0.42 |
| 1:2:534:ARG:HH11 | 1:2:815:ARG:NH2 | 2.17 | 0.42 |
| 1:2:585:ILE:HG23 | 1:2:586:THR:N | 2.35 | 0.42 |
| 1:2:645:SER:C | 1:2:646:ILE:HG13 | 2.40 | 0.42 |
| 2:3:310:ASN:HA | 2:3:311:SER:HA | 1.52 | 0.42 |
| 2:3:431:ALA:HB2 | 2:3:471:CYS:HB2 | 2.01 | 0.42 |
| 3:4:401:GLU:HG2 | 3:4:413:HIS:O | 2.19 | 0.42 |
| 3:4:552:PHE:HB3 | 3:4:553:THR:H | 1.62 | 0.42 |
| 3:4:727:LEU:HA | 3:4:728:TYR:C | 2.40 | 0.42 |
| 3:4:800:SER:HA | 3:4:803:ARG:HB2 | 2.01 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:4:820:GLU:HG3 | 3:4:823:GLN:CD | 2.39 | 0.42 |
| 4:5:166:ILE:HG13 | 4:5:292:VAL:HG21 | 2.01 | 0.42 |
| 5:6:122:PHE:HB2 | 5:6:124:VAL:CB | 2.48 | 0.42 |
| 5:6:292:GLY:O | 5:6:394:ARG:HA | 2.19 | 0.42 |
| 7:A:47:LEU:HD21 | 7:A:75:THR:CB | 2.48 | 0.42 |
| 9:C:174:LYS:O | 9:C:177:TYR:HB3 | 2.19 | 0.42 |
| 10:D:257:THR:HB | 10:D:258:VAL:O | 2.19 | 0.42 |
| 11:E:81:LEU:HD12 | 11:E:120:ILE:HG23 | 2.00 | 0.42 |
| 11:E:274:ILE:HG23 | 11:E:409:PHE:HD2 | 1.84 | 0.42 |
| 11:E:540:ARG:O | 11:E:580:LEU:HD13 | 2.19 | 0.42 |
| 1:2:236:GLU:OE2 | 11:E:361:LYS:HB2 | 2.20 | 0.42 |
| 1:2:258:LEU:HD12 | 1:2:261:ALA:HB3 | 1.99 | 0.42 |
| 1:2:806:THR:HG22 | 1:2:807:VAL:H | 1.85 | 0.42 |
| 2:3:100:LEU:HD21 | 2:3:157:PHE:CG | 2.54 | 0.42 |
| 2:3:437:SER:HA | 2:3:440:VAL:N | 2.24 | 0.42 |
| 3:4:572:THR:HG22 | 3:4:572:THR:O | 2.19 | 0.42 |
| 3:4:686:LEU:HD23 | 3:4:691:ASN:CG | 2.39 | 0.42 |
| 4:5:395:GLY:N | 4:5:409:ASP:HB2 | 2.35 | 0.42 |
| 1:2:446:VAL:HG13 | 5:6:301:ARG:HD2 | 2.01 | 0.42 |
| 5:6:726:GLU:C | 5:6:729:SER:H | 2.23 | 0.42 |
| 1:2:693:GLU:HG2 | 5:6:778:LYS:HD3 | 2.01 | 0.42 |
| 6:7:231:LYS:HG2 | 6:7:232:GLY:N | 2.35 | 0.42 |
| 6:7:499:LYS:HD2 | 6:7:506:MET:H | 1.85 | 0.42 |
| 6:7:580:PRO:HG2 | 6:7:679:PHE:O | 2.20 | 0.42 |
| 3:4:714:GLU:OE2 | 6:7:665:ILE:HD13 | 2.18 | 0.42 |
| 10:D:214:GLY:HA2 | 10:D:215:SER:HA | 1.45 | 0.42 |
| 11:E:348:LEU:HD21 | 11:E:401:LEU:HD21 | 2.01 | 0.42 |
| 1:2:246:TYR:CD2 | 1:2:300:PHE:HD1 | 2.37 | 0.42 |
| 1:2:325:THR:O | 1:2:326:ARG:C | 2.58 | 0.42 |
| 1:2:564:VAL:HG21 | 1:2:595:ALA:O | 2.19 | 0.42 |
| 2:3:300:SER:OG | 4:5:245:HIS:ND1 | 2.44 | 0.42 |
| 2:3:527:ARG:HG2 | 2:3:528:ASP:N | 2.35 | 0.42 |
| 3:4:266:GLN:OE1 | 3:4:440:ARG:NH2 | 2.53 | 0.42 |
| 3:4:328:LEU:O | 3:4:435:VAL:N | 2.52 | 0.42 |
| 3:4:704:LEU:HA | 3:4:704:LEU:HD12 | 1.89 | 0.42 |
| 3:4:704:LEU:HD12 | 3:4:832:ALA:HB2 | 2.01 | 0.42 |
| 4:5:143:ALA:HB3 | 4:5:161:ARG:HD3 | 2.01 | 0.42 |
| 4:5:392:LEU:HD23 | 4:5:392:LEU:HA | 1.77 | 0.42 |
| 4:5:388:ILE:HD11 | 4:5:425:LEU:HD11 | 2.02 | 0.42 |
| 4:5:411:ASN:HB2 | 4:5:550:PHE:HA | 2.01 | 0.42 |
| 4:5:579:ASN:O | 4:5:583:MET:HG2 | 2.19 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:6:124:VAL:HG22 | 5:6:132:VAL:HA | 2.00 | 0.42 |
| 5:6:530:VAL:HA | 5:6:533:ILE:CD1 | 2.43 | 0.42 |
| 5:6:625:ALA:HB3 | 5:6:626:GLY:CA | 2.45 | 0.42 |
| 5:6:956:GLU:HB2 | 5:6:960:LEU:HD13 | 2.02 | 0.42 |
| 6:7:134:TYR:HB2 | 6:7:141:VAL:CG1 | 2.48 | 0.42 |
| 9:C:79:MET:HB3 | 9:C:79:MET:HE2 | 1.96 | 0.42 |
| 11:E:25:CYS:CB | 11:E:26:GLN:HA | 2.34 | 0.42 |
| 1:2:540:LEU:HD23 | 1:2:680:LEU:HG | 2.02 | 0.42 |
| 3:4:243:LEU:HD13 | 3:4:303:VAL:HG13 | 2.02 | 0.42 |
| 3:4:281:VAL:HG22 | 3:4:297:GLU:CG | 2.49 | 0.42 |
| 3:4:433:ILE:HG21 | 3:4:468:LYS:C | 2.40 | 0.42 |
| 5:6:563:ILE:HD12 | 5:6:563:ILE:H | 1.84 | 0.42 |
| 6:7:17:LEU:HD21 | 6:7:113:PHE:CE1 | 2.54 | 0.42 |
| 6:7:107:GLN:HB2 | 6:7:238:LEU:O | 2.19 | 0.42 |
| 10:D:123:LYS:O | 10:D:126:LEU:HB3 | 2.20 | 0.42 |
| 1:2:574:VAL:HB | 5:6:666:ALA:HA | 2.01 | 0.42 |
| 2:3:493:GLN:NE2 | 2:3:509:ARG:HA | 2.35 | 0.42 |
| 2:3:716:ARG:NH1 | 2:3:722:ASN:HB3 | 2.32 | 0.42 |
| 3:4:318:ASN:OD1 | 6:7:341:ARG:NH1 | 2.46 | 0.42 |
| 3:4:337:PRO:HA | 5:6:375:ARG:HH11 | 1.84 | 0.42 |
| 3:4:593:GLY:C | 3:4:595:GLY:H | 2.22 | 0.42 |
| 4:5:244:ILE:O | 4:5:248:SER:OG | 2.36 | 0.42 |
| 4:5:484:LYS:N | 4:5:484:LYS:HD2 | 2.34 | 0.42 |
| 4:5:618:ALA:O | 4:5:622:LEU:HG | 2.19 | 0.42 |
| 5:6:711:LEU:HD12 | 5:6:712:PHE:H | 1.84 | 0.42 |
| 5:6:802:SER:O | 5:6:806:LEU:HG | 2.20 | 0.42 |
| 6:7:129:THR:OG1 | 6:7:130:LYS:N | 2.52 | 0.42 |
| 6:7:310:PHE:HE1 | 6:7:334:HIS:CG | 2.38 | 0.42 |
| 6:7:361:THR:OG1 | 6:7:362:GLY:N | 2.53 | 0.42 |
| 8:B:15:GLU:O | 8:B:18:PHE:HB3 | 2.19 | 0.42 |
| 10:D:218:MET:HG2 | 10:D:220:ASP:HB2 | 2.01 | 0.42 |
| 11:E:140:ILE:HB | 11:E:141:GLN:C | 2.40 | 0.42 |
| 11:E:148:VAL:CG1 | 11:E:150:ASP:HB2 | 2.48 | 0.42 |
| 1:2:279:THR:O | 1:2:283:TYR:N | 2.49 | 0.42 |
| 1:2:569:GLN:HA | 1:2:571:ALA:CB | 2.50 | 0.42 |
| 1:2:631:ILE:HB | 1:2:632:SER:H | 1.60 | 0.42 |
| 2:3:156:SER:OG | 2:3:157:PHE:N | 2.53 | 0.42 |
| 2:3:233:THR:C | 2:3:234:GLU:HG2 | 2.40 | 0.42 |
| 2:3:485:ALA:O | 2:3:488:GLU:HB3 | 2.20 | 0.42 |
| 3:4:243:LEU:HD21 | 3:4:245:ALA:HB2 | 2.02 | 0.42 |
| 3:4:501:ILE:HD11 | 3:4:752:SER:OG | 2.19 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:4:856:VAL:HG23 | 3:4:857:ILE:H | 1.82 | 0.42 |
| 4:5:349:PHE:HE2 | 4:5:354:GLU:H | 1.68 | 0.42 |
| 4:5:40:LEU:HA | 4:5:40:LEU:HD12 | 1.79 | 0.42 |
| 5:6:133:GLU:HA | 5:6:134:LYS:HA | 1.72 | 0.42 |
| 5:6:194:PRO:HG2 | 5:6:261:ARG:NH2 | 2.35 | 0.42 |
| 5:6:512:GLU:O | 5:6:515:GLU:HB3 | 2.19 | 0.42 |
| 6:7:493:LEU:HD21 | 6:7:533:ASP:OD1 | 2.19 | 0.42 |
| 8:B:26:LYS:HB2 | 8:B:88:VAL:HG11 | 2.01 | 0.42 |
| 9:C:182:GLU:HA | 9:C:185:LYS:HB2 | 2.01 | 0.42 |
| 11:E:410:VAL:HA | 11:E:420:SER:HA | 2.02 | 0.42 |
| 11:E:572:ILE:HD12 | 11:E:572:ILE:HA | 1.86 | 0.42 |
| 1:2:289:ILE:HG23 | 1:2:289:ILE:HD12 | 1.80 | 0.42 |
| 1:2:856:GLN:OE1 | 1:2:859:ARG:HD3 | 2.20 | 0.42 |
| 2:3:214:TYR:HD1 | 2:3:227:THR:HG22 | 1.84 | 0.42 |
| 2:3:706:ILE:HG21 | 6:7:620:HIS:NE2 | 2.31 | 0.42 |
| 3:4:248:LEU:HB3 | 3:4:254:THR:O | 2.19 | 0.42 |
| 3:4:467:LYS:HA | 3:4:468:LYS:HA | 1.85 | 0.42 |
| 3:4:522:LEU:HB2 | 3:4:541:LEU:HD11 | 2.02 | 0.42 |
| 3:4:830:ARG:HB3 | 3:4:834:LYS:HE2 | 2.01 | 0.42 |
| 4:5:347:THR:CB | 4:5:348:MET:HA | 2.49 | 0.42 |
| 4:5:444:SER:HA | 4:5:445:SER:HA | 1.77 | 0.42 |
| 5:6:543:VAL:HG23 | 5:6:713:PHE:HB3 | 2.02 | 0.42 |
| 6:7:139:LEU:CA | 6:7:142:ILE:HB | 2.47 | 0.42 |
| 6:7:81:ASP:OD1 | 6:7:81:ASP:N | 2.44 | 0.42 |
| 6:7:82:LEU:HD23 | 6:7:85:ILE:HD12 | 2.01 | 0.42 |
| 7:A:37:ILE:HA | 7:A:40:ILE:HD12 | 2.02 | 0.42 |
| 7:A:57:GLN:HG2 | 7:A:62:MET:HG2 | 2.01 | 0.42 |
| 10:D:199:LEU:HD13 | 10:D:202:MET:HE3 | 2.02 | 0.42 |
| 10:D:286:LEU:HD21 | 10:D:293:LEU:HD21 | 2.02 | 0.42 |
| 11:E:150:ASP:CB | 11:E:152:LEU:HB2 | 2.42 | 0.42 |
| 11:E:131:LEU:HD13 | 11:E:237:LEU:HD21 | 2.01 | 0.42 |
| 11:E:280:LEU:HG | 11:E:280:LEU:H | 1.54 | 0.42 |
| 11:E:283:ALA:HB1 | 11:E:284:TYR:CE2 | 2.55 | 0.42 |
| 11:E:327:PHE:CZ | 11:E:503:GLN:HG3 | 2.55 | 0.42 |
| 11:E:524:ILE:HD13 | 11:E:648:GLY:HA3 | 2.02 | 0.42 |
| 11:E:545:LEU:HD22 | 11:E:580:LEU:HD23 | 2.02 | 0.42 |
| 11:E:619:LYS:HB3 | 11:E:633:ARG:CG | 2.50 | 0.42 |
| 1:2:218:TYR:HD2 | 1:2:227:TYR:CE2 | 2.37 | 0.42 |
| 1:2:423:GLU:OE1 | 1:2:423:GLU:N | 2.52 | 0.42 |
| 1:2:790:TYR:HA | 1:2:793:LEU:HB2 | 2.02 | 0.42 |
| 1:2:830:SER:N | 1:2:833:ASP:OD2 | 2.41 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:3:122:ILE:HG22 | 2:3:123:PRO:HD3 | 2.02 | 0.42 |
| 2:3:228:PRO:HA | 2:3:229:ALA:HA | 1.75 | 0.42 |
| 4:5:258:LEU:HD21 | 4:5:276:MET:SD | 2.60 | 0.42 |
| 4:5:413:LEU:HD22 | 4:5:553:ILE:HG23 | 2.00 | 0.42 |
| 4:5:566:ILE:H | 4:5:566:ILE:HG13 | 1.72 | 0.42 |
| 5:6:173:GLN:OE1 | 5:6:173:GLN:N | 2.53 | 0.42 |
| 5:6:585:LEU:HA | 5:6:588:VAL:HG23 | 2.01 | 0.42 |
| 5:6:642:ASP:OD1 | 5:6:642:ASP:N | 2.51 | 0.42 |
| 3:4:909:ARG:NH2 | 5:6:685:VAL:HB | 2.35 | 0.42 |
| 5:6:767:LYS:HB3 | 5:6:767:LYS:HE3 | 1.76 | 0.42 |
| 5:6:834:SER:O | 5:6:838:VAL:HG23 | 2.20 | 0.42 |
| 5:6:919:LYS:HB2 | 5:6:939:TRP:HZ2 | 1.84 | 0.42 |
| 5:6:932:THR:OG1 | 5:6:933:ALA:N | 2.53 | 0.42 |
| 2:3:687:ARG:HE | 6:7:604:PRO:HA | 1.85 | 0.42 |
| 7:A:145:ASP:CA | 7:A:146:LEU:HB3 | 2.42 | 0.42 |
| 7:A:169:LYS:HA | 7:A:185:LYS:HD3 | 2.02 | 0.42 |
| 7:A:22:ARG:N | 7:A:23:SER:HA | 2.35 | 0.42 |
| 11:E:575:ASN:O | 11:E:576:THR:CB | 2.68 | 0.42 |
| 3:4:434:GLU:O | 3:4:466:VAL:HG13 | 2.20 | 0.41 |
| 3:4:626:GLY:N | 3:4:668:ARG:O | 2.48 | 0.41 |
| 3:4:795:THR:O | 3:4:799:GLU:HB2 | 2.20 | 0.41 |
| 3:4:808:HIS:O | 3:4:808:HIS:ND1 | 2.53 | 0.41 |
| 4:5:181:ILE:HG23 | 4:5:242:ILE:O | 2.20 | 0.41 |
| 4:5:337:VAL:HA | 4:5:338:GLU:HA | 1.70 | 0.41 |
| 5:6:794:ARG:HB2 | 5:6:795:ILE:C | 2.41 | 0.41 |
| 6:7:214:ARG:N | 6:7:215:TYR:HA | 2.34 | 0.41 |
| 6:7:401:VAL:HG12 | 6:7:405:ILE:HG13 | 2.02 | 0.41 |
| 8:B:184:PHE:HB2 | 9:C:180:SER:OG | 2.20 | 0.41 |
| 10:D:76:LEU:HD11 | 10:D:147:ARG:NE | 2.25 | 0.41 |
| 11:E:36:ILE:HG23 | 11:E:39:LEU:HD12 | 2.02 | 0.41 |
| 11:E:579:TYR:CZ | 11:E:634:ARG:HB3 | 2.49 | 0.41 |
| 1:2:273:LEU:O | 1:2:277:GLU:HG2 | 2.20 | 0.41 |
| 1:2:523:VAL:O | 1:2:535:GLY:HA3 | 2.21 | 0.41 |
| 1:2:544:ASP:H | 1:2:549:LYS:HE2 | 1.85 | 0.41 |
| 1:2:626:GLN:HG3 | 1:2:628:SER:N | 2.35 | 0.41 |
| 2:3:174:GLN:H | 2:3:174:GLN:CD | 2.24 | 0.41 |
| 2:3:211:TYR:CE1 | 6:7:6:PRO:HG2 | 2.56 | 0.41 |
| 2:3:234:GLU:H | 2:3:241:LEU:HD12 | 1.85 | 0.41 |
| 2:3:687:ARG:HB3 | 6:7:604:PRO:CB | 2.47 | 0.41 |
| 3:4:191:THR:HB | 3:4:275:THR:HG22 | 2.02 | 0.41 |
| 3:4:342:MET:HG3 | 5:6:417:PRO:HG3 | 2.02 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:4:410:GLN:HE21 | 6:7:345:PRO:CG | 2.33 | 0.41 |
| 3:4:633:GLU:HA | 3:4:675:ALA:HA | 2.01 | 0.41 |
| 1:2:640:LEU:HD21 | 4:5:271:PRO:HD3 | 2.02 | 0.41 |
| 5:6:126:SER:O | 5:6:130:GLY:HA3 | 2.19 | 0.41 |
| 5:6:533:ILE:HG22 | 5:6:587:TYR:CZ | 2.55 | 0.41 |
| 6:7:399:GLU:HA | 6:7:402:MET:HB2 | 2.02 | 0.41 |
| 6:7:28:PHE:O | 6:7:61:PRO:HB3 | 2.20 | 0.41 |
| 6:7:709:ASP:HB2 | 6:7:712:ASP:HB2 | 2.01 | 0.41 |
| 8:B:124:ARG:HD2 | 9:C:191:MET:O | 2.19 | 0.41 |
| 8:B:15:GLU:O | 8:B:18:PHE:N | 2.53 | 0.41 |
| 1:2:846:VAL:HG13 | 1:2:856:GLN:HG3 | 2.02 | 0.41 |
| 2:3:675:ALA:HB1 | 2:3:726:ALA:HB2 | 2.01 | 0.41 |
| 2:3:687:ARG:CG | 2:3:697:ILE:HG21 | 2.50 | 0.41 |
| 2:3:704:THR:O | 2:3:708:LEU:HD13 | 2.20 | 0.41 |
| 2:3:672:THR:OG1 | 2:3:721:VAL:O | 2.23 | 0.41 |
| 3:4:449:ARG:O | 3:4:451:ARG:N | 2.50 | 0.41 |
| 3:4:449:ARG:CG | 3:4:450:GLN:N | 2.77 | 0.41 |
| 4:5:408:GLY:HA2 | 4:5:409:ASP:HA | 1.44 | 0.41 |
| 4:5:87:ILE:N | 4:5:88:PRO:HD2 | 2.35 | 0.41 |
| 5:6:556:HIS:ND1 | 5:6:556:HIS:O | 2.53 | 0.41 |
| 1:2:550:SER:HB3 | 5:6:657:GLU:CD | 2.40 | 0.41 |
| 5:6:836:ILE:HA | 5:6:839:ASP:HB2 | 2.02 | 0.41 |
| 6:7:428:VAL:O | 6:7:432:LEU:HG | 2.21 | 0.41 |
| 8:B:144:LYS:O | 8:B:148:LEU:HB2 | 2.20 | 0.41 |
| 8:B:152:ARG:O | 8:B:156:VAL:HG23 | 2.20 | 0.41 |
| 9:C:22:TYR:CD2 | 9:C:71:PHE:HD1 | 2.38 | 0.41 |
| 9:C:27:LEU:HD12 | 9:C:35:GLY:HA3 | 2.02 | 0.41 |
| 10:D:260:ILE:HA | 10:D:261:PRO:HD3 | 1.60 | 0.41 |
| 11:E:36:ILE:HD11 | 11:E:429:THR:HG22 | 2.02 | 0.41 |
| 1:2:335:LYS:HA | 1:2:353:GLN:O | 2.19 | 0.41 |
| 1:2:476:TRP:CG | 1:2:769:TYR:HD1 | 2.39 | 0.41 |
| 2:3:462:MET:SD | 2:3:470:VAL:HG21 | 2.60 | 0.41 |
| 3:4:437:GLY:HA3 | 3:4:464:VAL:H | 1.86 | 0.41 |
| 3:4:506:LEU:HA | 3:4:509:ILE:HD12 | 2.02 | 0.41 |
| 3:4:621:LEU:HD23 | 3:4:621:LEU:HA | 1.92 | 0.41 |
| 3:4:598:ALA:HB2 | 3:4:640:SER:O | 2.20 | 0.41 |
| 3:4:692:ILE:HG21 | 3:4:699:LEU:CD1 | 2.51 | 0.41 |
| 4:5:297:ILE:N | 4:5:328:ILE:HG23 | 2.36 | 0.41 |
| 5:6:279:ILE:HG21 | 5:6:452:ILE:HD13 | 2.02 | 0.41 |
| 1:2:404:ARG:NH2 | 5:6:298:SER:O | 2.53 | 0.41 |
| 5:6:711:LEU:CD2 | 5:6:834:SER:HB2 | 2.51 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:6:945:GLU:HA | 5:6:948:LEU:CD1 | 2.50 | 0.41 |
| 6:7:82:LEU:CB | 6:7:207:LEU:HD23 | 2.48 | 0.41 |
| 6:7:570:LEU:HB2 | 6:7:585:ASN:HD21 | 1.85 | 0.41 |
| 7:A:14:LYS:HZ1 | 9:C:171:GLU:CD | 2.23 | 0.41 |
| 8:B:126:LEU:O | 8:B:130:ALA:N | 2.54 | 0.41 |
| 8:B:26:LYS:O | 8:B:88:VAL:HG12 | 2.20 | 0.41 |
| 9:C:127:LEU:HD23 | 9:C:131:ARG:HG2 | 2.01 | 0.41 |
| 9:C:98:HIS:HA | 9:C:102:SER:HB2 | 2.02 | 0.41 |
| 10:D:67:TRP:O | 10:D:70:GLU:HB3 | 2.20 | 0.41 |
| 11:E:36:ILE:HB | 11:E:279:SER:OG | 2.21 | 0.41 |
| 11:E:369:PRO:HD2 | 11:E:372:THR:HB | 2.01 | 0.41 |
| 12:F:7:DT:H5' | 12:F:7:DT:H6 | 1.85 | 0.41 |
| 1:2:327:ARG:NH2 | 4:5:269:GLU:OE1 | 2.54 | 0.41 |
| 1:2:525:LYS:HZ1 | 4:5:576:HIS:C | 2.24 | 0.41 |
| 1:2:586:THR:O | 1:2:586:THR:OG1 | 2.34 | 0.41 |
| 2:3:257:THR:HB | 2:3:273:SER:HB2 | 2.03 | 0.41 |
| 2:3:31:PHE:HZ | 2:3:38:TYR:HE2 | 1.68 | 0.41 |
| 2:3:350:ILE:HG23 | 2:3:659:TYR:HD1 | 1.85 | 0.41 |
| 3:4:225:TYR:HA | 3:4:226:TYR:HA | 1.67 | 0.41 |
| 3:4:252:LYS:CG | 3:4:253:GLN:HA | 2.46 | 0.41 |
| 3:4:314:MET:HA | 3:4:317:LEU:HG | 2.02 | 0.41 |
| 3:4:761:ILE:HG22 | 3:4:763:THR:H | 1.86 | 0.41 |
| 1:2:780:GLN:NE2 | 4:5:577:THR:O | 2.42 | 0.41 |
| 5:6:154:ASP:OD2 | 5:6:156:GLN:HB3 | 2.20 | 0.41 |
| 5:6:159:SER:O | 5:6:164:GLY:N | 2.54 | 0.41 |
| 5:6:398:THR:OG1 | 5:6:458:HIS:HB3 | 2.20 | 0.41 |
| 6:7:203:TYR:CZ | 6:7:339:LEU:HG | 2.56 | 0.41 |
| 6:7:409:ASP:O | 6:7:413:ARG:HB3 | 2.20 | 0.41 |
| 6:7:470:LEU:HD22 | 6:7:522:CYS:SG | 2.60 | 0.41 |
| 6:7:453:ASP:OD1 | 6:7:562:SER:HA | 2.20 | 0.41 |
| 6:7:713:VAL:HG12 | 6:7:717:LEU:CD1 | 2.50 | 0.41 |
| 7:A:110:MET:HG2 | 7:A:112:SER:N | 2.35 | 0.41 |
| 10:D:188:LEU:O | 10:D:192:LYS:HG2 | 2.20 | 0.41 |
| 1:2:249:LEU:HG | 1:2:257:ALA:HB2 | 2.03 | 0.41 |
| 1:2:506:TYR:HD2 | 1:2:695:LEU:HD12 | 1.85 | 0.41 |
| 1:2:562:ARG:HD2 | 1:2:600:ASP:O | 2.20 | 0.41 |
| 1:2:621:HIS:CD2 | 1:2:673:ILE:HG13 | 2.55 | 0.41 |
| 2:3:118:PRO:O | 2:3:122:ILE:HG22 | 2.20 | 0.41 |
| 2:3:500:ALA:H | 2:3:501:GLY:HA3 | 1.86 | 0.41 |
| 3:4:272:MET:HB3 | 3:4:303:VAL:HG21 | 2.02 | 0.41 |
| 3:4:319:PRO:O | 3:4:322:ILE:HG23 | 2.21 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:4:343:LYS:HG2 | 3:4:343:LYS:HZ3 | 1.74 | 0.41 |
| 3:4:754:ALA:O | 3:4:810:LYS:HG2 | 2.20 | 0.41 |
| 2:3:300:SER:O | 4:5:245:HIS:ND1 | 2.54 | 0.41 |
| 4:5:455:ARG:HG3 | 4:5:462:PHE:CD1 | 2.55 | 0.41 |
| 2:3:437:SER:O | 4:5:506:LYS:HA | 2.21 | 0.41 |
| 4:5:490:ARG:NH1 | 4:5:541:ASP:OD2 | 2.54 | 0.41 |
| 4:5:660:THR:CG2 | 4:5:677:VAL:HG13 | 2.51 | 0.41 |
| 5:6:102:LYS:HE2 | 5:6:102:LYS:HB2 | 1.90 | 0.41 |
| 5:6:403:VAL:HG12 | 5:6:404:VAL:N | 2.36 | 0.41 |
| 6:7:201:PHE:CE2 | 6:7:337:GLY:HA2 | 2.55 | 0.41 |
| 6:7:438:GLY:HA2 | 6:7:454:ILE:HG13 | 2.01 | 0.41 |
| 6:7:495:ALA:O | 6:7:548:ILE:HG21 | 2.20 | 0.41 |
| 10:D:175:LEU:HB2 | 10:D:180:ILE:HG23 | 2.02 | 0.41 |
| 11:E:285:ALA:CA | 11:E:288:TYR:HB3 | 2.51 | 0.41 |
| 11:E:288:TYR:HA | 11:E:291:LEU:HG | 2.01 | 0.41 |
| 11:E:30:PHE:HD1 | 11:E:61:ILE:CD1 | 2.33 | 0.41 |
| 1:2:433:ASN:HB2 | 1:2:434:TYR:HD2 | 1.86 | 0.41 |
| 1:2:445:PRO:HG3 | 5:6:304:LEU:HB3 | 2.01 | 0.41 |
| 1:2:479:GLU:OE1 | 1:2:479:GLU:N | 2.45 | 0.41 |
| 1:2:567:THR:CG2 | 1:2:568:GLY:N | 2.77 | 0.41 |
| 2:3:110:PHE:O | 2:3:114:ILE:HG13 | 2.20 | 0.41 |
| 2:3:43:ARG:HA | 2:3:43:ARG:HD2 | 1.84 | 0.41 |
| 2:3:488:GLU:HG3 | 2:3:494:THR:O | 2.20 | 0.41 |
| 2:3:545:LEU:HD13 | 2:3:547:PHE:CZ | 2.56 | 0.41 |
| 2:3:653:ILE:O | 2:3:656:LEU:HB3 | 2.20 | 0.41 |
| 2:3:714:LYS:O | 2:3:717:LEU:HD12 | 2.20 | 0.41 |
| 3:4:540:ILE:O | 3:4:543:GLN:HB3 | 2.20 | 0.41 |
| 3:4:683:ASN:HA | 3:4:684:PRO:HD3 | 1.94 | 0.41 |
| 3:4:901:SER:O | 3:4:905:GLU:HG2 | 2.21 | 0.41 |
| 4:5:286:VAL:CG1 | 4:5:292:VAL:HG11 | 2.51 | 0.41 |
| 4:5:27:ILE:O | 4:5:30:SER:HB3 | 2.20 | 0.41 |
| 4:5:343:TRP:CE3 | 4:5:344:ASN:HB3 | 2.56 | 0.41 |
| 5:6:539:GLY:O | 5:6:544:LYS:HE3 | 2.20 | 0.41 |
| 6:7:523:ILE:HD13 | 6:7:526:PHE:CE1 | 2.56 | 0.41 |
| 7:A:138:ILE:HD12 | 7:A:138:ILE:HA | 1.97 | 0.41 |
| 10:D:200:LYS:C | 10:D:202:MET:H | 2.23 | 0.41 |
| 10:D:87:LEU:O | 10:D:90:ARG:N | 2.54 | 0.41 |
| 10:D:94:GLN:O | 10:D:98:ILE:HG23 | 2.20 | 0.41 |
| 11:E:561:ASP:HA | 11:E:562:LYS:HA | 1.76 | 0.41 |
| 1:2:660:THR:O | 1:2:850:LYS:HB2 | 2.20 | 0.41 |
| 2:3:35:PHE:CE2 | 2:3:102:ASP:HB3 | 2.55 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:3:102:ASP:O | 2:3:105:GLU:HB2 | 2.21 | 0.41 |
| 4:5:136:GLN:CD | 4:5:280:ARG:HB2 | 2.41 | 0.41 |
| 5:6:266:SER:HB2 | 5:6:458:HIS:HD2 | 1.85 | 0.41 |
| 5:6:577:PRO:HD2 | 5:6:687:GLY:O | 2.21 | 0.41 |
| 6:7:611:LYS:O | 6:7:615:HIS:HB2 | 2.21 | 0.41 |
| 7:A:145:ASP:HB3 | 7:A:147:VAL:HG23 | 2.01 | 0.41 |
| 8:B:160:LEU:HD21 | 8:B:184:PHE:HE2 | 1.86 | 0.41 |
| 11:E:297:ASP:O | 11:E:301:ARG:N | 2.54 | 0.41 |
| 11:E:431:LEU:H | 11:E:431:LEU:HG | 1.62 | 0.41 |
| 11:E:569:LEU:O | 11:E:581:VAL:HA | 2.20 | 0.41 |
| 11:E:577:ASP:OD2 | 11:E:633:ARG:NH2 | 2.53 | 0.41 |
| 1:2:240:GLU:HB3 | 1:2:290:HIS:CE1 | 2.56 | 0.41 |
| 1:2:505:ILE:O | 13:2:901:ANP:N6 | 2.24 | 0.41 |
| 1:2:569:GLN:C | 1:2:571:ALA:HA | 2.42 | 0.41 |
| 1:2:802:SER:HA | 1:2:803:PHE:HA | 1.66 | 0.41 |
| 2:3:356:LYS:HB2 | 2:3:359:ILE:CG2 | 2.48 | 0.41 |
| 2:3:375:ASP:O | 2:3:379:LYS:HG3 | 2.21 | 0.41 |
| 2:3:528:ASP:O | 2:3:532:ASN:HB2 | 2.21 | 0.41 |
| 4:5:483:ASP:HB3 | 4:5:484:LYS:HD2 | 2.02 | 0.41 |
| 4:5:52:ASN:OD1 | 9:C:140:SER:HB3 | 2.21 | 0.41 |
| 4:5:599:MET:HE2 | 4:5:599:MET:HB2 | 1.90 | 0.41 |
| 4:5:601:ARG:HD2 | 4:5:601:ARG:HA | 1.82 | 0.41 |
| 4:5:422:LYS:NZ | 13:5:801:ANP:O3G | 2.54 | 0.41 |
| 6:7:429:LYS:HA | 6:7:432:LEU:HD12 | 2.02 | 0.41 |
| 6:7:486:LYS:HA | 6:7:486:LYS:HD3 | 1.90 | 0.41 |
| 6:7:537:ILE:HG23 | 6:7:541:MET:HE2 | 2.02 | 0.41 |
| 6:7:564:LEU:HD23 | 6:7:565:ALA:N | 2.36 | 0.41 |
| 6:7:650:PRO:HB3 | 6:7:706:ASP:HA | 2.03 | 0.41 |
| 6:7:668:ARG:HH22 | 6:7:686:PRO:CD | 2.33 | 0.41 |
| 6:7:688:THR:O | 6:7:692:ILE:HB | 2.21 | 0.41 |
| 6:7:699:LEU:HD13 | 6:7:715:GLU:HB3 | 2.01 | 0.41 |
| 7:A:31:MET:HG2 | 7:A:32:TYR:N | 2.36 | 0.41 |
| 9:C:95:LEU:O | 9:C:131:ARG:NH2 | 2.54 | 0.41 |
| 10:D:135:ARG:O | 10:D:139:VAL:HG23 | 2.20 | 0.41 |
| 1:2:439:ASN:O | 1:2:442:ASN:N | 2.39 | 0.41 |
| 2:3:716:ARG:HH22 | 2:3:724:VAL:HB | 1.86 | 0.41 |
| 3:4:375:ASP:HA | 3:4:376:CYS:C | 2.42 | 0.41 |
| 3:4:376:CYS:HA | 3:4:377:ASN:C | 2.42 | 0.41 |
| 4:5:557:LYS:HA | 4:5:557:LYS:HD2 | 1.79 | 0.41 |
| 5:6:656:MET:HG3 | 5:6:709:PHE:HE1 | 1.84 | 0.41 |
| 5:6:774:VAL:HG12 | 5:6:778:LYS:HZ3 | 1.85 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:7:89:GLN:HG3 | 6:7:102:LEU:HD12 | 2.03 | 0.41 |
| 6:7:110:ALA:HB2 | 6:7:238:LEU:N | 2.35 | 0.41 |
| 6:7:246:THR:HG21 | 6:7:316:GLN:NE2 | 2.36 | 0.41 |
| 6:7:464:VAL:HG11 | 6:7:600:MET:SD | 2.61 | 0.41 |
| 3:4:569:ASP:HB3 | 6:7:683:GLN:OE1 | 2.21 | 0.41 |
| 7:A:30:PRO:O | 7:A:122:ASN:ND2 | 2.42 | 0.41 |
| 7:A:102:TRP:CD1 | 8:B:3:LEU:HG | 2.56 | 0.41 |
| 8:B:32:THR:C | 8:B:62:ASN:HB2 | 2.40 | 0.41 |
| 9:C:172:MET:HG3 | 9:C:173:GLU:N | 2.36 | 0.41 |
| 1:2:759:PRO:HG2 | 1:2:762:LEU:HD12 | 2.02 | 0.41 |
| 1:2:803:PHE:HB3 | 1:2:805:ILE:N | 2.30 | 0.41 |
| 2:3:410:ASP:O | 2:3:413:THR:OG1 | 2.29 | 0.41 |
| 3:4:388:ARG:NH2 | 5:6:176:ARG:HB2 | 2.36 | 0.41 |
| 3:4:565:LEU:HD23 | 3:4:566:LEU:N | 2.35 | 0.41 |
| 4:5:163:SER:OG | 4:5:164:GLY:N | 2.54 | 0.41 |
| 4:5:494:HIS:HB3 | 4:5:549:ARG:NE | 2.36 | 0.41 |
| 4:5:564:ARG:O | 4:5:568:ILE:HG22 | 2.20 | 0.41 |
| 5:6:395:CYS:SG | 5:6:461:SER:HA | 2.62 | 0.41 |
| 5:6:836:ILE:O | 5:6:839:ASP:HB2 | 2.20 | 0.41 |
| 6:7:217:LYS:HG3 | 6:7:218:LYS:H | 1.86 | 0.41 |
| 6:7:499:LYS:NZ | 6:7:504:ASP:OD1 | 2.35 | 0.41 |
| 6:7:660:VAL:HG22 | 6:7:713:VAL:HG11 | 2.03 | 0.41 |
| 7:A:32:TYR:CB | 7:A:124:SER:HB3 | 2.51 | 0.41 |
| 7:A:46:ASN:OD1 | 7:A:50:ASN:ND2 | 2.52 | 0.41 |
| 7:A:87:LEU:HD13 | 9:C:4:TYR:OH | 2.21 | 0.41 |
| 8:B:79:LEU:O | 8:B:83:SER:N | 2.54 | 0.41 |
| 7:A:127:GLU:CD | 10:D:193:LEU:HD11 | 2.41 | 0.41 |
| 8:B:182:ARG:HA | 10:D:229:PHE:HE2 | 1.86 | 0.41 |
| 11:E:240:TYR:O | 11:E:241:TYR:HB3 | 2.21 | 0.41 |
| 11:E:34:LEU:O | 11:E:34:LEU:HD22 | 2.20 | 0.41 |
| 11:E:356:LYS:O | 11:E:360:HIS:ND1 | 2.45 | 0.41 |
| 11:E:368:ILE:HA | 11:E:369:PRO:HD3 | 1.92 | 0.41 |
| 11:E:60:PRO:HG3 | 11:E:478:TRP:HE1 | 1.85 | 0.41 |
| 11:E:97:GLU:HA | 11:E:98:ILE:C | 2.42 | 0.41 |
| 1:2:553:LEU:HD21 | 1:2:607:ASP:HB3 | 2.03 | 0.40 |
| 1:2:778:LEU:CD1 | 4:5:577:THR:CG2 | 2.99 | 0.40 |
| 2:3:197:ILE:O | 2:3:214:TYR:HB2 | 2.21 | 0.40 |
| 2:3:519:VAL:HB | 2:3:527:ARG:HH12 | 1.86 | 0.40 |
| 2:3:527:ARG:NH1 | 2:3:531:GLN:O | 2.54 | 0.40 |
| 2:3:654:PRO:HA | 2:3:657:ARG:CZ | 2.51 | 0.40 |
| 3:4:312:LYS:O | 3:4:316:GLU:HB3 | 2.22 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:3:315:ILE:HG22 | 4:5:255:PHE:CZ | 2.56 | 0.40 |
| 4:5:258:LEU:HD11 | 4:5:276:MET:HE3 | 2.03 | 0.40 |
| 4:5:378:ILE:HA | 13:5:801:ANP:N6 | 2.30 | 0.40 |
| 5:6:738:ARG:HD3 | 5:6:738:ARG:HA | 1.91 | 0.40 |
| 6:7:71:ALA:CB | 6:7:129:THR:HG21 | 2.51 | 0.40 |
| 6:7:222:SER:HB3 | 6:7:223:LYS:H | 1.67 | 0.40 |
| 6:7:451:ARG:HB2 | 6:7:453:ASP:H | 1.86 | 0.40 |
| 10:D:143:TYR:CZ | 10:D:147:ARG:HD2 | 2.56 | 0.40 |
| 11:E:127:ARG:O | 11:E:245:THR:HA | 2.20 | 0.40 |
| 11:E:380:MET:HB2 | 11:E:385:LYS:HE2 | 2.02 | 0.40 |
| 12:F:8:DT:H2' | 12:F:8:DT:H6 | 1.68 | 0.40 |
| 1:2:243:GLU:HA | 1:2:296:ARG:HB2 | 2.02 | 0.40 |
| 1:2:574:VAL:C | 1:2:576:LEU:H | 2.23 | 0.40 |
| 1:2:587:LYS:HB2 | 1:2:587:LYS:HE3 | 1.93 | 0.40 |
| 1:2:676:ARG:HD3 | 1:2:676:ARG:HA | 1.75 | 0.40 |
| 1:2:783:MET:SD | 1:2:783:MET:N | 2.94 | 0.40 |
| 3:4:228:LYS:HA | 3:4:231:ASN:HD22 | 1.86 | 0.40 |
| 3:4:370:ARG:HD2 | 3:4:378:GLU:O | 2.21 | 0.40 |
| 4:5:153:SER:O | 4:5:156:VAL:HG23 | 2.21 | 0.40 |
| 4:5:413:LEU:HD23 | 4:5:415:LEU:CD2 | 2.52 | 0.40 |
| 4:5:60:SER:HA | 4:5:136:GLN:O | 2.22 | 0.40 |
| 5:6:311:CYS:HA | 5:6:312:ASP:CB | 2.50 | 0.40 |
| 5:6:360:ARG:HA | 5:6:378:ASP:HA | 2.04 | 0.40 |
| 5:6:544:LYS:HE2 | 5:6:584:PHE:HE1 | 1.85 | 0.40 |
| 5:6:641:PHE:H | 5:6:682:ALA:HB2 | 1.86 | 0.40 |
| 6:7:110:ALA:CB | 6:7:238:LEU:HB2 | 2.51 | 0.40 |
| 6:7:368:ALA:HA | 6:7:369:GLY:HA2 | 1.79 | 0.40 |
| 6:7:523:ILE:O | 6:7:566:ALA:N | 2.36 | 0.40 |
| 6:7:544:GLN:O | 6:7:545:THR:OG1 | 2.24 | 0.40 |
| 6:7:700:ALA:O | 6:7:704:LEU:N | 2.54 | 0.40 |
| 7:A:150:ASP:O | 10:D:141:ARG:NE | 2.52 | 0.40 |
| 8:B:166:SER:HB3 | 10:D:227:PHE:HE1 | 1.86 | 0.40 |
| 10:D:150:LYS:HA | 10:D:153:LYS:HE2 | 2.02 | 0.40 |
| 10:D:69:ASN:OD1 | 10:D:293:LEU:HD13 | 2.22 | 0.40 |
| 11:E:64:TYR:OH | 11:E:90:ILE:HB | 2.21 | 0.40 |
| 1:2:247:ARG:HA | 1:2:247:ARG:HH11 | 1.86 | 0.40 |
| 1:2:606:ILE:HG22 | 1:2:609:PHE:HE1 | 1.86 | 0.40 |
| 1:2:803:PHE:CB | 1:2:805:ILE:H | 2.29 | 0.40 |
| 1:2:806:THR:H | 1:2:809:HIS:CB | 2.30 | 0.40 |
| 2:3:469:VAL:HA | 2:3:511:SER:O | 2.21 | 0.40 |
| 2:3:406:LEU:HD13 | 2:3:543:PHE:CE2 | 2.57 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:4:345:ALA:N | 3:4:360:ILE:HG13 | 2.36 | 0.40 |
| 3:4:442:ILE:HG22 | 3:4:443:PRO:O | 2.20 | 0.40 |
| 3:4:557:ARG:HE | 3:4:668:ARG:NH2 | 2.10 | 0.40 |
| 3:4:678:ILE:HD11 | 3:4:693:ASP:HA | 2.02 | 0.40 |
| 3:4:898:VAL:O | 3:4:903:ILE:HD11 | 2.22 | 0.40 |
| 4:5:437:VAL:HG23 | 4:5:472:ALA:HB2 | 2.03 | 0.40 |
| 5:6:640:GLU:HB3 | 5:6:643:LYS:HG2 | 2.04 | 0.40 |
| 2:3:245:TYR:CD2 | 6:7:356:LEU:HD22 | 2.56 | 0.40 |
| 6:7:397:VAL:HG12 | 6:7:640:GLU:HG2 | 2.02 | 0.40 |
| 6:7:495:ALA:O | 6:7:548:ILE:HG12 | 2.20 | 0.40 |
| 6:7:96:GLY:HA3 | 6:7:97:THR:HA | 1.92 | 0.40 |
| 8:B:18:PHE:HE1 | 10:D:135:ARG:CG | 2.35 | 0.40 |
| 11:E:71:TYR:CD2 | 11:E:96:LEU:HD13 | 2.55 | 0.40 |
| 1:2:514:ALA:HB1 | 1:2:679:ILE:HG21 | 2.03 | 0.40 |
| 13:2:901:ANP:HNB1 | 5:6:653:HIS:CE1 | 2.36 | 0.40 |
| 2:3:288:PRO:O | 2:3:464:LEU:HD11 | 2.22 | 0.40 |
| 2:3:372:TYR:CZ | 2:3:561:ILE:HA | 2.56 | 0.40 |
| 3:4:243:LEU:CG | 3:4:244:ASP:H | 2.34 | 0.40 |
| 3:4:505:ASP:HA | 3:4:508:LYS:HB3 | 2.02 | 0.40 |
| 3:4:865:LEU:HD21 | 3:4:903:ILE:HG23 | 2.03 | 0.40 |
| 4:5:94:ILE:HD12 | 4:5:135:PHE:HD2 | 1.87 | 0.40 |
| 4:5:24:ASN:O | 4:5:28:ILE:HG13 | 2.21 | 0.40 |
| 4:5:369:ILE:HD11 | 4:5:592:SER:C | 2.42 | 0.40 |
| 5:6:548:LEU:O | 5:6:552:LEU:HD13 | 2.21 | 0.40 |
| 5:6:585:LEU:HD21 | 5:6:679:LEU:CD2 | 2.51 | 0.40 |
| 5:6:610:ALA:N | 5:6:663:ILE:HD13 | 2.35 | 0.40 |
| 6:7:220:ILE:O | 6:7:222:SER:HB2 | 2.17 | 0.40 |
| 6:7:259:ALA:HB2 | 6:7:270:PHE:CE1 | 2.56 | 0.40 |
| 6:7:459:MET:CB | 6:7:597:LEU:HD21 | 2.38 | 0.40 |
| 6:7:81:ASP:O | 6:7:85:ILE:HG13 | 2.21 | 0.40 |
| 8:B:198:ALA:HB1 | 9:C:113:MET:CE | 2.52 | 0.40 |
| 8:B:95:THR:HG23 | 8:B:96:LYS:H | 1.86 | 0.40 |
| 11:E:313:PRO:HA | 11:E:415:TYR:CE2 | 2.57 | 0.40 |
| 11:E:28:VAL:CG2 | 11:E:57:GLN:HB3 | 2.51 | 0.40 |
| 1:2:284:PRO:HD2 | 11:E:365:ARG:HD3 | 2.03 | 0.40 |
| 1:2:359:ILE:HA | 1:2:360:ARG:HA | 1.79 | 0.40 |
| 1:2:691:ALA:O | 1:2:694:ARG:HB3 | 2.20 | 0.40 |
| 2:3:130:THR:HG22 | 2:3:153:TRP:HD1 | 1.86 | 0.40 |
| 2:3:245:TYR:C | 6:7:236:GLY:HA3 | 2.41 | 0.40 |
| 2:3:687:ARG:HG3 | 2:3:697:ILE:HG21 | 2.03 | 0.40 |
| 3:4:234:ARG:HB3 | 3:4:280:MET:CE | 2.48 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:4:408:ASP:HA | 3:4:409:GLY:HA2 | 1.66 | 0.40 |
| 3:4:520:SER:O | 3:4:523:ALA:HB3 | 2.22 | 0.40 |
| 3:4:760:PRO:HB2 | 3:4:809:ALA:HB1 | 2.03 | 0.40 |
| 4:5:370:LEU:HD23 | 4:5:666:LEU:HD22 | 2.03 | 0.40 |
| 4:5:605:TYR:HE2 | 4:5:668:LEU:HD11 | 1.87 | 0.40 |
| 5:6:152:TYR:HB3 | 5:6:268:PHE:CE2 | 2.55 | 0.40 |
| 6:7:139:LEU:HA | 6:7:142:ILE:CB | 2.49 | 0.40 |
| 2:3:53:ALA:CA | 6:7:218:LYS:HD2 | 2.51 | 0.40 |
| 6:7:360:TYR:CE2 | 6:7:363:PHE:HB2 | 2.57 | 0.40 |
| 6:7:441:ASP:N | 6:7:452:GLY:HA2 | 2.37 | 0.40 |
| 6:7:541:MET:HE1 | 6:7:563:ILE:HG21 | 2.04 | 0.40 |
| 6:7:650:PRO:CA | 6:7:706:ASP:HA | 2.50 | 0.40 |
| 7:A:106:GLY:N | 7:A:107:LEU:HD22 | 2.36 | 0.40 |
| 7:A:199:LEU:HA | 7:A:202:GLN:HB3 | 2.03 | 0.40 |
| 9:C:101:ASN:HB2 | 9:C:102:SER:C | 2.42 | 0.40 |
| 9:C:38:ILE:HD13 | 9:C:38:ILE:HG21 | 1.86 | 0.40 |
| 8:B:166:SER:HB3 | 10:D:227:PHE:CE1 | 2.57 | 0.40 |
| 10:D:98:ILE:HG22 | 10:D:129:MET:HG2 | 2.03 | 0.40 |
| 11:E:527:LEU:HD12 | 11:E:568:VAL:HB | 2.04 | 0.40 |
| 11:E:570:ALA:HB2 | 11:E:581:VAL:HG22 | 2.04 | 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 | 2 | 573/868 (66%) | 502 (88%) | 63 (11%) | 8 (1%) | 14 58 |
| 2 | 3 | 579/971 (60%) | 525 (91%) | 52 (9%) | 2 (0%) | 46 83 |
| 3 | 4 | 660/933 (71%) | 577 (87%) | 72 (11%) | 11 (2%) | 11 56 |
| 4 | 5 | 590/775 (76%) | 537 (91%) | 48 (8%) | 5 (1%) | 24 69 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 5 | 6 | 649/1017 (64%) | 571 (88%) | 72 (11%) | 6 (1%) | 21 | 67 |
| 6 | 7 | 652/845 (77%) | 566 (87%) | 76 (12%) | 10 (2%) | 13 | 58 |
| 7 | A | 206/208 (99%) | 185 (90%) | 20 (10%) | 1 (0%) | 34 | 77 |
| 8 | B | 177/213 (83%) | 156 (88%) | 21 (12%) | 0 | 100 | 100 |
| 9 | C | 151/194 (78%) | 140 (93%) | 11 (7%) | 0 | 100 | 100 |
| 10 | D | 215/294 (73%) | 193 (90%) | 19 (9%) | 3 (1%) | 14 | 58 |
| 11 | E | 543/650 (84%) | 488 (90%) | 50 (9%) | 5 (1%) | 21 | 67 |
| All | All | 4995/6968 (72%) | 4440 (89%) | 504 (10%) | 51 (1%) | 24 | 65 |

All (51) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | 4 | 429 | ALA |
| 4 | 5 | 596 | ILE |
| 6 | 7 | 26 | VAL |
| 6 | 7 | 222 | SER |
| 6 | 7 | 464 | VAL |
| 11 | E | 577 | ASP |
| 11 | E | 601 | ILE |
| 2 | 3 | 389 | VAL |
| 3 | 4 | 419 | VAL |
| 3 | 4 | 433 | ILE |
| 4 | 5 | 410 | ILE |
| 5 | 6 | 402 | ILE |
| 5 | 6 | 560 | VAL |
| 5 | 6 | 569 | ILE |
| 5 | 6 | 819 | ILE |
| 1 | 2 | 533 | ILE |
| 1 | 2 | 656 | ARG |
| 3 | 4 | 450 | GLN |
| 3 | 4 | 609 | VAL |
| 4 | 5 | 340 | SER |
| 10 | D | 219 | ILE |
| 1 | 2 | 291 | SER |
| 1 | 2 | 585 | ILE |
| 1 | 2 | 631 | ILE |
| 2 | 3 | 440 | VAL |
| 3 | 4 | 857 | ILE |
| 4 | 5 | 267 | VAL |
| 4 | 5 | 341 | SER |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | 6 | 106 | VAL |
| 5 | 6 | 321 | VAL |
| 6 | 7 | 502 | VAL |
| 7 | A | 27 | VAL |
| 10 | D | 210 | ASN |
| 3 | 4 | 373 | ARG |
| 6 | 7 | 255 | VAL |
| 6 | 7 | 374 | THR |
| 11 | E | 602 | LEU |
| 1 | 2 | 297 | ILE |
| 6 | 7 | 248 | VAL |
| 6 | 7 | 257 | VAL |
| 11 | E | 98 | ILE |
| 3 | 4 | 364 | VAL |
| 1 | 2 | 842 | VAL |
| 3 | 4 | 463 | VAL |
| 3 | 4 | 856 | VAL |
| 6 | 7 | 708 | VAL |
| 10 | D | 258 | VAL |
| 1 | 2 | 303 | ILE |
| 3 | 4 | 694 | LEU |
| 6 | 7 | 462 | PRO |
| 11 | E | 99 | ASP |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1 | 2 | 502/770 (65%) | 460 (92%) | 42 (8%) | 14 | 50 |
| 2 | 3 | 512/835 (61%) | 475 (93%) | 37 (7%) | 18 | 57 |
| 3 | 4 | 599/848 (71%) | 570 (95%) | 29 (5%) | 31 | 68 |
| 4 | 5 | 542/688 (79%) | 500 (92%) | 42 (8%) | 16 | 54 |
| 5 | 6 | 539/886 (61%) | 497 (92%) | 42 (8%) | 16 | 53 |
| 6 | 7 | 582/753 (77%) | 553 (95%) | 29 (5%) | 30 | 67 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|----|
| 7 | A | 193/193 (100%) | 182 (94%) | 11 (6%) | 25 | 64 |
| 8 | B | 171/198 (86%) | 162 (95%) | 9 (5%) | 28 | 66 |
| 9 | C | 144/173 (83%) | 136 (94%) | 8 (6%) | 26 | 65 |
| 10 | D | 213/279 (76%) | 207 (97%) | 6 (3%) | 51 | 79 |
| 11 | E | 499/586 (85%) | 479 (96%) | 20 (4%) | 38 | 72 |
| All | All | 4496/6209 (72%) | 4221 (94%) | 275 (6%) | 28 | 62 |

All (275) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 2 | 234 | LEU |
| 1 | 2 | 253 | LYS |
| 1 | 2 | 263 | CYS |
| 1 | 2 | 297 | ILE |
| 1 | 2 | 298 | SER |
| 1 | 2 | 384 | ASN |
| 1 | 2 | 391 | GLN |
| 1 | 2 | 432 | ASN |
| 1 | 2 | 437 | ASN |
| 1 | 2 | 446 | VAL |
| 1 | 2 | 454 | ASN |
| 1 | 2 | 501 | MET |
| 1 | 2 | 511 | ILE |
| 1 | 2 | 533 | ILE |
| 1 | 2 | 538 | ASN |
| 1 | 2 | 549 | LYS |
| 1 | 2 | 567 | THR |
| 1 | 2 | 577 | THR |
| 1 | 2 | 583 | ASP |
| 1 | 2 | 590 | THR |
| 1 | 2 | 624 | MET |
| 1 | 2 | 628 | SER |
| 1 | 2 | 630 | SER |
| 1 | 2 | 631 | ILE |
| 1 | 2 | 633 | LYS |
| 1 | 2 | 636 | ILE |
| 1 | 2 | 640 | LEU |
| 1 | 2 | 646 | ILE |
| 1 | 2 | 651 | ASN |
| 1 | 2 | 705 | ARG |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 2 | 706 | SER |
| 1 | 2 | 782 | ASP |
| 1 | 2 | 783 | MET |
| 1 | 2 | 787 | SER |
| 1 | 2 | 793 | LEU |
| 1 | 2 | 802 | SER |
| 1 | 2 | 805 | ILE |
| 1 | 2 | 806 | THR |
| 1 | 2 | 807 | VAL |
| 1 | 2 | 808 | ARG |
| 1 | 2 | 854 | ARG |
| 1 | 2 | 860 | SER |
| 2 | 3 | 108 | ARG |
| 2 | 3 | 137 | ASP |
| 2 | 3 | 154 | LYS |
| 2 | 3 | 169 | ARG |
| 2 | 3 | 170 | THR |
| 2 | 3 | 171 | LEU |
| 2 | 3 | 172 | THR |
| 2 | 3 | 190 | SER |
| 2 | 3 | 209 | PHE |
| 2 | 3 | 227 | THR |
| 2 | 3 | 275 | ASP |
| 2 | 3 | 291 | ARG |
| 2 | 3 | 300 | SER |
| 2 | 3 | 346 | ASP |
| 2 | 3 | 350 | ILE |
| 2 | 3 | 384 | MET |
| 2 | 3 | 395 | ASN |
| 2 | 3 | 402 | ASP |
| 2 | 3 | 423 | LEU |
| 2 | 3 | 435 | ARG |
| 2 | 3 | 438 | SER |
| 2 | 3 | 469 | VAL |
| 2 | 3 | 473 | ASP |
| 2 | 3 | 503 | HIS |
| 2 | 3 | 506 | LEU |
| 2 | 3 | 513 | ILE |
| 2 | 3 | 535 | LEU |
| 2 | 3 | 541 | SER |
| 2 | 3 | 542 | ARG |
| 2 | 3 | 553 | ILE |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | 3 | 563 | GLU |
| 2 | 3 | 564 | HIS |
| 2 | 3 | 656 | LEU |
| 2 | 3 | 657 | ARG |
| 2 | 3 | 691 | ASN |
| 2 | 3 | 732 | LEU |
| 2 | 3 | 733 | LEU |
| 3 | 4 | 243 | LEU |
| 3 | 4 | 261 | LEU |
| 3 | 4 | 279 | CYS |
| 3 | 4 | 311 | CYS |
| 3 | 4 | 321 | ASP |
| 3 | 4 | 371 | CYS |
| 3 | 4 | 389 | CYS |
| 3 | 4 | 416 | SER |
| 3 | 4 | 449 | ARG |
| 3 | 4 | 451 | ARG |
| 3 | 4 | 463 | VAL |
| 3 | 4 | 502 | THR |
| 3 | 4 | 563 | ASN |
| 3 | 4 | 569 | ASP |
| 3 | 4 | 591 | THR |
| 3 | 4 | 623 | LEU |
| 3 | 4 | 631 | ILE |
| 3 | 4 | 644 | VAL |
| 3 | 4 | 688 | VAL |
| 3 | 4 | 692 | ILE |
| 3 | 4 | 699 | LEU |
| 3 | 4 | 720 | LEU |
| 3 | 4 | 725 | THR |
| 3 | 4 | 727 | LEU |
| 3 | 4 | 762 | ILE |
| 3 | 4 | 770 | LEU |
| 3 | 4 | 772 | ARG |
| 3 | 4 | 810 | LYS |
| 3 | 4 | 856 | VAL |
| 4 | 5 | 21 | ASP |
| 4 | 5 | 35 | ILE |
| 4 | 5 | 36 | LEU |
| 4 | 5 | 48 | ASP |
| 4 | 5 | 84 | SER |
| 4 | 5 | 137 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | 5 | 141 | SER |
| 4 | 5 | 152 | ASP |
| 4 | 5 | 159 | ILE |
| 4 | 5 | 174 | SER |
| 4 | 5 | 179 | LEU |
| 4 | 5 | 190 | THR |
| 4 | 5 | 204 | THR |
| 4 | 5 | 210 | SER |
| 4 | 5 | 211 | CYS |
| 4 | 5 | 246 | GLU |
| 4 | 5 | 293 | THR |
| 4 | 5 | 321 | VAL |
| 4 | 5 | 331 | LEU |
| 4 | 5 | 337 | VAL |
| 4 | 5 | 339 | THR |
| 4 | 5 | 341 | SER |
| 4 | 5 | 344 | ASN |
| 4 | 5 | 347 | THR |
| 4 | 5 | 348 | MET |
| 4 | 5 | 370 | LEU |
| 4 | 5 | 384 | ILE |
| 4 | 5 | 410 | ILE |
| 4 | 5 | 430 | GLU |
| 4 | 5 | 439 | THR |
| 4 | 5 | 444 | SER |
| 4 | 5 | 454 | GLN |
| 4 | 5 | 462 | PHE |
| 4 | 5 | 511 | THR |
| 4 | 5 | 560 | HIS |
| 4 | 5 | 563 | GLU |
| 4 | 5 | 595 | SER |
| 4 | 5 | 640 | SER |
| 4 | 5 | 642 | GLU |
| 4 | 5 | 650 | ILE |
| 4 | 5 | 652 | GLN |
| 4 | 5 | 668 | LEU |
| 5 | 6 | 101 | LYS |
| 5 | 6 | 180 | PHE |
| 5 | 6 | 354 | LEU |
| 5 | 6 | 364 | ASN |
| 5 | 6 | 372 | SER |
| 5 | 6 | 376 | THR |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | 6 | 377 | LEU |
| 5 | 6 | 400 | VAL |
| 5 | 6 | 533 | ILE |
| 5 | 6 | 560 | VAL |
| 5 | 6 | 570 | ASN |
| 5 | 6 | 581 | LYS |
| 5 | 6 | 586 | LYS |
| 5 | 6 | 614 | ARG |
| 5 | 6 | 615 | ASP |
| 5 | 6 | 624 | GLU |
| 5 | 6 | 642 | ASP |
| 5 | 6 | 644 | MET |
| 5 | 6 | 647 | SER |
| 5 | 6 | 648 | ASP |
| 5 | 6 | 662 | SER |
| 5 | 6 | 688 | ARG |
| 5 | 6 | 692 | LYS |
| 5 | 6 | 719 | CYS |
| 5 | 6 | 723 | ILE |
| 5 | 6 | 752 | ARG |
| 5 | 6 | 781 | ARG |
| 5 | 6 | 783 | ASP |
| 5 | 6 | 822 | SER |
| 5 | 6 | 824 | ILE |
| 5 | 6 | 832 | ARG |
| 5 | 6 | 916 | ILE |
| 5 | 6 | 918 | ARG |
| 5 | 6 | 920 | ILE |
| 5 | 6 | 924 | ASP |
| 5 | 6 | 935 | ASP |
| 5 | 6 | 936 | ILE |
| 5 | 6 | 938 | ASP |
| 5 | 6 | 948 | LEU |
| 5 | 6 | 967 | ARG |
| 5 | 6 | 968 | LEU |
| 5 | 6 | 969 | VAL |
| 6 | 7 | 114 | THR |
| 6 | 7 | 116 | LEU |
| 6 | 7 | 127 | LEU |
| 6 | 7 | 222 | SER |
| 6 | 7 | 223 | LYS |
| 6 | 7 | 281 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | 7 | 344 | SER |
| 6 | 7 | 363 | PHE |
| 6 | 7 | 370 | LEU |
| 6 | 7 | 404 | LEU |
| 6 | 7 | 437 | VAL |
| 6 | 7 | 491 | VAL |
| 6 | 7 | 493 | LEU |
| 6 | 7 | 494 | THR |
| 6 | 7 | 497 | VAL |
| 6 | 7 | 503 | THR |
| 6 | 7 | 521 | CYS |
| 6 | 7 | 530 | ASP |
| 6 | 7 | 533 | ASP |
| 6 | 7 | 582 | ASP |
| 6 | 7 | 595 | ASP |
| 6 | 7 | 601 | LEU |
| 6 | 7 | 627 | ASP |
| 6 | 7 | 631 | THR |
| 6 | 7 | 636 | SER |
| 6 | 7 | 671 | SER |
| 6 | 7 | 723 | SER |
| 6 | 7 | 724 | LYS |
| 6 | 7 | 727 | LEU |
| 7 | A | 23 | SER |
| 7 | A | 25 | GLN |
| 7 | A | 44 | VAL |
| 7 | A | 104 | ASN |
| 7 | A | 107 | LEU |
| 7 | A | 109 | LEU |
| 7 | A | 149 | ILE |
| 7 | A | 151 | LEU |
| 7 | A | 160 | ASP |
| 7 | A | 165 | VAL |
| 7 | A | 183 | LEU |
| 8 | B | 20 | VAL |
| 8 | B | 31 | ILE |
| 8 | B | 54 | THR |
| 8 | B | 87 | ILE |
| 8 | B | 95 | THR |
| 8 | B | 118 | ASN |
| 8 | B | 160 | LEU |
| 8 | B | 175 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | B | 189 | MET |
| 9 | C | 24 | ILE |
| 9 | C | 53 | ILE |
| 9 | C | 79 | MET |
| 9 | C | 95 | LEU |
| 9 | C | 112 | ILE |
| 9 | C | 120 | LEU |
| 9 | C | 125 | SER |
| 9 | C | 163 | SER |
| 10 | D | 124 | LEU |
| 10 | D | 127 | LEU |
| 10 | D | 129 | MET |
| 10 | D | 257 | THR |
| 10 | D | 259 | THR |
| 10 | D | 260 | ILE |
| 11 | E | 27 | LEU |
| 11 | E | 32 | SER |
| 11 | E | 33 | CYS |
| 11 | E | 34 | LEU |
| 11 | E | 57 | GLN |
| 11 | E | 99 | ASP |
| 11 | E | 123 | LEU |
| 11 | E | 142 | CYS |
| 11 | E | 250 | SER |
| 11 | E | 280 | LEU |
| 11 | E | 284 | TYR |
| 11 | E | 314 | ASP |
| 11 | E | 326 | LEU |
| 11 | E | 333 | SER |
| 11 | E | 362 | MET |
| 11 | E | 396 | LEU |
| 11 | E | 492 | LEU |
| 11 | E | 529 | VAL |
| 11 | E | 601 | ILE |
| 11 | E | 637 | LEU |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 2 | 238 | ASN |
| 1 | 2 | 641 | GLN |
| 1 | 2 | 651 | ASN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 2 | 780 | GLN |
| 1 | 2 | 856 | GLN |
| 2 | 3 | 51 | ASN |
| 2 | 3 | 351 | ASN |
| 2 | 3 | 417 | GLN |
| 2 | 3 | 532 | ASN |
| 3 | 4 | 400 | GLN |
| 3 | 4 | 582 | HIS |
| 4 | 5 | 140 | ASN |
| 4 | 5 | 253 | GLN |
| 4 | 5 | 411 | ASN |
| 4 | 5 | 454 | GLN |
| 4 | 5 | 561 | ASN |
| 4 | 5 | 581 | ASN |
| 4 | 5 | 676 | HIS |
| 5 | 6 | 458 | HIS |
| 5 | 6 | 570 | ASN |
| 5 | 6 | 653 | HIS |
| 5 | 6 | 735 | HIS |
| 6 | 7 | 657 | ASN |
| 8 | B | 128 | ASN |
| 9 | C | 101 | ASN |
| 11 | E | 155 | GLN |
| 11 | E | 269 | ASN |
| 11 | E | 286 | GLN |
| 11 | E | 493 | ASN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

3 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 13 | ANP | 2 | 901 | - | 29,33,33 | 2.84 | 6 (20%) | 26,52,52 | 1.37 | 3 (11%) |
| 13 | ANP | 3 | 1001 | - | 29,33,33 | 2.95 | 6 (20%) | 26,52,52 | 1.20 | 3 (11%) |
| 13 | ANP | 5 | 801 | - | 29,33,33 | 2.13 | 5 (17%) | 26,52,52 | 1.14 | 1 (3%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|------------|---------|
| 13 | ANP | 2 | 901 | - | - | 0/13/38/38 | 0/3/3/3 |
| 13 | ANP | 3 | 1001 | - | - | 1/13/38/38 | 0/3/3/3 |
| 13 | ANP | 5 | 801 | - | - | 0/13/38/38 | 0/3/3/3 |

All (17) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 13 | 2 | 901 | ANP | PB-O3A | -3.00 | 1.55 | 1.59 |
| 13 | 3 | 1001 | ANP | PB-O2B | -2.93 | 1.48 | 1.56 |
| 13 | 5 | 801 | ANP | PB-O3A | -2.91 | 1.55 | 1.59 |
| 13 | 3 | 1001 | ANP | PB-O3A | -2.82 | 1.55 | 1.59 |
| 13 | 3 | 1001 | ANP | PG-O2G | -2.72 | 1.49 | 1.56 |
| 13 | 5 | 801 | ANP | PB-O2B | -2.47 | 1.50 | 1.56 |
| 13 | 2 | 901 | ANP | PG-O2G | -2.42 | 1.50 | 1.56 |
| 13 | 2 | 901 | ANP | PB-O2B | -2.40 | 1.50 | 1.56 |
| 13 | 5 | 801 | ANP | PG-N3B | 2.15 | 1.69 | 1.63 |
| 13 | 2 | 901 | ANP | PG-N3B | 2.38 | 1.69 | 1.63 |
| 13 | 3 | 1001 | ANP | PG-N3B | 2.39 | 1.69 | 1.63 |
| 13 | 5 | 801 | ANP | PG-O1G | 3.69 | 1.50 | 1.46 |
| 13 | 2 | 901 | ANP | PB-O1B | 8.63 | 1.55 | 1.46 |
| 13 | 5 | 801 | ANP | PB-O1B | 9.35 | 1.56 | 1.46 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 13 | 3 | 1001 | ANP | PB-O1B | 9.64 | 1.56 | 1.46 |
| 13 | 3 | 1001 | ANP | PG-O1G | 11.03 | 1.58 | 1.46 |
| 13 | 2 | 901 | ANP | PG-O1G | 11.13 | 1.58 | 1.46 |

All (7) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 13 | 2 | 901 | ANP | PA-O3A-PB | -5.62 | 112.30 | 132.71 |
| 13 | 5 | 801 | ANP | PA-O3A-PB | -4.40 | 116.73 | 132.71 |
| 13 | 3 | 1001 | ANP | PA-O3A-PB | -3.95 | 118.36 | 132.71 |
| 13 | 3 | 1001 | ANP | O3G-PG-O1G | -2.56 | 106.85 | 113.58 |
| 13 | 2 | 901 | ANP | O3G-PG-O1G | -2.19 | 107.81 | 113.58 |
| 13 | 3 | 1001 | ANP | O3A-PB-N3B | 2.19 | 112.09 | 106.07 |
| 13 | 2 | 901 | ANP | O3A-PB-N3B | 2.23 | 112.21 | 106.07 |

There are no chirality outliers.

All (1) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|---------------|
| 13 | 3 | 1001 | ANP | O1B-PB-N3B-PG |

There are no ring outliers.

3 monomers are involved in 28 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 13 | 2 | 901 | ANP | 9 | 0 |
| 13 | 3 | 1001 | ANP | 10 | 0 |
| 13 | 5 | 801 | ANP | 9 | 0 |

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.