



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 04:26 pm GMT

PDB ID : 2QZP
Title : Crystal structure of mutation of an acylptide hydrolase/esterase from *Aeropyrum pernix* K1
Authors : Zhang, H.F.; Zheng, B.S.; Rao, Z.
Deposited on : 2007-08-17
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

| | | |
|--------------------------------|---|--|
| MolProbity | : | 4.02b-467 |
| Xtriage (Phenix) | : | 1.9-1692 |
| EDS | : | trunk28620 |
| Percentile statistics | : | 20161228.v01 (using entries in the PDB archive December 28th 2016) |
| Refmac | : | 5.8.0135 |
| CCP4 | : | 6.5.0 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | recalc28949 |

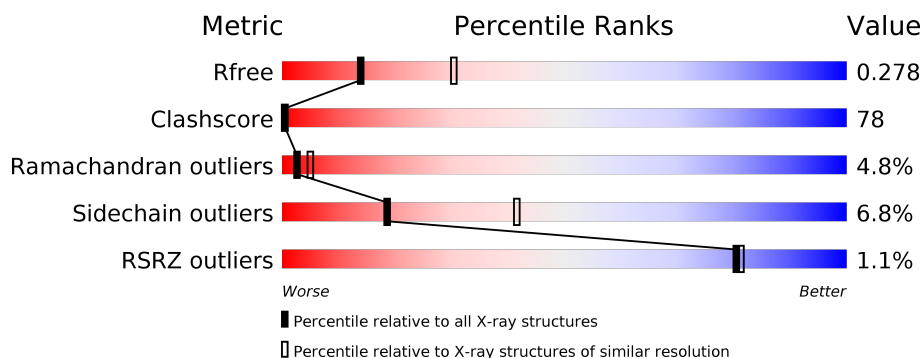
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 100719 | 2259 (2.70-2.70) |
| Clashscore | 112137 | 2590 (2.70-2.70) |
| Ramachandran outliers | 110173 | 2550 (2.70-2.70) |
| Sidechain outliers | 110143 | 2550 (2.70-2.70) |
| RSRZ outliers | 101464 | 2275 (2.70-2.70) |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | A | 562 | <div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 22%, yellow 70%, orange 7%, red 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 22% 70% 7% • </div> </div> |
| 1 | B | 562 | <div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 20%, yellow 72%, orange 8%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 20% 72% 8% </div> </div> |

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8881 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Acylamino-acid-releasing enzyme.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | A | 560 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4255 | 2685 | 750 | 808 | 12 | | | |
| 1 | B | 561 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4260 | 2688 | 751 | 809 | 12 | | | |

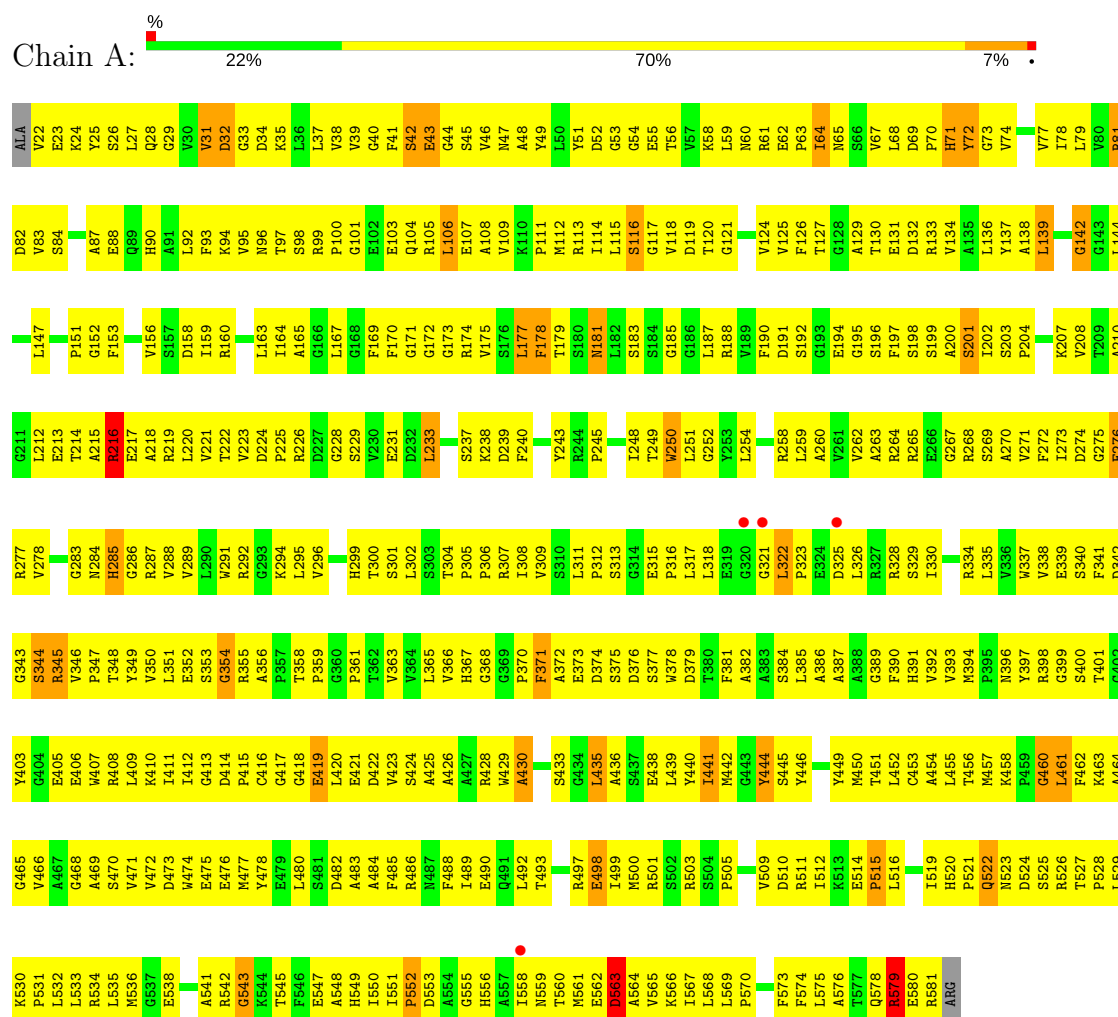
- Molecule 2 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 2 | A | 154 | Total | O | 0 | 0 |
| | | | 154 | 154 | | |
| 2 | B | 212 | Total | O | 0 | 0 |
| | | | 212 | 212 | | |

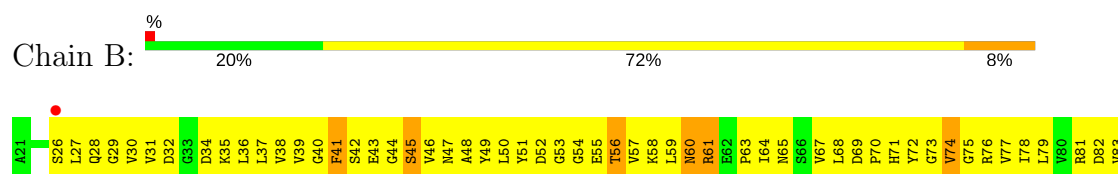
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: Acylamino-acid-releasing enzyme



• Molecule 1: Acylamino-acid-releasing enzyme



| | | | | | | | |
|------|------|------|------|------|------|------|------|
| R526 | G465 | Y403 | D342 | A280 | A218 | E146 | S84 |
| TS27 | V466 | G404 | G343 | P281 | R219 | L147 | R65 |
| P528 | A467 | E405 | S344 | Q282 | R219 | A148 | G86 |
| L529 | G468 | E406 | R345 | Q283 | V221 | R149 | A87 |
| K530 | A469 | W407 | V346 | N284 | T222 | L150 | E88 |
| P531 | S470 | R408 | P347 | H285 | V223 | Q89 | H90 |
| L532 | W471 | L409 | | H286 | D224 | F153 | A91 |
| L533 | V472 | K410 | V350 | R287 | P225 | | L92 |
| R534 | D473 | I411 | L351 | V288 | R226 | V156 | F93 |
| L535 | W474 | | E352 | V289 | D227 | S157 | K94 |
| M536 | E475 | D414 | S353 | L290 | | D158 | V95 |
| G537 | E476 | P415 | G354 | W291 | V230 | I159 | I96 |
| E538 | M477 | G416 | R355 | R292 | E231 | R160 | |
| L539 | Y478 | G417 | A356 | G293 | D232 | G161 | R99 |
| L540 | E479 | G418 | P357 | K294 | L233 | D162 | P100 |
| A541 | L480 | E419 | T358 | L295 | E234 | L163 | G101 |
| R542 | S481 | L420 | P359 | V296 | L235 | I164 | E102 |
| G543 | D482 | E421 | G360 | | P236 | | E103 |
| K544 | A483 | D422 | P361 | H299 | | G168 | Q104 |
| T545 | A484 | V423 | T362 | T300 | D239 | F169 | R105 |
| F546 | F485 | S424 | V363 | S301 | F240 | F170 | L106 |
| E547 | R486 | A425 | V364 | L302 | S241 | G171 | E107 |
| A548 | N487 | | L365 | S303 | S242 | G172 | E107 |
| H549 | F488 | R428 | V366 | T304 | Y243 | G173 | A108 |
| I550 | I489 | W429 | H367 | P305 | R244 | R174 | V109 |
| I551 | E490 | A430 | G368 | P306 | P245 | V175 | K110 |
| P552 | Q491 | R431 | G369 | R307 | T246 | S176 | P111 |
| D553 | L492 | E432 | S371 | P370 | A247 | S177 | M112 |
| A554 | T493 | S433 | A372 | V309 | L248 | F178 | R113 |
| G555 | G494 | G434 | S373 | S310 | T249 | T179 | I114 |
| H556 | G495 | L435 | E374 | L311 | W250 | S180 | L115 |
| A557 | S496 | A436 | D374 | P312 | L251 | N181 | S116 |
| L558 | R497 | S437 | S375 | S313 | G252 | L182 | G117 |
| N559 | E498 | E438 | D376 | G314 | Y253 | | V118 |
| M561 | M500 | Y440 | W377 | E315 | P255 | G186 | T120 |
| E562 | R501 | T441 | D379 | P316 | D256 | G187 | G121 |
| D563 | S502 | M442 | T380 | L317 | G257 | R188 | E122 |
| A564 | R503 | G443 | F381 | E319 | R258 | V189 | A123 |
| V565 | S504 | Y444 | A382 | | L259 | | V124 |
| K566 | P505 | S445 | A383 | L322 | A260 | G195 | F126 |
| I567 | I506 | Y446 | S384 | P323 | V261 | F197 | T127 |
| L568 | N507 | G447 | L385 | E324 | A263 | S198 | T130 |
| P569 | H508 | G448 | A386 | D325 | R264 | S199 | E131 |
| P570 | V509 | Y449 | A387 | L326 | R265 | A200 | D132 |
| A571 | D510 | M450 | A388 | R327 | E266 | S201 | R133 |
| V572 | R511 | T451 | G389 | R328 | I202 | I203 | V134 |
| F573 | I512 | L452 | F390 | S329 | G267 | S203 | A135 |
| F574 | K513 | C453 | H391 | T330 | R268 | S204 | L136 |
| | E514 | A454 | V392 | A331 | S269 | G205 | Y137 |
| TS77 | P515 | L455 | V393 | G332 | A270 | M206 | A138 |
| Q578 | L516 | T456 | M394 | S333 | V271 | K207 | V208 |
| R579 | A517 | M457 | P395 | R334 | F272 | V208 | L139 |
| E580 | L518 | K458 | N396 | L335 | L273 | T209 | D140 |
| R581 | I519 | P459 | Y397 | V336 | D274 | G210 | G142 |
| ARG | H520 | G460 | R398 | V337 | G275 | A211 | G143 |
| | P521 | L461 | G399 | V338 | E276 | G211 | L144 |
| | Q522 | F462 | S400 | E339 | R277 | E213 | R145 |
| | N523 | K463 | T401 | F341 | V278 | | |
| | | A464 | G402 | | E279 | | |

4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 63.12Å 102.18Å 163.59Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 48.11 – 2.70 48.11 – 2.50 | Depositor EDS |
| % Data completeness (in resolution range) | 92.0 (48.11-2.70) 90.3 (48.11-2.50) | Depositor EDS |
| R_{merge} | 0.18 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.58 (at 2.51Å) | Xtriage |
| Refinement program | CNS 1.0 | Depositor |
| R, R_{free} | 0.226 , 0.277 0.226 , 0.278 | Depositor DCC |
| R_{free} test set | 1393 reflections (5.07%) | DCC |
| Wilson B-factor (Å ²) | 32.5 | Xtriage |
| Anisotropy | 0.373 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.33 , 81.0 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.88 | EDS |
| Total number of atoms | 8881 | wwPDB-VP |
| Average B, all atoms (Å ²) | 30.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | A | 0.47 | 0/4346 | 0.76 | 0/5892 |
| 1 | B | 0.46 | 0/4351 | 0.75 | 1/5899 (0.0%) |
| All | All | 0.46 | 0/8697 | 0.75 | 1/11791 (0.0%) |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | B | 374 | ASP | N-CA-C | -5.06 | 97.33 | 111.00 |

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 4255 | 0 | 4219 | 642 | 0 |
| 1 | B | 4260 | 0 | 4224 | 704 | 0 |
| 2 | A | 154 | 0 | 0 | 93 | 0 |
| 2 | B | 212 | 0 | 0 | 137 | 0 |
| All | All | 8881 | 0 | 8443 | 1329 | 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 78.

All (1329) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:497:ARG:HH11 | 1:B:497:ARG:HB2 | 0.94 | 1.11 |
| 1:A:552:PRO:HD3 | 1:B:547:GLU:HB2 | 1.30 | 1.11 |
| 1:A:346:VAL:HG21 | 1:A:422:ASP:HB3 | 1.32 | 1.09 |
| 1:B:334:ARG:HH21 | 1:B:350:VAL:HG11 | 1.03 | 1.09 |
| 1:A:547:GLU:HB3 | 1:B:552:PRO:HD3 | 1.18 | 1.07 |
| 1:B:92:LEU:HD12 | 1:B:109:VAL:HG21 | 1.34 | 1.03 |
| 1:B:90:HIS:HB2 | 1:B:114:ILE:HD13 | 1.42 | 1.00 |
| 1:A:530:LYS:HB3 | 1:A:531:PRO:HD3 | 1.41 | 1.00 |
| 1:B:376:ASP:HA | 2:B:791:HOH:O | 1.60 | 1.00 |
| 1:B:323:PRO:HB2 | 1:B:326:LEU:HB2 | 1.42 | 0.99 |
| 1:B:497:ARG:HB2 | 1:B:497:ARG:NH1 | 1.79 | 0.98 |
| 1:B:347:PRO:O | 1:B:396:ASN:HB2 | 1.63 | 0.98 |
| 1:B:212:LEU:HD23 | 1:B:219:ARG:HH12 | 1.26 | 0.96 |
| 1:B:201:SER:HB3 | 2:B:767:HOH:O | 1.65 | 0.96 |
| 1:A:558:ILE:HD12 | 1:A:563:ASP:HB3 | 1.45 | 0.95 |
| 1:B:322:LEU:HD12 | 1:B:323:PRO:HD2 | 1.49 | 0.94 |
| 1:B:567:ILE:HD12 | 1:B:568:LEU:N | 1.82 | 0.94 |
| 1:B:497:ARG:HH11 | 1:B:497:ARG:CB | 1.81 | 0.93 |
| 1:A:522:GLN:HA | 1:A:529:LEU:HD22 | 1.45 | 0.93 |
| 1:A:471:VAL:HG12 | 2:A:657:HOH:O | 1.68 | 0.92 |
| 1:A:558:ILE:HG23 | 1:A:563:ASP:HB2 | 1.51 | 0.92 |
| 1:B:212:LEU:HD23 | 1:B:219:ARG:NH1 | 1.85 | 0.91 |
| 1:A:529:LEU:HD11 | 1:A:550:ILE:HD12 | 1.51 | 0.90 |
| 1:B:530:LYS:HB3 | 1:B:531:PRO:HD3 | 1.51 | 0.90 |
| 1:B:42:SER:HA | 1:B:561:MET:SD | 2.12 | 0.90 |
| 1:B:88:GLU:HG2 | 1:B:113:ARG:NH1 | 1.85 | 0.90 |
| 1:B:363:VAL:HG22 | 1:B:440:TYR:HB2 | 1.52 | 0.89 |
| 1:A:449:TYR:HA | 2:A:709:HOH:O | 1.71 | 0.88 |
| 1:A:69:ASP:HB2 | 1:A:118:VAL:HG22 | 1.56 | 0.88 |
| 1:A:68:LEU:HD12 | 1:A:78:ILE:HG21 | 1.52 | 0.88 |
| 1:B:325:ASP:HA | 1:B:328:ARG:HB2 | 1.56 | 0.88 |
| 1:A:65:ASN:HD21 | 1:A:82:ASP:HB2 | 1.37 | 0.88 |
| 1:B:334:ARG:NH2 | 1:B:350:VAL:HG11 | 1.87 | 0.88 |
| 1:A:547:GLU:CB | 1:B:552:PRO:HD3 | 2.03 | 0.88 |
| 1:B:509:VAL:HA | 1:B:512:ILE:HD13 | 1.56 | 0.87 |
| 1:A:574:PHE:HA | 2:A:602:HOH:O | 1.74 | 0.87 |
| 1:A:127:THR:HB | 2:A:677:HOH:O | 1.73 | 0.87 |
| 1:B:208:VAL:HB | 1:B:223:VAL:HB | 1.56 | 0.87 |
| 1:B:528:PRO:HG3 | 2:B:756:HOH:O | 1.75 | 0.86 |
| 1:A:545:THR:HB | 2:A:613:HOH:O | 1.73 | 0.86 |
| 1:A:457:MET:HB2 | 2:A:696:HOH:O | 1.75 | 0.86 |
| 1:B:49:TYR:HA | 1:B:57:VAL:O | 1.74 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:505:PRO:HG2 | 2:B:731:HOH:O | 1.76 | 0.86 |
| 1:B:520:HIS:HD2 | 1:B:521:PRO:HD2 | 1.40 | 0.86 |
| 1:B:539:LEU:HB2 | 2:B:678:HOH:O | 1.75 | 0.86 |
| 1:A:515:PRO:HA | 2:A:613:HOH:O | 1.76 | 0.85 |
| 1:B:303:SER:O | 1:B:304:THR:HG23 | 1.74 | 0.85 |
| 1:B:26:SER:HB3 | 1:B:39:VAL:HB | 1.58 | 0.85 |
| 1:A:569:LEU:HB3 | 1:A:570:PRO:HD3 | 1.57 | 0.85 |
| 1:A:412:ILE:HB | 2:A:721:HOH:O | 1.77 | 0.84 |
| 1:B:127:THR:HG23 | 1:B:156:VAL:HG23 | 1.59 | 0.84 |
| 1:B:278:VAL:HG11 | 1:B:295:LEU:HD12 | 1.56 | 0.84 |
| 1:A:215:ALA:HB1 | 1:A:406:GLU:HB2 | 1.57 | 0.84 |
| 1:A:558:ILE:HG22 | 1:A:560:THR:O | 1.78 | 0.84 |
| 1:A:547:GLU:HB3 | 1:B:552:PRO:CD | 2.07 | 0.84 |
| 1:A:273:ILE:O | 1:A:276:GLU:HB2 | 1.77 | 0.83 |
| 1:B:561:MET:HA | 2:B:589:HOH:O | 1.76 | 0.83 |
| 1:B:338:VAL:HG11 | 1:B:425:ALA:O | 1.78 | 0.83 |
| 1:B:484:ALA:HB3 | 2:B:604:HOH:O | 1.79 | 0.83 |
| 1:A:194:GLU:HB2 | 1:A:212:LEU:HD21 | 1.60 | 0.83 |
| 1:A:548:ALA:HB3 | 1:B:550:ILE:HD13 | 1.58 | 0.83 |
| 1:B:463:LYS:HB2 | 2:B:658:HOH:O | 1.77 | 0.82 |
| 1:B:458:LYS:HE3 | 2:B:778:HOH:O | 1.79 | 0.82 |
| 1:A:116:SER:N | 2:A:677:HOH:O | 2.13 | 0.82 |
| 1:A:452:LEU:HD22 | 2:A:709:HOH:O | 1.78 | 0.82 |
| 1:A:532:LEU:HD13 | 1:A:532:LEU:O | 1.79 | 0.82 |
| 1:B:70:PRO:HB2 | 1:B:74:VAL:HG21 | 1.61 | 0.82 |
| 1:A:94:LYS:O | 1:A:94:LYS:HG3 | 1.79 | 0.82 |
| 1:B:420:LEU:HD21 | 1:B:458:LYS:HD3 | 1.59 | 0.82 |
| 1:B:284:ASN:HD22 | 1:B:376:ASP:C | 1.83 | 0.81 |
| 1:B:302:LEU:HG | 2:B:600:HOH:O | 1.79 | 0.81 |
| 1:A:177:LEU:HD21 | 1:A:208:VAL:HG11 | 1.62 | 0.81 |
| 1:A:138:ALA:HB2 | 1:A:147:LEU:HD21 | 1.63 | 0.81 |
| 1:A:458:LYS:HD3 | 1:A:461:LEU:HD13 | 1.63 | 0.80 |
| 1:B:102:GLU:HA | 2:B:621:HOH:O | 1.79 | 0.80 |
| 1:A:322:LEU:HD23 | 1:A:323:PRO:HD2 | 1.63 | 0.80 |
| 1:A:23:GLU:HA | 2:A:730:HOH:O | 1.80 | 0.80 |
| 1:B:158:ASP:O | 1:B:159:ILE:HD13 | 1.80 | 0.80 |
| 1:B:374:ASP:CG | 1:B:394:MET:HB3 | 2.01 | 0.80 |
| 1:B:406:GLU:HG2 | 1:B:410:LYS:HE2 | 1.64 | 0.80 |
| 1:A:545:THR:HG23 | 1:B:553:ASP:OD1 | 1.80 | 0.80 |
| 1:B:570:PRO:HD2 | 2:B:594:HOH:O | 1.82 | 0.79 |
| 1:B:44:GLY:O | 1:B:560:THR:HG22 | 1.83 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:78:ILE:HD13 | 1:B:124:VAL:HG13 | 1.63 | 0.79 |
| 1:A:38:VAL:HG12 | 1:A:39:VAL:N | 1.97 | 0.79 |
| 1:B:281:PRO:O | 1:B:285:HIS:HE1 | 1.66 | 0.78 |
| 1:A:238:LYS:HG2 | 2:A:614:HOH:O | 1.84 | 0.78 |
| 1:B:376:ASP:HB2 | 2:B:616:HOH:O | 1.82 | 0.78 |
| 1:A:558:ILE:HG23 | 1:A:563:ASP:CB | 2.14 | 0.78 |
| 1:A:32:ASP:HB2 | 1:A:35:LYS:HB2 | 1.64 | 0.78 |
| 1:A:44:GLY:HA2 | 1:A:561:MET:H | 1.49 | 0.78 |
| 1:B:353:SER:HB3 | 1:B:356:ALA:HB3 | 1.66 | 0.78 |
| 1:A:406:GLU:O | 1:A:410:LYS:HG3 | 1.85 | 0.77 |
| 1:A:469:ALA:O | 1:A:527:THR:HG21 | 1.84 | 0.77 |
| 1:B:522:GLN:HA | 1:B:529:LEU:HD22 | 1.64 | 0.77 |
| 1:B:569:LEU:HB3 | 1:B:570:PRO:HD3 | 1.66 | 0.77 |
| 1:B:574:PHE:HA | 2:B:784:HOH:O | 1.84 | 0.77 |
| 1:A:83:VAL:HA | 2:A:717:HOH:O | 1.84 | 0.77 |
| 1:B:406:GLU:O | 1:B:410:LYS:HG3 | 1.85 | 0.77 |
| 1:A:138:ALA:CB | 1:A:147:LEU:HD21 | 2.13 | 0.77 |
| 1:A:562:GLU:O | 1:A:564:ALA:N | 2.17 | 0.77 |
| 1:B:268:ARG:HA | 2:B:614:HOH:O | 1.83 | 0.77 |
| 1:A:61:ARG:NH1 | 1:A:101:GLY:HA3 | 1.99 | 0.77 |
| 1:A:519:ILE:HA | 1:A:549:HIS:HB2 | 1.66 | 0.77 |
| 1:A:523:ASN:ND2 | 1:A:553:ASP:HA | 1.99 | 0.77 |
| 1:A:417:GLY:N | 1:A:419:GLU:OE2 | 2.18 | 0.77 |
| 1:B:323:PRO:HG2 | 1:B:326:LEU:HD12 | 1.67 | 0.77 |
| 1:B:387:ALA:HB2 | 2:B:643:HOH:O | 1.83 | 0.77 |
| 1:A:334:ARG:HH21 | 1:A:350:VAL:HG11 | 1.50 | 0.76 |
| 1:A:90:HIS:HD2 | 1:A:114:ILE:H | 1.32 | 0.76 |
| 1:A:215:ALA:N | 1:A:405:GLU:HB3 | 2.01 | 0.75 |
| 1:A:420:LEU:HD21 | 2:A:696:HOH:O | 1.84 | 0.75 |
| 1:B:567:ILE:HD11 | 1:B:568:LEU:HD22 | 1.69 | 0.75 |
| 1:B:520:HIS:ND1 | 1:B:532:LEU:HG | 2.01 | 0.75 |
| 1:A:552:PRO:CD | 1:B:547:GLU:HB2 | 2.14 | 0.75 |
| 1:A:411:ILE:HD11 | 1:A:446:TYR:OH | 1.87 | 0.74 |
| 1:A:194:GLU:HB3 | 1:A:214:THR:CG2 | 2.16 | 0.74 |
| 1:B:139:LEU:HD13 | 1:B:144:LEU:HB2 | 1.69 | 0.74 |
| 1:B:542:ARG:HG3 | 1:B:542:ARG:HH11 | 1.49 | 0.74 |
| 1:A:428:ARG:HG3 | 2:A:622:HOH:O | 1.87 | 0.74 |
| 1:B:480:LEU:HB2 | 2:B:756:HOH:O | 1.88 | 0.74 |
| 1:A:534:ARG:O | 1:A:538:GLU:HG2 | 1.88 | 0.74 |
| 1:A:309:VAL:HA | 1:A:316:PRO:HA | 1.68 | 0.73 |
| 1:B:59:LEU:O | 1:B:95:VAL:HG11 | 1.87 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:311:LEU:HG | 2:A:670:HOH:O | 1.87 | 0.73 |
| 1:B:239:ASP:HB2 | 1:B:275:GLY:O | 1.87 | 0.73 |
| 1:B:579:ARG:C | 1:B:581:ARG:H | 1.91 | 0.73 |
| 1:A:136:LEU:HD21 | 1:A:164:ILE:HG21 | 1.70 | 0.73 |
| 1:A:526:ARG:HH11 | 1:A:556:HIS:HD2 | 1.34 | 0.73 |
| 1:B:265:ARG:HB3 | 2:B:696:HOH:O | 1.87 | 0.73 |
| 1:A:194:GLU:HB3 | 1:A:214:THR:HG21 | 1.70 | 0.73 |
| 1:B:428:ARG:HG2 | 2:B:592:HOH:O | 1.88 | 0.73 |
| 1:B:445:SER:H | 1:B:469:ALA:HB3 | 1.54 | 0.73 |
| 1:A:529:LEU:HD23 | 1:B:540:LEU:HD13 | 1.70 | 0.72 |
| 1:A:65:ASN:ND2 | 1:A:82:ASP:HB2 | 2.04 | 0.72 |
| 1:B:90:HIS:CB | 1:B:114:ILE:HD13 | 2.20 | 0.72 |
| 1:B:485:PHE:HA | 1:B:488:PHE:HB3 | 1.72 | 0.72 |
| 1:B:503:ARG:O | 1:B:505:PRO:HD3 | 1.89 | 0.72 |
| 1:B:477:MET:HG3 | 1:B:528:PRO:HD2 | 1.72 | 0.72 |
| 1:B:133:ARG:HD3 | 1:B:149:ARG:HE | 1.54 | 0.72 |
| 1:B:177:LEU:CD2 | 1:B:223:VAL:HG21 | 2.19 | 0.72 |
| 1:B:496:SER:HB3 | 2:B:619:HOH:O | 1.89 | 0.72 |
| 1:A:251:LEU:HD13 | 1:A:259:LEU:HD11 | 1.71 | 0.71 |
| 1:B:519:ILE:HD13 | 2:B:594:HOH:O | 1.90 | 0.71 |
| 1:B:71:HIS:O | 1:B:74:VAL:HG13 | 1.89 | 0.71 |
| 1:A:271:VAL:HB | 1:A:278:VAL:HB | 1.71 | 0.71 |
| 1:A:419:GLU:HG3 | 2:A:643:HOH:O | 1.90 | 0.71 |
| 1:B:347:PRO:O | 1:B:396:ASN:CB | 2.38 | 0.71 |
| 1:B:573:PHE:HB2 | 2:B:653:HOH:O | 1.90 | 0.71 |
| 1:B:95:VAL:HA | 2:B:742:HOH:O | 1.90 | 0.71 |
| 1:A:549:HIS:CE1 | 1:A:570:PRO:HB3 | 2.26 | 0.71 |
| 1:A:361:PRO:HA | 1:A:438:GLU:CG | 2.21 | 0.71 |
| 1:B:381:PHE:CZ | 1:B:567:ILE:HD13 | 2.25 | 0.71 |
| 1:B:374:ASP:OD2 | 1:B:394:MET:HB3 | 1.90 | 0.71 |
| 1:B:417:GLY:O | 1:B:421:GLU:HG2 | 1.89 | 0.71 |
| 1:A:350:VAL:O | 1:A:351:LEU:HD23 | 1.89 | 0.71 |
| 1:B:364:VAL:HG22 | 2:B:775:HOH:O | 1.91 | 0.71 |
| 1:B:475:GLU:O | 1:B:479:GLU:HG3 | 1.88 | 0.71 |
| 1:B:472:VAL:HG12 | 1:B:506:ILE:HB | 1.71 | 0.71 |
| 1:B:451:THR:CG2 | 1:B:467:ALA:HB2 | 2.21 | 0.71 |
| 1:B:577:THR:HB | 2:B:784:HOH:O | 1.89 | 0.71 |
| 1:B:160:ARG:HB3 | 1:B:202:ILE:HG21 | 1.74 | 0.70 |
| 1:A:338:VAL:O | 1:A:345:ARG:HA | 1.91 | 0.70 |
| 1:A:308:ILE:HB | 1:A:318:LEU:HB2 | 1.73 | 0.70 |
| 1:B:45:SER:HA | 1:B:560:THR:HA | 1.72 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:363:VAL:HG12 | 2:A:693:HOH:O | 1.92 | 0.70 |
| 1:A:71:HIS:O | 1:A:74:VAL:HG23 | 1.91 | 0.70 |
| 1:A:284:ASN:ND2 | 1:A:377:SER:OG | 2.25 | 0.70 |
| 1:A:309:VAL:HG12 | 1:A:316:PRO:HA | 1.73 | 0.70 |
| 1:B:30:VAL:HG23 | 1:B:289:VAL:CG1 | 2.21 | 0.70 |
| 1:B:362:THR:HG22 | 1:B:363:VAL:N | 2.06 | 0.70 |
| 1:B:356:ALA:HB2 | 1:B:389:GLY:O | 1.92 | 0.70 |
| 1:B:564:ALA:O | 1:B:567:ILE:HD11 | 1.92 | 0.70 |
| 1:A:129:ALA:CB | 1:A:134:VAL:HG22 | 2.21 | 0.70 |
| 1:B:164:ILE:HB | 1:B:180:SER:HB3 | 1.74 | 0.70 |
| 1:B:373:GLU:OE2 | 1:B:396:ASN:HB3 | 1.91 | 0.70 |
| 1:B:331:ALA:HB3 | 1:B:352:GLU:HB3 | 1.73 | 0.69 |
| 1:A:335:LEU:HD12 | 1:A:348:THR:O | 1.93 | 0.69 |
| 1:B:51:TYR:HE2 | 1:B:317:LEU:HB3 | 1.58 | 0.69 |
| 1:B:79:LEU:HD11 | 1:B:95:VAL:HG21 | 1.74 | 0.69 |
| 1:A:346:VAL:HG13 | 1:A:407:TRP:HZ2 | 1.58 | 0.69 |
| 1:A:90:HIS:HB2 | 1:A:114:ILE:HD13 | 1.75 | 0.69 |
| 1:B:565:VAL:C | 1:B:567:ILE:H | 1.93 | 0.69 |
| 1:A:441:ILE:HD13 | 1:A:442:MET:N | 2.06 | 0.69 |
| 1:A:511:ARG:O | 2:A:630:HOH:O | 2.10 | 0.69 |
| 1:A:439:LEU:N | 2:A:729:HOH:O | 2.24 | 0.69 |
| 1:B:178:PHE:HB3 | 2:B:706:HOH:O | 1.93 | 0.69 |
| 1:B:208:VAL:HG23 | 1:B:223:VAL:O | 1.93 | 0.69 |
| 1:A:528:PRO:HD3 | 2:A:644:HOH:O | 1.91 | 0.69 |
| 1:B:245:PRO:HA | 2:B:696:HOH:O | 1.93 | 0.69 |
| 1:B:324:GLU:O | 1:B:327:ARG:HB3 | 1.92 | 0.69 |
| 1:A:130:THR:OG1 | 1:A:132:ASP:OD1 | 2.10 | 0.68 |
| 1:B:327:ARG:O | 2:B:720:HOH:O | 2.11 | 0.68 |
| 1:A:174:ARG:HE | 1:A:409:LEU:HD11 | 1.59 | 0.68 |
| 1:B:35:LYS:HG2 | 1:B:52:ASP:OD1 | 1.93 | 0.68 |
| 1:A:200:ALA:HB3 | 2:A:639:HOH:O | 1.92 | 0.68 |
| 1:A:405:GLU:OE1 | 1:A:409:LEU:HG | 1.93 | 0.68 |
| 1:A:163:LEU:C | 1:A:164:ILE:HD12 | 2.13 | 0.68 |
| 1:A:474:TRP:HB2 | 1:A:500:MET:HB3 | 1.75 | 0.68 |
| 1:A:175:VAL:HG23 | 1:A:196:SER:HB3 | 1.76 | 0.68 |
| 1:B:169:PHE:CZ | 1:B:175:VAL:HG22 | 2.28 | 0.68 |
| 1:B:329:SER:HB2 | 1:B:387:ALA:HA | 1.76 | 0.68 |
| 1:A:352:GLU:HA | 1:A:391:HIS:ND1 | 2.09 | 0.68 |
| 1:A:361:PRO:HA | 1:A:438:GLU:HG2 | 1.76 | 0.68 |
| 1:A:27:LEU:HD21 | 1:A:289:VAL:HG22 | 1.76 | 0.68 |
| 1:B:477:MET:HA | 2:B:756:HOH:O | 1.93 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:92:LEU:O | 1:B:106:LEU:HD12 | 1.94 | 0.68 |
| 1:B:526:ARG:NH2 | 1:B:557:ALA:HB2 | 2.08 | 0.68 |
| 1:B:218:ALA:HB1 | 1:B:248:ILE:HD11 | 1.76 | 0.67 |
| 1:B:526:ARG:HA | 2:B:680:HOH:O | 1.94 | 0.67 |
| 1:A:42:SER:HB2 | 2:A:649:HOH:O | 1.94 | 0.67 |
| 1:B:222:THR:O | 1:B:230:VAL:HG13 | 1.95 | 0.67 |
| 1:B:59:LEU:HD13 | 1:B:77:VAL:HG21 | 1.76 | 0.67 |
| 1:B:218:ALA:HB1 | 1:B:248:ILE:CD1 | 2.25 | 0.67 |
| 1:A:27:LEU:HD23 | 1:A:287:ARG:O | 1.93 | 0.67 |
| 1:A:368:GLY:HA2 | 2:A:686:HOH:O | 1.95 | 0.67 |
| 1:B:295:LEU:O | 1:B:311:LEU:HG | 1.95 | 0.67 |
| 1:B:485:PHE:O | 1:B:489:ILE:HG12 | 1.95 | 0.67 |
| 1:B:440:TYR:OH | 1:B:463:LYS:HD3 | 1.94 | 0.66 |
| 1:B:91:ALA:HB3 | 1:B:93:PHE:CZ | 2.30 | 0.66 |
| 1:B:221:VAL:HB | 1:B:230:VAL:HG12 | 1.77 | 0.66 |
| 1:A:90:HIS:O | 1:A:111:PRO:HA | 1.96 | 0.66 |
| 1:A:386:ALA:HA | 1:A:390:PHE:O | 1.95 | 0.66 |
| 1:B:438:GLU:HA | 2:B:714:HOH:O | 1.95 | 0.66 |
| 1:B:449:TYR:HB2 | 2:B:685:HOH:O | 1.94 | 0.66 |
| 1:A:498:GLU:HA | 1:A:501:ARG:HD2 | 1.77 | 0.66 |
| 1:B:559:ASN:O | 1:B:560:THR:HG23 | 1.95 | 0.66 |
| 1:A:423:VAL:HA | 2:A:651:HOH:O | 1.95 | 0.66 |
| 1:A:58:LYS:O | 1:A:100:PRO:HB3 | 1.96 | 0.66 |
| 1:A:81:ARG:HB2 | 1:A:81:ARG:HH11 | 1.61 | 0.66 |
| 1:A:353:SER:O | 1:A:356:ALA:N | 2.29 | 0.66 |
| 1:A:529:LEU:HD11 | 1:A:550:ILE:CD1 | 2.25 | 0.66 |
| 1:B:159:ILE:HD12 | 1:B:164:ILE:HG23 | 1.78 | 0.66 |
| 1:A:322:LEU:HD23 | 1:A:323:PRO:CD | 2.25 | 0.66 |
| 1:A:548:ALA:O | 1:B:549:HIS:HA | 1.95 | 0.66 |
| 1:A:551:ILE:HG23 | 1:A:552:PRO:HD2 | 1.77 | 0.66 |
| 1:B:421:GLU:HA | 1:B:421:GLU:OE2 | 1.96 | 0.66 |
| 1:B:574:PHE:O | 1:B:577:THR:HB | 1.96 | 0.66 |
| 1:A:480:LEU:HD21 | 1:A:530:LYS:HD2 | 1.78 | 0.66 |
| 1:A:567:ILE:HG13 | 1:A:567:ILE:O | 1.95 | 0.66 |
| 1:B:424:SER:HB3 | 1:B:428:ARG:NH1 | 2.11 | 0.66 |
| 1:A:125:VAL:HA | 1:A:137:TYR:O | 1.96 | 0.65 |
| 1:A:392:VAL:HG22 | 2:A:720:HOH:O | 1.95 | 0.65 |
| 1:A:45:SER:HB2 | 1:A:63:PRO:HB3 | 1.76 | 0.65 |
| 1:B:153:PHE:HE1 | 1:B:488:PHE:HB2 | 1.61 | 0.65 |
| 1:A:308:ILE:O | 1:A:318:LEU:N | 2.23 | 0.65 |
| 1:B:171:GLY:O | 1:B:173:GLY:N | 2.30 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:90:HIS:N | 1:A:112:MET:O | 2.21 | 0.65 |
| 1:A:555:GLY:HA3 | 2:A:663:HOH:O | 1.96 | 0.65 |
| 1:B:99:ARG:HB2 | 1:B:102:GLU:OE2 | 1.96 | 0.65 |
| 1:B:410:LYS:HG2 | 2:B:695:HOH:O | 1.95 | 0.65 |
| 1:A:302:LEU:HD13 | 1:A:351:LEU:HD21 | 1.78 | 0.65 |
| 1:B:523:ASN:ND2 | 1:B:553:ASP:HA | 2.11 | 0.65 |
| 1:A:579:ARG:HB2 | 1:A:579:ARG:NH1 | 2.12 | 0.65 |
| 1:B:103:GLU:HB2 | 2:B:687:HOH:O | 1.97 | 0.65 |
| 1:B:458:LYS:HB3 | 1:B:461:LEU:HD22 | 1.79 | 0.65 |
| 1:B:532:LEU:O | 1:B:536:MET:HG3 | 1.97 | 0.65 |
| 1:B:469:ALA:HB1 | 1:B:556:HIS:CE1 | 2.31 | 0.65 |
| 1:A:563:ASP:HA | 1:A:566:LYS:CG | 2.27 | 0.65 |
| 1:A:63:PRO:HA | 2:A:595:HOH:O | 1.97 | 0.65 |
| 1:B:278:VAL:HG11 | 1:B:295:LEU:CD1 | 2.27 | 0.64 |
| 1:B:136:LEU:O | 1:B:147:LEU:N | 2.31 | 0.64 |
| 1:B:29:GLY:CA | 1:B:289:VAL:HG21 | 2.28 | 0.64 |
| 1:A:353:SER:O | 1:A:355:ARG:N | 2.30 | 0.64 |
| 1:B:100:PRO:O | 1:B:102:GLU:HG3 | 1.96 | 0.64 |
| 1:B:133:ARG:HA | 1:B:483:ALA:CB | 2.27 | 0.64 |
| 1:B:137:TYR:HA | 1:B:146:GLU:HA | 1.80 | 0.64 |
| 1:B:362:THR:CG2 | 1:B:363:VAL:N | 2.60 | 0.64 |
| 1:A:88:GLU:HG3 | 1:A:113:ARG:HH12 | 1.61 | 0.64 |
| 1:A:223:VAL:HA | 1:A:229:SER:O | 1.98 | 0.64 |
| 1:A:263:ALA:O | 1:A:269:SER:HB2 | 1.97 | 0.64 |
| 1:A:325:ASP:HA | 1:A:328:ARG:HB3 | 1.79 | 0.64 |
| 1:A:337:TRP:CZ3 | 1:A:347:PRO:HB3 | 2.33 | 0.64 |
| 1:B:69:ASP:O | 1:B:118:VAL:HG13 | 1.97 | 0.64 |
| 1:B:201:SER:N | 2:B:652:HOH:O | 2.30 | 0.64 |
| 1:A:438:GLU:HB2 | 2:A:729:HOH:O | 1.96 | 0.64 |
| 1:A:525:SER:C | 2:A:644:HOH:O | 2.35 | 0.64 |
| 1:A:526:ARG:HD2 | 1:A:556:HIS:CD2 | 2.32 | 0.64 |
| 1:A:61:ARG:HH12 | 1:A:101:GLY:HA3 | 1.62 | 0.64 |
| 1:B:181:ASN:HB2 | 1:B:185:GLY:O | 1.97 | 0.64 |
| 1:A:272:PHE:CE2 | 1:A:277:ARG:HD3 | 2.33 | 0.64 |
| 1:A:38:VAL:CG1 | 1:A:39:VAL:N | 2.61 | 0.64 |
| 1:A:415:PRO:O | 1:A:503:ARG:HD2 | 1.98 | 0.64 |
| 1:B:46:VAL:HG23 | 2:B:764:HOH:O | 1.98 | 0.64 |
| 1:A:172:GLY:O | 1:A:409:LEU:HD22 | 1.98 | 0.64 |
| 1:B:251:LEU:HG | 2:B:652:HOH:O | 1.97 | 0.64 |
| 1:B:201:SER:CB | 1:B:252:GLY:HA2 | 2.28 | 0.64 |
| 1:B:411:ILE:CD1 | 1:B:419:GLU:HG2 | 2.27 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:90:HIS:HB2 | 1:B:114:ILE:CD1 | 2.23 | 0.64 |
| 1:A:129:ALA:HB2 | 1:A:134:VAL:HG22 | 1.80 | 0.64 |
| 1:A:200:ALA:CB | 2:A:639:HOH:O | 2.46 | 0.64 |
| 1:A:214:THR:C | 1:A:405:GLU:HB3 | 2.18 | 0.64 |
| 1:B:361:PRO:HA | 1:B:438:GLU:HG2 | 1.80 | 0.64 |
| 1:B:373:GLU:OE1 | 1:B:396:ASN:ND2 | 2.31 | 0.64 |
| 1:A:164:ILE:HD13 | 1:A:181:ASN:C | 2.18 | 0.63 |
| 1:A:370:PRO:O | 1:A:372:ALA:N | 2.29 | 0.63 |
| 1:A:511:ARG:HG2 | 2:A:630:HOH:O | 1.98 | 0.63 |
| 1:B:137:TYR:CD2 | 1:B:146:GLU:HG3 | 2.32 | 0.63 |
| 1:A:493:THR:O | 1:A:499:ILE:HD12 | 1.97 | 0.63 |
| 1:B:90:HIS:HD2 | 1:B:114:ILE:H | 1.47 | 0.63 |
| 1:B:180:SER:HA | 2:B:750:HOH:O | 1.98 | 0.63 |
| 1:B:92:LEU:HD12 | 1:B:109:VAL:CG2 | 2.22 | 0.63 |
| 1:B:104:GLN:HG2 | 2:B:620:HOH:O | 1.98 | 0.63 |
| 1:B:428:ARG:O | 1:B:431:ARG:HB2 | 1.98 | 0.63 |
| 1:B:471:VAL:HG11 | 1:B:474:TRP:CH2 | 2.33 | 0.63 |
| 1:A:133:ARG:HA | 1:A:483:ALA:CB | 2.28 | 0.63 |
| 1:A:93:PHE:C | 2:A:589:HOH:O | 2.36 | 0.63 |
| 1:B:441:ILE:HG21 | 2:B:615:HOH:O | 1.96 | 0.63 |
| 1:B:411:ILE:HD11 | 1:B:446:TYR:OH | 1.99 | 0.63 |
| 1:A:62:GLU:HB2 | 1:A:81:ARG:HH21 | 1.64 | 0.63 |
| 1:B:186:GLY:O | 1:B:187:LEU:HB2 | 1.98 | 0.63 |
| 1:B:171:GLY:C | 1:B:173:GLY:H | 2.00 | 0.63 |
| 1:B:472:VAL:CG1 | 1:B:506:ILE:HB | 2.29 | 0.63 |
| 1:B:542:ARG:HG3 | 1:B:542:ARG:NH1 | 2.14 | 0.63 |
| 1:B:278:VAL:HG13 | 1:B:312:PRO:HB3 | 1.80 | 0.62 |
| 1:B:340:SER:HB3 | 2:B:722:HOH:O | 1.98 | 0.62 |
| 1:B:61:ARG:HB2 | 1:B:103:GLU:OE1 | 1.99 | 0.62 |
| 1:A:109:VAL:HG12 | 2:A:594:HOH:O | 1.99 | 0.62 |
| 1:A:475:GLU:HB3 | 2:A:627:HOH:O | 2.00 | 0.62 |
| 1:B:99:ARG:NH2 | 1:B:102:GLU:HB3 | 2.13 | 0.62 |
| 1:B:264:ARG:O | 1:B:264:ARG:HG3 | 1.97 | 0.62 |
| 1:B:78:ILE:HD13 | 1:B:124:VAL:CG1 | 2.30 | 0.62 |
| 1:A:523:ASN:HD21 | 1:A:553:ASP:HA | 1.61 | 0.62 |
| 1:B:91:ALA:HB1 | 1:B:105:ARG:HE | 1.65 | 0.62 |
| 1:B:116:SER:C | 2:B:596:HOH:O | 2.38 | 0.62 |
| 1:A:45:SER:OG | 1:A:47:ASN:ND2 | 2.30 | 0.62 |
| 1:B:523:ASN:HB2 | 1:B:554:ALA:O | 1.99 | 0.62 |
| 1:A:58:LYS:HE2 | 1:A:60:ASN:O | 1.99 | 0.62 |
| 1:B:345:ARG:HD2 | 2:B:684:HOH:O | 2.00 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:539:LEU:HD13 | 1:B:546:PHE:CG | 2.34 | 0.62 |
| 1:B:68:LEU:O | 1:B:70:PRO:HD3 | 2.00 | 0.62 |
| 1:A:328:ARG:HH11 | 1:A:328:ARG:HG2 | 1.64 | 0.62 |
| 1:B:29:GLY:HA2 | 1:B:289:VAL:HG21 | 1.82 | 0.62 |
| 1:B:420:LEU:CD2 | 1:B:458:LYS:HD3 | 2.29 | 0.62 |
| 1:A:90:HIS:HB2 | 1:A:114:ILE:CD1 | 2.30 | 0.62 |
| 1:B:133:ARG:NH1 | 1:B:146:GLU:OE2 | 2.32 | 0.62 |
| 1:A:251:LEU:HD12 | 1:A:252:GLY:N | 2.13 | 0.61 |
| 1:A:283:GLY:HA2 | 1:A:376:ASP:OD2 | 2.00 | 0.61 |
| 1:A:45:SER:HB2 | 2:A:595:HOH:O | 1.99 | 0.61 |
| 1:A:470:SER:O | 1:A:527:THR:HB | 2.00 | 0.61 |
| 1:B:115:LEU:HB2 | 1:B:127:THR:OG1 | 2.00 | 0.61 |
| 1:A:346:VAL:HG22 | 1:A:407:TRP:CH2 | 2.36 | 0.61 |
| 1:A:341:PHE:CD2 | 1:A:421:GLU:HB3 | 2.35 | 0.61 |
| 1:B:373:GLU:HA | 1:B:373:GLU:OE1 | 1.99 | 0.61 |
| 1:A:273:ILE:HG13 | 1:A:295:LEU:HD11 | 1.82 | 0.61 |
| 1:A:499:ILE:HD11 | 2:A:732:HOH:O | 2.01 | 0.61 |
| 1:B:160:ARG:NH2 | 2:B:715:HOH:O | 2.33 | 0.61 |
| 1:A:419:GLU:CD | 1:A:420:LEU:H | 2.03 | 0.61 |
| 1:B:370:PRO:O | 1:B:372:ALA:N | 2.33 | 0.61 |
| 1:A:340:SER:HB2 | 1:A:344:SER:O | 1.99 | 0.61 |
| 1:B:31:VAL:HG12 | 1:B:32:ASP:N | 2.15 | 0.61 |
| 1:B:559:ASN:HB2 | 2:B:762:HOH:O | 2.00 | 0.61 |
| 1:A:558:ILE:HG12 | 2:A:583:HOH:O | 2.01 | 0.61 |
| 1:A:547:GLU:OE2 | 1:A:574:PHE:HB2 | 2.00 | 0.61 |
| 1:B:323:PRO:CG | 1:B:326:LEU:HD12 | 2.31 | 0.61 |
| 1:A:533:LEU:CD1 | 1:B:536:MET:HB3 | 2.30 | 0.61 |
| 1:A:497:ARG:O | 1:A:499:ILE:N | 2.34 | 0.61 |
| 1:B:399:GLY:HA2 | 1:B:408:ARG:O | 2.01 | 0.61 |
| 1:B:55:GLU:C | 2:B:735:HOH:O | 2.38 | 0.61 |
| 1:A:533:LEU:HD11 | 1:B:536:MET:HB3 | 1.81 | 0.61 |
| 1:B:127:THR:HG23 | 1:B:156:VAL:CG2 | 2.29 | 0.60 |
| 1:B:347:PRO:HG2 | 1:B:396:ASN:HB2 | 1.83 | 0.60 |
| 1:B:45:SER:HB2 | 1:B:63:PRO:HB3 | 1.83 | 0.60 |
| 1:B:282:GLN:HB3 | 2:B:700:HOH:O | 1.99 | 0.60 |
| 1:B:567:ILE:CD1 | 1:B:568:LEU:HD22 | 2.32 | 0.60 |
| 1:A:264:ARG:NH2 | 1:A:373:GLU:OE2 | 2.33 | 0.60 |
| 1:A:562:GLU:C | 1:A:564:ALA:H | 2.05 | 0.60 |
| 1:B:30:VAL:H | 1:B:289:VAL:HG11 | 1.64 | 0.60 |
| 1:B:26:SER:O | 1:B:308:ILE:HD11 | 2.01 | 0.60 |
| 1:A:296:VAL:HG13 | 1:A:309:VAL:O | 2.02 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:160:ARG:N | 1:A:202:ILE:HD12 | 2.16 | 0.60 |
| 1:A:41:PHE:CE2 | 1:A:561:MET:HA | 2.37 | 0.60 |
| 1:B:90:HIS:CD2 | 1:B:114:ILE:HD13 | 2.35 | 0.60 |
| 1:A:533:LEU:HD21 | 1:B:536:MET:SD | 2.42 | 0.60 |
| 1:A:309:VAL:HG12 | 1:A:316:PRO:CA | 2.32 | 0.60 |
| 1:A:468:GLY:HA2 | 1:A:519:ILE:O | 2.02 | 0.60 |
| 1:A:41:PHE:CZ | 1:A:561:MET:HA | 2.35 | 0.60 |
| 1:B:135:ALA:HB3 | 1:B:137:TYR:CZ | 2.37 | 0.60 |
| 1:B:517:ALA:HB2 | 1:B:574:PHE:CD1 | 2.37 | 0.60 |
| 1:B:530:LYS:HB3 | 1:B:531:PRO:CD | 2.27 | 0.60 |
| 1:A:334:ARG:HG3 | 2:A:694:HOH:O | 2.01 | 0.60 |
| 1:B:330:ILE:HD12 | 2:B:720:HOH:O | 2.02 | 0.60 |
| 1:A:385:LEU:HD13 | 2:A:720:HOH:O | 2.00 | 0.60 |
| 1:B:361:PRO:O | 1:B:390:PHE:HA | 2.02 | 0.59 |
| 1:B:325:ASP:CA | 1:B:328:ARG:HB2 | 2.30 | 0.59 |
| 1:B:410:LYS:HE3 | 2:B:786:HOH:O | 2.02 | 0.59 |
| 1:A:171:GLY:O | 1:A:174:ARG:HB2 | 2.02 | 0.59 |
| 1:B:175:VAL:HB | 1:B:196:SER:HB3 | 1.84 | 0.59 |
| 1:A:356:ALA:HB2 | 1:A:389:GLY:O | 2.01 | 0.59 |
| 1:A:267:GLY:HA2 | 1:A:375:SER:HB2 | 1.83 | 0.59 |
| 1:A:55:GLU:HA | 2:A:604:HOH:O | 2.03 | 0.59 |
| 1:B:451:THR:HG21 | 1:B:467:ALA:HB2 | 1.85 | 0.59 |
| 1:A:558:ILE:CG2 | 1:A:560:THR:O | 2.51 | 0.59 |
| 1:B:361:PRO:HG3 | 1:B:438:GLU:CD | 2.23 | 0.59 |
| 1:B:471:VAL:HG11 | 1:B:474:TRP:CZ3 | 2.37 | 0.59 |
| 1:A:480:LEU:HD21 | 1:A:530:LYS:CD | 2.32 | 0.59 |
| 1:A:37:LEU:HD23 | 1:A:70:PRO:HG3 | 1.85 | 0.59 |
| 1:A:530:LYS:CB | 1:A:531:PRO:HD3 | 2.24 | 0.59 |
| 1:A:109:VAL:HG12 | 1:A:109:VAL:O | 2.02 | 0.59 |
| 1:A:306:PRO:HD3 | 1:A:378:TRP:HB3 | 1.83 | 0.59 |
| 1:B:565:VAL:C | 1:B:567:ILE:N | 2.56 | 0.59 |
| 1:A:526:ARG:HH11 | 1:A:556:HIS:CD2 | 2.18 | 0.59 |
| 1:B:145:ARG:HG3 | 2:B:748:HOH:O | 2.01 | 0.58 |
| 1:B:302:LEU:HD13 | 1:B:351:LEU:CD1 | 2.33 | 0.58 |
| 1:B:251:LEU:CD1 | 1:B:259:LEU:HD11 | 2.33 | 0.58 |
| 1:B:246:THR:HG22 | 1:B:264:ARG:O | 2.03 | 0.58 |
| 1:B:456:THR:CG2 | 1:B:512:ILE:HD11 | 2.32 | 0.58 |
| 1:B:46:VAL:HB | 1:B:64:ILE:O | 2.03 | 0.58 |
| 1:A:475:GLU:HA | 1:A:500:MET:HE2 | 1.85 | 0.58 |
| 1:B:414:ASP:HA | 1:B:503:ARG:HH12 | 1.66 | 0.58 |
| 1:B:210:ALA:HA | 1:B:251:LEU:HD23 | 1.84 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:307:ARG:NH2 | 2:B:595:HOH:O | 2.33 | 0.58 |
| 1:A:165:ALA:CB | 2:A:653:HOH:O | 2.51 | 0.58 |
| 1:A:455:LEU:HD23 | 2:A:682:HOH:O | 2.03 | 0.58 |
| 1:A:465:GLY:O | 1:A:516:LEU:HA | 2.04 | 0.58 |
| 1:B:250:TRP:HZ3 | 1:B:260:ALA:HB3 | 1.67 | 0.58 |
| 1:B:324:GLU:OE2 | 1:B:327:ARG:NH1 | 2.33 | 0.58 |
| 1:B:390:PHE:CE1 | 1:B:579:ARG:NH2 | 2.72 | 0.58 |
| 1:B:61:ARG:HB2 | 1:B:103:GLU:CD | 2.24 | 0.58 |
| 1:B:28:GLN:HG3 | 1:B:67:VAL:CG2 | 2.33 | 0.58 |
| 1:A:177:LEU:HB3 | 1:A:190:PHE:HB2 | 1.86 | 0.58 |
| 1:B:248:ILE:H | 1:B:248:ILE:HD12 | 1.69 | 0.58 |
| 1:A:40:GLY:C | 1:A:42:SER:H | 2.07 | 0.58 |
| 1:B:27:LEU:CD1 | 1:B:38:VAL:HG12 | 2.33 | 0.58 |
| 1:B:284:ASN:ND2 | 1:B:376:ASP:C | 2.54 | 0.58 |
| 1:B:528:PRO:O | 1:B:532:LEU:HD23 | 2.03 | 0.58 |
| 1:A:159:ILE:HG23 | 1:A:163:LEU:O | 2.03 | 0.58 |
| 1:A:160:ARG:HD3 | 1:A:202:ILE:HG22 | 1.85 | 0.58 |
| 1:A:38:VAL:CG1 | 1:A:39:VAL:H | 2.17 | 0.58 |
| 1:B:133:ARG:HA | 1:B:483:ALA:HB2 | 1.85 | 0.58 |
| 1:B:497:ARG:O | 1:B:500:MET:N | 2.37 | 0.58 |
| 1:A:120:THR:HB | 2:A:617:HOH:O | 2.04 | 0.57 |
| 1:A:403:TYR:HD1 | 2:A:618:HOH:O | 1.87 | 0.57 |
| 1:B:60:ASN:O | 1:B:101:GLY:HA2 | 2.05 | 0.57 |
| 1:B:201:SER:HB2 | 1:B:252:GLY:HA2 | 1.86 | 0.57 |
| 1:A:217:GLU:HG2 | 1:A:245:PRO:O | 2.05 | 0.57 |
| 1:B:295:LEU:HB2 | 1:B:311:LEU:HB2 | 1.85 | 0.57 |
| 1:B:343:GLY:N | 2:B:722:HOH:O | 2.37 | 0.57 |
| 1:A:44:GLY:HA2 | 1:A:561:MET:CB | 2.34 | 0.57 |
| 1:A:51:TYR:CZ | 1:A:53:GLY:HA2 | 2.39 | 0.57 |
| 1:B:266:GLU:HG2 | 1:B:337:TRP:HZ2 | 1.69 | 0.57 |
| 1:B:477:MET:HB3 | 2:B:642:HOH:O | 2.05 | 0.57 |
| 1:B:477:MET:CE | 1:B:489:ILE:HD11 | 2.34 | 0.57 |
| 1:B:326:LEU:HA | 1:B:355:ARG:HH11 | 1.67 | 0.57 |
| 1:A:187:LEU:HD12 | 1:A:188:ARG:H | 1.68 | 0.57 |
| 1:A:412:ILE:HD13 | 1:A:492:LEU:HD12 | 1.86 | 0.57 |
| 1:B:233:LEU:HD23 | 1:B:234:GLU:N | 2.20 | 0.57 |
| 1:A:187:LEU:HD12 | 1:A:188:ARG:N | 2.20 | 0.57 |
| 1:A:267:GLY:HA2 | 1:A:375:SER:CB | 2.34 | 0.57 |
| 1:A:372:ALA:O | 1:A:401:THR:N | 2.34 | 0.57 |
| 1:A:38:VAL:HG12 | 1:A:39:VAL:H | 1.65 | 0.57 |
| 1:B:271:VAL:O | 1:B:277:ARG:HA | 2.03 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:198:SER:HB3 | 1:B:213:GLU:OE2 | 2.04 | 0.57 |
| 1:B:47:ASN:HA | 2:B:679:HOH:O | 2.04 | 0.57 |
| 1:B:551:ILE:HB | 1:B:554:ALA:HB2 | 1.87 | 0.57 |
| 1:A:251:LEU:HD12 | 1:A:251:LEU:C | 2.24 | 0.57 |
| 1:A:323:PRO:HD2 | 1:A:326:LEU:HD12 | 1.86 | 0.57 |
| 1:A:569:LEU:HG | 1:A:573:PHE:HE2 | 1.70 | 0.57 |
| 1:B:329:SER:HB3 | 1:B:355:ARG:HE | 1.69 | 0.57 |
| 1:B:464:ALA:CB | 1:B:578:GLN:HG3 | 2.35 | 0.57 |
| 1:A:169:PHE:HE2 | 1:A:371:PHE:CD1 | 2.22 | 0.57 |
| 1:A:449:TYR:HB2 | 1:A:471:VAL:HG23 | 1.86 | 0.57 |
| 1:A:113:ARG:NH2 | 1:A:525:SER:OG | 2.38 | 0.56 |
| 1:A:446:TYR:HB3 | 2:A:686:HOH:O | 2.05 | 0.56 |
| 1:B:68:LEU:HG | 1:B:78:ILE:HB | 1.87 | 0.56 |
| 1:A:419:GLU:O | 1:A:423:VAL:HG23 | 2.06 | 0.56 |
| 1:A:526:ARG:HD2 | 1:A:556:HIS:CG | 2.40 | 0.56 |
| 1:B:304:THR:O | 1:B:378:TRP:HB2 | 2.06 | 0.56 |
| 1:A:174:ARG:HH21 | 1:A:405:GLU:CD | 2.08 | 0.56 |
| 1:A:342:ASP:CG | 1:A:398:ARG:HH22 | 2.08 | 0.56 |
| 1:A:473:ASP:N | 2:A:657:HOH:O | 2.38 | 0.56 |
| 1:B:127:THR:HA | 1:B:135:ALA:O | 2.06 | 0.56 |
| 1:A:363:VAL:HA | 1:A:440:TYR:O | 2.05 | 0.56 |
| 1:B:420:LEU:HD22 | 1:B:453:CYS:SG | 2.46 | 0.56 |
| 1:A:305:PRO:HA | 1:A:378:TRP:CG | 2.41 | 0.56 |
| 1:A:429:TRP:CD1 | 1:A:433:SER:HB2 | 2.40 | 0.56 |
| 1:B:240:PHE:HE1 | 1:B:263:ALA:HB2 | 1.70 | 0.56 |
| 1:B:361:PRO:HA | 1:B:438:GLU:CG | 2.34 | 0.56 |
| 1:B:516:LEU:HD12 | 1:B:517:ALA:H | 1.70 | 0.56 |
| 1:A:519:ILE:HG12 | 1:A:549:HIS:CD2 | 2.40 | 0.56 |
| 1:B:198:SER:HB3 | 1:B:213:GLU:CD | 2.26 | 0.56 |
| 1:B:99:ARG:CZ | 1:B:102:GLU:HB3 | 2.36 | 0.56 |
| 1:B:455:LEU:HD22 | 1:B:514:GLU:HB2 | 1.88 | 0.56 |
| 1:A:393:VAL:HG11 | 1:A:426:ALA:HB1 | 1.88 | 0.56 |
| 1:A:441:ILE:HB | 1:A:462:PHE:CD1 | 2.41 | 0.56 |
| 1:A:486:ARG:HG3 | 1:A:486:ARG:HH11 | 1.71 | 0.56 |
| 1:B:517:ALA:HB2 | 1:B:574:PHE:CE1 | 2.41 | 0.56 |
| 1:B:90:HIS:O | 1:B:111:PRO:HA | 2.05 | 0.56 |
| 1:A:305:PRO:HD3 | 1:A:322:LEU:HD12 | 1.88 | 0.56 |
| 1:B:456:THR:HG23 | 1:B:512:ILE:HD11 | 1.87 | 0.56 |
| 1:A:106:LEU:HA | 2:A:698:HOH:O | 2.04 | 0.56 |
| 1:A:164:ILE:O | 1:A:179:THR:HA | 2.06 | 0.56 |
| 1:A:347:PRO:HG3 | 1:A:403:TYR:CD2 | 2.41 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:458:LYS:O | 1:A:460:GLY:N | 2.39 | 0.56 |
| 1:A:46:VAL:N | 2:A:595:HOH:O | 2.38 | 0.56 |
| 1:B:271:VAL:O | 1:B:277:ARG:HD2 | 2.06 | 0.56 |
| 1:B:331:ALA:HB3 | 1:B:352:GLU:CB | 2.36 | 0.56 |
| 1:A:550:ILE:O | 1:B:547:GLU:HA | 2.06 | 0.55 |
| 1:A:219:ARG:HH11 | 1:A:219:ARG:HG3 | 1.71 | 0.55 |
| 1:A:445:SER:HA | 1:A:469:ALA:O | 2.06 | 0.55 |
| 1:A:520:HIS:O | 1:A:550:ILE:HA | 2.06 | 0.55 |
| 1:B:350:VAL:HG21 | 1:B:429:TRP:CH2 | 2.41 | 0.55 |
| 1:B:453:CYS:HB2 | 2:B:731:HOH:O | 2.07 | 0.55 |
| 1:A:92:LEU:O | 1:A:106:LEU:HG | 2.04 | 0.55 |
| 1:A:178:PHE:CD1 | 1:A:178:PHE:C | 2.80 | 0.55 |
| 1:A:563:ASP:OD2 | 2:A:585:HOH:O | 2.18 | 0.55 |
| 1:B:471:VAL:HG23 | 2:B:685:HOH:O | 2.05 | 0.55 |
| 1:A:25:TYR:HB3 | 1:A:38:VAL:HG11 | 1.88 | 0.55 |
| 1:A:426:ALA:HB2 | 2:A:651:HOH:O | 2.06 | 0.55 |
| 1:B:123:ALA:HA | 1:B:139:LEU:O | 2.06 | 0.55 |
| 1:B:268:ARG:NH1 | 1:B:282:GLN:CD | 2.60 | 0.55 |
| 1:B:326:LEU:HB3 | 2:B:794:HOH:O | 2.05 | 0.55 |
| 1:B:455:LEU:CD2 | 1:B:514:GLU:HB2 | 2.37 | 0.55 |
| 1:A:399:GLY:O | 1:A:408:ARG:HG3 | 2.06 | 0.55 |
| 1:A:478:TYR:HE1 | 1:A:486:ARG:O | 1.90 | 0.55 |
| 1:A:499:ILE:HG23 | 1:A:503:ARG:HG3 | 1.89 | 0.55 |
| 1:A:532:LEU:HD13 | 1:A:532:LEU:C | 2.26 | 0.55 |
| 1:A:541:ALA:C | 1:A:543:GLY:H | 2.09 | 0.55 |
| 1:B:51:TYR:CZ | 1:B:53:GLY:HA2 | 2.42 | 0.55 |
| 1:A:379:ASP:OD1 | 1:A:381:PHE:N | 2.38 | 0.55 |
| 1:A:474:TRP:CD1 | 1:A:500:MET:HA | 2.42 | 0.55 |
| 1:B:255:PRO:O | 1:B:257:GLY:N | 2.39 | 0.55 |
| 1:B:496:SER:CB | 2:B:619:HOH:O | 2.52 | 0.55 |
| 1:B:59:LEU:HD22 | 2:B:727:HOH:O | 2.07 | 0.55 |
| 1:A:579:ARG:HG2 | 1:A:580:GLU:HG3 | 1.88 | 0.55 |
| 1:B:169:PHE:CE2 | 1:B:175:VAL:HG22 | 2.40 | 0.55 |
| 1:B:259:LEU:HD11 | 2:B:767:HOH:O | 2.06 | 0.55 |
| 1:B:246:THR:CG2 | 1:B:402:GLY:O | 2.55 | 0.55 |
| 1:A:169:PHE:HE2 | 1:A:371:PHE:HD1 | 1.54 | 0.55 |
| 1:A:215:ALA:CB | 1:A:406:GLU:HB2 | 2.35 | 0.55 |
| 1:A:418:GLY:O | 1:A:421:GLU:HB2 | 2.07 | 0.55 |
| 1:A:550:ILE:HB | 1:B:548:ALA:H | 1.71 | 0.55 |
| 1:B:219:ARG:HG3 | 1:B:220:LEU:N | 2.22 | 0.55 |
| 1:A:237:SER:HB3 | 1:A:276:GLU:N | 2.21 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:510:ASP:CG | 1:A:542:ARG:HE | 2.10 | 0.55 |
| 1:B:373:GLU:HB3 | 2:B:739:HOH:O | 2.05 | 0.55 |
| 1:B:451:THR:HG21 | 1:B:466:VAL:C | 2.27 | 0.55 |
| 1:A:173:GLY:O | 1:A:408:ARG:NH1 | 2.38 | 0.55 |
| 1:A:449:TYR:HB2 | 1:A:471:VAL:CG2 | 2.36 | 0.55 |
| 1:A:472:VAL:HG21 | 1:A:535:LEU:HD13 | 1.88 | 0.55 |
| 1:A:159:ILE:HD12 | 1:A:164:ILE:HG13 | 1.89 | 0.54 |
| 1:A:269:SER:OG | 1:A:285:HIS:CD2 | 2.60 | 0.54 |
| 1:A:563:ASP:HA | 1:A:566:LYS:HB2 | 1.88 | 0.54 |
| 1:B:220:LEU:HG | 1:B:240:PHE:CE2 | 2.43 | 0.54 |
| 1:B:250:TRP:CD2 | 1:B:287:ARG:HA | 2.42 | 0.54 |
| 1:B:355:ARG:HG3 | 1:B:387:ALA:HA | 1.88 | 0.54 |
| 1:B:406:GLU:HA | 2:B:763:HOH:O | 2.07 | 0.54 |
| 1:A:284:ASN:HB2 | 1:A:300:THR:HG23 | 1.89 | 0.54 |
| 1:A:519:ILE:HG22 | 1:A:567:ILE:HG22 | 1.89 | 0.54 |
| 1:B:90:HIS:CD2 | 1:B:114:ILE:H | 2.25 | 0.54 |
| 1:B:300:THR:O | 1:B:301:SER:HB2 | 2.06 | 0.54 |
| 1:B:357:PRO:O | 1:B:360:GLY:HA3 | 2.07 | 0.54 |
| 1:B:359:PRO:HB3 | 1:B:434:GLY:O | 2.07 | 0.54 |
| 1:B:458:LYS:O | 1:B:461:LEU:HB2 | 2.07 | 0.54 |
| 1:A:322:LEU:HD22 | 1:A:323:PRO:O | 2.07 | 0.54 |
| 1:B:411:ILE:HD12 | 1:B:419:GLU:HG2 | 1.87 | 0.54 |
| 1:B:35:LYS:HE2 | 1:B:52:ASP:OD2 | 2.07 | 0.54 |
| 1:B:52:ASP:C | 1:B:54:GLY:H | 2.11 | 0.54 |
| 1:A:307:ARG:HB2 | 1:A:318:LEU:O | 2.08 | 0.54 |
| 1:A:353:SER:O | 1:A:354:GLY:C | 2.45 | 0.54 |
| 1:A:346:VAL:HG13 | 1:A:407:TRP:CZ2 | 2.40 | 0.54 |
| 1:A:220:LEU:HB3 | 1:A:233:LEU:HD12 | 1.89 | 0.54 |
| 1:A:549:HIS:HD1 | 1:B:549:HIS:CE1 | 2.25 | 0.54 |
| 1:B:562:GLU:HG3 | 2:B:724:HOH:O | 2.07 | 0.54 |
| 1:B:91:ALA:HB1 | 1:B:105:ARG:NE | 2.22 | 0.54 |
| 1:A:59:LEU:O | 1:A:101:GLY:N | 2.41 | 0.54 |
| 1:A:249:THR:HG22 | 1:A:250:TRP:HB3 | 1.88 | 0.54 |
| 1:A:24:LYS:O | 1:A:40:GLY:HA2 | 2.08 | 0.54 |
| 1:A:175:VAL:HB | 1:A:197:PHE:H | 1.73 | 0.54 |
| 1:A:309:VAL:HG12 | 1:A:316:PRO:HB3 | 1.90 | 0.54 |
| 1:A:379:ASP:OD1 | 1:A:381:PHE:CD1 | 2.61 | 0.54 |
| 1:B:171:GLY:C | 1:B:173:GLY:N | 2.61 | 0.54 |
| 1:B:376:ASP:CB | 2:B:616:HOH:O | 2.46 | 0.54 |
| 1:B:397:TYR:HD1 | 1:B:419:GLU:HB3 | 1.71 | 0.54 |
| 1:B:60:ASN:CG | 2:B:679:HOH:O | 2.46 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:105:ARG:O | 1:A:107:GLU:N | 2.40 | 0.54 |
| 1:B:245:PRO:HB2 | 1:B:263:ALA:HB1 | 1.90 | 0.54 |
| 1:B:323:PRO:CB | 1:B:326:LEU:HD12 | 2.37 | 0.54 |
| 1:A:308:ILE:N | 1:A:318:LEU:O | 2.33 | 0.54 |
| 1:B:408:ARG:O | 1:B:411:ILE:HG22 | 2.08 | 0.54 |
| 1:B:421:GLU:O | 1:B:425:ALA:N | 2.39 | 0.54 |
| 1:B:570:PRO:HA | 2:B:653:HOH:O | 2.07 | 0.54 |
| 1:B:164:ILE:HD11 | 1:B:182:LEU:HA | 1.89 | 0.54 |
| 1:B:565:VAL:O | 1:B:568:LEU:N | 2.40 | 0.54 |
| 1:A:23:GLU:HG2 | 2:A:600:HOH:O | 2.08 | 0.53 |
| 1:A:536:MET:HE1 | 1:A:550:ILE:HD11 | 1.89 | 0.53 |
| 1:A:578:GLN:O | 1:A:579:ARG:C | 2.46 | 0.53 |
| 1:B:205:GLY:O | 1:B:206:MET:HB2 | 2.08 | 0.53 |
| 1:B:30:VAL:N | 1:B:289:VAL:HG11 | 2.23 | 0.53 |
| 1:A:258:ARG:HD2 | 1:A:273:ILE:CG2 | 2.38 | 0.53 |
| 1:B:178:PHE:C | 1:B:178:PHE:CD1 | 2.81 | 0.53 |
| 1:B:177:LEU:HD22 | 1:B:223:VAL:HG21 | 1.89 | 0.53 |
| 1:B:490:GLU:O | 1:B:495:GLY:N | 2.27 | 0.53 |
| 1:B:522:GLN:HB3 | 1:B:551:ILE:O | 2.07 | 0.53 |
| 1:A:175:VAL:CG2 | 1:A:196:SER:HB3 | 2.38 | 0.53 |
| 1:A:96:ASN:HD21 | 1:A:98:SER:HB2 | 1.73 | 0.53 |
| 1:B:114:ILE:HD12 | 1:B:114:ILE:N | 2.23 | 0.53 |
| 1:B:249:THR:N | 1:B:262:VAL:O | 2.42 | 0.53 |
| 1:A:292:ARG:O | 1:A:294:LYS:HD2 | 2.08 | 0.53 |
| 1:A:334:ARG:NH2 | 1:A:350:VAL:HG11 | 2.22 | 0.53 |
| 1:A:37:LEU:HD12 | 1:A:49:TYR:O | 2.08 | 0.53 |
| 1:A:579:ARG:HG2 | 1:A:580:GLU:N | 2.22 | 0.53 |
| 1:A:115:LEU:O | 1:A:116:SER:HB3 | 2.07 | 0.53 |
| 1:A:174:ARG:NH2 | 1:A:405:GLU:OE2 | 2.41 | 0.53 |
| 1:A:351:LEU:CD1 | 1:A:382:ALA:HB1 | 2.38 | 0.53 |
| 1:A:469:ALA:HA | 1:A:520:HIS:CE1 | 2.44 | 0.53 |
| 1:A:46:VAL:O | 1:A:64:ILE:HG12 | 2.09 | 0.53 |
| 1:B:92:LEU:C | 1:B:106:LEU:HD12 | 2.29 | 0.53 |
| 1:B:195:GLY:HA3 | 1:B:213:GLU:O | 2.08 | 0.53 |
| 1:A:22:VAL:HG21 | 1:A:323:PRO:HD3 | 1.90 | 0.53 |
| 1:A:442:MET:HG3 | 1:A:466:VAL:HB | 1.89 | 0.53 |
| 1:A:456:THR:HG22 | 1:A:512:ILE:HG12 | 1.90 | 0.53 |
| 1:A:524:ASP:OD1 | 1:A:556:HIS:HB2 | 2.09 | 0.53 |
| 1:B:509:VAL:HA | 1:B:512:ILE:CD1 | 2.35 | 0.53 |
| 1:A:115:LEU:HB2 | 2:A:677:HOH:O | 2.08 | 0.53 |
| 1:A:379:ASP:OD1 | 1:A:381:PHE:HD1 | 1.92 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:58:LYS:HD3 | 2:A:736:HOH:O | 2.08 | 0.53 |
| 1:A:62:GLU:HB2 | 1:A:81:ARG:NH2 | 2.23 | 0.53 |
| 1:B:423:VAL:HG21 | 1:B:450:MET:HG2 | 1.90 | 0.53 |
| 1:A:194:GLU:HB3 | 1:A:214:THR:HG22 | 1.91 | 0.53 |
| 1:A:348:THR:HG21 | 1:A:393:VAL:HG13 | 1.90 | 0.53 |
| 1:B:31:VAL:CG1 | 1:B:32:ASP:N | 2.71 | 0.53 |
| 1:B:42:SER:OG | 1:B:43:GLU:N | 2.42 | 0.53 |
| 1:A:151:PRO:HB2 | 1:A:170:PHE:CD2 | 2.44 | 0.53 |
| 1:A:169:PHE:CE2 | 1:A:371:PHE:HD1 | 2.27 | 0.53 |
| 1:A:497:ARG:C | 1:A:499:ILE:H | 2.13 | 0.53 |
| 1:A:328:ARG:NH1 | 1:A:328:ARG:HG2 | 2.23 | 0.52 |
| 1:A:350:VAL:HA | 2:A:652:HOH:O | 2.09 | 0.52 |
| 1:A:125:VAL:HG13 | 1:A:137:TYR:O | 2.09 | 0.52 |
| 1:A:84:SER:OG | 1:A:87:ALA:HB3 | 2.10 | 0.52 |
| 1:B:493:THR:O | 1:B:494:GLY:C | 2.47 | 0.52 |
| 1:B:133:ARG:HD2 | 1:B:146:GLU:OE2 | 2.09 | 0.52 |
| 1:B:539:LEU:HD13 | 1:B:546:PHE:CD1 | 2.44 | 0.52 |
| 1:A:106:LEU:HD11 | 2:A:589:HOH:O | 2.09 | 0.52 |
| 1:A:551:ILE:N | 1:A:551:ILE:HD12 | 2.25 | 0.52 |
| 1:B:209:THR:O | 1:B:210:ALA:HB2 | 2.09 | 0.52 |
| 1:B:366:VAL:HG12 | 2:B:588:HOH:O | 2.07 | 0.52 |
| 1:A:198:SER:HB3 | 1:A:213:GLU:OE2 | 2.09 | 0.52 |
| 1:A:392:VAL:HG12 | 1:A:393:VAL:N | 2.25 | 0.52 |
| 1:A:442:MET:HE2 | 1:A:444:TYR:HE1 | 1.74 | 0.52 |
| 1:A:441:ILE:HB | 1:A:462:PHE:CE1 | 2.45 | 0.52 |
| 1:A:463:LYS:HB2 | 2:A:729:HOH:O | 2.09 | 0.52 |
| 1:B:325:ASP:HA | 1:B:328:ARG:NE | 2.24 | 0.52 |
| 1:B:579:ARG:C | 1:B:581:ARG:N | 2.59 | 0.52 |
| 1:B:59:LEU:HA | 1:B:100:PRO:HB3 | 1.90 | 0.52 |
| 1:A:132:ASP:O | 1:A:133:ARG:HB3 | 2.09 | 0.52 |
| 1:A:415:PRO:HD3 | 1:A:492:LEU:O | 2.08 | 0.52 |
| 1:B:246:THR:HG21 | 1:B:402:GLY:O | 2.10 | 0.52 |
| 1:A:309:VAL:HG12 | 1:A:316:PRO:CB | 2.39 | 0.52 |
| 1:A:353:SER:HB2 | 1:A:386:ALA:HA | 1.92 | 0.52 |
| 1:B:501:ARG:O | 1:B:507:ASN:OD1 | 2.27 | 0.52 |
| 1:A:304:THR:HG23 | 2:A:654:HOH:O | 2.10 | 0.52 |
| 1:A:339:GLU:OE2 | 1:A:343:GLY:HA2 | 2.09 | 0.52 |
| 1:A:463:LYS:O | 1:A:514:GLU:HB3 | 2.09 | 0.52 |
| 1:A:530:LYS:HB3 | 1:A:531:PRO:CD | 2.28 | 0.52 |
| 1:B:159:ILE:CD1 | 1:B:164:ILE:HG23 | 2.39 | 0.52 |
| 1:B:472:VAL:HG23 | 1:B:532:LEU:HD22 | 1.92 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:564:ALA:HB2 | 2:B:729:HOH:O | 2.10 | 0.52 |
| 1:B:246:THR:HG22 | 1:B:265:ARG:HA | 1.91 | 0.52 |
| 1:A:202:ILE:HG13 | 2:A:653:HOH:O | 2.09 | 0.51 |
| 1:B:145:ARG:HD3 | 2:B:664:HOH:O | 2.09 | 0.51 |
| 1:B:281:PRO:HG3 | 2:B:595:HOH:O | 2.09 | 0.51 |
| 1:B:37:LEU:HD23 | 1:B:70:PRO:HG3 | 1.91 | 0.51 |
| 1:A:133:ARG:HD2 | 2:A:609:HOH:O | 2.10 | 0.51 |
| 1:A:129:ALA:HB1 | 1:A:134:VAL:HG22 | 1.91 | 0.51 |
| 1:A:341:PHE:C | 1:A:343:GLY:H | 2.13 | 0.51 |
| 1:A:497:ARG:O | 1:A:500:MET:N | 2.43 | 0.51 |
| 1:A:471:VAL:HG11 | 1:A:474:TRP:CZ3 | 2.46 | 0.51 |
| 1:B:397:TYR:CD1 | 1:B:419:GLU:HB3 | 2.45 | 0.51 |
| 1:B:497:ARG:N | 2:B:648:HOH:O | 2.42 | 0.51 |
| 1:A:482:ASP:OD1 | 1:A:485:PHE:HD1 | 1.93 | 0.51 |
| 1:A:172:GLY:C | 1:A:174:ARG:N | 2.63 | 0.51 |
| 1:A:181:ASN:HB3 | 1:A:185:GLY:H | 1.75 | 0.51 |
| 1:A:299:HIS:CG | 1:A:300:THR:N | 2.77 | 0.51 |
| 1:B:136:LEU:O | 1:B:147:LEU:HB2 | 2.10 | 0.51 |
| 1:B:72:TYR:CE2 | 1:B:289:VAL:HG13 | 2.46 | 0.51 |
| 1:B:463:LYS:O | 2:B:689:HOH:O | 2.19 | 0.51 |
| 1:B:579:ARG:O | 1:B:581:ARG:N | 2.43 | 0.51 |
| 1:A:202:ILE:HG22 | 1:A:203:SER:N | 2.26 | 0.51 |
| 1:A:284:ASN:ND2 | 1:A:376:ASP:O | 2.43 | 0.51 |
| 1:A:87:ALA:HA | 1:A:523:ASN:O | 2.11 | 0.51 |
| 1:B:139:LEU:HD12 | 1:B:143:GLY:C | 2.31 | 0.51 |
| 1:B:411:ILE:HD12 | 1:B:419:GLU:CG | 2.41 | 0.51 |
| 1:B:487:ASN:O | 1:B:491:GLN:HG3 | 2.10 | 0.51 |
| 1:B:78:ILE:HD11 | 1:B:124:VAL:HG22 | 1.93 | 0.51 |
| 1:A:27:LEU:HB3 | 2:A:605:HOH:O | 2.10 | 0.51 |
| 1:A:286:GLY:O | 1:A:287:ARG:C | 2.48 | 0.51 |
| 1:B:225:PRO:HB2 | 2:B:738:HOH:O | 2.11 | 0.51 |
| 1:A:399:GLY:HA2 | 1:A:408:ARG:O | 2.10 | 0.51 |
| 1:A:350:VAL:HG12 | 1:A:351:LEU:N | 2.26 | 0.51 |
| 1:B:344:SER:N | 2:B:722:HOH:O | 2.43 | 0.51 |
| 1:A:385:LEU:HB3 | 2:A:720:HOH:O | 2.11 | 0.51 |
| 1:A:174:ARG:HH21 | 1:A:405:GLU:CG | 2.23 | 0.51 |
| 1:A:474:TRP:CB | 1:A:500:MET:HB3 | 2.40 | 0.51 |
| 1:A:63:PRO:HB3 | 2:A:595:HOH:O | 2.11 | 0.51 |
| 1:A:81:ARG:O | 1:A:90:HIS:HA | 2.11 | 0.51 |
| 1:B:362:THR:CG2 | 1:B:363:VAL:H | 2.23 | 0.51 |
| 1:B:401:THR:HG22 | 1:B:408:ARG:CD | 2.41 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:477:MET:HE1 | 1:B:489:ILE:HD11 | 1.91 | 0.51 |
| 1:B:82:ASP:OD1 | 1:B:84:SER:OG | 2.22 | 0.50 |
| 1:A:371:PHE:N | 1:A:371:PHE:CD2 | 2.78 | 0.50 |
| 1:B:139:LEU:HD12 | 1:B:143:GLY:O | 2.11 | 0.50 |
| 1:B:430:ALA:O | 1:B:436:ALA:N | 2.38 | 0.50 |
| 1:A:202:ILE:CG1 | 2:A:653:HOH:O | 2.58 | 0.50 |
| 1:A:415:PRO:O | 1:A:416:CYS:HB3 | 2.11 | 0.50 |
| 1:A:472:VAL:HG21 | 1:A:535:LEU:HD22 | 1.93 | 0.50 |
| 1:A:551:ILE:CG2 | 1:A:552:PRO:HD2 | 2.41 | 0.50 |
| 1:B:451:THR:O | 2:B:615:HOH:O | 2.18 | 0.50 |
| 1:B:476:GLU:HA | 1:B:479:GLU:CD | 2.31 | 0.50 |
| 1:B:482:ASP:HB2 | 2:B:604:HOH:O | 2.12 | 0.50 |
| 1:A:207:LYS:HE2 | 1:A:224:ASP:HB2 | 1.93 | 0.50 |
| 1:A:29:GLY:O | 1:A:37:LEU:HB3 | 2.11 | 0.50 |
| 1:A:569:LEU:O | 1:A:573:PHE:CD2 | 2.65 | 0.50 |
| 1:B:109:VAL:CG2 | 1:B:139:LEU:HD22 | 2.41 | 0.50 |
| 1:B:314:GLY:HA3 | 2:B:595:HOH:O | 2.09 | 0.50 |
| 1:B:353:SER:HB3 | 1:B:356:ALA:CB | 2.38 | 0.50 |
| 1:A:160:ARG:NH1 | 1:A:203:SER:HA | 2.27 | 0.50 |
| 1:A:268:ARG:HA | 1:A:283:GLY:O | 2.11 | 0.50 |
| 1:B:362:THR:OG1 | 1:B:391:HIS:HB2 | 2.11 | 0.50 |
| 1:B:76:ARG:NH2 | 2:B:725:HOH:O | 2.32 | 0.50 |
| 1:B:393:VAL:HB | 2:B:775:HOH:O | 2.11 | 0.50 |
| 1:B:476:GLU:O | 1:B:480:LEU:HG | 2.12 | 0.50 |
| 1:B:35:LYS:HB2 | 1:B:50:LEU:HD22 | 1.93 | 0.50 |
| 1:B:56:THR:N | 2:B:735:HOH:O | 2.43 | 0.50 |
| 1:B:81:ARG:HB3 | 1:B:93:PHE:CE1 | 2.47 | 0.50 |
| 1:A:365:LEU:HB2 | 2:A:693:HOH:O | 2.12 | 0.50 |
| 1:A:399:GLY:N | 1:A:407:TRP:O | 2.45 | 0.50 |
| 1:B:250:TRP:CZ3 | 1:B:260:ALA:HB3 | 2.46 | 0.50 |
| 1:B:371:PHE:CE2 | 1:B:408:ARG:NH1 | 2.79 | 0.50 |
| 1:B:35:LYS:CG | 1:B:52:ASP:OD1 | 2.60 | 0.50 |
| 1:A:249:THR:HG22 | 1:A:250:TRP:N | 2.25 | 0.50 |
| 1:A:294:LYS:O | 1:A:296:VAL:HG23 | 2.12 | 0.50 |
| 1:A:366:VAL:HG12 | 1:A:367:HIS:O | 2.12 | 0.50 |
| 1:B:34:ASP:O | 1:B:35:LYS:HG2 | 2.10 | 0.50 |
| 1:B:455:LEU:CD1 | 1:B:516:LEU:HD13 | 2.42 | 0.50 |
| 1:A:94:LYS:HB3 | 1:A:106:LEU:HD21 | 1.94 | 0.50 |
| 1:A:413:GLY:HA2 | 1:A:493:THR:HA | 1.93 | 0.50 |
| 1:A:308:ILE:O | 1:A:317:LEU:N | 2.44 | 0.49 |
| 1:A:536:MET:CE | 1:A:550:ILE:HD11 | 2.41 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:508:HIS:C | 1:B:510:ASP:N | 2.64 | 0.49 |
| 1:A:441:ILE:C | 1:A:441:ILE:HD13 | 2.31 | 0.49 |
| 1:A:529:LEU:CD1 | 1:A:550:ILE:HD12 | 2.33 | 0.49 |
| 1:B:268:ARG:HH12 | 1:B:282:GLN:CD | 2.15 | 0.49 |
| 1:B:431:ARG:HH11 | 1:B:431:ARG:HG3 | 1.77 | 0.49 |
| 1:A:240:PHE:HD1 | 1:A:272:PHE:CD1 | 2.31 | 0.49 |
| 1:A:60:ASN:ND2 | 1:A:62:GLU:O | 2.37 | 0.49 |
| 1:B:251:LEU:HD11 | 1:B:259:LEU:HD11 | 1.93 | 0.49 |
| 1:B:543:GLY:O | 1:B:544:LYS:C | 2.50 | 0.49 |
| 1:A:468:GLY:C | 1:A:470:SER:N | 2.61 | 0.49 |
| 1:A:522:GLN:HG2 | 1:A:552:PRO:HA | 1.94 | 0.49 |
| 1:A:71:HIS:HB2 | 1:A:119:ASP:O | 2.11 | 0.49 |
| 1:B:405:GLU:HG3 | 1:B:409:LEU:HG | 1.95 | 0.49 |
| 1:B:451:THR:HG21 | 1:B:466:VAL:O | 2.12 | 0.49 |
| 1:B:49:TYR:CA | 1:B:57:VAL:O | 2.54 | 0.49 |
| 1:A:408:ARG:O | 1:A:411:ILE:HG22 | 2.13 | 0.49 |
| 1:A:416:CYS:SG | 1:A:416:CYS:O | 2.70 | 0.49 |
| 1:A:68:LEU:HB2 | 1:A:78:ILE:HB | 1.94 | 0.49 |
| 1:B:311:LEU:HB3 | 1:B:312:PRO:HA | 1.95 | 0.49 |
| 1:B:486:ARG:O | 1:B:490:GLU:HG3 | 2.12 | 0.49 |
| 1:B:153:PHE:CE1 | 1:B:488:PHE:HB2 | 2.45 | 0.49 |
| 1:A:44:GLY:HA2 | 1:A:561:MET:N | 2.22 | 0.49 |
| 1:B:243:TYR:CZ | 1:B:270:ALA:HB2 | 2.47 | 0.49 |
| 1:B:431:ARG:HG3 | 1:B:431:ARG:NH1 | 2.28 | 0.49 |
| 1:A:160:ARG:HH22 | 1:A:204:PRO:HG3 | 1.78 | 0.49 |
| 1:A:309:VAL:HA | 1:A:317:LEU:H | 1.77 | 0.49 |
| 1:A:87:ALA:O | 1:A:525:SER:OG | 2.24 | 0.49 |
| 1:B:242:SER:C | 1:B:244:ARG:H | 2.15 | 0.49 |
| 1:B:365:LEU:HD23 | 1:B:394:MET:HG2 | 1.94 | 0.49 |
| 1:A:142:GLY:HA3 | 2:A:636:HOH:O | 2.11 | 0.49 |
| 1:B:90:HIS:CG | 1:B:114:ILE:HD13 | 2.46 | 0.49 |
| 1:A:174:ARG:NE | 1:A:409:LEU:HD11 | 2.25 | 0.49 |
| 1:A:489:ILE:O | 1:A:490:GLU:C | 2.50 | 0.49 |
| 1:B:209:THR:HG23 | 1:B:233:LEU:HD12 | 1.95 | 0.49 |
| 1:B:36:LEU:HD11 | 1:B:296:VAL:HG11 | 1.94 | 0.49 |
| 1:A:124:VAL:N | 1:A:139:LEU:O | 2.38 | 0.49 |
| 1:A:224:ASP:OD1 | 1:A:225:PRO:HD2 | 2.12 | 0.49 |
| 1:A:475:GLU:OE1 | 1:A:497:ARG:HG3 | 2.13 | 0.49 |
| 1:B:280:ALA:CB | 1:B:285:HIS:CE1 | 2.96 | 0.49 |
| 1:B:522:GLN:HG3 | 1:B:523:ASN:N | 2.27 | 0.49 |
| 1:B:506:ILE:CD1 | 1:B:535:LEU:HA | 2.43 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:65:ASN:HD21 | 1:B:82:ASP:HB2 | 1.77 | 0.49 |
| 1:A:74:VAL:HG11 | 1:A:121:GLY:CA | 2.43 | 0.48 |
| 1:A:240:PHE:CE1 | 1:A:245:PRO:HG3 | 2.47 | 0.48 |
| 1:A:305:PRO:HD2 | 2:A:654:HOH:O | 2.11 | 0.48 |
| 1:B:411:ILE:HD13 | 1:B:419:GLU:HG2 | 1.94 | 0.48 |
| 1:B:71:HIS:HA | 2:B:666:HOH:O | 2.13 | 0.48 |
| 1:A:194:GLU:CB | 1:A:212:LEU:HD21 | 2.38 | 0.48 |
| 1:A:277:ARG:HD2 | 1:A:278:VAL:H | 1.77 | 0.48 |
| 1:B:239:ASP:HA | 1:B:242:SER:OG | 2.13 | 0.48 |
| 1:A:341:PHE:CG | 1:A:342:ASP:N | 2.82 | 0.48 |
| 1:A:579:ARG:CB | 1:A:579:ARG:NH1 | 2.75 | 0.48 |
| 1:B:379:ASP:HB3 | 1:B:382:ALA:CB | 2.43 | 0.48 |
| 1:B:459:PRO:HG3 | 2:B:605:HOH:O | 2.13 | 0.48 |
| 1:B:516:LEU:HD21 | 1:B:518:LEU:HD21 | 1.94 | 0.48 |
| 1:A:136:LEU:HD11 | 1:A:156:VAL:HG22 | 1.96 | 0.48 |
| 1:A:194:GLU:OE2 | 1:A:219:ARG:NH2 | 2.47 | 0.48 |
| 1:A:274:ASP:C | 1:A:276:GLU:H | 2.17 | 0.48 |
| 1:B:453:CYS:N | 2:B:731:HOH:O | 2.46 | 0.48 |
| 1:B:68:LEU:HD12 | 1:B:78:ILE:CD1 | 2.43 | 0.48 |
| 1:A:563:ASP:HA | 1:A:566:LYS:CB | 2.43 | 0.48 |
| 1:B:272:PHE:CE2 | 1:B:277:ARG:HB2 | 2.48 | 0.48 |
| 1:B:40:GLY:HA3 | 1:B:49:TYR:HE1 | 1.79 | 0.48 |
| 1:B:445:SER:C | 1:B:447:GLY:N | 2.66 | 0.48 |
| 1:A:384:SER:O | 1:A:387:ALA:HB3 | 2.13 | 0.48 |
| 1:A:361:PRO:HB3 | 1:A:438:GLU:OE2 | 2.14 | 0.48 |
| 1:B:68:LEU:HD12 | 1:B:124:VAL:HG13 | 1.95 | 0.48 |
| 1:A:192:SER:HB3 | 1:A:195:GLY:O | 2.13 | 0.48 |
| 1:A:258:ARG:HB3 | 1:A:273:ILE:HG23 | 1.96 | 0.48 |
| 1:A:26:SER:OG | 1:A:28:GLN:NE2 | 2.46 | 0.48 |
| 1:A:264:ARG:NE | 1:A:373:GLU:OE2 | 2.45 | 0.48 |
| 1:A:374:ASP:N | 1:A:396:ASN:OD1 | 2.35 | 0.48 |
| 1:B:376:ASP:HA | 2:B:600:HOH:O | 2.12 | 0.48 |
| 1:A:129:ALA:CB | 1:A:484:ALA:HB2 | 2.43 | 0.48 |
| 1:A:330:ILE:HD12 | 1:A:330:ILE:N | 2.29 | 0.48 |
| 1:A:452:LEU:HB3 | 1:A:505:PRO:HG2 | 1.95 | 0.48 |
| 1:A:549:HIS:ND1 | 1:A:570:PRO:HB3 | 2.29 | 0.48 |
| 1:B:449:TYR:N | 2:B:685:HOH:O | 2.47 | 0.48 |
| 1:B:519:ILE:HD13 | 1:B:567:ILE:O | 2.13 | 0.48 |
| 1:B:28:GLN:HG3 | 1:B:67:VAL:HG21 | 1.96 | 0.48 |
| 1:A:173:GLY:O | 1:A:408:ARG:NH2 | 2.47 | 0.48 |
| 1:A:174:ARG:NH2 | 1:A:195:GLY:HA2 | 2.29 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:222:THR:HB | 1:A:231:GLU:CG | 2.43 | 0.48 |
| 1:A:414:ASP:CG | 1:A:414:ASP:O | 2.51 | 0.48 |
| 1:A:553:ASP:OD1 | 1:B:545:THR:CG2 | 2.61 | 0.48 |
| 1:B:365:LEU:HD11 | 1:B:381:PHE:HB3 | 1.96 | 0.48 |
| 1:B:367:HIS:CE1 | 1:B:400:SER:OG | 2.67 | 0.48 |
| 1:B:457:MET:C | 1:B:459:PRO:HD2 | 2.34 | 0.48 |
| 1:B:442:MET:HG3 | 1:B:466:VAL:CG1 | 2.44 | 0.48 |
| 1:B:468:GLY:HA2 | 1:B:519:ILE:O | 2.13 | 0.48 |
| 1:A:497:ARG:C | 1:A:499:ILE:N | 2.67 | 0.48 |
| 1:B:282:GLN:NE2 | 2:B:660:HOH:O | 2.46 | 0.48 |
| 1:B:294:LYS:HG2 | 2:B:705:HOH:O | 2.13 | 0.48 |
| 1:B:38:VAL:CG1 | 1:B:308:ILE:HD13 | 2.44 | 0.48 |
| 1:B:411:ILE:HG12 | 1:B:492:LEU:HD11 | 1.95 | 0.48 |
| 1:B:458:LYS:N | 1:B:459:PRO:CD | 2.77 | 0.48 |
| 1:B:568:LEU:O | 1:B:572:VAL:HG23 | 2.14 | 0.48 |
| 1:A:415:PRO:HG3 | 1:A:493:THR:HG22 | 1.95 | 0.47 |
| 1:A:474:TRP:HD1 | 1:A:500:MET:HA | 1.79 | 0.47 |
| 1:A:569:LEU:HB3 | 1:A:570:PRO:CD | 2.36 | 0.47 |
| 1:A:90:HIS:HD2 | 1:A:114:ILE:N | 2.08 | 0.47 |
| 1:B:325:ASP:C | 1:B:328:ARG:H | 2.17 | 0.47 |
| 1:B:333:SER:HA | 1:B:350:VAL:O | 2.14 | 0.47 |
| 1:B:520:HIS:CB | 2:B:744:HOH:O | 2.62 | 0.47 |
| 1:A:372:ALA:O | 1:A:373:GLU:HB3 | 2.14 | 0.47 |
| 1:A:521:PRO:CB | 1:A:555:GLY:O | 2.62 | 0.47 |
| 1:A:532:LEU:HD12 | 1:A:536:MET:HE3 | 1.96 | 0.47 |
| 1:B:406:GLU:HG2 | 1:B:410:LYS:CE | 2.41 | 0.47 |
| 1:B:451:THR:HA | 2:B:615:HOH:O | 2.14 | 0.47 |
| 1:B:158:ASP:C | 1:B:159:ILE:HD13 | 2.34 | 0.47 |
| 1:B:322:LEU:O | 1:B:323:PRO:O | 2.33 | 0.47 |
| 1:B:27:LEU:HD12 | 1:B:38:VAL:HG12 | 1.94 | 0.47 |
| 1:B:475:GLU:O | 1:B:478:TYR:HB3 | 2.14 | 0.47 |
| 1:A:224:ASP:O | 1:A:228:GLY:HA2 | 2.14 | 0.47 |
| 1:A:515:PRO:CA | 2:A:613:HOH:O | 2.47 | 0.47 |
| 1:B:212:LEU:CD2 | 1:B:219:ARG:HH12 | 2.12 | 0.47 |
| 1:B:550:ILE:N | 1:B:550:ILE:HD12 | 2.29 | 0.47 |
| 1:A:309:VAL:CA | 1:A:316:PRO:HA | 2.41 | 0.47 |
| 1:B:70:PRO:HA | 1:B:119:ASP:HB3 | 1.97 | 0.47 |
| 1:B:248:ILE:N | 1:B:248:ILE:HD12 | 2.28 | 0.47 |
| 1:B:504:SER:O | 1:B:506:ILE:N | 2.48 | 0.47 |
| 1:B:520:HIS:CE1 | 2:B:618:HOH:O | 2.67 | 0.47 |
| 1:B:551:ILE:HB | 1:B:554:ALA:CB | 2.43 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:385:LEU:O | 1:B:390:PHE:N | 2.45 | 0.47 |
| 1:B:477:MET:HA | 1:B:528:PRO:HG3 | 1.96 | 0.47 |
| 1:A:254:LEU:HD11 | 1:A:295:LEU:HD21 | 1.96 | 0.47 |
| 1:A:430:ALA:HB1 | 1:A:436:ALA:HB2 | 1.97 | 0.47 |
| 1:B:112:MET:HB2 | 1:B:130:THR:HG22 | 1.97 | 0.47 |
| 1:B:477:MET:CA | 2:B:756:HOH:O | 2.58 | 0.47 |
| 1:B:480:LEU:CB | 2:B:756:HOH:O | 2.52 | 0.47 |
| 1:A:104:GLN:NE2 | 2:A:699:HOH:O | 2.47 | 0.47 |
| 1:A:219:ARG:HH12 | 1:A:221:VAL:CG1 | 2.27 | 0.47 |
| 1:A:468:GLY:O | 1:A:469:ALA:C | 2.53 | 0.47 |
| 1:B:250:TRP:CE3 | 1:B:287:ARG:HA | 2.50 | 0.47 |
| 1:B:309:VAL:HG12 | 1:B:316:PRO:CA | 2.45 | 0.47 |
| 1:A:258:ARG:HD2 | 1:A:273:ILE:HG21 | 1.97 | 0.47 |
| 1:A:346:VAL:HG22 | 1:A:407:TRP:CZ2 | 2.50 | 0.47 |
| 1:A:367:HIS:HE1 | 1:A:396:ASN:HA | 1.80 | 0.47 |
| 1:B:495:GLY:O | 1:B:496:SER:O | 2.33 | 0.47 |
| 1:B:476:GLU:CG | 1:B:531:PRO:HG3 | 2.45 | 0.47 |
| 1:A:237:SER:O | 1:A:275:GLY:HA3 | 2.14 | 0.47 |
| 1:A:267:GLY:CA | 1:A:375:SER:HB2 | 2.45 | 0.47 |
| 1:A:452:LEU:HB2 | 2:A:709:HOH:O | 2.14 | 0.47 |
| 1:B:445:SER:HA | 1:B:469:ALA:O | 2.15 | 0.47 |
| 1:B:472:VAL:HG23 | 2:B:683:HOH:O | 2.14 | 0.47 |
| 1:A:519:ILE:CG2 | 1:A:567:ILE:HG22 | 2.44 | 0.47 |
| 1:A:62:GLU:HB2 | 1:A:81:ARG:HE | 1.80 | 0.47 |
| 1:B:280:ALA:HB3 | 1:B:285:HIS:CE1 | 2.50 | 0.47 |
| 1:B:367:HIS:HD2 | 1:B:368:GLY:O | 1.98 | 0.47 |
| 1:B:441:ILE:HD13 | 2:B:615:HOH:O | 2.15 | 0.47 |
| 1:B:47:ASN:HB2 | 2:B:656:HOH:O | 2.15 | 0.47 |
| 1:B:495:GLY:O | 1:B:496:SER:C | 2.54 | 0.47 |
| 1:B:89:GLN:HA | 1:B:112:MET:O | 2.15 | 0.47 |
| 1:A:151:PRO:HD2 | 1:A:170:PHE:CZ | 2.49 | 0.46 |
| 1:A:366:VAL:HG13 | 1:A:397:TYR:CE2 | 2.50 | 0.46 |
| 1:B:141:GLY:C | 1:B:143:GLY:H | 2.18 | 0.46 |
| 1:B:431:ARG:HA | 1:B:436:ALA:HB3 | 1.98 | 0.46 |
| 1:A:160:ARG:NH2 | 1:A:204:PRO:HG3 | 2.30 | 0.46 |
| 1:A:45:SER:CB | 2:A:595:HOH:O | 2.59 | 0.46 |
| 1:B:133:ARG:HD2 | 2:B:608:HOH:O | 2.16 | 0.46 |
| 1:B:567:ILE:C | 1:B:567:ILE:HD12 | 2.32 | 0.46 |
| 1:A:305:PRO:O | 1:A:306:PRO:C | 2.52 | 0.46 |
| 1:A:302:LEU:HG | 1:A:376:ASP:OD1 | 2.15 | 0.46 |
| 1:A:532:LEU:O | 1:A:536:MET:HG3 | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:332:GLY:H | 1:B:352:GLU:HB2 | 1.80 | 0.46 |
| 1:B:520:HIS:CD2 | 1:B:521:PRO:HD2 | 2.32 | 0.46 |
| 1:A:270:ALA:HB3 | 2:A:588:HOH:O | 2.15 | 0.46 |
| 1:A:399:GLY:CA | 1:A:408:ARG:HA | 2.46 | 0.46 |
| 1:A:88:GLU:HG3 | 1:A:113:ARG:NH1 | 2.29 | 0.46 |
| 1:B:134:VAL:HB | 1:B:150:LEU:HB2 | 1.97 | 0.46 |
| 1:B:178:PHE:HB2 | 1:B:187:LEU:HD11 | 1.96 | 0.46 |
| 1:B:251:LEU:HD12 | 1:B:259:LEU:HD11 | 1.97 | 0.46 |
| 1:B:458:LYS:O | 1:B:461:LEU:CB | 2.63 | 0.46 |
| 1:B:41:PHE:HZ | 1:B:558:ILE:HG22 | 1.80 | 0.46 |
| 1:A:172:GLY:C | 1:A:174:ARG:H | 2.18 | 0.46 |
| 1:A:486:ARG:HG3 | 1:A:486:ARG:NH1 | 2.29 | 0.46 |
| 1:A:510:ASP:HB2 | 2:A:607:HOH:O | 2.16 | 0.46 |
| 1:B:160:ARG:HD2 | 1:B:202:ILE:CG2 | 2.46 | 0.46 |
| 1:A:93:PHE:HA | 1:A:104:GLN:O | 2.16 | 0.46 |
| 1:A:272:PHE:HD2 | 1:A:277:ARG:HA | 1.80 | 0.46 |
| 1:A:398:ARG:HD3 | 1:A:410:LYS:HB3 | 1.97 | 0.46 |
| 1:B:323:PRO:HG2 | 1:B:326:LEU:CD1 | 2.43 | 0.46 |
| 1:B:51:TYR:CE2 | 1:B:53:GLY:HA2 | 2.51 | 0.46 |
| 1:B:88:GLU:HG2 | 1:B:113:ARG:HH12 | 1.74 | 0.46 |
| 1:A:138:ALA:HB2 | 1:A:147:LEU:CD2 | 2.38 | 0.46 |
| 1:A:222:THR:HG22 | 1:A:222:THR:O | 2.16 | 0.46 |
| 1:A:240:PHE:CZ | 1:A:245:PRO:HG3 | 2.51 | 0.46 |
| 1:A:265:ARG:HD3 | 2:A:598:HOH:O | 2.15 | 0.46 |
| 1:A:579:ARG:CB | 1:A:579:ARG:HH11 | 2.28 | 0.46 |
| 1:B:125:VAL:HA | 1:B:138:ALA:HA | 1.96 | 0.46 |
| 1:B:379:ASP:O | 1:B:380:THR:C | 2.53 | 0.46 |
| 1:A:277:ARG:HD2 | 1:A:278:VAL:N | 2.31 | 0.46 |
| 1:A:444:TYR:O | 1:A:445:SER:HB3 | 2.16 | 0.46 |
| 1:A:474:TRP:HZ3 | 1:A:477:MET:HE1 | 1.80 | 0.46 |
| 1:B:51:TYR:CE2 | 1:B:317:LEU:HB3 | 2.43 | 0.46 |
| 1:B:464:ALA:HB2 | 1:B:578:GLN:HG3 | 1.98 | 0.46 |
| 1:B:448:GLY:HA3 | 1:B:470:SER:HB3 | 1.97 | 0.46 |
| 1:B:577:THR:CB | 2:B:784:HOH:O | 2.57 | 0.46 |
| 1:A:354:GLY:C | 1:A:356:ALA:H | 2.18 | 0.46 |
| 1:A:574:PHE:O | 1:A:578:GLN:HG2 | 2.15 | 0.46 |
| 1:B:30:VAL:CG2 | 1:B:290:LEU:O | 2.64 | 0.46 |
| 1:B:347:PRO:HG2 | 1:B:396:ASN:CB | 2.45 | 0.46 |
| 1:B:458:LYS:HB3 | 1:B:461:LEU:CD2 | 2.45 | 0.46 |
| 1:B:75:GLY:O | 1:B:96:ASN:OD1 | 2.34 | 0.46 |
| 1:A:400:SER:C | 2:A:618:HOH:O | 2.53 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:95:VAL:CG2 | 1:A:103:GLU:HG2 | 2.45 | 0.45 |
| 1:B:251:LEU:HD11 | 1:B:259:LEU:HD21 | 1.98 | 0.45 |
| 1:B:235:LEU:HD13 | 1:B:274:ASP:C | 2.37 | 0.45 |
| 1:B:279:GLU:HB2 | 1:B:312:PRO:O | 2.15 | 0.45 |
| 1:B:334:ARG:NH2 | 1:B:429:TRP:HH2 | 2.14 | 0.45 |
| 1:B:48:ALA:O | 1:B:58:LYS:HA | 2.17 | 0.45 |
| 1:A:178:PHE:O | 1:A:178:PHE:CD1 | 2.70 | 0.45 |
| 1:A:420:LEU:HD11 | 1:A:454:ALA:HA | 1.97 | 0.45 |
| 1:A:47:ASN:HB3 | 1:A:60:ASN:OD1 | 2.17 | 0.45 |
| 1:A:558:ILE:HD12 | 1:A:563:ASP:CB | 2.31 | 0.45 |
| 1:B:178:PHE:HD2 | 2:B:706:HOH:O | 1.99 | 0.45 |
| 1:B:307:ARG:HB2 | 1:B:319:GLU:CB | 2.46 | 0.45 |
| 1:A:446:TYR:O | 1:A:449:TYR:HB3 | 2.15 | 0.45 |
| 1:B:255:PRO:C | 1:B:257:GLY:H | 2.19 | 0.45 |
| 1:B:326:LEU:HD23 | 1:B:355:ARG:NH1 | 2.31 | 0.45 |
| 1:A:129:ALA:HA | 1:A:134:VAL:HA | 1.99 | 0.45 |
| 1:B:327:ARG:NH2 | 2:B:651:HOH:O | 2.48 | 0.45 |
| 1:B:445:SER:C | 1:B:447:GLY:H | 2.19 | 0.45 |
| 1:B:482:ASP:O | 1:B:486:ARG:HG3 | 2.17 | 0.45 |
| 1:A:475:GLU:HG2 | 1:A:500:MET:HB2 | 1.98 | 0.45 |
| 1:B:61:ARG:N | 1:B:103:GLU:OE2 | 2.50 | 0.45 |
| 1:B:27:LEU:HD13 | 1:B:38:VAL:HG12 | 1.98 | 0.45 |
| 1:B:551:ILE:HD11 | 1:B:567:ILE:HG22 | 1.98 | 0.45 |
| 1:B:91:ALA:CB | 1:B:105:ARG:NE | 2.79 | 0.45 |
| 1:B:92:LEU:CD1 | 1:B:109:VAL:HG11 | 2.46 | 0.45 |
| 1:B:95:VAL:HG13 | 2:B:742:HOH:O | 2.15 | 0.45 |
| 1:A:160:ARG:HD3 | 1:A:202:ILE:CG2 | 2.46 | 0.45 |
| 1:A:346:VAL:HG22 | 1:A:407:TRP:HH2 | 1.81 | 0.45 |
| 1:A:463:LYS:CB | 2:A:729:HOH:O | 2.63 | 0.45 |
| 1:A:44:GLY:CA | 1:A:561:MET:H | 2.24 | 0.45 |
| 1:A:579:ARG:HB2 | 1:A:579:ARG:CZ | 2.46 | 0.45 |
| 1:B:164:ILE:O | 1:B:179:THR:HA | 2.16 | 0.45 |
| 1:B:233:LEU:HD22 | 1:B:235:LEU:HG | 1.99 | 0.45 |
| 1:B:444:TYR:HA | 1:B:468:GLY:O | 2.17 | 0.45 |
| 1:A:251:LEU:HA | 1:A:260:ALA:O | 2.17 | 0.45 |
| 1:A:34:ASP:O | 1:A:291:TRP:NE1 | 2.50 | 0.45 |
| 1:A:440:TYR:HE2 | 1:A:578:GLN:HB3 | 1.82 | 0.45 |
| 1:B:219:ARG:HD2 | 1:B:232:ASP:OD1 | 2.16 | 0.45 |
| 1:B:376:ASP:C | 2:B:600:HOH:O | 2.55 | 0.45 |
| 1:B:424:SER:CB | 2:B:778:HOH:O | 2.65 | 0.45 |
| 1:B:522:GLN:HE21 | 1:B:523:ASN:CG | 2.19 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:22:VAL:HG12 | 1:A:23:GLU:N | 2.32 | 0.45 |
| 1:A:239:ASP:O | 1:A:243:TYR:N | 2.48 | 0.45 |
| 1:A:370:PRO:HG3 | 1:A:411:ILE:HD13 | 1.99 | 0.45 |
| 1:A:421:GLU:OE2 | 1:A:458:LYS:CE | 2.65 | 0.45 |
| 1:A:475:GLU:HA | 1:A:500:MET:CE | 2.47 | 0.45 |
| 1:A:68:LEU:HD12 | 1:A:78:ILE:CG2 | 2.35 | 0.45 |
| 1:B:29:GLY:HA3 | 1:B:289:VAL:HG21 | 1.99 | 0.45 |
| 1:B:398:ARG:NH2 | 1:B:407:TRP:HZ3 | 2.13 | 0.45 |
| 1:B:479:GLU:HG2 | 2:B:617:HOH:O | 2.16 | 0.45 |
| 1:B:411:ILE:CG1 | 1:B:492:LEU:HD11 | 2.46 | 0.45 |
| 1:B:520:HIS:HB2 | 2:B:744:HOH:O | 2.17 | 0.45 |
| 1:B:520:HIS:HD2 | 1:B:521:PRO:CD | 2.21 | 0.45 |
| 1:A:547:GLU:HB2 | 1:B:550:ILE:O | 2.17 | 0.45 |
| 1:A:125:VAL:O | 1:A:126:PHE:HB3 | 2.16 | 0.45 |
| 1:A:262:VAL:O | 1:A:262:VAL:HG12 | 2.17 | 0.45 |
| 1:A:263:ALA:O | 1:A:269:SER:CB | 2.65 | 0.45 |
| 1:A:335:LEU:HD13 | 1:A:349:TYR:CE1 | 2.51 | 0.45 |
| 1:B:226:ARG:NE | 2:B:769:HOH:O | 2.49 | 0.45 |
| 1:B:476:GLU:HA | 1:B:479:GLU:CG | 2.47 | 0.45 |
| 1:B:476:GLU:HA | 1:B:479:GLU:HG3 | 1.99 | 0.45 |
| 1:B:565:VAL:O | 1:B:567:ILE:N | 2.50 | 0.45 |
| 1:B:569:LEU:CB | 1:B:570:PRO:HD3 | 2.42 | 0.45 |
| 1:A:179:THR:H | 1:A:187:LEU:CD1 | 2.30 | 0.45 |
| 1:B:448:GLY:HA3 | 1:B:470:SER:HA | 1.99 | 0.45 |
| 1:B:415:PRO:O | 1:B:503:ARG:HG3 | 2.17 | 0.45 |
| 1:A:163:LEU:HB3 | 1:A:202:ILE:HD13 | 1.98 | 0.44 |
| 1:A:417:GLY:H | 1:A:419:GLU:CD | 2.19 | 0.44 |
| 1:B:156:VAL:HG23 | 2:B:596:HOH:O | 2.16 | 0.44 |
| 1:B:38:VAL:HG11 | 1:B:308:ILE:HD13 | 1.99 | 0.44 |
| 1:A:25:TYR:HB3 | 1:A:38:VAL:CG1 | 2.46 | 0.44 |
| 1:B:330:ILE:HG23 | 1:B:351:LEU:HD21 | 1.99 | 0.44 |
| 1:B:364:VAL:HA | 1:B:393:VAL:O | 2.17 | 0.44 |
| 1:A:224:ASP:HA | 1:A:225:PRO:HD3 | 1.83 | 0.44 |
| 1:A:520:HIS:N | 1:A:549:HIS:O | 2.35 | 0.44 |
| 1:B:340:SER:CA | 2:B:722:HOH:O | 2.65 | 0.44 |
| 1:B:551:ILE:HG23 | 1:B:566:LYS:HD3 | 1.98 | 0.44 |
| 1:A:109:VAL:HA | 2:A:728:HOH:O | 2.17 | 0.44 |
| 1:A:217:GLU:HG2 | 1:A:218:ALA:H | 1.82 | 0.44 |
| 1:A:393:VAL:HG22 | 2:A:652:HOH:O | 2.16 | 0.44 |
| 1:A:424:SER:HB3 | 1:A:461:LEU:HD21 | 1.99 | 0.44 |
| 1:B:221:VAL:HG12 | 1:B:232:ASP:HA | 2.00 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:401:THR:HG22 | 1:B:408:ARG:HD3 | 1.97 | 0.44 |
| 1:B:40:GLY:N | 1:B:47:ASN:O | 2.32 | 0.44 |
| 1:B:571:ALA:HA | 2:B:723:HOH:O | 2.16 | 0.44 |
| 1:A:304:THR:HA | 1:A:305:PRO:HD3 | 1.82 | 0.44 |
| 1:A:488:PHE:HZ | 2:A:672:HOH:O | 2.00 | 0.44 |
| 1:A:509:VAL:O | 1:A:509:VAL:HG12 | 2.17 | 0.44 |
| 1:B:226:ARG:HG3 | 1:B:226:ARG:HH11 | 1.82 | 0.44 |
| 1:B:240:PHE:CE1 | 1:B:263:ALA:HB2 | 2.52 | 0.44 |
| 1:B:340:SER:N | 2:B:722:HOH:O | 2.43 | 0.44 |
| 1:A:219:ARG:NH1 | 1:A:221:VAL:HG12 | 2.33 | 0.44 |
| 1:A:31:VAL:HB | 1:A:74:VAL:O | 2.16 | 0.44 |
| 1:A:367:HIS:HD2 | 1:A:372:ALA:HB3 | 1.81 | 0.44 |
| 1:A:499:ILE:O | 1:A:503:ARG:HB2 | 2.17 | 0.44 |
| 1:A:576:ALA:O | 1:A:579:ARG:HB3 | 2.18 | 0.44 |
| 1:B:135:ALA:HB2 | 2:B:608:HOH:O | 2.17 | 0.44 |
| 1:B:239:ASP:HA | 1:B:242:SER:HG | 1.82 | 0.44 |
| 1:B:243:TYR:O | 1:B:244:ARG:C | 2.56 | 0.44 |
| 1:B:456:THR:HG22 | 1:B:512:ILE:CD1 | 2.47 | 0.44 |
| 1:A:379:ASP:OD1 | 1:A:379:ASP:C | 2.56 | 0.44 |
| 1:A:451:THR:O | 1:A:455:LEU:HG | 2.18 | 0.44 |
| 1:B:301:SER:HA | 1:B:376:ASP:O | 2.18 | 0.44 |
| 1:B:371:PHE:HD2 | 1:B:408:ARG:HH11 | 1.61 | 0.44 |
| 1:B:59:LEU:HB3 | 2:B:727:HOH:O | 2.17 | 0.44 |
| 1:A:374:ASP:CG | 1:A:394:MET:HB3 | 2.39 | 0.44 |
| 1:A:442:MET:CE | 1:A:444:TYR:HE1 | 2.31 | 0.44 |
| 1:A:51:TYR:CE2 | 1:A:53:GLY:HA2 | 2.53 | 0.44 |
| 1:B:465:GLY:O | 1:B:516:LEU:HD12 | 2.18 | 0.44 |
| 1:B:549:HIS:CE1 | 2:B:686:HOH:O | 2.70 | 0.44 |
| 1:A:117:GLY:HA2 | 1:A:126:PHE:HA | 2.00 | 0.44 |
| 1:A:430:ALA:HB3 | 1:A:439:LEU:HD11 | 2.00 | 0.44 |
| 1:A:440:TYR:HD2 | 1:A:464:ALA:HB3 | 1.82 | 0.44 |
| 1:A:475:GLU:CA | 1:A:500:MET:HE2 | 2.48 | 0.44 |
| 1:A:72:TYR:OH | 1:A:289:VAL:HG12 | 2.18 | 0.44 |
| 1:B:523:ASN:ND2 | 1:B:553:ASP:CA | 2.81 | 0.44 |
| 1:A:195:GLY:HA3 | 1:A:213:GLU:O | 2.18 | 0.43 |
| 1:A:309:VAL:HB | 1:A:315:GLU:O | 2.18 | 0.43 |
| 1:A:174:ARG:NH2 | 1:A:405:GLU:HG2 | 2.33 | 0.43 |
| 1:A:499:ILE:CD1 | 2:A:732:HOH:O | 2.63 | 0.43 |
| 1:A:503:ARG:HA | 2:A:601:HOH:O | 2.17 | 0.43 |
| 1:A:61:ARG:NH1 | 1:A:101:GLY:CA | 2.74 | 0.43 |
| 1:B:118:VAL:HG21 | 1:B:159:ILE:HG12 | 1.99 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:264:ARG:HA | 1:B:269:SER:HA | 2.00 | 0.43 |
| 1:B:48:ALA:N | 2:B:679:HOH:O | 2.50 | 0.43 |
| 1:A:62:GLU:CB | 1:A:81:ARG:HH21 | 2.31 | 0.43 |
| 1:B:170:PHE:HD1 | 1:B:189:VAL:HG11 | 1.83 | 0.43 |
| 1:B:169:PHE:CZ | 1:B:175:VAL:CG2 | 2.99 | 0.43 |
| 1:B:251:LEU:CD2 | 2:B:652:HOH:O | 2.66 | 0.43 |
| 1:B:477:MET:HE2 | 1:B:489:ILE:HD11 | 2.00 | 0.43 |
| 1:B:86:GLY:CA | 1:B:555:GLY:HA3 | 2.48 | 0.43 |
| 1:A:165:ALA:HB2 | 2:A:653:HOH:O | 2.16 | 0.43 |
| 1:A:438:GLU:HG3 | 1:A:440:TYR:HE1 | 1.83 | 0.43 |
| 1:A:565:VAL:O | 1:A:569:LEU:HB2 | 2.18 | 0.43 |
| 1:A:79:LEU:HD11 | 1:A:95:VAL:HG21 | 1.99 | 0.43 |
| 1:B:209:THR:CA | 1:B:222:THR:HG22 | 2.48 | 0.43 |
| 1:B:210:ALA:O | 1:B:211:GLY:C | 2.55 | 0.43 |
| 1:B:198:SER:HB2 | 1:B:248:ILE:O | 2.18 | 0.43 |
| 1:B:270:ALA:HB1 | 1:B:277:ARG:CZ | 2.48 | 0.43 |
| 1:B:431:ARG:NH2 | 2:B:714:HOH:O | 2.47 | 0.43 |
| 1:B:472:VAL:CG2 | 1:B:532:LEU:HD22 | 2.48 | 0.43 |
| 1:B:487:ASN:HA | 1:B:490:GLU:OE1 | 2.17 | 0.43 |
| 1:B:580:GLU:O | 1:B:581:ARG:HB2 | 2.18 | 0.43 |
| 1:A:130:THR:O | 1:A:131:GLU:C | 2.56 | 0.43 |
| 1:A:164:ILE:HD13 | 1:A:181:ASN:CA | 2.47 | 0.43 |
| 1:A:248:ILE:N | 1:A:248:ILE:HD12 | 2.33 | 0.43 |
| 1:A:40:GLY:C | 1:A:42:SER:N | 2.72 | 0.43 |
| 1:A:469:ALA:HB1 | 1:A:556:HIS:CE1 | 2.54 | 0.43 |
| 1:A:469:ALA:HB1 | 1:A:556:HIS:ND1 | 2.32 | 0.43 |
| 1:B:224:ASP:HB3 | 1:B:227:ASP:OD1 | 2.18 | 0.43 |
| 1:B:487:ASN:O | 1:B:487:ASN:OD1 | 2.37 | 0.43 |
| 1:A:277:ARG:NH1 | 1:A:277:ARG:HG2 | 2.33 | 0.43 |
| 1:A:366:VAL:HG11 | 1:A:450:MET:HG3 | 2.00 | 0.43 |
| 1:A:578:GLN:O | 1:A:581:ARG:N | 2.52 | 0.43 |
| 1:B:207:LYS:HG2 | 1:B:222:THR:HB | 1.99 | 0.43 |
| 1:B:371:PHE:HA | 1:B:399:GLY:O | 2.19 | 0.43 |
| 1:B:414:ASP:OD2 | 1:B:418:GLY:N | 2.30 | 0.43 |
| 1:B:42:SER:HA | 1:B:561:MET:CE | 2.48 | 0.43 |
| 1:B:493:THR:HA | 2:B:629:HOH:O | 2.18 | 0.43 |
| 1:B:79:LEU:HD11 | 1:B:95:VAL:CG2 | 2.45 | 0.43 |
| 1:A:74:VAL:HG11 | 1:A:121:GLY:HA3 | 2.00 | 0.43 |
| 1:A:33:GLY:H | 1:A:73:GLY:HA2 | 1.83 | 0.43 |
| 1:A:421:GLU:O | 1:A:424:SER:HB2 | 2.19 | 0.43 |
| 1:A:509:VAL:O | 1:A:509:VAL:CG1 | 2.66 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:331:ALA:HB3 | 1:B:352:GLU:C | 2.38 | 0.43 |
| 1:B:472:VAL:HG21 | 1:B:532:LEU:HA | 2.01 | 0.43 |
| 1:B:473:ASP:OD1 | 1:B:475:GLU:N | 2.49 | 0.43 |
| 1:B:494:GLY:O | 1:B:496:SER:N | 2.51 | 0.43 |
| 1:B:472:VAL:O | 1:B:505:PRO:HD2 | 2.18 | 0.43 |
| 1:B:522:GLN:HB3 | 1:B:550:ILE:HG22 | 1.99 | 0.43 |
| 1:B:523:ASN:HD21 | 1:B:553:ASP:HA | 1.82 | 0.43 |
| 1:A:106:LEU:CD2 | 2:A:698:HOH:O | 2.66 | 0.43 |
| 1:A:178:PHE:HB2 | 1:A:187:LEU:HD11 | 2.01 | 0.43 |
| 1:B:240:PHE:O | 1:B:245:PRO:CD | 2.67 | 0.43 |
| 1:B:419:GLU:O | 1:B:423:VAL:HG23 | 2.19 | 0.43 |
| 1:A:197:PHE:HD2 | 1:A:210:ALA:HB1 | 1.84 | 0.43 |
| 1:A:214:THR:C | 1:A:216:ARG:N | 2.70 | 0.43 |
| 1:A:381:PHE:O | 1:A:385:LEU:HB2 | 2.18 | 0.43 |
| 1:A:460:GLY:O | 1:A:461:LEU:C | 2.57 | 0.43 |
| 1:A:77:VAL:HG23 | 1:A:97:THR:CG2 | 2.49 | 0.43 |
| 1:B:137:TYR:CD1 | 1:B:137:TYR:N | 2.86 | 0.43 |
| 1:B:209:THR:OG1 | 1:B:253:TYR:OH | 2.32 | 0.43 |
| 1:B:246:THR:CG2 | 1:B:265:ARG:HA | 2.49 | 0.43 |
| 1:B:299:HIS:CG | 1:B:300:THR:N | 2.86 | 0.43 |
| 1:B:300:THR:O | 1:B:301:SER:CB | 2.67 | 0.43 |
| 1:B:377:SER:N | 2:B:600:HOH:O | 2.51 | 0.43 |
| 1:B:520:HIS:CE1 | 1:B:529:LEU:HA | 2.54 | 0.43 |
| 1:B:30:VAL:HG23 | 1:B:289:VAL:HG12 | 1.99 | 0.43 |
| 1:A:167:LEU:CD2 | 1:A:197:PHE:HB2 | 2.49 | 0.43 |
| 1:A:71:HIS:HB2 | 1:A:120:THR:HA | 2.01 | 0.43 |
| 1:A:78:ILE:HG23 | 2:A:589:HOH:O | 2.19 | 0.43 |
| 1:B:205:GLY:O | 1:B:206:MET:CB | 2.67 | 0.43 |
| 1:B:334:ARG:NH2 | 1:B:429:TRP:CH2 | 2.87 | 0.43 |
| 1:B:489:ILE:HG13 | 2:B:642:HOH:O | 2.18 | 0.43 |
| 1:B:73:GLY:O | 1:B:74:VAL:C | 2.57 | 0.43 |
| 1:B:59:LEU:CD1 | 1:B:77:VAL:HG21 | 2.46 | 0.43 |
| 1:A:138:ALA:HB3 | 1:A:147:LEU:HD21 | 1.98 | 0.42 |
| 1:A:167:LEU:HD11 | 1:A:199:SER:HA | 2.01 | 0.42 |
| 1:A:188:ARG:HH11 | 1:A:188:ARG:HG3 | 1.84 | 0.42 |
| 1:A:350:VAL:HG22 | 2:A:652:HOH:O | 2.19 | 0.42 |
| 1:B:203:SER:O | 1:B:206:MET:N | 2.46 | 0.42 |
| 1:B:31:VAL:HG21 | 1:B:37:LEU:HD22 | 2.00 | 0.42 |
| 1:B:324:GLU:HA | 1:B:324:GLU:OE1 | 2.19 | 0.42 |
| 1:A:120:THR:O | 1:A:120:THR:HG22 | 2.19 | 0.42 |
| 1:A:32:ASP:CB | 1:A:35:LYS:HD2 | 2.49 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:218:ALA:HB1 | 1:B:248:ILE:HD12 | 1.97 | 0.42 |
| 1:B:26:SER:OG | 1:B:28:GLN:NE2 | 2.51 | 0.42 |
| 1:B:401:THR:HG22 | 1:B:408:ARG:HD2 | 2.01 | 0.42 |
| 1:B:526:ARG:HH21 | 1:B:557:ALA:HB2 | 1.81 | 0.42 |
| 1:B:50:LEU:CD1 | 1:B:59:LEU:HD21 | 2.48 | 0.42 |
| 1:A:203:SER:CB | 1:A:204:PRO:CD | 2.97 | 0.42 |
| 1:A:288:VAL:CG1 | 1:A:295:LEU:HD22 | 2.49 | 0.42 |
| 1:A:351:LEU:HD12 | 1:A:382:ALA:HB1 | 2.00 | 0.42 |
| 1:B:428:ARG:O | 1:B:431:ARG:N | 2.49 | 0.42 |
| 1:B:450:MET:HA | 1:B:453:CYS:HB3 | 2.01 | 0.42 |
| 1:B:84:SER:HB3 | 1:B:89:GLN:HB2 | 2.01 | 0.42 |
| 1:A:203:SER:HB2 | 1:A:204:PRO:CD | 2.49 | 0.42 |
| 1:A:312:PRO:O | 1:A:313:SER:C | 2.58 | 0.42 |
| 1:A:342:ASP:OD1 | 1:A:342:ASP:N | 2.50 | 0.42 |
| 1:A:440:TYR:HE2 | 1:A:578:GLN:CB | 2.32 | 0.42 |
| 1:B:330:ILE:HB | 2:B:720:HOH:O | 2.19 | 0.42 |
| 1:B:536:MET:HA | 2:B:678:HOH:O | 2.19 | 0.42 |
| 1:A:35:LYS:HG2 | 1:A:52:ASP:OD2 | 2.20 | 0.42 |
| 1:A:196:SER:OG | 1:A:405:GLU:OE2 | 2.36 | 0.42 |
| 1:A:96:ASN:HD22 | 1:A:99:ARG:HG3 | 1.84 | 0.42 |
| 1:B:123:ALA:CB | 1:B:182:LEU:HD11 | 2.50 | 0.42 |
| 1:B:359:PRO:O | 1:B:437:SER:HB3 | 2.19 | 0.42 |
| 1:B:574:PHE:CB | 2:B:723:HOH:O | 2.67 | 0.42 |
| 1:A:158:ASP:HB2 | 1:A:201:SER:HA | 2.02 | 0.42 |
| 1:A:170:PHE:HB2 | 2:A:662:HOH:O | 2.20 | 0.42 |
| 1:B:501:ARG:NH1 | 2:B:749:HOH:O | 2.52 | 0.42 |
| 1:B:70:PRO:HB2 | 1:B:74:VAL:CG2 | 2.41 | 0.42 |
| 1:A:152:GLY:O | 1:A:153:PHE:C | 2.57 | 0.42 |
| 1:A:29:GLY:HA2 | 1:A:289:VAL:HG11 | 2.02 | 0.42 |
| 1:A:393:VAL:CG1 | 1:A:426:ALA:HB1 | 2.49 | 0.42 |
| 1:A:359:PRO:HA | 1:A:435:LEU:HA | 2.02 | 0.42 |
| 1:A:48:ALA:HB2 | 1:A:67:VAL:HG21 | 2.01 | 0.42 |
| 1:A:532:LEU:CD1 | 1:A:536:MET:CE | 2.98 | 0.42 |
| 1:A:579:ARG:CG | 1:A:580:GLU:N | 2.82 | 0.42 |
| 1:A:98:SER:C | 1:A:100:PRO:HD3 | 2.39 | 0.42 |
| 1:B:476:GLU:OE1 | 1:B:531:PRO:HA | 2.20 | 0.42 |
| 1:A:371:PHE:CE1 | 1:A:408:ARG:NH1 | 2.88 | 0.42 |
| 1:B:392:VAL:HG12 | 1:B:394:MET:HG3 | 2.02 | 0.42 |
| 1:B:418:GLY:O | 1:B:421:GLU:HB2 | 2.19 | 0.42 |
| 1:A:315:GLU:OE1 | 1:A:315:GLU:HA | 2.18 | 0.42 |
| 1:A:44:GLY:HA2 | 1:A:561:MET:HB3 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:469:ALA:HB1 | 1:A:556:HIS:HD1 | 1.85 | 0.42 |
| 1:A:84:SER:CB | 1:A:87:ALA:HB3 | 2.50 | 0.42 |
| 1:B:209:THR:HA | 1:B:222:THR:HG22 | 2.02 | 0.42 |
| 1:B:305:PRO:HA | 1:B:306:PRO:HD3 | 1.92 | 0.42 |
| 1:B:428:ARG:O | 1:B:429:TRP:C | 2.58 | 0.42 |
| 1:B:443:GLY:HA2 | 2:B:601:HOH:O | 2.19 | 0.42 |
| 1:B:79:LEU:N | 1:B:93:PHE:O | 2.43 | 0.42 |
| 1:A:212:LEU:HG | 1:A:214:THR:HG23 | 2.01 | 0.42 |
| 1:A:367:HIS:N | 2:A:584:HOH:O | 2.53 | 0.42 |
| 1:B:133:ARG:NE | 1:B:149:ARG:HH21 | 2.18 | 0.42 |
| 1:B:322:LEU:O | 1:B:323:PRO:C | 2.59 | 0.42 |
| 1:B:76:ARG:HA | 1:B:96:ASN:HA | 2.01 | 0.42 |
| 1:A:92:LEU:HB3 | 1:A:106:LEU:HD12 | 2.02 | 0.41 |
| 1:B:168:GLY:HA3 | 2:B:706:HOH:O | 2.20 | 0.41 |
| 1:B:240:PHE:HD1 | 1:B:272:PHE:CD1 | 2.37 | 0.41 |
| 1:B:569:LEU:HD12 | 1:B:569:LEU:HA | 1.83 | 0.41 |
| 1:A:264:ARG:HA | 1:A:269:SER:HA | 2.02 | 0.41 |
| 1:B:176:SER:HA | 2:B:746:HOH:O | 2.19 | 0.41 |
| 1:B:300:THR:OG1 | 1:B:301:SER:N | 2.53 | 0.41 |
| 1:B:302:LEU:HD13 | 1:B:351:LEU:HD13 | 2.02 | 0.41 |
| 1:B:315:GLU:HA | 1:B:316:PRO:HD2 | 1.75 | 0.41 |
| 1:B:520:HIS:HA | 1:B:521:PRO:HD3 | 1.81 | 0.41 |
| 1:B:71:HIS:O | 1:B:72:TYR:C | 2.58 | 0.41 |
| 1:A:296:VAL:HA | 2:A:670:HOH:O | 2.20 | 0.41 |
| 1:A:532:LEU:CD1 | 1:A:536:MET:HE3 | 2.50 | 0.41 |
| 1:B:201:SER:HB3 | 2:B:652:HOH:O | 2.20 | 0.41 |
| 1:B:227:ASP:OD1 | 1:B:227:ASP:N | 2.42 | 0.41 |
| 1:B:264:ARG:HG2 | 1:B:264:ARG:HH11 | 1.85 | 0.41 |
| 1:B:419:GLU:OE2 | 1:B:420:LEU:N | 2.45 | 0.41 |
| 1:A:373:GLU:HB2 | 1:A:396:ASN:OD1 | 2.20 | 0.41 |
| 1:B:457:MET:O | 1:B:459:PRO:HD2 | 2.20 | 0.41 |
| 1:A:219:ARG:NH1 | 1:A:221:VAL:CG1 | 2.84 | 0.41 |
| 1:A:169:PHE:CE2 | 1:A:371:PHE:CD1 | 3.04 | 0.41 |
| 1:B:133:ARG:HE | 1:B:133:ARG:HB3 | 1.50 | 0.41 |
| 1:B:291:TRP:O | 1:B:292:ARG:HB2 | 2.19 | 0.41 |
| 1:B:309:VAL:HA | 1:B:316:PRO:HA | 2.02 | 0.41 |
| 1:B:397:TYR:CB | 1:B:422:ASP:HB2 | 2.49 | 0.41 |
| 1:B:86:GLY:O | 1:B:555:GLY:HA3 | 2.21 | 0.41 |
| 1:B:567:ILE:HD12 | 1:B:568:LEU:CA | 2.47 | 0.41 |
| 1:B:569:LEU:HB3 | 1:B:570:PRO:CD | 2.43 | 0.41 |
| 1:A:108:ALA:O | 1:A:144:LEU:HB2 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:198:SER:CB | 1:A:213:GLU:OE2 | 2.68 | 0.41 |
| 1:A:421:GLU:O | 1:A:425:ALA:N | 2.53 | 0.41 |
| 1:B:30:VAL:H | 1:B:289:VAL:CG1 | 2.33 | 0.41 |
| 1:B:31:VAL:HG22 | 1:B:74:VAL:CG2 | 2.51 | 0.41 |
| 1:B:325:ASP:O | 1:B:328:ARG:HB2 | 2.21 | 0.41 |
| 1:B:411:ILE:HG13 | 1:B:411:ILE:O | 2.21 | 0.41 |
| 1:B:456:THR:HG22 | 1:B:512:ILE:HD11 | 2.00 | 0.41 |
| 1:A:226:ARG:HD3 | 1:A:226:ARG:HA | 1.93 | 0.41 |
| 1:A:25:TYR:HA | 1:A:39:VAL:O | 2.20 | 0.41 |
| 1:A:569:LEU:H | 1:A:570:PRO:CD | 2.33 | 0.41 |
| 1:B:78:ILE:CD1 | 1:B:124:VAL:HG22 | 2.50 | 0.41 |
| 1:B:328:ARG:NH1 | 2:B:682:HOH:O | 2.54 | 0.41 |
| 1:B:444:TYR:OH | 1:B:521:PRO:HG2 | 2.21 | 0.41 |
| 1:A:26:SER:HA | 2:A:725:HOH:O | 2.21 | 0.41 |
| 1:A:393:VAL:HA | 2:A:652:HOH:O | 2.21 | 0.41 |
| 1:A:367:HIS:CE1 | 1:A:396:ASN:HA | 2.56 | 0.41 |
| 1:A:551:ILE:HD13 | 1:A:567:ILE:HG22 | 2.03 | 0.41 |
| 1:B:125:VAL:HG13 | 1:B:137:TYR:O | 2.20 | 0.41 |
| 1:B:263:ALA:O | 1:B:269:SER:HA | 2.21 | 0.41 |
| 1:B:514:GLU:HA | 1:B:515:PRO:HD3 | 1.90 | 0.41 |
| 1:B:476:GLU:CD | 1:B:531:PRO:HG3 | 2.41 | 0.41 |
| 1:A:190:PHE:CD1 | 1:A:190:PHE:N | 2.88 | 0.41 |
| 1:A:194:GLU:CB | 1:A:214:THR:HG22 | 2.51 | 0.41 |
| 1:A:224:ASP:O | 1:A:228:GLY:N | 2.53 | 0.41 |
| 1:A:358:THR:HA | 1:A:359:PRO:C | 2.39 | 0.41 |
| 1:A:562:GLU:O | 1:A:565:VAL:N | 2.52 | 0.41 |
| 1:B:29:GLY:HA2 | 1:B:289:VAL:HG11 | 2.03 | 0.41 |
| 1:B:31:VAL:CG1 | 1:B:32:ASP:H | 2.34 | 0.41 |
| 1:B:504:SER:C | 1:B:506:ILE:H | 2.24 | 0.41 |
| 1:B:522:GLN:NE2 | 2:B:663:HOH:O | 2.53 | 0.41 |
| 1:A:158:ASP:CB | 1:A:201:SER:HA | 2.50 | 0.41 |
| 1:A:322:LEU:HB2 | 2:A:697:HOH:O | 2.21 | 0.41 |
| 1:A:329:SER:HB2 | 1:A:387:ALA:HA | 2.02 | 0.41 |
| 1:A:398:ARG:HB2 | 1:A:410:LYS:HB2 | 2.03 | 0.41 |
| 1:A:451:THR:HG21 | 1:A:466:VAL:C | 2.42 | 0.41 |
| 1:B:145:ARG:NH1 | 2:B:624:HOH:O | 2.53 | 0.41 |
| 1:B:272:PHE:HA | 1:B:276:GLU:O | 2.21 | 0.41 |
| 1:B:491:GLN:NE2 | 2:B:747:HOH:O | 2.53 | 0.41 |
| 1:B:522:GLN:OE1 | 1:B:552:PRO:HA | 2.21 | 0.41 |
| 1:A:59:LEU:O | 1:A:101:GLY:HA2 | 2.20 | 0.41 |
| 1:A:119:ASP:OD1 | 1:A:120:THR:N | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:270:ALA:HB1 | 1:A:277:ARG:NE | 2.36 | 0.41 |
| 1:A:309:VAL:CG1 | 1:A:316:PRO:HA | 2.46 | 0.41 |
| 1:A:476:GLU:C | 1:A:478:TYR:N | 2.74 | 0.41 |
| 1:B:156:VAL:CG1 | 1:B:159:ILE:HD11 | 2.51 | 0.41 |
| 1:B:280:ALA:HB1 | 1:B:285:HIS:CE1 | 2.56 | 0.41 |
| 1:B:357:PRO:O | 1:B:360:GLY:CA | 2.69 | 0.41 |
| 1:B:511:ARG:NH1 | 2:B:605:HOH:O | 2.37 | 0.41 |
| 1:B:520:HIS:O | 1:B:550:ILE:HA | 2.21 | 0.41 |
| 1:B:534:ARG:HD3 | 1:B:534:ARG:HA | 1.80 | 0.41 |
| 1:B:538:GLU:O | 1:B:541:ALA:N | 2.54 | 0.41 |
| 1:B:77:VAL:O | 1:B:94:LYS:HA | 2.20 | 0.41 |
| 1:A:136:LEU:CD1 | 1:A:156:VAL:HG22 | 2.51 | 0.40 |
| 1:A:413:GLY:H | 1:A:492:LEU:C | 2.24 | 0.40 |
| 1:A:474:TRP:CZ3 | 1:A:477:MET:HE1 | 2.56 | 0.40 |
| 1:A:520:HIS:HA | 1:A:521:PRO:HD3 | 1.80 | 0.40 |
| 1:A:521:PRO:HG2 | 1:A:555:GLY:O | 2.21 | 0.40 |
| 1:B:364:VAL:CG1 | 1:B:395:PRO:HD3 | 2.51 | 0.40 |
| 1:B:453:CYS:CB | 2:B:731:HOH:O | 2.66 | 0.40 |
| 1:B:93:PHE:CD1 | 1:B:93:PHE:N | 2.89 | 0.40 |
| 1:A:163:LEU:HD23 | 1:A:202:ILE:HD13 | 2.03 | 0.40 |
| 1:A:249:THR:HB | 1:A:262:VAL:O | 2.21 | 0.40 |
| 1:A:284:ASN:ND2 | 1:A:376:ASP:C | 2.75 | 0.40 |
| 1:A:95:VAL:O | 1:A:95:VAL:HG12 | 2.22 | 0.40 |
| 1:B:199:SER:OG | 1:B:251:LEU:HB3 | 2.22 | 0.40 |
| 1:B:210:ALA:HA | 1:B:251:LEU:CD2 | 2.51 | 0.40 |
| 1:B:278:VAL:CG1 | 1:B:312:PRO:HB3 | 2.49 | 0.40 |
| 1:B:397:TYR:HB2 | 1:B:422:ASP:HB2 | 2.03 | 0.40 |
| 1:B:440:TYR:CZ | 1:B:463:LYS:HD3 | 2.56 | 0.40 |
| 1:B:567:ILE:HA | 2:B:594:HOH:O | 2.21 | 0.40 |
| 1:B:95:VAL:HB | 2:B:727:HOH:O | 2.20 | 0.40 |
| 1:A:117:GLY:HA3 | 1:A:126:PHE:CB | 2.51 | 0.40 |
| 1:A:147:LEU:HD22 | 2:A:695:HOH:O | 2.21 | 0.40 |
| 1:A:219:ARG:NH1 | 1:A:219:ARG:HG3 | 2.36 | 0.40 |
| 1:A:428:ARG:CG | 2:A:622:HOH:O | 2.58 | 0.40 |
| 1:A:497:ARG:HD3 | 1:A:501:ARG:HE | 1.85 | 0.40 |
| 1:B:371:PHE:CD2 | 1:B:408:ARG:NH1 | 2.79 | 0.40 |
| 1:B:379:ASP:HB3 | 1:B:382:ALA:HB3 | 2.03 | 0.40 |
| 1:B:398:ARG:HG2 | 1:B:419:GLU:HA | 2.02 | 0.40 |
| 1:B:429:TRP:O | 1:B:431:ARG:N | 2.54 | 0.40 |
| 1:A:188:ARG:CG | 1:A:188:ARG:HH11 | 2.35 | 0.40 |
| 1:A:23:GLU:HG3 | 1:A:23:GLU:H | 1.69 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:420:LEU:O | 1:A:424:SER:N | 2.54 | 0.40 |
| 1:B:432:GLU:HG3 | 2:B:759:HOH:O | 2.21 | 0.40 |
| 1:B:444:TYR:O | 1:B:447:GLY:N | 2.50 | 0.40 |
| 1:B:60:ASN:O | 1:B:61:ARG:HG2 | 2.21 | 0.40 |
| 1:A:98:SER:O | 1:A:100:PRO:HD3 | 2.21 | 0.40 |
| 1:A:305:PRO:CD | 1:A:322:LEU:HD12 | 2.50 | 0.40 |
| 1:A:444:TYR:N | 1:A:444:TYR:CD1 | 2.90 | 0.40 |
| 1:A:575:LEU:HD23 | 1:A:575:LEU:HA | 1.93 | 0.40 |
| 1:B:131:GLU:O | 1:B:131:GLU:OE2 | 2.40 | 0.40 |
| 1:B:133:ARG:CD | 2:B:608:HOH:O | 2.70 | 0.40 |
| 1:B:281:PRO:HB2 | 1:B:299:HIS:CE1 | 2.57 | 0.40 |
| 1:B:334:ARG:HD2 | 2:B:661:HOH:O | 2.22 | 0.40 |
| 1:B:266:GLU:HA | 1:B:403:TYR:CE2 | 2.57 | 0.40 |
| 1:B:385:LEU:HD11 | 1:B:442:MET:CE | 2.51 | 0.40 |
| 1:B:520:HIS:O | 1:B:550:ILE:HG23 | 2.21 | 0.40 |
| 1:B:521:PRO:HA | 1:B:554:ALA:HB3 | 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 X-ray entries followed by that with respect to entries of similar resolution.

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|-----------|-----------|----------|-------------|---|
| 1 | A | 558/562 (99%) | 445 (80%) | 90 (16%) | 23 (4%) | 3 | 7 |
| 1 | B | 559/562 (100%) | 432 (77%) | 96 (17%) | 31 (6%) | 2 | 3 |
| All | All | 1117/1124 (99%) | 877 (78%) | 186 (17%) | 54 (5%) | 2 | 5 |

All (54) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 43 | GLU |
| 1 | A | 72 | TYR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 563 | ASP |
| 1 | B | 206 | MET |
| 1 | B | 232 | ASP |
| 1 | B | 371 | PHE |
| 1 | B | 496 | SER |
| 1 | A | 106 | LEU |
| 1 | A | 321 | GLY |
| 1 | A | 354 | GLY |
| 1 | A | 371 | PHE |
| 1 | A | 498 | GLU |
| 1 | A | 543 | GLY |
| 1 | A | 568 | LEU |
| 1 | B | 45 | SER |
| 1 | B | 60 | ASN |
| 1 | B | 107 | GLU |
| 1 | B | 172 | GLY |
| 1 | B | 187 | LEU |
| 1 | B | 210 | ALA |
| 1 | B | 211 | GLY |
| 1 | B | 256 | ASP |
| 1 | B | 580 | GLU |
| 1 | A | 42 | SER |
| 1 | A | 216 | ARG |
| 1 | B | 323 | PRO |
| 1 | B | 498 | GLU |
| 1 | B | 505 | PRO |
| 1 | B | 522 | GLN |
| 1 | B | 544 | LYS |
| 1 | A | 116 | SER |
| 1 | B | 61 | ARG |
| 1 | B | 74 | VAL |
| 1 | B | 121 | GLY |
| 1 | B | 122 | GLU |
| 1 | B | 380 | THR |
| 1 | B | 430 | ALA |
| 1 | B | 560 | THR |
| 1 | B | 562 | GLU |
| 1 | A | 31 | VAL |
| 1 | A | 32 | ASP |
| 1 | A | 276 | GLU |
| 1 | A | 579 | ARG |
| 1 | B | 292 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 430 | ALA |
| 1 | B | 301 | SER |
| 1 | B | 417 | GLY |
| 1 | A | 54 | GLY |
| 1 | A | 64 | ILE |
| 1 | A | 142 | GLY |
| 1 | A | 460 | GLY |
| 1 | A | 515 | PRO |
| 1 | B | 306 | PRO |
| 1 | B | 472 | VAL |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 1 | A | 448/449 (100%) | 418 (93%) | 30 (7%) | 19 | 42 |
| 1 | B | 448/449 (100%) | 417 (93%) | 31 (7%) | 18 | 41 |
| All | All | 896/898 (100%) | 835 (93%) | 61 (7%) | 18 | 41 |

All (61) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 43 | GLU |
| 1 | A | 56 | THR |
| 1 | A | 71 | HIS |
| 1 | A | 81 | ARG |
| 1 | A | 139 | LEU |
| 1 | A | 177 | LEU |
| 1 | A | 178 | PHE |
| 1 | A | 181 | ASN |
| 1 | A | 183 | SER |
| 1 | A | 191 | ASP |
| 1 | A | 201 | SER |
| 1 | A | 216 | ARG |
| 1 | A | 233 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 250 | TRP |
| 1 | A | 285 | HIS |
| 1 | A | 301 | SER |
| 1 | A | 322 | LEU |
| 1 | A | 344 | SER |
| 1 | A | 345 | ARG |
| 1 | A | 419 | GLU |
| 1 | A | 435 | LEU |
| 1 | A | 441 | ILE |
| 1 | A | 444 | TYR |
| 1 | A | 453 | CYS |
| 1 | A | 461 | LEU |
| 1 | A | 522 | GLN |
| 1 | A | 552 | PRO |
| 1 | A | 559 | ASN |
| 1 | A | 563 | ASP |
| 1 | A | 579 | ARG |
| 1 | B | 41 | PHE |
| 1 | B | 56 | THR |
| 1 | B | 83 | VAL |
| 1 | B | 99 | ARG |
| 1 | B | 133 | ARG |
| 1 | B | 137 | TYR |
| 1 | B | 162 | ASP |
| 1 | B | 178 | PHE |
| 1 | B | 219 | ARG |
| 1 | B | 222 | THR |
| 1 | B | 236 | PRO |
| 1 | B | 256 | ASP |
| 1 | B | 304 | THR |
| 1 | B | 315 | GLU |
| 1 | B | 322 | LEU |
| 1 | B | 327 | ARG |
| 1 | B | 328 | ARG |
| 1 | B | 336 | VAL |
| 1 | B | 341 | PHE |
| 1 | B | 358 | THR |
| 1 | B | 384 | SER |
| 1 | B | 411 | ILE |
| 1 | B | 419 | GLU |
| 1 | B | 428 | ARG |
| 1 | B | 445 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 456 | THR |
| 1 | B | 482 | ASP |
| 1 | B | 497 | ARG |
| 1 | B | 522 | GLN |
| 1 | B | 560 | THR |
| 1 | B | 568 | LEU |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 28 | GLN |
| 1 | A | 90 | HIS |
| 1 | A | 96 | ASN |
| 1 | A | 104 | GLN |
| 1 | A | 284 | ASN |
| 1 | A | 285 | HIS |
| 1 | A | 523 | ASN |
| 1 | B | 28 | GLN |
| 1 | B | 65 | ASN |
| 1 | B | 90 | HIS |
| 1 | B | 96 | ASN |
| 1 | B | 104 | GLN |
| 1 | B | 284 | ASN |
| 1 | B | 299 | HIS |
| 1 | B | 367 | HIS |
| 1 | B | 396 | ASN |
| 1 | B | 507 | ASN |
| 1 | B | 520 | HIS |
| 1 | B | 522 | GLN |
| 1 | B | 523 | 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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1 | A | 560/562 (99%) | -0.10 | 4 (0%) 87 88 | 7, 26, 44, 73 | 0 |
| 1 | B | 561/562 (99%) | 0.13 | 8 (1%) 75 76 | 9, 32, 51, 71 | 0 |
| All | All | 1121/1124 (99%) | 0.01 | 12 (1%) 80 81 | 7, 28, 49, 73 | 0 |

All (12) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | A | 558 | ILE | 3.9 |
| 1 | B | 295 | LEU | 3.8 |
| 1 | A | 325 | ASP | 2.9 |
| 1 | B | 261 | VAL | 2.7 |
| 1 | B | 558 | ILE | 2.7 |
| 1 | B | 296 | VAL | 2.7 |
| 1 | B | 579 | ARG | 2.7 |
| 1 | A | 320 | GLY | 2.6 |
| 1 | A | 321 | GLY | 2.2 |
| 1 | B | 26 | SER | 2.1 |
| 1 | B | 235 | LEU | 2.1 |
| 1 | B | 262 | VAL | 2.0 |

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.