



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:23 PM GMT

PDB ID : 1AHU
Title : STRUCTURE OF THE OCTAMERIC FLAVOENZYME VANILLYL-ALCOHOL OXIDASE IN COMPLEX WITH P-CRESOL
Authors : Mattevi, A.
Deposited on : 1997-04-10
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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

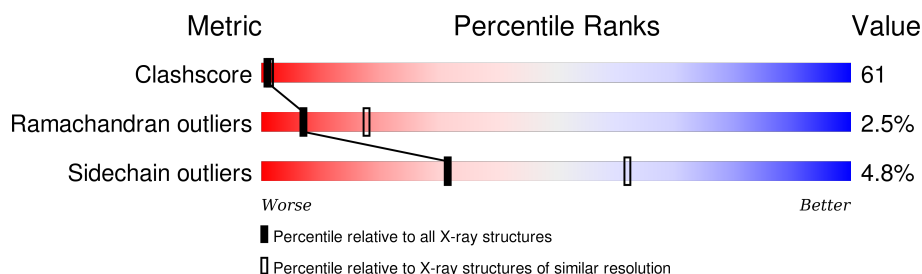
1 Overall quality at a glance

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)) |
|-----------------------|-----------------------------|---|
| Clashscore | 102246 | 2422 (2.70-2.70) |
| Ramachandran outliers | 100387 | 2382 (2.70-2.70) |
| Sidechain outliers | 100360 | 2382 (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.

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | A | 560 |  26% 56% 16% .. |
| 1 | B | 560 |  25% 57% 16% .. |

2 Entry composition [i](#)

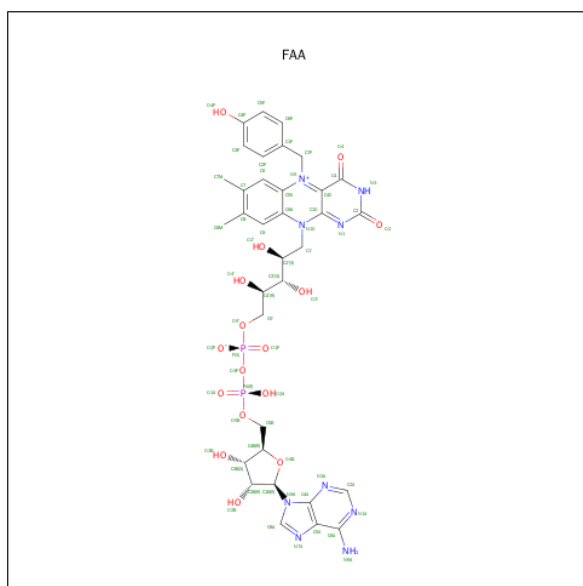
There are 3 unique types of molecules in this entry. The entry contains 9011 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 VANILLYL-ALCOHOL OXIDASE.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | A | 555 | Total | C | N | O | S | 37 | 0 | 0 |
| | | | 4391 | 2817 | 751 | 799 | 24 | | | |
| 1 | B | 555 | Total | C | N | O | S | 37 | 0 | 0 |
| | | | 4391 | 2817 | 751 | 799 | 24 | | | |

- Molecule 2 is N5-(4-HYDROXYBENZYL)FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAA) (formula: $C_{34}H_{39}N_9O_{16}P_2$).



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 2 | A | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 61 | 34 | 9 | 16 | 2 | | |
| 2 | B | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 61 | 34 | 9 | 16 | 2 | | |

- Molecule 3 is water.

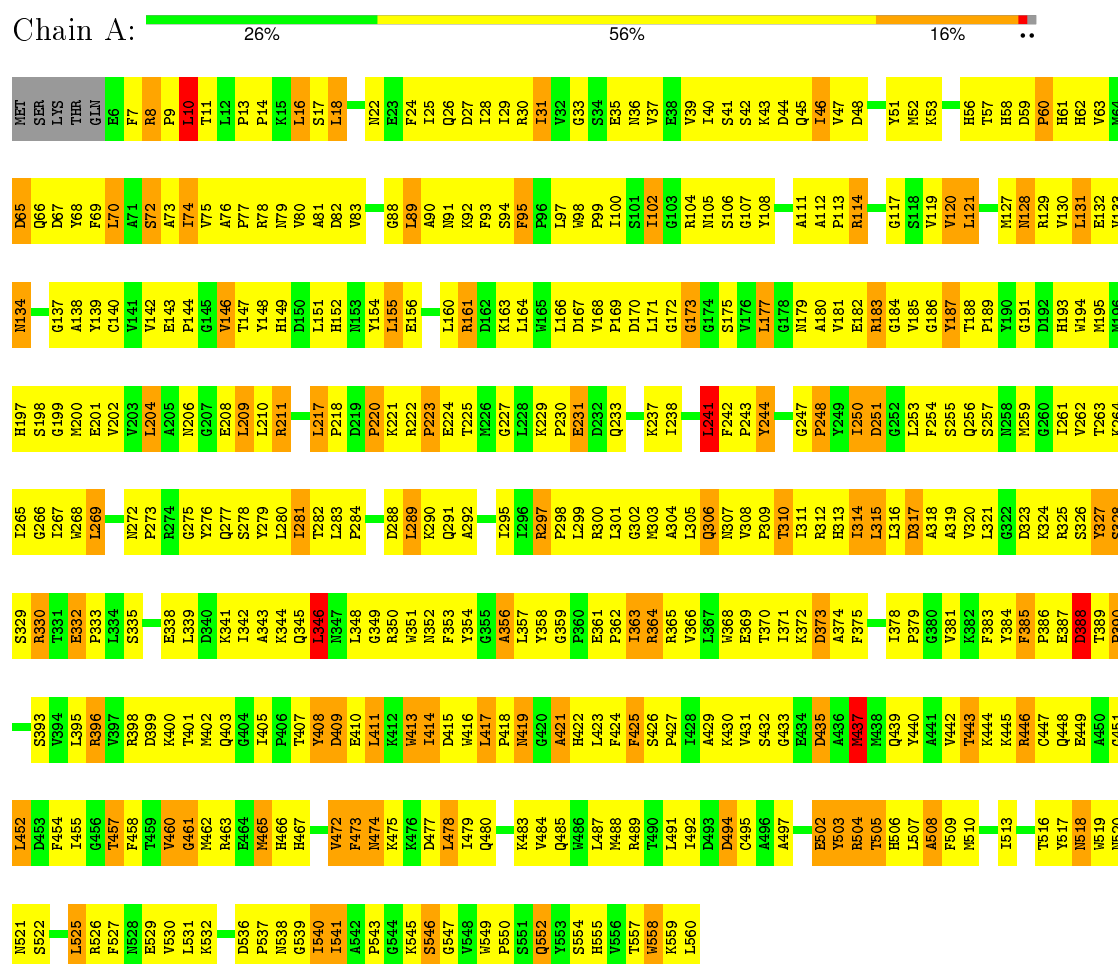
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 3 | A | 55 | Total 55 | O 55 | 0 | 0 |
| 3 | B | 52 | Total 52 | O 52 | 1 | 0 |

3 Residue-property plots

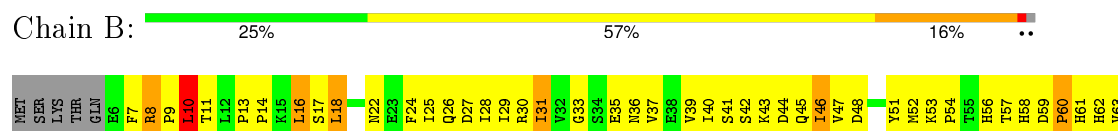
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

• Molecule 1: VANILLYL-ALCOHOL OXIDASE



• Molecule 1: VANILLYL-ALCOHOL OXIDASE



| | | | | | | | |
|------|------|------|------|------|------|------|------|
| T516 | E449 | D388 | S326 | T263 | H197 | M134 | M64 |
| T517 | A450 | T389 | Y327 | K264 | S198 | | D65 |
| M518 | G451 | P390 | S328 | I265 | G199 | G137 | Q66 |
| M519 | L452 | | S329 | G266 | M200 | | D67 |
| M520 | D453 | S393 | R330 | I267 | E201 | Y139 | A138 |
| M521 | F454 | V394 | T331 | W268 | E202 | C140 | F69 |
| S522 | L455 | L395 | E332 | L269 | V203 | W141 | L70 |
| | G456 | R396 | F333 | M270 | L204 | V142 | A71 |
| | T457 | V397 | L334 | P271 | L205 | E143 | S72 |
| L525 | F458 | R398 | S335 | M272 | G207 | P144 | A73 |
| R526 | T459 | D399 | | P273 | G145 | V146 | G174 |
| F527 | V460 | K400 | E338 | R274 | E208 | T147 | V75 |
| M528 | G461 | T401 | L339 | G275 | L209 | A148 | A76 |
| E529 | M462 | M402 | E340 | Y276 | L210 | Y149 | F77 |
| V530 | R463 | Q403 | K341 | Q277 | R211 | H151 | M78 |
| L531 | E464 | G404 | I342 | S278 | | D150 | N79 |
| K532 | M465 | I405 | A343 | Y279 | K214 | L151 | W80 |
| | H466 | P406 | K344 | L280 | | H152 | A81 |
| D536 | H467 | T407 | G345 | I281 | L217 | M153 | D82 |
| P537 | | Y408 | I346 | T282 | P218 | Y154 | V83 |
| M538 | V472 | D409 | K347 | L283 | D219 | E156 | |
| G539 | F473 | E410 | L348 | P284 | K220 | | L89 |
| I540 | M474 | L411 | G349 | | K221 | | A90 |
| I541 | K475 | K412 | R350 | D288 | R222 | L160 | N91 |
| A542 | V476 | M413 | R351 | L289 | R223 | R161 | Q92 |
| P543 | D477 | I414 | R352 | K290 | E224 | D162 | F93 |
| G544 | L478 | D415 | F353 | Q291 | T225 | K163 | S94 |
| K545 | L479 | W416 | Y354 | A292 | M226 | L164 | F95 |
| S546 | Q480 | L417 | G355 | | G227 | W165 | P96 |
| | | P418 | A356 | I295 | L228 | L166 | L97 |
| W549 | K483 | M419 | L357 | T296 | K229 | D167 | W98 |
| P550 | V484 | G420 | Y358 | R297 | P230 | V168 | P99 |
| S551 | Q485 | A421 | G359 | P298 | E231 | P169 | I100 |
| Q552 | D486 | R422 | P360 | L299 | D232 | D170 | S101 |
| Y553 | L487 | I423 | P361 | R300 | Q233 | L171 | I102 |
| M554 | M488 | F424 | P362 | L301 | | G172 | G103 |
| H555 | R489 | F425 | I363 | G302 | K237 | G173 | R104 |
| V556 | T490 | S426 | R364 | K303 | L238 | G174 | M105 |
| T557 | L491 | P427 | R365 | A304 | | S175 | S106 |
| W558 | L492 | I428 | Y366 | L305 | L241 | V176 | G107 |
| K559 | D493 | A429 | L367 | Q306 | F242 | L177 | Y108 |
| | C495 | V431 | K368 | N307 | P243 | G178 | |
| | L496 | S432 | T370 | V308 | Y244 | M179 | A111 |
| | A497 | G433 | I371 | P309 | | A180 | A112 |
| | | E434 | K372 | T310 | G247 | V181 | P113 |
| | | D435 | D373 | I311 | P248 | E182 | R114 |
| | | A436 | A374 | R312 | Y249 | R183 | |
| | | K437 | F375 | H313 | I250 | G184 | G117 |
| | | M438 | | I314 | D251 | V185 | S118 |
| G501 | | Q439 | I378 | L315 | G252 | G186 | V119 |
| B502 | | Y440 | P379 | L316 | L253 | Y187 | L121 |
| Y503 | | A441 | F379 | D317 | F254 | T188 | |
| R504 | | M442 | G380 | A318 | S255 | P189 | M127 |
| T505 | | V442 | V381 | A319 | Q256 | Y190 | N128 |
| H506 | | T443 | K382 | V320 | S257 | G191 | R129 |
| A508 | | K444 | F383 | L321 | W258 | D192 | M129 |
| P509 | | K445 | V384 | G322 | K259 | H193 | V130 |
| M510 | | R446 | F385 | K323 | G260 | W194 | L131 |
| B511 | | C447 | P386 | K324 | L261 | M195 | E132 |
| Q512 | | Q448 | | R325 | V262 | M196 | V133 |
| I513 | | | | | | | |

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

| Property | Value | Source |
|--|---|-----------|
| Space group | I 4 | Depositor |
| Cell constants a, b, c, α , β , γ | 128.82Å 128.82Å 130.79Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 30.00 – 2.70 | Depositor |
| % Data completeness (in resolution range) | 95.4 (30.00-2.70) | Depositor |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | 0.97 | Depositor |
| Refinement program | TNT V. 5-E | Depositor |
| R, R_{free} | 0.221 , 0.290 | Depositor |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| Total number of atoms | 9011 | wwPDB-VP |
| Average B, all atoms (Å ²) | 27.0 | wwPDB-VP |

5 Model quality

5.1 Standard geometry

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

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 | 0.73 | 0/4511 | 1.74 | 110/6131 (1.8%) |
| 1 | B | 0.73 | 0/4511 | 1.74 | 108/6131 (1.8%) |
| All | All | 0.73 | 0/9022 | 1.74 | 218/12262 (1.8%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | A | 2 | 0 |
| 1 | B | 2 | 0 |
| All | All | 4 | 0 |

There are no bond length outliers.

All (218) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1 | A | 330 | ARG | NE-CZ-NH1 | -11.34 | 114.63 | 120.30 |
| 1 | B | 330 | ARG | NE-CZ-NH1 | -11.24 | 114.68 | 120.30 |
| 1 | A | 536 | ASP | C-N-CD | -9.85 | 98.92 | 120.60 |
| 1 | B | 536 | ASP | C-N-CD | -9.85 | 98.93 | 120.60 |
| 1 | B | 417 | LEU | CA-CB-CG | -9.34 | 93.83 | 115.30 |
| 1 | A | 417 | LEU | CA-CB-CG | -9.31 | 93.88 | 115.30 |
| 1 | B | 457 | THR | CB-CA-C | -8.82 | 87.78 | 111.60 |
| 1 | A | 457 | THR | CB-CA-C | -8.82 | 87.80 | 111.60 |
| 1 | B | 452 | LEU | CA-CB-CG | -8.62 | 95.47 | 115.30 |
| 1 | A | 452 | LEU | CA-CB-CG | -8.60 | 95.53 | 115.30 |
| 1 | A | 187 | TYR | N-CA-C | 8.46 | 133.84 | 111.00 |
| 1 | B | 187 | TYR | N-CA-C | 8.44 | 133.79 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | B | 209 | LEU | CA-CB-CG | 8.06 | 133.84 | 115.30 |
| 1 | A | 209 | LEU | CA-CB-CG | 8.05 | 133.82 | 115.30 |
| 1 | B | 129 | ARG | N-CA-C | 8.03 | 132.68 | 111.00 |
| 1 | A | 129 | ARG | N-CA-C | 8.02 | 132.65 | 111.00 |
| 1 | A | 8 | ARG | CB-CA-C | -7.94 | 94.53 | 110.40 |
| 1 | B | 8 | ARG | CB-CA-C | -7.93 | 94.53 | 110.40 |
| 1 | B | 31 | ILE | CB-CA-C | -7.89 | 95.82 | 111.60 |
| 1 | A | 31 | ILE | CB-CA-C | -7.88 | 95.84 | 111.60 |
| 1 | A | 472 | VAL | CB-CA-C | -7.84 | 96.51 | 111.40 |
| 1 | B | 505 | THR | CB-CA-C | -7.83 | 90.45 | 111.60 |
| 1 | B | 472 | VAL | CB-CA-C | -7.83 | 96.52 | 111.40 |
| 1 | A | 505 | THR | CB-CA-C | -7.82 | 90.48 | 111.60 |
| 1 | B | 330 | ARG | NE-CZ-NH2 | 7.81 | 124.20 | 120.30 |
| 1 | B | 16 | LEU | CA-CB-CG | -7.80 | 97.36 | 115.30 |
| 1 | A | 16 | LEU | CA-CB-CG | -7.80 | 97.36 | 115.30 |
| 1 | A | 366 | VAL | CB-CA-C | -7.79 | 96.61 | 111.40 |
| 1 | A | 330 | ARG | NE-CZ-NH2 | 7.77 | 124.18 | 120.30 |
| 1 | B | 366 | VAL | CB-CA-C | -7.77 | 96.64 | 111.40 |
| 1 | B | 183 | ARG | NE-CZ-NH2 | -7.68 | 116.46 | 120.30 |
| 1 | A | 183 | ARG | NE-CZ-NH2 | -7.59 | 116.50 | 120.30 |
| 1 | A | 315 | LEU | CB-CG-CD2 | -7.55 | 98.16 | 111.00 |
| 1 | B | 315 | LEU | CB-CG-CD2 | -7.53 | 98.20 | 111.00 |
| 1 | A | 67 | ASP | N-CA-CB | -7.38 | 97.31 | 110.60 |
| 1 | B | 67 | ASP | N-CA-CB | -7.36 | 97.36 | 110.60 |
| 1 | A | 183 | ARG | NE-CZ-NH1 | 7.26 | 123.93 | 120.30 |
| 1 | A | 444 | LYS | N-CA-CB | -7.22 | 97.61 | 110.60 |
| 1 | B | 444 | LYS | N-CA-CB | -7.20 | 97.64 | 110.60 |
| 1 | B | 183 | ARG | NE-CZ-NH1 | 7.20 | 123.90 | 120.30 |
| 1 | B | 128 | ASN | CB-CA-C | -7.05 | 96.31 | 110.40 |
| 1 | A | 128 | ASN | CB-CA-C | -7.03 | 96.34 | 110.40 |
| 1 | B | 155 | LEU | CA-CB-CG | -6.84 | 99.57 | 115.30 |
| 1 | A | 155 | LEU | CA-CB-CG | -6.83 | 99.58 | 115.30 |
| 1 | B | 264 | LYS | CB-CA-C | -6.82 | 96.76 | 110.40 |
| 1 | A | 264 | LYS | CB-CA-C | -6.81 | 96.78 | 110.40 |
| 1 | A | 452 | LEU | N-CA-C | 6.80 | 129.37 | 111.00 |
| 1 | B | 452 | LEU | N-CA-C | 6.80 | 129.36 | 111.00 |
| 1 | A | 541 | ILE | CB-CA-C | -6.80 | 98.00 | 111.60 |
| 1 | B | 541 | ILE | CB-CA-C | -6.78 | 98.04 | 111.60 |
| 1 | A | 558 | TRP | N-CA-C | 6.76 | 129.25 | 111.00 |
| 1 | B | 204 | LEU | CB-CG-CD2 | -6.76 | 99.51 | 111.00 |
| 1 | B | 558 | TRP | N-CA-C | 6.74 | 129.21 | 111.00 |
| 1 | A | 417 | LEU | C-N-CD | -6.74 | 105.77 | 120.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | A | 204 | LEU | CB-CG-CD2 | -6.74 | 99.55 | 111.00 |
| 1 | B | 417 | LEU | C-N-CD | -6.73 | 105.80 | 120.60 |
| 1 | A | 129 | ARG | CB-CG-CD | -6.70 | 94.19 | 111.60 |
| 1 | B | 129 | ARG | CB-CG-CD | -6.69 | 94.20 | 111.60 |
| 1 | B | 10 | LEU | CA-CB-CG | 6.67 | 130.65 | 115.30 |
| 1 | A | 10 | LEU | CA-CB-CG | 6.66 | 130.61 | 115.30 |
| 1 | A | 560 | LEU | CB-CG-CD2 | -6.57 | 99.83 | 111.00 |
| 1 | B | 560 | LEU | CB-CG-CD2 | -6.57 | 99.83 | 111.00 |
| 1 | A | 130 | VAL | N-CA-C | -6.50 | 93.44 | 111.00 |
| 1 | B | 130 | VAL | N-CA-C | -6.50 | 93.44 | 111.00 |
| 1 | A | 419 | ASN | CB-CA-C | 6.48 | 123.36 | 110.40 |
| 1 | B | 411 | LEU | CA-CB-CG | 6.48 | 130.20 | 115.30 |
| 1 | B | 419 | ASN | CB-CA-C | 6.46 | 123.32 | 110.40 |
| 1 | B | 495 | CYS | CA-CB-SG | -6.46 | 102.38 | 114.00 |
| 1 | A | 89 | LEU | CB-CG-CD2 | -6.45 | 100.03 | 111.00 |
| 1 | B | 89 | LEU | CB-CG-CD2 | -6.45 | 100.03 | 111.00 |
| 1 | A | 411 | LEU | CA-CB-CG | 6.45 | 130.12 | 115.30 |
| 1 | B | 89 | LEU | CA-CB-CG | -6.44 | 100.48 | 115.30 |
| 1 | A | 495 | CYS | CA-CB-SG | -6.44 | 102.41 | 114.00 |
| 1 | A | 460 | VAL | CG1-CB-CG2 | 6.44 | 121.20 | 110.90 |
| 1 | A | 89 | LEU | CA-CB-CG | -6.43 | 100.50 | 115.30 |
| 1 | A | 177 | LEU | CB-CG-CD1 | 6.43 | 121.93 | 111.00 |
| 1 | B | 177 | LEU | CB-CG-CD1 | 6.42 | 121.92 | 111.00 |
| 1 | B | 460 | VAL | CG1-CB-CG2 | 6.42 | 121.17 | 110.90 |
| 1 | B | 430 | LYS | CB-CA-C | -6.40 | 97.60 | 110.40 |
| 1 | B | 473 | PHE | N-CA-C | -6.38 | 93.78 | 111.00 |
| 1 | A | 473 | PHE | N-CA-C | -6.37 | 93.79 | 111.00 |
| 1 | A | 430 | LYS | CB-CA-C | -6.36 | 97.69 | 110.40 |
| 1 | A | 424 | PHE | CB-CA-C | -6.31 | 97.79 | 110.40 |
| 1 | B | 424 | PHE | CB-CA-C | -6.28 | 97.84 | 110.40 |
| 1 | B | 385 | PHE | N-CA-C | -6.25 | 94.12 | 111.00 |
| 1 | A | 385 | PHE | N-CA-C | -6.25 | 94.14 | 111.00 |
| 1 | A | 477 | ASP | CB-CG-OD1 | 6.24 | 123.92 | 118.30 |
| 1 | B | 477 | ASP | CB-CG-OD1 | 6.22 | 123.90 | 118.30 |
| 1 | A | 217 | LEU | CA-CB-CG | -6.21 | 101.01 | 115.30 |
| 1 | B | 540 | ILE | CB-CA-C | -6.20 | 99.21 | 111.60 |
| 1 | B | 217 | LEU | CA-CB-CG | -6.19 | 101.06 | 115.30 |
| 1 | A | 540 | ILE | CB-CA-C | -6.18 | 99.24 | 111.60 |
| 1 | A | 411 | LEU | CB-CA-C | -6.17 | 98.48 | 110.20 |
| 1 | B | 411 | LEU | CB-CA-C | -6.13 | 98.55 | 110.20 |
| 1 | A | 317 | ASP | CB-CG-OD1 | -6.12 | 112.80 | 118.30 |
| 1 | B | 317 | ASP | CB-CG-OD1 | -6.10 | 112.81 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | B | 306 | GLN | N-CA-C | 6.06 | 127.36 | 111.00 |
| 1 | B | 18 | LEU | CA-CB-CG | -6.05 | 101.39 | 115.30 |
| 1 | A | 18 | LEU | CA-CB-CG | -6.04 | 101.40 | 115.30 |
| 1 | A | 306 | GLN | N-CA-C | 6.04 | 127.30 | 111.00 |
| 1 | A | 462 | MET | CB-CA-C | -6.03 | 98.33 | 110.40 |
| 1 | B | 462 | MET | CB-CA-C | -6.01 | 98.37 | 110.40 |
| 1 | B | 332 | GLU | N-CA-CB | 6.01 | 121.42 | 110.60 |
| 1 | A | 332 | GLU | N-CA-CB | 6.01 | 121.41 | 110.60 |
| 1 | B | 121 | LEU | CB-CG-CD1 | -6.00 | 100.80 | 111.00 |
| 1 | A | 121 | LEU | CB-CG-CD1 | -6.00 | 100.80 | 111.00 |
| 1 | B | 269 | LEU | CA-CB-CG | -6.00 | 101.50 | 115.30 |
| 1 | A | 269 | LEU | CA-CB-CG | -5.98 | 101.55 | 115.30 |
| 1 | B | 465 | MET | CB-CA-C | -5.96 | 98.48 | 110.40 |
| 1 | A | 241 | LEU | CA-CB-CG | 5.96 | 129.01 | 115.30 |
| 1 | A | 465 | MET | CB-CA-C | -5.96 | 98.48 | 110.40 |
| 1 | B | 114 | ARG | NE-CZ-NH2 | -5.95 | 117.32 | 120.30 |
| 1 | B | 241 | LEU | CA-CB-CG | 5.95 | 128.99 | 115.30 |
| 1 | A | 346 | LEU | CB-CG-CD1 | 5.91 | 121.05 | 111.00 |
| 1 | B | 346 | LEU | CB-CG-CD1 | 5.90 | 121.02 | 111.00 |
| 1 | B | 437 | MET | N-CA-CB | -5.88 | 100.02 | 110.60 |
| 1 | A | 114 | ARG | NE-CZ-NH2 | -5.87 | 117.36 | 120.30 |
| 1 | A | 437 | MET | N-CA-CB | -5.84 | 100.08 | 110.60 |
| 1 | A | 74 | ILE | CB-CA-C | -5.84 | 99.92 | 111.60 |
| 1 | A | 388 | ASP | CB-CG-OD1 | -5.82 | 113.06 | 118.30 |
| 1 | B | 74 | ILE | CB-CA-C | -5.82 | 99.96 | 111.60 |
| 1 | A | 446 | ARG | NE-CZ-NH2 | 5.80 | 123.20 | 120.30 |
| 1 | B | 504 | ARG | NE-CZ-NH1 | -5.80 | 117.40 | 120.30 |
| 1 | A | 504 | ARG | NE-CZ-NH1 | -5.78 | 117.41 | 120.30 |
| 1 | B | 259 | MET | CA-CB-CG | -5.77 | 103.49 | 113.30 |
| 1 | A | 259 | MET | CA-CB-CG | -5.76 | 103.50 | 113.30 |
| 1 | B | 388 | ASP | CB-CG-OD1 | -5.76 | 113.12 | 118.30 |
| 1 | A | 518 | ASN | N-CA-C | 5.75 | 126.54 | 111.00 |
| 1 | B | 518 | ASN | N-CA-C | 5.75 | 126.52 | 111.00 |
| 1 | A | 494 | ASP | CB-CA-C | -5.73 | 98.95 | 110.40 |
| 1 | B | 494 | ASP | CB-CA-C | -5.72 | 98.95 | 110.40 |
| 1 | B | 289 | LEU | CB-CG-CD2 | 5.72 | 120.72 | 111.00 |
| 1 | A | 289 | LEU | CB-CG-CD2 | 5.71 | 120.71 | 111.00 |
| 1 | A | 297 | ARG | N-CA-C | 5.71 | 126.41 | 111.00 |
| 1 | B | 297 | ARG | N-CA-C | 5.70 | 126.40 | 111.00 |
| 1 | B | 244 | TYR | N-CA-C | 5.69 | 126.36 | 111.00 |
| 1 | B | 446 | ARG | NE-CZ-NH2 | 5.69 | 123.14 | 120.30 |
| 1 | B | 120 | VAL | CB-CA-C | 5.69 | 122.21 | 111.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | A | 244 | TYR | N-CA-C | 5.68 | 126.35 | 111.00 |
| 1 | A | 120 | VAL | CB-CA-C | 5.64 | 122.12 | 111.40 |
| 1 | A | 267 | ILE | CB-CA-C | -5.57 | 100.45 | 111.60 |
| 1 | B | 227 | GLY | N-CA-C | 5.55 | 126.99 | 113.10 |
| 1 | B | 396 | ARG | CG-CD-NE | -5.55 | 100.14 | 111.80 |
| 1 | B | 267 | ILE | CB-CA-C | -5.54 | 100.51 | 111.60 |
| 1 | A | 227 | GLY | N-CA-C | 5.54 | 126.95 | 113.10 |
| 1 | B | 8 | ARG | N-CA-CB | -5.53 | 100.64 | 110.60 |
| 1 | B | 425 | PHE | CB-CA-C | 5.52 | 121.44 | 110.40 |
| 1 | A | 396 | ARG | CG-CD-NE | -5.52 | 100.22 | 111.80 |
| 1 | A | 425 | PHE | CB-CA-C | 5.51 | 121.42 | 110.40 |
| 1 | A | 388 | ASP | CB-CG-OD2 | 5.51 | 123.26 | 118.30 |
| 1 | A | 8 | ARG | N-CA-CB | -5.50 | 100.69 | 110.60 |
| 1 | B | 503 | TYR | CB-CG-CD1 | 5.48 | 124.29 | 121.00 |
| 1 | A | 502 | GLU | CA-CB-CG | -5.48 | 101.35 | 113.40 |
| 1 | B | 241 | LEU | CB-CG-CD1 | 5.47 | 120.30 | 111.00 |
| 1 | B | 502 | GLU | CA-CB-CG | -5.47 | 101.37 | 113.40 |
| 1 | B | 327 | TYR | CA-CB-CG | 5.46 | 123.77 | 113.40 |
| 1 | B | 388 | ASP | CB-CG-OD2 | 5.45 | 123.21 | 118.30 |
| 1 | B | 304 | ALA | N-CA-C | -5.45 | 96.28 | 111.00 |
| 1 | A | 241 | LEU | CB-CG-CD1 | 5.45 | 120.26 | 111.00 |
| 1 | A | 304 | ALA | N-CA-C | -5.44 | 96.31 | 111.00 |
| 1 | B | 146 | VAL | CB-CA-C | -5.44 | 101.07 | 111.40 |
| 1 | A | 503 | TYR | CB-CG-CD1 | 5.43 | 124.26 | 121.00 |
| 1 | B | 474 | ASN | N-CA-CB | -5.43 | 100.82 | 110.60 |
| 1 | A | 327 | TYR | CA-CB-CG | 5.42 | 123.70 | 113.40 |
| 1 | A | 421 | ALA | N-CA-C | -5.42 | 96.37 | 111.00 |
| 1 | B | 421 | ALA | N-CA-C | -5.41 | 96.40 | 111.00 |
| 1 | A | 146 | VAL | CB-CA-C | -5.41 | 101.13 | 111.40 |
| 1 | A | 474 | ASN | N-CA-CB | -5.41 | 100.87 | 110.60 |
| 1 | B | 131 | LEU | CA-CB-CG | -5.38 | 102.94 | 115.30 |
| 1 | A | 131 | LEU | CA-CB-CG | -5.37 | 102.95 | 115.30 |
| 1 | A | 415 | ASP | N-CA-C | 5.36 | 125.46 | 111.00 |
| 1 | B | 415 | ASP | N-CA-C | 5.35 | 125.45 | 111.00 |
| 1 | A | 173 | GLY | N-CA-C | 5.34 | 126.46 | 113.10 |
| 1 | B | 173 | GLY | N-CA-C | 5.34 | 126.44 | 113.10 |
| 1 | B | 461 | GLY | N-CA-C | -5.32 | 99.80 | 113.10 |
| 1 | A | 461 | GLY | N-CA-C | -5.31 | 99.83 | 113.10 |
| 1 | A | 396 | ARG | NE-CZ-NH2 | -5.30 | 117.65 | 120.30 |
| 1 | B | 301 | LEU | CA-CB-CG | 5.30 | 127.48 | 115.30 |
| 1 | B | 250 | ILE | CB-CA-C | -5.29 | 101.03 | 111.60 |
| 1 | A | 250 | ILE | CB-CA-C | -5.28 | 101.04 | 111.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | A | 364 | ARG | CG-CD-NE | -5.28 | 100.72 | 111.80 |
| 1 | B | 396 | ARG | NE-CZ-NH2 | -5.27 | 117.66 | 120.30 |
| 1 | A | 301 | LEU | CA-CB-CG | 5.27 | 127.42 | 115.30 |
| 1 | B | 364 | ARG | CG-CD-NE | -5.24 | 100.80 | 111.80 |
| 1 | B | 332 | GLU | CB-CA-C | 5.22 | 120.85 | 110.40 |
| 1 | A | 472 | VAL | N-CA-C | -5.21 | 96.92 | 111.00 |
| 1 | A | 332 | GLU | CB-CA-C | 5.21 | 120.82 | 110.40 |
| 1 | B | 472 | VAL | N-CA-C | -5.19 | 96.97 | 111.00 |
| 1 | A | 414 | ILE | CG1-CB-CG2 | 5.19 | 122.82 | 111.40 |
| 1 | B | 414 | ILE | CG1-CB-CG2 | 5.18 | 122.81 | 111.40 |
| 1 | A | 102 | ILE | N-CA-C | 5.18 | 124.98 | 111.00 |
| 1 | A | 72 | SER | N-CA-C | -5.17 | 97.05 | 111.00 |
| 1 | A | 211 | ARG | N-CA-C | -5.16 | 97.06 | 111.00 |
| 1 | B | 102 | ILE | N-CA-C | 5.16 | 124.94 | 111.00 |
| 1 | A | 317 | ASP | CB-CG-OD2 | 5.15 | 122.94 | 118.30 |
| 1 | B | 211 | ARG | N-CA-C | -5.15 | 97.10 | 111.00 |
| 1 | B | 72 | SER | N-CA-C | -5.14 | 97.12 | 111.00 |
| 1 | B | 525 | LEU | CA-CB-CG | -5.10 | 103.57 | 115.30 |
| 1 | A | 546 | SER | CB-CA-C | 5.09 | 119.77 | 110.10 |
| 1 | B | 281 | ILE | N-CA-C | -5.09 | 97.26 | 111.00 |
| 1 | B | 546 | SER | CB-CA-C | 5.09 | 119.76 | 110.10 |
| 1 | A | 396 | ARG | CA-CB-CG | -5.08 | 102.22 | 113.40 |
| 1 | A | 161 | ARG | CB-CA-C | -5.08 | 100.24 | 110.40 |
| 1 | B | 396 | ARG | CA-CB-CG | -5.08 | 102.22 | 113.40 |
| 1 | A | 281 | ILE | N-CA-C | -5.08 | 97.29 | 111.00 |
| 1 | B | 161 | ARG | CB-CA-C | -5.08 | 100.25 | 110.40 |
| 1 | B | 317 | ASP | CB-CG-OD2 | 5.07 | 122.86 | 118.30 |
| 1 | B | 310 | THR | N-CA-C | -5.07 | 97.32 | 111.00 |
| 1 | A | 525 | LEU | CA-CB-CG | -5.06 | 103.66 | 115.30 |
| 1 | A | 217 | LEU | CB-CG-CD2 | -5.06 | 102.40 | 111.00 |
| 1 | A | 310 | THR | N-CA-C | -5.06 | 97.34 | 111.00 |
| 1 | A | 314 | ILE | CG1-CB-CG2 | 5.05 | 122.52 | 111.40 |
| 1 | B | 314 | ILE | CG1-CB-CG2 | 5.05 | 122.51 | 111.40 |
| 1 | B | 217 | LEU | CB-CG-CD2 | -5.04 | 102.44 | 111.00 |
| 1 | B | 225 | THR | CA-CB-CG2 | -5.03 | 105.36 | 112.40 |
| 1 | A | 225 | THR | CA-CB-CG2 | -5.02 | 105.37 | 112.40 |
| 1 | A | 70 | LEU | N-CA-CB | -5.01 | 100.37 | 110.40 |
| 1 | A | 356 | ALA | N-CA-CB | 5.00 | 117.10 | 110.10 |

All (4) chirality outliers are listed below:

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
|-----|-------|-----|------|------|

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 1 | A | 187 | TYR | CA |
| 1 | A | 332 | GLU | CA |
| 1 | B | 187 | TYR | CA |
| 1 | B | 332 | GLU | CA |

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 4391 | 0 | 4330 | 531 | 0 |
| 1 | B | 4391 | 0 | 4330 | 548 | 0 |
| 2 | A | 61 | 0 | 35 | 13 | 0 |
| 2 | B | 61 | 0 | 35 | 13 | 0 |
| 3 | A | 55 | 0 | 0 | 9 | 0 |
| 3 | B | 52 | 0 | 0 | 9 | 0 |
| All | All | 9011 | 0 | 8730 | 1058 | 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 61.

All (1058) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:600:FAA:H8A | 2:A:600:FAA:H51A | 1.21 | 1.13 |
| 1:A:309:PRO:HG2 | 1:A:460:VAL:HB | 1.32 | 1.11 |
| 2:B:600:FAA:H51A | 2:B:600:FAA:H8A | 1.21 | 1.10 |
| 1:A:555:HIS:HB3 | 1:A:559:LYS:HE3 | 1.32 | 1.07 |
| 1:A:507:LEU:HA | 1:A:510:MET:HE3 | 1.37 | 1.06 |
| 1:B:309:PRO:HG2 | 1:B:460:VAL:HB | 1.32 | 1.05 |
| 1:B:555:HIS:HB3 | 1:B:559:LYS:HE3 | 1.32 | 1.05 |
| 1:B:507:LEU:HA | 1:B:510:MET:HE3 | 1.44 | 0.98 |
| 1:A:56:HIS:HA | 1:A:111:ALA:HB3 | 1.44 | 0.97 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:56:HIS:HA | 1:B:111:ALA:HB3 | 1.44 | 0.96 |
| 1:B:280:LEU:HD12 | 1:B:281:ILE:H | 1.31 | 0.95 |
| 1:A:280:LEU:HD12 | 1:A:281:ILE:H | 1.31 | 0.95 |
| 1:B:61:HIS:HB3 | 1:B:421:ALA:HB1 | 1.49 | 0.94 |
| 1:A:200:MET:HE2 | 1:A:251:ASP:HB3 | 1.51 | 0.93 |
| 1:A:61:HIS:HB3 | 1:A:421:ALA:HB1 | 1.49 | 0.92 |
| 1:A:253:LEU:HD11 | 1:B:253:LEU:HD21 | 1.51 | 0.91 |
| 1:A:414:ILE:HD11 | 2:A:600:FAA:HM71 | 1.54 | 0.90 |
| 1:B:200:MET:HE2 | 1:B:251:ASP:HB3 | 1.51 | 0.90 |
| 1:A:61:HIS:HE1 | 3:A:641:HOH:O | 1.54 | 0.90 |
| 1:B:419:ASN:O | 1:B:474:ASN:HA | 1.72 | 0.89 |
| 1:B:555:HIS:CB | 1:B:559:LYS:HE3 | 2.02 | 0.88 |
| 1:A:555:HIS:CB | 1:A:559:LYS:HE3 | 2.02 | 0.88 |
| 1:B:554:SER:HB3 | 1:B:557:THR:HB | 1.56 | 0.88 |
| 1:A:480:GLN:HA | 1:A:483:LYS:CD | 2.04 | 0.88 |
| 1:A:309:PRO:HG2 | 1:A:460:VAL:CB | 2.04 | 0.88 |
| 1:B:425:PHE:CE2 | 1:B:427:PRO:HG3 | 2.09 | 0.88 |
| 1:B:414:ILE:HD11 | 2:B:600:FAA:HM71 | 1.54 | 0.88 |
| 1:B:133:VAL:HG21 | 1:B:154:TYR:CE1 | 2.09 | 0.87 |
| 1:A:419:ASN:O | 1:A:474:ASN:HA | 1.72 | 0.87 |
| 1:B:480:GLN:HA | 1:B:483:LYS:CD | 2.04 | 0.87 |
| 1:B:507:LEU:HA | 1:B:510:MET:CE | 2.05 | 0.87 |
| 1:A:133:VAL:HG21 | 1:A:154:TYR:CE1 | 2.09 | 0.87 |
| 1:A:507:LEU:HA | 1:A:510:MET:CE | 2.05 | 0.87 |
| 1:A:425:PHE:CE2 | 1:A:427:PRO:HG3 | 2.09 | 0.87 |
| 1:B:309:PRO:HG2 | 1:B:460:VAL:CB | 2.04 | 0.86 |
| 1:B:289:LEU:HD23 | 1:B:437:MET:HE3 | 1.59 | 0.85 |
| 1:B:480:GLN:HA | 1:B:483:LYS:HD2 | 1.58 | 0.85 |
| 1:A:554:SER:HB3 | 1:A:557:THR:HB | 1.56 | 0.85 |
| 1:B:463:ARG:HD2 | 3:B:630:HOH:O | 1.76 | 0.84 |
| 1:A:56:HIS:HA | 1:A:111:ALA:CB | 2.09 | 0.83 |
| 1:A:289:LEU:HD23 | 1:A:437:MET:HE3 | 1.61 | 0.82 |
| 1:A:80:VAL:HG11 | 1:A:209:LEU:HD21 | 1.61 | 0.82 |
| 1:A:61:HIS:NE2 | 1:A:422:HIS:ND1 | 2.28 | 0.82 |
| 1:A:369:GLU:O | 1:A:373:ASP:HB3 | 1.79 | 0.82 |
| 1:A:425:PHE:CZ | 1:A:427:PRO:HG3 | 2.14 | 0.82 |
| 1:A:480:GLN:HA | 1:A:483:LYS:HD2 | 1.59 | 0.82 |
| 1:A:378:ILE:HB | 1:A:381:VAL:HG21 | 1.62 | 0.82 |
| 1:A:247:GLY:O | 1:B:183:ARG:NH2 | 2.11 | 0.82 |
| 2:B:600:FAA:H8A | 2:B:600:FAA:C5B | 2.07 | 0.82 |
| 1:B:56:HIS:HA | 1:B:111:ALA:CB | 2.09 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:369:GLU:O | 1:B:373:ASP:HB3 | 1.79 | 0.82 |
| 1:B:425:PHE:CZ | 1:B:427:PRO:HG3 | 2.14 | 0.81 |
| 1:B:61:HIS:NE2 | 1:B:422:HIS:ND1 | 2.28 | 0.81 |
| 1:A:132:GLU:HG2 | 1:A:133:VAL:N | 1.95 | 0.81 |
| 1:B:80:VAL:HG11 | 1:B:209:LEU:HD21 | 1.61 | 0.81 |
| 1:A:309:PRO:CG | 1:A:460:VAL:HB | 2.10 | 0.81 |
| 1:B:378:ILE:HB | 1:B:381:VAL:HG21 | 1.62 | 0.81 |
| 2:A:600:FAA:H8A | 2:A:600:FAA:C5B | 2.07 | 0.80 |
| 2:B:600:FAA:C8A | 2:B:600:FAA:H51A | 2.09 | 0.80 |
| 1:A:187:TYR:O | 1:A:307:ASN:HB2 | 1.82 | 0.80 |
| 1:B:156:GLU:HB2 | 1:B:161:ARG:HH21 | 1.46 | 0.80 |
| 1:B:316:LEU:O | 1:B:320:VAL:HG23 | 1.81 | 0.80 |
| 1:B:187:TYR:O | 1:B:307:ASN:HB2 | 1.82 | 0.80 |
| 1:A:316:LEU:O | 1:A:320:VAL:HG23 | 1.81 | 0.80 |
| 1:A:479:ILE:O | 1:A:483:LYS:HG3 | 1.81 | 0.79 |
| 1:A:156:GLU:HB2 | 1:A:161:ARG:HH21 | 1.46 | 0.79 |
| 1:B:479:ILE:O | 1:B:483:LYS:HG3 | 1.81 | 0.79 |
| 1:A:445:LYS:O | 1:A:449:GLU:HG3 | 1.82 | 0.79 |
| 1:B:132:GLU:HG2 | 1:B:133:VAL:N | 1.95 | 0.79 |
| 1:B:445:LYS:O | 1:B:449:GLU:HG3 | 1.82 | 0.79 |
| 1:A:40:ILE:HD11 | 1:A:57:THR:HG22 | 1.64 | 0.79 |
| 1:B:40:ILE:HD11 | 1:B:57:THR:HG22 | 1.64 | 0.79 |
| 1:B:309:PRO:CG | 1:B:460:VAL:HB | 2.10 | 0.78 |
| 1:B:480:GLN:O | 1:B:484:VAL:HG23 | 1.84 | 0.78 |
| 1:A:341:LYS:O | 1:A:345:GLN:HG3 | 1.83 | 0.78 |
| 1:A:177:LEU:HD12 | 1:A:265:ILE:HG22 | 1.66 | 0.78 |
| 1:B:45:GLN:HA | 3:B:642:HOH:O | 1.83 | 0.78 |
| 1:B:289:LEU:HB2 | 1:B:351:TRP:NE1 | 1.98 | 0.78 |
| 1:A:480:GLN:O | 1:A:484:VAL:HG23 | 1.84 | 0.78 |
| 1:B:91:ASN:ND2 | 1:B:538:ASN:HD22 | 1.82 | 0.78 |
| 1:A:289:LEU:HB2 | 1:A:351:TRP:NE1 | 1.98 | 0.78 |
| 1:B:550:PRO:HB2 | 1:B:552:GLN:HG2 | 1.66 | 0.78 |
| 1:B:177:LEU:HD12 | 1:B:265:ILE:HG22 | 1.65 | 0.77 |
| 1:B:341:LYS:O | 1:B:345:GLN:HG3 | 1.83 | 0.77 |
| 1:B:79:ASN:ND2 | 1:B:81:ALA:HB3 | 2.00 | 0.77 |
| 1:A:91:ASN:ND2 | 1:A:538:ASN:HD22 | 1.82 | 0.77 |
| 1:A:253:LEU:HD21 | 1:B:253:LEU:HD11 | 1.67 | 0.77 |
| 1:B:300:ARG:HA | 1:B:305:LEU:HB2 | 1.67 | 0.77 |
| 1:A:300:ARG:HA | 1:A:305:LEU:HB2 | 1.67 | 0.76 |
| 1:A:77:PRO:HB2 | 1:A:127:MET:CE | 2.15 | 0.76 |
| 2:A:600:FAA:H51A | 2:A:600:FAA:C8A | 2.09 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:98:TRP:HB3 | 1:B:120:VAL:HG22 | 1.67 | 0.76 |
| 1:B:51:TYR:CE1 | 1:B:171:LEU:HD13 | 2.21 | 0.76 |
| 1:A:51:TYR:CE1 | 1:A:171:LEU:HD13 | 2.21 | 0.76 |
| 1:B:77:PRO:HB2 | 1:B:127:MET:CE | 2.15 | 0.76 |
| 1:A:61:HIS:HA | 1:A:475:LYS:HE2 | 1.68 | 0.75 |
| 1:A:555:HIS:CG | 1:A:559:LYS:HE3 | 2.22 | 0.75 |
| 1:A:550:PRO:HB2 | 1:A:552:GLN:HG2 | 1.66 | 0.75 |
| 1:B:414:ILE:HG23 | 3:B:636:HOH:O | 1.85 | 0.75 |
| 1:B:61:HIS:HA | 1:B:475:LYS:HE2 | 1.68 | 0.75 |
| 1:A:79:ASN:ND2 | 1:A:81:ALA:HB3 | 2.00 | 0.75 |
| 1:B:485:GLN:O | 1:B:489:ARG:HG3 | 1.86 | 0.75 |
| 1:A:43:LYS:O | 1:A:45:GLN:HG2 | 1.87 | 0.75 |
| 1:B:555:HIS:CG | 1:B:559:LYS:HE3 | 2.21 | 0.75 |
| 1:B:341:LYS:O | 1:B:344:LYS:HG2 | 1.87 | 0.75 |
| 1:A:229:LYS:O | 1:A:233:GLN:HG3 | 1.86 | 0.75 |
| 1:B:229:LYS:O | 1:B:233:GLN:HG3 | 1.86 | 0.75 |
| 1:B:47:VAL:HG11 | 3:B:640:HOH:O | 1.86 | 0.75 |
| 1:A:289:LEU:HB2 | 1:A:351:TRP:CD1 | 2.22 | 0.74 |
| 1:B:280:LEU:HD12 | 1:B:281:ILE:N | 2.02 | 0.74 |
| 1:B:555:HIS:HB3 | 1:B:559:LYS:CE | 2.15 | 0.74 |
| 1:B:10:LEU:HD21 | 1:B:42:SER:CA | 2.18 | 0.74 |
| 1:A:98:TRP:HB3 | 1:A:120:VAL:HG22 | 1.67 | 0.74 |
| 1:B:43:LYS:O | 1:B:45:GLN:HG2 | 1.86 | 0.74 |
| 1:B:289:LEU:HB2 | 1:B:351:TRP:CD1 | 2.22 | 0.74 |
| 1:A:485:GLN:O | 1:A:489:ARG:HG3 | 1.86 | 0.74 |
| 1:A:280:LEU:HD12 | 1:A:281:ILE:N | 2.02 | 0.73 |
| 1:B:505:THR:OG1 | 1:B:513:ILE:HD12 | 1.88 | 0.73 |
| 1:A:10:LEU:HD21 | 1:A:42:SER:CA | 2.18 | 0.73 |
| 1:B:399:ASP:O | 1:B:403:GLN:HG2 | 1.88 | 0.73 |
| 1:B:505:THR:HG21 | 1:B:509:PHE:HB2 | 1.69 | 0.73 |
| 1:A:399:ASP:O | 1:A:403:GLN:HG2 | 1.88 | 0.73 |
| 1:A:341:LYS:O | 1:A:344:LYS:HG2 | 1.87 | 0.73 |
| 1:B:202:VAL:HG23 | 1:B:261:ILE:O | 1.88 | 0.73 |
| 1:A:95:PHE:CE1 | 1:A:119:VAL:HG23 | 2.24 | 0.73 |
| 1:A:505:THR:HG21 | 1:A:509:PHE:HB2 | 1.69 | 0.73 |
| 1:A:202:VAL:HG23 | 1:A:261:ILE:C | 2.09 | 0.73 |
| 1:B:537:PRO:HD2 | 1:B:538:ASN:H | 1.54 | 0.72 |
| 1:B:95:PHE:CE1 | 1:B:119:VAL:HG23 | 2.24 | 0.72 |
| 1:A:217:LEU:HB2 | 1:B:517:TYR:CE1 | 2.24 | 0.72 |
| 1:A:505:THR:OG1 | 1:A:513:ILE:HD12 | 1.88 | 0.72 |
| 1:A:170:ASP:OD2 | 2:A:600:FAA:H7P1 | 1.89 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:460:VAL:HG13 | 1:B:465:MET:HG2 | 1.72 | 0.72 |
| 1:B:202:VAL:HG23 | 1:B:261:ILE:C | 2.09 | 0.72 |
| 1:A:445:LYS:O | 1:A:448:GLN:HB3 | 1.89 | 0.72 |
| 1:A:361:GLU:HG2 | 1:A:361:GLU:O | 1.90 | 0.72 |
| 1:A:284:PRO:HD2 | 1:A:288:ASP:OD2 | 1.89 | 0.72 |
| 1:A:202:VAL:HG23 | 1:A:261:ILE:O | 1.88 | 0.72 |
| 1:B:363:ILE:HD12 | 1:B:363:ILE:N | 2.05 | 0.72 |
| 1:B:170:ASP:OD2 | 2:B:600:FAA:H7P1 | 1.88 | 0.72 |
| 1:B:284:PRO:HD2 | 1:B:288:ASP:OD2 | 1.89 | 0.72 |
| 1:B:332:GLU:HB3 | 1:B:333:PRO:CD | 2.19 | 0.72 |
| 1:B:292:ALA:O | 1:B:295:ILE:HB | 1.90 | 0.71 |
| 1:A:332:GLU:HB3 | 1:A:333:PRO:CD | 2.19 | 0.71 |
| 1:A:537:PRO:HD2 | 1:A:538:ASN:H | 1.54 | 0.71 |
| 1:A:460:VAL:HG13 | 1:A:465:MET:HG2 | 1.72 | 0.71 |
| 1:B:433:GLY:O | 1:B:437:MET:HB2 | 1.91 | 0.71 |
| 1:A:537:PRO:HD2 | 3:A:612:HOH:O | 1.89 | 0.71 |
| 1:A:79:ASN:HD21 | 1:A:81:ALA:HB3 | 1.55 | 0.71 |
| 1:B:445:LYS:O | 1:B:448:GLN:HB3 | 1.89 | 0.71 |
| 1:B:550:PRO:CB | 1:B:552:GLN:HE21 | 2.03 | 0.71 |
| 1:A:313:HIS:HB2 | 1:A:351:TRP:CZ3 | 2.26 | 0.71 |
| 1:B:61:HIS:NE2 | 1:B:422:HIS:CE1 | 2.59 | 0.71 |
| 1:A:433:GLY:O | 1:A:437:MET:HB2 | 1.91 | 0.71 |
| 1:A:363:ILE:HD12 | 1:A:363:ILE:N | 2.05 | 0.71 |
| 1:A:519:TRP:CZ3 | 1:B:211:ARG:HG3 | 2.26 | 0.70 |
| 1:B:79:ASN:HD21 | 1:B:81:ALA:HB3 | 1.55 | 0.70 |
| 1:A:68:TYR:HA | 3:A:645:HOH:O | 1.91 | 0.70 |
| 1:B:351:TRP:HA | 1:B:351:TRP:CE3 | 2.26 | 0.70 |
| 1:B:361:GLU:HG2 | 1:B:361:GLU:O | 1.90 | 0.70 |
| 1:B:200:MET:CE | 1:B:251:ASP:HB3 | 2.22 | 0.70 |
| 1:A:555:HIS:HB3 | 1:A:559:LYS:CE | 2.15 | 0.70 |
| 1:A:292:ALA:O | 1:A:295:ILE:HB | 1.90 | 0.70 |
| 1:A:60:PRO:O | 1:A:62:HIS:ND1 | 2.24 | 0.70 |
| 1:A:550:PRO:CB | 1:A:552:GLN:HE21 | 2.04 | 0.70 |
| 1:A:61:HIS:NE2 | 1:A:422:HIS:CE1 | 2.59 | 0.69 |
| 1:A:134:ASN:OD1 | 1:A:137:GLY:N | 2.23 | 0.69 |
| 1:A:351:TRP:CE3 | 1:A:351:TRP:HA | 2.26 | 0.69 |
| 1:A:91:ASN:HD22 | 1:A:538:ASN:HD22 | 1.40 | 0.69 |
| 1:A:247:GLY:C | 1:B:183:ARG:HH22 | 1.95 | 0.69 |
| 1:B:313:HIS:HB2 | 1:B:351:TRP:CZ3 | 2.26 | 0.69 |
| 1:B:324:LYS:HB2 | 1:B:416:TRP:CE2 | 2.28 | 0.69 |
| 1:B:505:THR:HG22 | 1:B:506:HIS:N | 2.08 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:378:ILE:HB | 1:B:381:VAL:CG2 | 2.23 | 0.68 |
| 1:B:312:ARG:NH1 | 1:B:317:ASP:OD1 | 2.27 | 0.68 |
| 1:B:156:GLU:OE1 | 1:B:161:ARG:NH2 | 2.27 | 0.68 |
| 1:A:505:THR:HG22 | 1:A:506:HIS:N | 2.08 | 0.68 |
| 1:A:312:ARG:NH1 | 1:A:317:ASP:OD1 | 2.27 | 0.68 |
| 1:A:324:LYS:HB2 | 1:A:416:TRP:CE2 | 2.28 | 0.68 |
| 1:A:416:TRP:C | 1:A:417:LEU:HD23 | 2.13 | 0.68 |
| 1:A:156:GLU:OE1 | 1:A:161:ARG:NH2 | 2.27 | 0.68 |
| 1:B:10:LEU:HD21 | 1:B:42:SER:HA | 1.75 | 0.68 |
| 1:B:363:ILE:H | 1:B:363:ILE:HD12 | 1.58 | 0.68 |
| 1:B:217:LEU:HD12 | 1:B:218:PRO:CD | 2.23 | 0.68 |
| 1:B:177:LEU:HG | 1:B:265:ILE:CG2 | 2.24 | 0.67 |
| 1:B:416:TRP:C | 1:B:417:LEU:HD23 | 2.13 | 0.67 |
| 1:A:177:LEU:HG | 1:A:265:ILE:CG2 | 2.24 | 0.67 |
| 1:A:339:LEU:O | 1:A:343:ALA:N | 2.24 | 0.67 |
| 1:A:10:LEU:HD21 | 1:A:42:SER:HA | 1.75 | 0.67 |
| 1:A:378:ILE:HB | 1:A:381:VAL:CG2 | 2.24 | 0.67 |
| 1:B:91:ASN:HD22 | 1:B:538:ASN:HD22 | 1.40 | 0.67 |
| 1:A:217:LEU:HD12 | 1:A:218:PRO:CD | 2.24 | 0.67 |
| 1:A:237:LYS:HD2 | 1:B:500:TRP:NE1 | 2.10 | 0.67 |
| 1:A:200:MET:CE | 1:A:251:ASP:HB3 | 2.22 | 0.67 |
| 1:A:77:PRO:HB2 | 1:A:127:MET:HE3 | 1.75 | 0.67 |
| 1:B:417:LEU:HB3 | 1:B:418:PRO:HD2 | 1.77 | 0.67 |
| 1:B:48:ASP:OD1 | 1:B:66:GLN:NE2 | 2.28 | 0.67 |
| 1:B:77:PRO:HB2 | 1:B:127:MET:HE3 | 1.75 | 0.67 |
| 1:A:211:ARG:HG3 | 1:B:519:TRP:CZ3 | 2.30 | 0.67 |
| 1:A:97:LEU:CD2 | 1:A:119:VAL:HB | 2.25 | 0.67 |
| 1:B:97:LEU:CD2 | 1:B:119:VAL:HB | 2.25 | 0.66 |
| 1:A:363:ILE:H | 1:A:363:ILE:HD12 | 1.58 | 0.66 |
| 1:B:505:THR:HG22 | 1:B:506:HIS:H | 1.61 | 0.66 |
| 1:A:505:THR:HG22 | 1:A:506:HIS:H | 1.60 | 0.66 |
| 1:A:417:LEU:HB3 | 1:A:418:PRO:HD2 | 1.77 | 0.66 |
| 1:A:48:ASP:OD1 | 1:A:66:GLN:NE2 | 2.28 | 0.66 |
| 1:A:283:LEU:HB2 | 1:A:351:TRP:HB2 | 1.77 | 0.66 |
| 1:A:531:LEU:HD22 | 1:B:531:LEU:HD22 | 1.78 | 0.66 |
| 1:B:283:LEU:HB2 | 1:B:351:TRP:HB2 | 1.78 | 0.65 |
| 1:B:312:ARG:NH2 | 1:B:410:GLU:OE1 | 2.29 | 0.65 |
| 1:A:503:TYR:HD2 | 3:A:654:HOH:O | 1.78 | 0.65 |
| 1:A:312:ARG:NH2 | 1:A:410:GLU:OE1 | 2.29 | 0.65 |
| 1:B:65:ASP:OD1 | 1:B:65:ASP:N | 2.29 | 0.65 |
| 1:B:339:LEU:O | 1:B:343:ALA:N | 2.24 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:339:LEU:O | 1:A:342:ILE:N | 2.30 | 0.65 |
| 1:B:35:GLU:HA | 1:B:35:GLU:OE1 | 1.96 | 0.65 |
| 1:A:429:ALA:HB2 | 1:A:439:GLN:NE2 | 2.11 | 0.65 |
| 1:B:339:LEU:O | 1:B:342:ILE:N | 2.30 | 0.65 |
| 1:A:446:ARG:NH1 | 1:A:449:GLU:OE1 | 2.30 | 0.65 |
| 1:B:445:LYS:HD3 | 3:B:620:HOH:O | 1.96 | 0.65 |
| 1:A:43:LYS:C | 1:A:45:GLN:H | 1.99 | 0.65 |
| 1:B:134:ASN:OD1 | 1:B:137:GLY:N | 2.23 | 0.65 |
| 1:B:429:ALA:HB2 | 1:B:439:GLN:NE2 | 2.11 | 0.65 |
| 1:A:62:HIS:HE1 | 1:A:475:LYS:HD3 | 1.61 | 0.64 |
| 1:B:177:LEU:CD1 | 1:B:265:ILE:HG22 | 2.28 | 0.64 |
| 1:B:324:LYS:HA | 1:B:416:TRP:CH2 | 2.32 | 0.64 |
| 1:A:58:HIS:HD2 | 1:A:59:ASP:C | 2.00 | 0.64 |
| 1:A:299:LEU:HB3 | 1:A:305:LEU:HG | 1.79 | 0.64 |
| 1:B:550:PRO:HB3 | 1:B:552:GLN:HE21 | 1.62 | 0.64 |
| 1:A:65:ASP:N | 1:A:65:ASP:OD1 | 2.29 | 0.64 |
| 1:A:457:THR:HG22 | 1:A:458:PHE:N | 2.11 | 0.64 |
| 1:A:160:LEU:O | 1:A:163:LYS:N | 2.30 | 0.64 |
| 1:A:324:LYS:HA | 1:A:416:TRP:CH2 | 2.32 | 0.64 |
| 1:B:277:GLN:HB3 | 1:B:357:LEU:HD12 | 1.78 | 0.64 |
| 1:A:277:GLN:HB3 | 1:A:357:LEU:HD12 | 1.78 | 0.64 |
| 1:A:183:ARG:NH2 | 1:A:256:GLN:HB2 | 2.13 | 0.64 |
| 1:B:60:PRO:O | 1:B:62:HIS:ND1 | 2.24 | 0.64 |
| 1:B:58:HIS:HD2 | 1:B:59:ASP:C | 2.00 | 0.64 |
| 1:B:446:ARG:NH1 | 1:B:449:GLU:OE1 | 2.30 | 0.64 |
| 1:A:35:GLU:OE1 | 1:A:35:GLU:HA | 1.96 | 0.64 |
| 1:A:62:HIS:CE1 | 1:A:475:LYS:HD3 | 2.33 | 0.64 |
| 1:B:62:HIS:HE1 | 1:B:475:LYS:HD3 | 1.61 | 0.64 |
| 1:B:183:ARG:NH2 | 1:B:256:GLN:HB2 | 2.13 | 0.64 |
| 1:B:43:LYS:C | 1:B:45:GLN:H | 1.99 | 0.64 |
| 1:B:166:LEU:HD23 | 1:B:269:LEU:HD22 | 1.78 | 0.64 |
| 1:B:62:HIS:CE1 | 1:B:475:LYS:HD3 | 2.33 | 0.64 |
| 1:B:299:LEU:HB3 | 1:B:305:LEU:HG | 1.80 | 0.63 |
| 1:B:439:GLN:O | 1:B:442:VAL:HB | 1.98 | 0.63 |
| 2:B:600:FAA:C4 | 2:B:600:FAA:C2P | 2.76 | 0.63 |
| 1:A:188:THR:HB | 1:A:189:PRO:HD2 | 1.81 | 0.63 |
| 1:B:416:TRP:O | 1:B:417:LEU:HD23 | 1.99 | 0.63 |
| 1:B:222:ARG:HB2 | 1:B:223:PRO:HD2 | 1.79 | 0.63 |
| 1:A:166:LEU:HD23 | 1:A:269:LEU:HD22 | 1.79 | 0.63 |
| 1:A:451:GLY:O | 1:A:452:LEU:HD23 | 1.98 | 0.63 |
| 1:A:138:ALA:O | 1:B:463:ARG:NH2 | 2.27 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:506:HIS:ND1 | 1:B:507:LEU:N | 2.46 | 0.63 |
| 1:B:457:THR:HG22 | 1:B:458:PHE:N | 2.11 | 0.63 |
| 2:A:600:FAA:C2P | 2:A:600:FAA:C4 | 2.76 | 0.63 |
| 1:B:78:ARG:HD3 | 1:B:82:ASP:OD2 | 1.98 | 0.63 |
| 1:B:201:GLU:HG2 | 1:B:263:THR:OG1 | 1.99 | 0.62 |
| 1:B:302:GLY:O | 1:B:303:MET:HB2 | 1.98 | 0.62 |
| 1:A:302:GLY:O | 1:A:303:MET:HB2 | 1.98 | 0.62 |
| 1:B:411:LEU:O | 1:B:414:ILE:HB | 1.99 | 0.62 |
| 1:B:451:GLY:O | 1:B:452:LEU:HD23 | 1.98 | 0.62 |
| 1:A:194:TRP:O | 1:A:197:HIS:HD2 | 1.81 | 0.62 |
| 1:A:550:PRO:HB3 | 1:A:552:GLN:HE21 | 1.62 | 0.62 |
| 1:B:399:ASP:OD1 | 1:B:403:GLN:NE2 | 2.32 | 0.62 |
| 1:A:506:HIS:ND1 | 1:A:507:LEU:N | 2.46 | 0.62 |
| 1:A:222:ARG:HB2 | 1:A:223:PRO:HD2 | 1.79 | 0.62 |
| 1:A:506:HIS:CE1 | 1:A:508:ALA:H | 2.18 | 0.62 |
| 1:A:62:HIS:N | 1:A:62:HIS:ND1 | 2.47 | 0.62 |
| 1:B:200:MET:O | 1:B:211:ARG:HA | 1.99 | 0.62 |
| 1:A:532:LYS:NZ | 1:A:541:ILE:O | 2.32 | 0.62 |
| 1:A:201:GLU:HG2 | 1:A:263:THR:OG1 | 1.99 | 0.62 |
| 1:B:194:TRP:O | 1:B:197:HIS:HD2 | 1.81 | 0.62 |
| 1:A:399:ASP:OD1 | 1:A:403:GLN:NE2 | 2.32 | 0.62 |
| 1:A:177:LEU:CD1 | 1:A:265:ILE:HG22 | 2.28 | 0.62 |
| 1:A:480:GLN:O | 1:A:483:LYS:HB2 | 1.99 | 0.62 |
| 1:A:295:ILE:O | 1:A:298:PRO:HD2 | 2.00 | 0.62 |
| 1:B:480:GLN:O | 1:B:483:LYS:HB2 | 1.99 | 0.62 |
| 1:B:149:HIS:O | 1:B:152:HIS:HB3 | 2.00 | 0.62 |
| 1:A:78:ARG:HD3 | 1:A:82:ASP:OD2 | 1.99 | 0.62 |
| 1:B:309:PRO:HG2 | 1:B:460:VAL:CG2 | 2.30 | 0.62 |
| 1:A:197:HIS:HA | 1:A:266:GLY:O | 2.00 | 0.62 |
| 1:B:389:THR:HB | 1:B:390:PRO:HD2 | 1.82 | 0.62 |
| 1:B:506:HIS:CE1 | 1:B:508:ALA:H | 2.17 | 0.62 |
| 1:A:200:MET:O | 1:A:211:ARG:HA | 1.99 | 0.62 |
| 1:A:439:GLN:O | 1:A:442:VAL:HB | 1.98 | 0.61 |
| 1:A:309:PRO:HG2 | 1:A:460:VAL:CG2 | 2.30 | 0.61 |
| 1:A:416:TRP:O | 1:A:417:LEU:HD23 | 1.99 | 0.61 |
| 1:A:253:LEU:CD1 | 1:B:253:LEU:HD21 | 2.29 | 0.61 |
| 1:A:411:LEU:O | 1:A:414:ILE:HB | 1.99 | 0.61 |
| 1:B:295:ILE:O | 1:B:298:PRO:HD2 | 2.00 | 0.61 |
| 1:B:197:HIS:HA | 1:B:266:GLY:O | 2.00 | 0.61 |
| 1:A:149:HIS:O | 1:A:152:HIS:HB3 | 2.00 | 0.61 |
| 1:A:389:THR:HB | 1:A:390:PRO:HD2 | 1.82 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:283:LEU:O | 1:A:349:GLY:HA3 | 2.01 | 0.61 |
| 1:B:74:ILE:HG22 | 1:B:75:VAL:N | 2.16 | 0.61 |
| 1:B:306:GLN:OE1 | 1:B:357:LEU:HA | 2.01 | 0.61 |
| 1:B:283:LEU:O | 1:B:349:GLY:HA3 | 2.01 | 0.61 |
| 1:A:51:TYR:CZ | 1:A:171:LEU:HD13 | 2.36 | 0.61 |
| 1:A:306:GLN:OE1 | 1:A:357:LEU:HA | 2.01 | 0.61 |
| 1:A:43:LYS:O | 1:A:45:GLN:N | 2.33 | 0.60 |
| 1:B:188:THR:HB | 1:B:189:PRO:HD2 | 1.81 | 0.60 |
| 1:A:279:TYR:HA | 1:A:395:LEU:HD21 | 1.83 | 0.60 |
| 1:A:206:ASN:OD1 | 1:A:208:GLU:N | 2.30 | 0.60 |
| 1:B:102:ILE:HG12 | 1:B:175:SER:HB2 | 1.83 | 0.60 |
| 1:B:507:LEU:HD23 | 1:B:510:MET:HE3 | 1.82 | 0.60 |
| 1:B:43:LYS:O | 1:B:45:GLN:N | 2.33 | 0.60 |
| 1:B:51:TYR:CZ | 1:B:171:LEU:HD13 | 2.36 | 0.60 |
| 1:B:532:LYS:NZ | 1:B:541:ILE:O | 2.32 | 0.60 |
| 1:A:102:ILE:HG12 | 1:A:175:SER:HB2 | 1.83 | 0.60 |
| 1:A:414:ILE:HD11 | 2:A:600:FAA:C8M | 2.31 | 0.60 |
| 1:B:62:HIS:N | 1:B:62:HIS:ND1 | 2.47 | 0.60 |
| 1:A:40:ILE:CD1 | 1:A:57:THR:HG22 | 2.31 | 0.60 |
| 1:A:517:TYR:CE1 | 1:B:217:LEU:HB2 | 2.37 | 0.60 |
| 1:B:506:HIS:ND1 | 1:B:508:ALA:N | 2.48 | 0.60 |
| 1:A:108:TYR:HD1 | 1:A:505:THR:C | 2.05 | 0.60 |
| 1:B:279:TYR:HA | 1:B:395:LEU:HD21 | 1.83 | 0.60 |
| 1:B:108:TYR:HD1 | 1:B:505:THR:C | 2.05 | 0.59 |
| 1:A:79:ASN:O | 1:A:82:ASP:HB2 | 2.02 | 0.59 |
| 1:A:74:ILE:HG22 | 1:A:75:VAL:N | 2.16 | 0.59 |
| 1:B:79:ASN:O | 1:B:82:ASP:HB2 | 2.02 | 0.59 |
| 1:B:94:SER:HA | 1:B:540:ILE:HD11 | 1.85 | 0.59 |
| 1:B:24:PHE:O | 1:B:28:ILE:HG13 | 2.02 | 0.59 |
| 1:B:177:LEU:HG | 1:B:265:ILE:HG21 | 1.85 | 0.59 |
| 1:B:539:GLY:O | 1:B:543:PRO:HG3 | 2.03 | 0.59 |
| 1:B:160:LEU:O | 1:B:163:LYS:N | 2.30 | 0.59 |
| 1:B:210:LEU:HD23 | 1:B:211:ARG:N | 2.18 | 0.59 |
| 1:A:237:LYS:HD2 | 1:B:500:TRP:HE1 | 1.68 | 0.59 |
| 1:B:414:ILE:HD11 | 2:B:600:FAA:C8M | 2.32 | 0.59 |
| 1:B:189:PRO:HD3 | 1:B:307:ASN:HB3 | 1.84 | 0.59 |
| 1:B:273:PRO:O | 1:B:359:GLY:HA2 | 2.03 | 0.59 |
| 1:A:189:PRO:HD3 | 1:A:307:ASN:HB3 | 1.84 | 0.59 |
| 1:A:24:PHE:O | 1:A:28:ILE:HG13 | 2.02 | 0.59 |
| 1:A:173:GLY:N | 1:A:408:TYR:HE1 | 2.01 | 0.59 |
| 1:A:210:LEU:HD23 | 1:A:211:ARG:N | 2.18 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:539:GLY:O | 1:A:543:PRO:HG3 | 2.03 | 0.59 |
| 1:A:10:LEU:CD2 | 1:A:42:SER:HA | 2.32 | 0.59 |
| 1:A:361:GLU:HB3 | 1:A:362:PRO:HD3 | 1.85 | 0.59 |
| 1:B:361:GLU:HB3 | 1:B:362:PRO:HD3 | 1.85 | 0.59 |
| 1:A:309:PRO:HB2 | 1:A:353:PHE:HE1 | 1.68 | 0.58 |
| 1:A:183:ARG:NH2 | 1:B:247:GLY:O | 2.35 | 0.58 |
| 1:A:94:SER:HA | 1:A:540:ILE:HD11 | 1.84 | 0.58 |
| 1:B:309:PRO:HB2 | 1:B:353:PHE:HE1 | 1.68 | 0.58 |
| 1:A:156:GLU:HB2 | 1:A:161:ARG:NH2 | 2.17 | 0.58 |
| 1:B:223:PRO:HD2 | 1:B:224:GLU:OE2 | 2.04 | 0.58 |
| 1:A:502:GLU:HG2 | 1:A:503:TYR:N | 2.17 | 0.58 |
| 1:B:502:GLU:HG2 | 1:B:503:TYR:H | 1.69 | 0.58 |
| 1:A:273:PRO:O | 1:A:359:GLY:HA2 | 2.03 | 0.58 |
| 1:A:502:GLU:HG2 | 1:A:503:TYR:H | 1.69 | 0.58 |
| 1:B:502:GLU:HG2 | 1:B:503:TYR:N | 2.17 | 0.58 |
| 1:A:95:PHE:O | 1:A:540:ILE:HD12 | 2.03 | 0.58 |
| 1:A:324:LYS:HB2 | 1:A:416:TRP:CD2 | 2.39 | 0.58 |
| 1:B:324:LYS:HB2 | 1:B:416:TRP:CD2 | 2.39 | 0.58 |
| 1:A:223:PRO:HD2 | 1:A:224:GLU:OE2 | 2.04 | 0.58 |
| 1:B:62:HIS:CG | 1:B:66:GLN:HG3 | 2.39 | 0.58 |
| 1:B:330:ARG:NH1 | 1:B:338:GLU:OE1 | 2.37 | 0.58 |
| 1:A:330:ARG:NH1 | 1:A:338:GLU:OE1 | 2.37 | 0.58 |
| 1:B:10:LEU:CD2 | 1:B:42:SER:HA | 2.32 | 0.58 |
| 1:A:104:ARG:C | 1:A:106:SER:H | 2.07 | 0.58 |
| 1:B:173:GLY:N | 1:B:408:TYR:HE1 | 2.01 | 0.58 |
| 1:B:487:LEU:HD11 | 1:B:491:LEU:HD11 | 1.86 | 0.58 |
| 1:B:95:PHE:O | 1:B:540:ILE:HD12 | 2.03 | 0.58 |
| 1:A:62:HIS:CG | 1:A:66:GLN:HG3 | 2.39 | 0.57 |
| 1:A:241:LEU:HB3 | 1:B:463:ARG:O | 2.04 | 0.57 |
| 1:A:414:ILE:CD1 | 2:A:600:FAA:HM71 | 2.31 | 0.57 |
| 1:A:177:LEU:HG | 1:A:265:ILE:HG21 | 1.85 | 0.57 |
| 1:B:210:LEU:HD23 | 1:B:210:LEU:C | 2.25 | 0.57 |
| 1:B:156:GLU:HB2 | 1:B:161:ARG:NH2 | 2.17 | 0.57 |
| 1:A:210:LEU:C | 1:A:210:LEU:HD23 | 2.25 | 0.57 |
| 1:B:40:ILE:CD1 | 1:B:57:THR:HG22 | 2.31 | 0.57 |
| 1:B:78:ARG:HB2 | 1:B:82:ASP:OD2 | 2.04 | 0.57 |
| 1:B:480:GLN:HA | 1:B:483:LYS:CG | 2.34 | 0.57 |
| 1:A:354:TYR:CD2 | 1:A:395:LEU:HD13 | 2.40 | 0.57 |
| 1:B:488:MET:O | 1:B:492:ILE:HG13 | 2.05 | 0.57 |
| 1:B:338:GLU:O | 1:B:342:ILE:HG13 | 2.04 | 0.57 |
| 1:A:338:GLU:O | 1:A:342:ILE:HG13 | 2.04 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:276:TYR:HE2 | 1:B:403:GLN:NE2 | 2.02 | 0.57 |
| 1:B:417:LEU:HD23 | 1:B:417:LEU:N | 2.19 | 0.57 |
| 1:A:480:GLN:HA | 1:A:483:LYS:CG | 2.34 | 0.57 |
| 1:A:78:ARG:HB2 | 1:A:82:ASP:OD2 | 2.04 | 0.57 |
| 1:A:248:PRO:HG3 | 1:B:257:SER:CB | 2.34 | 0.57 |
| 1:A:552:GLN:CD | 1:A:552:GLN:H | 2.08 | 0.57 |
| 1:B:429:ALA:O | 1:B:465:MET:N | 2.37 | 0.57 |
| 1:A:276:TYR:HE2 | 1:A:403:GLN:NE2 | 2.02 | 0.57 |
| 1:A:359:GLY:O | 1:A:364:ARG:NE | 2.38 | 0.57 |
| 1:B:359:GLY:O | 1:B:364:ARG:NE | 2.38 | 0.57 |
| 1:B:224:GLU:CD | 1:B:224:GLU:H | 2.08 | 0.57 |
| 1:A:325:ARG:C | 1:A:327:TYR:H | 2.08 | 0.57 |
| 1:A:312:ARG:NH1 | 1:A:316:LEU:HG | 2.20 | 0.56 |
| 1:A:506:HIS:ND1 | 1:A:508:ALA:N | 2.48 | 0.56 |
| 1:A:507:LEU:HD23 | 1:A:510:MET:HE3 | 1.87 | 0.56 |
| 1:B:104:ARG:C | 1:B:106:SER:H | 2.07 | 0.56 |
| 1:A:238:ILE:HD11 | 1:B:429:ALA:HA | 1.87 | 0.56 |
| 1:A:478:LEU:CD1 | 1:A:478:LEU:H | 2.19 | 0.56 |
| 1:A:488:MET:O | 1:A:492:ILE:HG13 | 2.05 | 0.56 |
| 1:A:407:THR:OG1 | 1:A:408:TYR:N | 2.37 | 0.56 |
| 1:A:487:LEU:HD11 | 1:A:491:LEU:HD11 | 1.86 | 0.56 |
| 1:B:324:LYS:HA | 1:B:416:TRP:CZ3 | 2.41 | 0.56 |
| 1:A:324:LYS:HA | 1:A:416:TRP:CZ3 | 2.41 | 0.56 |
| 1:B:312:ARG:NH1 | 1:B:316:LEU:HG | 2.20 | 0.56 |
| 1:B:354:TYR:CD2 | 1:B:395:LEU:HD13 | 2.40 | 0.56 |
| 1:B:52:MET:O | 1:B:53:LYS:HG3 | 2.06 | 0.56 |
| 1:A:167:ASP:OD1 | 1:A:186:GLY:HA3 | 2.05 | 0.56 |
| 1:A:177:LEU:HG | 1:A:265:ILE:HG22 | 1.86 | 0.56 |
| 1:B:177:LEU:HG | 1:B:265:ILE:HG22 | 1.86 | 0.56 |
| 1:A:52:MET:O | 1:A:53:LYS:HG3 | 2.06 | 0.56 |
| 1:B:169:PRO:HG3 | 1:B:193:HIS:HE1 | 1.71 | 0.56 |
| 1:A:224:GLU:H | 1:A:224:GLU:CD | 2.08 | 0.56 |
| 1:B:62:HIS:H | 1:B:62:HIS:HD1 | 1.51 | 0.55 |
| 1:B:167:ASP:OD1 | 1:B:186:GLY:HA3 | 2.05 | 0.55 |
| 1:A:169:PRO:HG3 | 1:A:193:HIS:HE1 | 1.71 | 0.55 |
| 1:B:9:PRO:HA | 1:B:40:ILE:O | 2.07 | 0.55 |
| 1:A:39:VAL:HG22 | 1:A:73:ALA:HB2 | 1.89 | 0.55 |
| 1:B:478:LEU:CD1 | 1:B:478:LEU:H | 2.19 | 0.55 |
| 1:A:300:ARG:HE | 1:A:309:PRO:HD2 | 1.72 | 0.55 |
| 1:A:132:GLU:HG2 | 1:A:133:VAL:H | 1.71 | 0.55 |
| 1:B:282:THR:C | 1:B:283:LEU:HD23 | 2.27 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:552:GLN:H | 1:B:552:GLN:CD | 2.08 | 0.55 |
| 1:A:494:ASP:O | 1:A:497:ALA:HB3 | 2.06 | 0.55 |
| 1:B:300:ARG:HE | 1:B:309:PRO:HD2 | 1.72 | 0.55 |
| 1:B:385:PHE:O | 1:B:388:ASP:N | 2.40 | 0.55 |
| 1:A:62:HIS:HD1 | 1:A:62:HIS:H | 1.51 | 0.55 |
| 1:A:152:HIS:CE1 | 1:A:161:ARG:NH2 | 2.75 | 0.55 |
| 1:A:332:GLU:HB3 | 1:A:333:PRO:HD2 | 1.89 | 0.55 |
| 1:B:494:ASP:O | 1:B:497:ALA:HB3 | 2.06 | 0.55 |
| 1:B:325:ARG:C | 1:B:327:TYR:H | 2.08 | 0.55 |
| 1:B:407:THR:OG1 | 1:B:408:TYR:N | 2.37 | 0.54 |
| 1:A:429:ALA:O | 1:A:465:MET:N | 2.37 | 0.54 |
| 1:A:237:LYS:HD2 | 1:B:500:TRP:CD1 | 2.42 | 0.54 |
| 1:A:522:SER:O | 1:A:526:ARG:HG2 | 2.08 | 0.54 |
| 1:A:104:ARG:O | 1:A:106:SER:N | 2.38 | 0.54 |
| 1:B:458:PHE:CD1 | 1:B:458:PHE:N | 2.74 | 0.54 |
| 1:B:206:ASN:OD1 | 1:B:208:GLU:N | 2.30 | 0.54 |
| 1:A:282:THR:C | 1:A:283:LEU:HD23 | 2.27 | 0.54 |
| 1:A:9:PRO:HA | 1:A:40:ILE:O | 2.07 | 0.54 |
| 1:A:97:LEU:HD23 | 1:A:119:VAL:HB | 1.90 | 0.54 |
| 1:A:429:ALA:HB2 | 1:A:439:GLN:HE22 | 1.73 | 0.54 |
| 1:B:522:SER:O | 1:B:526:ARG:HG2 | 2.08 | 0.54 |
| 1:B:152:HIS:CE1 | 1:B:161:ARG:NH2 | 2.75 | 0.54 |
| 1:B:97:LEU:HD23 | 1:B:119:VAL:HB | 1.90 | 0.54 |
| 1:A:458:PHE:CD1 | 1:A:458:PHE:N | 2.75 | 0.54 |
| 1:B:61:HIS:CB | 1:B:421:ALA:HB1 | 2.31 | 0.54 |
| 1:B:414:ILE:CD1 | 2:B:600:FAA:HM71 | 2.31 | 0.54 |
| 1:B:39:VAL:HG22 | 1:B:73:ALA:HB2 | 1.89 | 0.54 |
| 1:A:59:ASP:N | 1:A:112:ALA:HB2 | 2.23 | 0.53 |
| 1:A:385:PHE:O | 1:A:388:ASP:N | 2.40 | 0.53 |
| 1:B:142:VAL:HB | 1:B:146:VAL:HG21 | 1.90 | 0.53 |
| 1:A:315:LEU:HA | 1:A:318:ALA:HB3 | 1.90 | 0.53 |
| 1:A:181:VAL:O | 1:A:255:SER:HB2 | 2.08 | 0.53 |
| 1:A:102:ILE:HG21 | 1:A:104:ARG:HD2 | 1.90 | 0.53 |
| 1:B:156:GLU:CB | 1:B:161:ARG:HE | 2.21 | 0.53 |
| 1:A:422:HIS:HD1 | 1:A:422:HIS:H | 1.57 | 0.53 |
| 1:B:300:ARG:CA | 1:B:305:LEU:HB2 | 2.37 | 0.53 |
| 1:A:185:VAL:HG12 | 1:A:186:GLY:N | 2.24 | 0.53 |
| 1:B:185:VAL:HG12 | 1:B:186:GLY:N | 2.24 | 0.53 |
| 1:B:315:LEU:HA | 1:B:318:ALA:HB3 | 1.90 | 0.53 |
| 1:B:315:LEU:O | 1:B:319:ALA:N | 2.29 | 0.53 |
| 1:A:58:HIS:C | 1:A:112:ALA:HB2 | 2.29 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:351:TRP:O | 1:B:352:ASN:OD1 | 2.27 | 0.53 |
| 1:B:36:ASN:HB3 | 1:B:76:ALA:HB3 | 1.91 | 0.53 |
| 1:B:59:ASP:N | 1:B:112:ALA:HB2 | 2.23 | 0.53 |
| 1:B:429:ALA:HB2 | 1:B:439:GLN:HE22 | 1.73 | 0.53 |
| 1:B:181:VAL:O | 1:B:255:SER:HB2 | 2.08 | 0.53 |
| 2:A:600:FAA:C10 | 2:A:600:FAA:C6P | 2.87 | 0.53 |
| 1:A:504:ARG:NH2 | 2:A:600:FAA:O3' | 2.41 | 0.53 |
| 1:B:422:HIS:H | 1:B:422:HIS:HD1 | 1.57 | 0.53 |
| 1:A:289:LEU:HD23 | 1:A:437:MET:CE | 2.36 | 0.53 |
| 1:B:543:PRO:HB3 | 1:B:550:PRO:CG | 2.39 | 0.53 |
| 1:A:36:ASN:HB3 | 1:A:76:ALA:HB3 | 1.90 | 0.53 |
| 1:A:202:VAL:HG23 | 1:A:261:ILE:N | 2.24 | 0.52 |
| 1:A:24:PHE:CE1 | 1:A:28:ILE:HD12 | 2.44 | 0.52 |
| 1:A:156:GLU:CB | 1:A:161:ARG:HE | 2.21 | 0.52 |
| 1:A:363:ILE:HD11 | 1:B:366:VAL:HG11 | 1.90 | 0.52 |
| 1:B:99:PRO:HA | 1:B:121:LEU:HB3 | 1.91 | 0.52 |
| 1:B:238:ILE:O | 1:B:238:ILE:HG22 | 2.09 | 0.52 |
| 1:A:238:ILE:O | 1:A:238:ILE:HG22 | 2.09 | 0.52 |
| 1:B:504:ARG:NH2 | 2:B:600:FAA:O3' | 2.41 | 0.52 |
| 1:B:348:LEU:HB3 | 1:B:352:ASN:HD21 | 1.74 | 0.52 |
| 1:A:171:LEU:HD12 | 3:A:602:HOH:O | 2.09 | 0.52 |
| 1:B:297:ARG:HB2 | 1:B:431:VAL:HG12 | 1.91 | 0.52 |
| 1:B:58:HIS:C | 1:B:112:ALA:HB2 | 2.29 | 0.52 |
| 2:B:600:FAA:C6P | 2:B:600:FAA:C10 | 2.87 | 0.52 |
| 1:A:316:LEU:HD11 | 1:A:413:TRP:CD1 | 2.44 | 0.52 |
| 1:A:463:ARG:NH2 | 1:B:138:ALA:O | 2.38 | 0.52 |
| 1:A:142:VAL:HB | 1:A:146:VAL:HG21 | 1.90 | 0.52 |
| 1:B:426:SER:O | 1:B:502:GLU:HG3 | 2.10 | 0.52 |
| 1:A:348:LEU:HB3 | 1:A:352:ASN:HD21 | 1.74 | 0.52 |
| 1:A:543:PRO:HB3 | 1:A:550:PRO:CG | 2.39 | 0.52 |
| 1:B:202:VAL:HG23 | 1:B:261:ILE:N | 2.24 | 0.52 |
| 1:B:332:GLU:HB3 | 1:B:333:PRO:HD2 | 1.89 | 0.52 |
| 1:A:99:PRO:HA | 1:A:121:LEU:HB3 | 1.92 | 0.52 |
| 1:B:426:SER:N | 1:B:427:PRO:HD3 | 2.22 | 0.52 |
| 1:A:95:PHE:CD1 | 1:A:119:VAL:HG23 | 2.45 | 0.52 |
| 1:A:107:GLY:HA2 | 1:A:422:HIS:O | 2.10 | 0.52 |
| 1:A:297:ARG:HB2 | 1:A:431:VAL:HG12 | 1.91 | 0.52 |
| 1:B:520:ASN:O | 1:B:521:ASN:HB2 | 2.09 | 0.52 |
| 1:A:426:SER:N | 1:A:427:PRO:HD3 | 2.22 | 0.52 |
| 1:B:316:LEU:HD11 | 1:B:413:TRP:CD1 | 2.44 | 0.52 |
| 1:A:57:THR:O | 1:A:70:LEU:HD12 | 2.10 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:409:ASP:OD1 | 1:A:409:ASP:N | 2.43 | 0.52 |
| 1:A:300:ARG:CA | 1:A:305:LEU:HB2 | 2.37 | 0.52 |
| 1:A:253:LEU:HD21 | 1:B:253:LEU:CD1 | 2.39 | 0.51 |
| 1:B:289:LEU:HD23 | 1:B:437:MET:CE | 2.36 | 0.51 |
| 1:B:24:PHE:CE1 | 1:B:28:ILE:HD12 | 2.44 | 0.51 |
| 1:B:409:ASP:OD1 | 1:B:409:ASP:N | 2.43 | 0.51 |
| 1:B:104:ARG:O | 1:B:106:SER:N | 2.38 | 0.51 |
| 1:A:351:TRP:O | 1:A:352:ASN:OD1 | 2.27 | 0.51 |
| 1:B:317:ASP:O | 1:B:321:LEU:HG | 2.10 | 0.51 |
| 1:A:108:TYR:HE1 | 1:A:505:THR:HA | 1.75 | 0.51 |
| 1:B:107:GLY:HA2 | 1:B:422:HIS:O | 2.10 | 0.51 |
| 1:B:108:TYR:HE1 | 1:B:505:THR:HA | 1.75 | 0.51 |
| 1:B:57:THR:O | 1:B:70:LEU:HD12 | 2.10 | 0.51 |
| 1:B:275:GLY:HA3 | 1:B:359:GLY:O | 2.11 | 0.51 |
| 1:A:385:PHE:HB3 | 1:A:386:PRO:HD2 | 1.92 | 0.51 |
| 1:A:269:LEU:O | 1:B:463:ARG:NH2 | 2.44 | 0.51 |
| 1:B:102:ILE:HG21 | 1:B:104:ARG:HD2 | 1.90 | 0.51 |
| 1:B:132:GLU:HG2 | 1:B:133:VAL:H | 1.71 | 0.51 |
| 1:A:317:ASP:O | 1:A:321:LEU:HG | 2.10 | 0.51 |
| 1:B:217:LEU:HD12 | 1:B:218:PRO:HD2 | 1.92 | 0.51 |
| 1:B:444:LYS:HE3 | 3:B:608:HOH:O | 2.10 | 0.51 |
| 1:B:511:ASP:HB2 | 3:B:612:HOH:O | 2.11 | 0.51 |
| 1:B:543:PRO:HB3 | 1:B:550:PRO:HG2 | 1.93 | 0.51 |
| 1:B:160:LEU:HD23 | 1:B:163:LYS:HD2 | 1.93 | 0.51 |
| 1:B:385:PHE:HB3 | 1:B:386:PRO:HD2 | 1.92 | 0.51 |
| 1:A:315:LEU:O | 1:A:319:ALA:N | 2.29 | 0.51 |
| 1:A:520:ASN:O | 1:A:521:ASN:HB2 | 2.09 | 0.51 |
| 1:B:502:GLU:HG2 | 1:B:504:ARG:H | 1.75 | 0.51 |
| 1:B:45:GLN:HG2 | 1:B:46:ILE:N | 2.25 | 0.51 |
| 1:B:95:PHE:CD1 | 1:B:119:VAL:HG23 | 2.45 | 0.51 |
| 1:A:275:GLY:HA3 | 1:A:359:GLY:O | 2.11 | 0.51 |
| 1:A:160:LEU:HD23 | 1:A:163:LYS:HD2 | 1.93 | 0.51 |
| 1:A:323:ASP:OD1 | 1:A:326:SER:N | 2.34 | 0.51 |
| 1:A:61:HIS:CB | 1:A:421:ALA:HB1 | 2.31 | 0.51 |
| 1:A:527:PHE:O | 1:A:530:VAL:HB | 2.11 | 0.51 |
| 1:A:479:ILE:N | 1:A:479:ILE:HD12 | 2.26 | 0.51 |
| 1:B:479:ILE:N | 1:B:479:ILE:HD12 | 2.26 | 0.50 |
| 1:B:383:PHE:C | 1:B:384:TYR:CD1 | 2.85 | 0.50 |
| 1:A:443:THR:HB | 1:A:454:PHE:HE2 | 1.76 | 0.50 |
| 1:B:108:TYR:CD1 | 1:B:505:THR:C | 2.85 | 0.50 |
| 1:A:194:TRP:HH2 | 1:A:200:MET:HE1 | 1.76 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:537:PRO:CD | 1:B:538:ASN:H | 2.22 | 0.50 |
| 1:A:45:GLN:HG2 | 1:A:46:ILE:N | 2.25 | 0.50 |
| 1:B:276:TYR:CE2 | 1:B:403:GLN:NE2 | 2.79 | 0.50 |
| 1:A:383:PHE:C | 1:A:384:TYR:CD1 | 2.85 | 0.50 |
| 1:B:155:LEU:HD23 | 1:B:155:LEU:N | 2.19 | 0.50 |
| 1:A:426:SER:C | 1:A:502:GLU:HG3 | 2.32 | 0.50 |
| 1:B:443:THR:HB | 1:B:454:PHE:HE2 | 1.76 | 0.50 |
| 1:A:346:LEU:HB3 | 1:A:348:LEU:CD1 | 2.42 | 0.50 |
| 1:A:437:MET:HE3 | 1:A:437:MET:HA | 1.93 | 0.50 |
| 1:A:426:SER:O | 1:A:502:GLU:HG3 | 2.10 | 0.50 |
| 1:A:74:ILE:CG2 | 1:A:75:VAL:N | 2.75 | 0.50 |
| 1:B:45:GLN:CG | 1:B:46:ILE:N | 2.74 | 0.50 |
| 1:A:543:PRO:HB3 | 1:A:550:PRO:HG2 | 1.93 | 0.50 |
| 1:A:417:LEU:CB | 1:A:418:PRO:HD2 | 2.38 | 0.50 |
| 1:B:426:SER:C | 1:B:502:GLU:HG3 | 2.32 | 0.50 |
| 1:A:437:MET:O | 1:A:440:TYR:HB3 | 2.12 | 0.50 |
| 1:A:80:VAL:CG1 | 1:A:209:LEU:HD21 | 2.38 | 0.50 |
| 1:A:400:LYS:HB3 | 1:A:405:ILE:HB | 1.94 | 0.50 |
| 1:A:502:GLU:HG2 | 1:A:504:ARG:H | 1.75 | 0.50 |
| 1:B:194:TRP:O | 1:B:197:HIS:CD2 | 2.64 | 0.50 |
| 1:B:437:MET:O | 1:B:440:TYR:HB3 | 2.12 | 0.50 |
| 1:A:217:LEU:HD12 | 1:A:218:PRO:HD2 | 1.92 | 0.50 |
| 1:B:218:PRO:O | 1:B:220:PRO:HD3 | 2.12 | 0.50 |
| 1:A:378:ILE:HG22 | 1:A:381:VAL:HG23 | 1.94 | 0.50 |
| 1:A:156:GLU:HB2 | 1:A:161:ARG:HE | 1.76 | 0.50 |
| 1:B:24:PHE:CE1 | 1:B:28:ILE:CD1 | 2.95 | 0.50 |
| 1:B:527:PHE:O | 1:B:530:VAL:HB | 2.11 | 0.50 |
| 1:A:276:TYR:CE2 | 1:A:403:GLN:NE2 | 2.79 | 0.50 |
| 1:A:217:LEU:HD12 | 1:A:218:PRO:HD3 | 1.93 | 0.50 |
| 1:B:354:TYR:HD2 | 1:B:395:LEU:HD13 | 1.76 | 0.50 |
| 1:A:45:GLN:C | 1:A:47:VAL:N | 2.65 | 0.49 |
| 1:B:400:LYS:HB3 | 1:B:405:ILE:HB | 1.94 | 0.49 |
| 1:B:45:GLN:O | 1:B:47:VAL:N | 2.45 | 0.49 |
| 1:A:354:TYR:HD2 | 1:A:395:LEU:HD13 | 1.76 | 0.49 |
| 1:B:74:ILE:CG2 | 1:B:75:VAL:N | 2.75 | 0.49 |
| 1:A:194:TRP:O | 1:A:197:HIS:CD2 | 2.64 | 0.49 |
| 1:B:45:GLN:C | 1:B:47:VAL:N | 2.65 | 0.49 |
| 1:A:537:PRO:CD | 1:A:538:ASN:H | 2.22 | 0.49 |
| 1:A:45:GLN:O | 1:A:47:VAL:N | 2.45 | 0.49 |
| 1:A:439:GLN:OE1 | 1:A:467:HIS:HB2 | 2.13 | 0.49 |
| 1:B:37:VAL:HA | 1:B:74:ILE:O | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:530:VAL:HG13 | 3:A:628:HOH:O | 2.11 | 0.49 |
| 1:A:388:ASP:OD1 | 1:A:388:ASP:N | 2.45 | 0.49 |
| 1:A:505:THR:CG2 | 1:A:509:PHE:HB2 | 2.41 | 0.49 |
| 1:B:426:SER:H | 1:B:502:GLU:CD | 2.16 | 0.49 |
| 1:B:346:LEU:HB3 | 1:B:348:LEU:CD1 | 2.42 | 0.49 |
| 1:B:332:GLU:CB | 1:B:333:PRO:CD | 2.89 | 0.49 |
| 1:B:217:LEU:HD12 | 1:B:218:PRO:HD3 | 1.93 | 0.49 |
| 1:A:18:LEU:HG | 1:A:22:ASN:ND2 | 2.28 | 0.49 |
| 1:B:439:GLN:OE1 | 1:B:467:HIS:HB2 | 2.13 | 0.49 |
| 1:A:221:LYS:O | 1:A:222:ARG:HB3 | 2.13 | 0.49 |
| 1:A:24:PHE:CE1 | 1:A:28:ILE:CD1 | 2.95 | 0.49 |
| 1:B:18:LEU:HB3 | 3:B:622:HOH:O | 2.11 | 0.49 |
| 1:A:61:HIS:CD2 | 1:A:422:HIS:H | 2.31 | 0.49 |
| 1:B:457:THR:CG2 | 1:B:458:PHE:N | 2.75 | 0.49 |
| 1:B:384:TYR:O | 1:B:385:PHE:HD1 | 1.95 | 0.49 |
| 1:A:426:SER:H | 1:A:502:GLU:CD | 2.16 | 0.49 |
| 1:B:431:VAL:HG22 | 1:B:465:MET:HG3 | 1.95 | 0.49 |
| 1:A:156:GLU:CA | 1:A:161:ARG:HE | 2.26 | 0.49 |
| 1:A:229:LYS:HB3 | 1:A:231:GLU:CD | 2.34 | 0.49 |
| 1:B:378:ILE:HG22 | 1:B:381:VAL:HG23 | 1.94 | 0.48 |
| 1:A:457:THR:CG2 | 1:A:458:PHE:N | 2.75 | 0.48 |
| 1:A:384:TYR:O | 1:A:385:PHE:HD1 | 1.95 | 0.48 |
| 1:A:16:LEU:HG | 1:A:17:SER:N | 2.27 | 0.48 |
| 1:A:37:VAL:HA | 1:A:74:ILE:O | 2.12 | 0.48 |
| 1:B:197:HIS:HB2 | 1:B:265:ILE:HD11 | 1.95 | 0.48 |
| 1:B:80:VAL:CG1 | 1:B:209:LEU:HD21 | 2.38 | 0.48 |
| 1:B:156:GLU:HB2 | 1:B:161:ARG:HE | 1.76 | 0.48 |
| 1:A:65:ASP:O | 1:A:68:TYR:HB2 | 2.13 | 0.48 |
| 1:A:387:GLU:HB2 | 3:A:606:HOH:O | 2.13 | 0.48 |
| 1:A:218:PRO:O | 1:A:220:PRO:HD3 | 2.12 | 0.48 |
| 1:B:221:LYS:O | 1:B:222:ARG:HB3 | 2.13 | 0.48 |
| 1:B:18:LEU:HG | 1:B:22:ASN:ND2 | 2.28 | 0.48 |
| 1:B:61:HIS:CD2 | 1:B:422:HIS:H | 2.31 | 0.48 |
| 1:B:16:LEU:HG | 1:B:17:SER:N | 2.27 | 0.48 |
| 1:B:323:ASP:OD1 | 1:B:326:SER:N | 2.35 | 0.48 |
| 1:A:454:PHE:HZ | 1:A:467:HIS:CE1 | 2.32 | 0.48 |
| 2:A:600:FAA:C4 | 2:A:600:FAA:C1P | 2.82 | 0.48 |
| 1:B:454:PHE:HZ | 1:B:467:HIS:CE1 | 2.32 | 0.48 |
| 1:B:229:LYS:HB3 | 1:B:231:GLU:CD | 2.34 | 0.48 |
| 1:A:7:PHE:HA | 1:A:22:ASN:OD1 | 2.14 | 0.48 |
| 1:A:108:TYR:CD1 | 1:A:505:THR:C | 2.85 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:156:GLU:CA | 1:B:161:ARG:HE | 2.26 | 0.48 |
| 1:B:90:ALA:HB1 | 1:B:540:ILE:HG23 | 1.96 | 0.48 |
| 1:B:143:GLU:HB3 | 1:B:144:PRO:HD2 | 1.96 | 0.48 |
| 1:B:56:HIS:HB2 | 1:B:74:ILE:HD13 | 1.96 | 0.48 |
| 1:B:65:ASP:O | 1:B:68:TYR:HB2 | 2.13 | 0.48 |
| 1:A:452:LEU:HA | 1:A:452:LEU:HD23 | 1.31 | 0.48 |
| 1:A:22:ASN:O | 1:A:25:ILE:HG22 | 2.14 | 0.48 |
| 1:A:431:VAL:HG22 | 1:A:465:MET:HG3 | 1.95 | 0.48 |
| 1:A:177:LEU:C | 1:A:177:LEU:HD23 | 2.33 | 0.48 |
| 1:A:197:HIS:HB2 | 1:A:265:ILE:HD11 | 1.95 | 0.48 |
| 1:B:330:ARG:HH22 | 1:B:335:SER:HB3 | 1.79 | 0.48 |
| 1:A:385:PHE:HB3 | 1:A:386:PRO:CD | 2.44 | 0.48 |
| 1:A:36:ASN:OD1 | 1:A:76:ALA:HB3 | 2.14 | 0.48 |
| 1:A:97:LEU:HD22 | 1:A:119:VAL:HB | 1.94 | 0.48 |
| 1:A:90:ALA:HB1 | 1:A:540:ILE:HG23 | 1.96 | 0.48 |
| 1:B:385:PHE:HB3 | 1:B:386:PRO:CD | 2.43 | 0.48 |
| 1:B:388:ASP:OD1 | 1:B:388:ASP:N | 2.45 | 0.48 |
| 1:B:36:ASN:OD1 | 1:B:76:ALA:HB3 | 2.14 | 0.48 |
| 1:B:173:GLY:H | 1:B:408:TYR:HE1 | 1.62 | 0.47 |
| 1:B:177:LEU:C | 1:B:177:LEU:HD23 | 2.33 | 0.47 |
| 1:B:97:LEU:HD22 | 1:B:119:VAL:HB | 1.94 | 0.47 |
| 1:A:502:GLU:HB3 | 1:A:513:ILE:HD13 | 1.96 | 0.47 |
| 1:B:200:MET:HE2 | 1:B:251:ASP:CB | 2.36 | 0.47 |
| 1:A:242:PHE:HA | 1:A:243:PRO:HD3 | 1.38 | 0.47 |
| 1:A:330:ARG:HH22 | 1:A:335:SER:HB3 | 1.79 | 0.47 |
| 1:A:338:GLU:O | 1:A:341:LYS:HB2 | 2.14 | 0.47 |
| 1:B:276:TYR:OH | 1:B:399:ASP:O | 2.24 | 0.47 |
| 1:B:417:LEU:CB | 1:B:418:PRO:HD2 | 2.38 | 0.47 |
| 1:A:398:ARG:HB3 | 1:A:402:MET:HE2 | 1.96 | 0.47 |
| 1:B:398:ARG:HB3 | 1:B:402:MET:HE2 | 1.96 | 0.47 |
| 1:B:148:TYR:HB2 | 1:B:172:GLY:O | 2.15 | 0.47 |
| 1:B:427:PRO:HD2 | 1:B:467:HIS:O | 2.15 | 0.47 |
| 1:B:198:SER:O | 1:B:266:GLY:HA3 | 2.14 | 0.47 |
| 1:B:155:LEU:HD23 | 1:B:155:LEU:HA | 1.38 | 0.47 |
| 1:A:147:THR:HB | 1:A:173:GLY:O | 2.15 | 0.47 |
| 1:A:248:PRO:HD3 | 1:B:256:GLN:O | 2.14 | 0.47 |
| 1:B:401:THR:C | 1:B:403:GLN:H | 2.18 | 0.47 |
| 1:B:332:GLU:HB3 | 1:B:333:PRO:HD3 | 1.96 | 0.47 |
| 1:A:427:PRO:HD2 | 1:A:467:HIS:O | 2.15 | 0.47 |
| 1:A:330:ARG:NH1 | 1:A:338:GLU:CD | 2.68 | 0.47 |
| 1:A:45:GLN:CG | 1:A:46:ILE:N | 2.74 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:463:ARG:NH2 | 1:B:269:LEU:O | 2.47 | 0.47 |
| 1:B:147:THR:HB | 1:B:173:GLY:O | 2.15 | 0.47 |
| 1:A:198:SER:O | 1:A:266:GLY:HA3 | 2.14 | 0.47 |
| 1:A:143:GLU:HB3 | 1:A:144:PRO:HD2 | 1.96 | 0.47 |
| 1:A:201:GLU:HG2 | 1:A:263:THR:HG1 | 1.79 | 0.47 |
| 1:B:168:VAL:HA | 1:B:169:PRO:HD3 | 1.66 | 0.47 |
| 1:B:22:ASN:O | 1:B:25:ILE:HG22 | 2.14 | 0.47 |
| 1:B:7:PHE:HA | 1:B:22:ASN:OD1 | 2.14 | 0.47 |
| 1:A:100:ILE:HG13 | 1:A:100:ILE:O | 2.14 | 0.47 |
| 1:B:295:ILE:HD12 | 1:B:378:ILE:HD11 | 1.97 | 0.47 |
| 1:B:339:LEU:HD12 | 1:B:350:ARG:CZ | 2.45 | 0.47 |
| 1:B:272:ASN:HA | 1:B:273:PRO:HD3 | 1.55 | 0.47 |
| 1:A:148:TYR:HB2 | 1:A:172:GLY:O | 2.15 | 0.47 |
| 1:B:480:GLN:HG3 | 1:B:483:LYS:HD2 | 1.97 | 0.47 |
| 1:A:25:ILE:CG2 | 1:A:26:GLN:N | 2.78 | 0.47 |
| 1:A:525:LEU:O | 1:A:529:GLU:HG3 | 2.15 | 0.47 |
| 1:B:505:THR:CG2 | 1:B:509:PHE:HB2 | 2.41 | 0.47 |
| 1:B:338:GLU:O | 1:B:341:LYS:HB2 | 2.14 | 0.47 |
| 1:A:401:THR:C | 1:A:403:GLN:H | 2.17 | 0.47 |
| 1:B:502:GLU:HB3 | 1:B:513:ILE:HD13 | 1.96 | 0.46 |
| 1:A:290:LYS:O | 1:A:290:LYS:HG3 | 2.15 | 0.46 |
| 1:A:339:LEU:HD12 | 1:A:350:ARG:CZ | 2.45 | 0.46 |
| 1:A:295:ILE:HD12 | 1:A:378:ILE:HD11 | 1.97 | 0.46 |
| 1:A:10:LEU:HD21 | 1:A:42:SER:N | 2.31 | 0.46 |
| 1:A:182:GLU:OE1 | 1:A:256:GLN:HG2 | 2.15 | 0.46 |
| 1:A:269:LEU:HA | 1:A:269:LEU:HD23 | 1.77 | 0.46 |
| 1:A:332:GLU:CB | 1:A:333:PRO:CD | 2.89 | 0.46 |
| 1:A:244:TYR:CD1 | 1:A:244:TYR:N | 2.82 | 0.46 |
| 1:A:198:SER:HB2 | 1:A:268:TRP:CZ2 | 2.50 | 0.46 |
| 1:B:10:LEU:HD21 | 1:B:42:SER:N | 2.31 | 0.46 |
| 1:B:238:ILE:HA | 1:B:241:LEU:HD22 | 1.98 | 0.46 |
| 1:B:139:TYR:HE2 | 1:B:241:LEU:CD1 | 2.29 | 0.46 |
| 1:B:127:MET:O | 1:B:143:GLU:HB3 | 2.16 | 0.46 |
| 1:B:198:SER:HB2 | 1:B:268:TRP:CZ2 | 2.50 | 0.46 |
| 1:A:90:ALA:O | 1:A:94:SER:N | 2.48 | 0.46 |
| 1:A:204:LEU:HD22 | 1:B:527:PHE:CE1 | 2.50 | 0.46 |
| 1:A:173:GLY:H | 1:A:408:TYR:HE1 | 1.62 | 0.46 |
| 1:B:460:VAL:HG12 | 1:B:461:GLY:O | 2.15 | 0.46 |
| 1:B:132:GLU:CG | 1:B:133:VAL:N | 2.72 | 0.46 |
| 1:B:182:GLU:OE1 | 1:B:256:GLN:HG2 | 2.15 | 0.46 |
| 1:A:127:MET:O | 1:A:143:GLU:HB3 | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:93:PHE:O | 1:B:94:SER:HB2 | 2.16 | 0.46 |
| 1:A:332:GLU:HB3 | 1:A:333:PRO:HD3 | 1.96 | 0.46 |
| 1:A:423:LEU:CD2 | 1:A:488:MET:HE2 | 2.45 | 0.46 |
| 1:A:36:ASN:CB | 1:A:76:ALA:HB3 | 2.46 | 0.46 |
| 1:B:16:LEU:HD12 | 1:B:16:LEU:HA | 1.50 | 0.46 |
| 1:A:139:TYR:HE2 | 1:A:241:LEU:CD1 | 2.29 | 0.46 |
| 1:B:549:TRP:HA | 1:B:550:PRO:HD3 | 1.75 | 0.46 |
| 1:A:550:PRO:HB2 | 1:A:552:GLN:HE21 | 1.80 | 0.46 |
| 1:A:45:GLN:C | 1:A:47:VAL:H | 2.18 | 0.46 |
| 1:B:371:ILE:O | 1:B:374:ALA:N | 2.49 | 0.46 |
| 1:A:56:HIS:HB2 | 1:A:74:ILE:HD13 | 1.96 | 0.46 |
| 1:A:480:GLN:HG3 | 1:A:483:LYS:HD2 | 1.97 | 0.46 |
| 1:B:480:GLN:HA | 1:B:483:LYS:HG3 | 1.98 | 0.46 |
| 1:B:437:MET:HE3 | 1:B:437:MET:HA | 1.96 | 0.46 |
| 1:A:13:PRO:HD3 | 1:A:117:GLY:O | 2.16 | 0.46 |
| 1:B:525:LEU:O | 1:B:529:GLU:HG3 | 2.15 | 0.46 |
| 1:A:305:LEU:HD23 | 1:A:305:LEU:HA | 1.82 | 0.46 |
| 1:B:330:ARG:NH1 | 1:B:338:GLU:CD | 2.68 | 0.46 |
| 1:B:346:LEU:HB3 | 1:B:348:LEU:HD11 | 1.98 | 0.46 |
| 1:A:93:PHE:O | 1:A:94:SER:HB2 | 2.16 | 0.46 |
| 1:A:217:LEU:HD12 | 1:A:217:LEU:HA | 1.33 | 0.46 |
| 1:A:72:SER:HB3 | 1:A:117:GLY:O | 2.16 | 0.46 |
| 1:A:237:LYS:HG3 | 1:A:238:ILE:HG12 | 1.98 | 0.46 |
| 1:B:156:GLU:HA | 1:B:161:ARG:HE | 1.81 | 0.46 |
| 1:B:45:GLN:C | 1:B:47:VAL:H | 2.18 | 0.46 |
| 1:B:550:PRO:CB | 1:B:552:GLN:NE2 | 2.77 | 0.46 |
| 1:B:11:THR:HG22 | 1:B:117:GLY:HA3 | 1.98 | 0.46 |
| 1:A:280:LEU:HD12 | 1:A:353:PHE:O | 2.16 | 0.46 |
| 1:B:484:VAL:O | 1:B:487:LEU:HB3 | 2.16 | 0.46 |
| 1:A:330:ARG:NH1 | 1:A:338:GLU:OE2 | 2.49 | 0.46 |
| 1:A:167:ASP:OD2 | 1:A:191:GLY:HA2 | 2.16 | 0.46 |
| 1:A:244:TYR:OH | 1:B:195:MET:HG2 | 2.16 | 0.46 |
| 1:A:371:ILE:O | 1:A:374:ALA:N | 2.49 | 0.46 |
| 1:A:62:HIS:CD2 | 1:A:66:GLN:HB2 | 2.51 | 0.45 |
| 1:B:480:GLN:HA | 1:B:483:LYS:CE | 2.46 | 0.45 |
| 1:B:244:TYR:N | 1:B:244:TYR:CD1 | 2.82 | 0.45 |
| 1:B:242:PHE:HA | 1:B:243:PRO:HD3 | 1.38 | 0.45 |
| 1:A:299:LEU:HB2 | 1:A:305:LEU:HD12 | 1.98 | 0.45 |
| 1:B:280:LEU:HD12 | 1:B:353:PHE:O | 2.16 | 0.45 |
| 1:A:484:VAL:O | 1:A:487:LEU:HB3 | 2.16 | 0.45 |
| 1:B:132:GLU:O | 1:B:140:CYS:HA | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:132:GLU:O | 1:A:140:CYS:HA | 2.16 | 0.45 |
| 1:A:295:ILE:CG2 | 1:A:375:PHE:CE1 | 3.00 | 0.45 |
| 1:A:156:GLU:HA | 1:A:161:ARG:HE | 1.81 | 0.45 |
| 1:A:40:ILE:HD11 | 1:A:57:THR:CG2 | 2.42 | 0.45 |
| 1:B:90:ALA:O | 1:B:94:SER:N | 2.48 | 0.45 |
| 1:B:100:ILE:O | 1:B:100:ILE:HG13 | 2.14 | 0.45 |
| 1:B:62:HIS:HD1 | 1:B:62:HIS:N | 2.12 | 0.45 |
| 1:A:480:GLN:HA | 1:A:483:LYS:CE | 2.46 | 0.45 |
| 1:B:277:GLN:O | 1:B:356:ALA:HA | 2.17 | 0.45 |
| 1:B:13:PRO:HD3 | 1:B:117:GLY:O | 2.16 | 0.45 |
| 1:A:460:VAL:HG12 | 1:A:461:GLY:O | 2.15 | 0.45 |
| 1:B:507:LEU:HA | 1:B:510:MET:HE2 | 1.94 | 0.45 |
| 1:B:290:LYS:O | 1:B:290:LYS:HG3 | 2.15 | 0.45 |
| 1:A:93:PHE:CD1 | 1:A:93:PHE:N | 2.85 | 0.45 |
| 1:B:18:LEU:HD12 | 1:B:18:LEU:HA | 1.65 | 0.45 |
| 1:A:506:HIS:CG | 1:A:507:LEU:N | 2.84 | 0.45 |
| 1:B:299:LEU:HB2 | 1:B:305:LEU:HD12 | 1.98 | 0.45 |
| 1:B:59:ASP:HA | 1:B:60:PRO:HD3 | 1.80 | 0.45 |
| 1:B:330:ARG:NH1 | 1:B:338:GLU:OE2 | 2.49 | 0.45 |
| 1:B:201:GLU:HG2 | 1:B:263:THR:HG1 | 1.80 | 0.45 |
| 1:B:393:SER:HB3 | 1:B:396:ARG:HG3 | 1.98 | 0.45 |
| 1:B:506:HIS:CG | 1:B:507:LEU:N | 2.84 | 0.45 |
| 1:B:40:ILE:O | 1:B:40:ILE:HG22 | 2.16 | 0.45 |
| 1:B:25:ILE:CG2 | 1:B:26:GLN:N | 2.78 | 0.45 |
| 1:A:11:THR:HG22 | 1:A:117:GLY:HA3 | 1.98 | 0.45 |
| 1:B:72:SER:HB3 | 1:B:117:GLY:O | 2.16 | 0.45 |
| 1:A:480:GLN:HA | 1:A:483:LYS:HG3 | 1.98 | 0.45 |
| 1:A:183:ARG:HH22 | 1:B:247:GLY:C | 2.19 | 0.45 |
| 1:B:167:ASP:OD2 | 1:B:191:GLY:HA2 | 2.16 | 0.45 |
| 1:A:40:ILE:HG22 | 1:A:40:ILE:O | 2.16 | 0.45 |
| 1:B:40:ILE:HD11 | 1:B:57:THR:CG2 | 2.42 | 0.45 |
| 1:A:417:LEU:N | 1:A:417:LEU:HD23 | 2.19 | 0.45 |
| 1:A:277:GLN:O | 1:A:356:ALA:HA | 2.17 | 0.45 |
| 2:B:600:FAA:C1P | 2:B:600:FAA:C4 | 2.82 | 0.45 |
| 1:B:180:ALA:O | 1:B:194:TRP:HE3 | 2.00 | 0.45 |
| 1:B:194:TRP:HH2 | 1:B:200:MET:HE1 | 1.81 | 0.45 |
| 1:B:389:THR:HB | 1:B:390:PRO:CD | 2.47 | 0.45 |
| 1:A:384:TYR:N | 1:A:384:TYR:CD1 | 2.85 | 0.45 |
| 1:A:309:PRO:CB | 1:A:353:PHE:HE1 | 2.29 | 0.45 |
| 1:A:248:PRO:HG3 | 1:B:257:SER:HB3 | 1.97 | 0.45 |
| 1:B:536:ASP:HA | 1:B:537:PRO:HD3 | 1.47 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:550:PRO:HB2 | 1:B:552:GLN:HE21 | 1.80 | 0.45 |
| 1:A:139:TYR:CE2 | 1:A:241:LEU:CD1 | 3.00 | 0.44 |
| 1:B:426:SER:HB2 | 1:B:502:GLU:HG3 | 1.99 | 0.44 |
| 1:B:93:PHE:N | 1:B:93:PHE:CD1 | 2.85 | 0.44 |
| 1:B:237:LYS:HG3 | 1:B:238:ILE:HG12 | 1.98 | 0.44 |
| 1:A:151:LEU:O | 1:A:155:LEU:HG | 2.17 | 0.44 |
| 1:A:426:SER:HB2 | 1:A:502:GLU:HG3 | 1.99 | 0.44 |
| 1:A:308:VAL:HG13 | 1:A:460:VAL:O | 2.17 | 0.44 |
| 1:B:102:ILE:HD13 | 1:B:102:ILE:HA | 1.71 | 0.44 |
| 1:B:295:ILE:CG2 | 1:B:375:PHE:CE1 | 3.00 | 0.44 |
| 1:A:487:LEU:CD1 | 1:A:491:LEU:HD11 | 2.47 | 0.44 |
| 1:B:283:LEU:O | 1:B:349:GLY:CA | 2.66 | 0.44 |
| 1:B:346:LEU:HB2 | 1:B:348:LEU:HD12 | 1.99 | 0.44 |
| 1:A:220:PRO:HD2 | 3:A:620:HOH:O | 2.17 | 0.44 |
| 1:B:142:VAL:HB | 1:B:146:VAL:CG2 | 2.47 | 0.44 |
| 1:B:139:TYR:CE2 | 1:B:241:LEU:CD1 | 2.99 | 0.44 |
| 1:B:309:PRO:CB | 1:B:353:PHE:HE1 | 2.29 | 0.44 |
| 1:B:513:ILE:O | 1:B:516:THR:HG23 | 2.18 | 0.44 |
| 1:B:131:LEU:HD11 | 1:B:143:GLU:HG3 | 2.00 | 0.44 |
| 1:B:487:LEU:CD1 | 1:B:491:LEU:HD11 | 2.47 | 0.44 |
| 1:B:36:ASN:CB | 1:B:76:ALA:HB3 | 2.46 | 0.44 |
| 1:B:270:MET:HA | 1:B:271:PRO:HD2 | 1.78 | 0.44 |
| 1:A:513:ILE:O | 1:A:516:THR:HG23 | 2.17 | 0.44 |
| 1:B:313:HIS:HB2 | 1:B:351:TRP:CH2 | 2.52 | 0.44 |
| 1:A:313:HIS:HB2 | 1:A:351:TRP:CH2 | 2.52 | 0.44 |
| 1:A:131:LEU:HD11 | 1:A:143:GLU:HG3 | 2.00 | 0.44 |
| 1:B:478:LEU:CD1 | 1:B:478:LEU:N | 2.80 | 0.44 |
| 1:B:384:TYR:CD1 | 1:B:384:TYR:N | 2.85 | 0.44 |
| 1:A:121:LEU:HA | 1:A:121:LEU:HD12 | 1.44 | 0.44 |
| 1:A:16:LEU:HA | 1:A:16:LEU:HD12 | 1.50 | 0.44 |
| 1:A:408:TYR:O | 1:A:411:LEU:HD12 | 2.18 | 0.44 |
| 1:A:506:HIS:CE1 | 1:A:507:LEU:HB2 | 2.53 | 0.44 |
| 1:B:408:TYR:O | 1:B:411:LEU:HD12 | 2.18 | 0.44 |
| 1:B:62:HIS:CD2 | 1:B:66:GLN:HB2 | 2.51 | 0.44 |
| 1:A:300:ARG:HE | 1:A:309:PRO:CD | 2.31 | 0.44 |
| 1:A:291:GLN:O | 1:A:295:ILE:HG13 | 2.18 | 0.44 |
| 1:A:142:VAL:HB | 1:A:146:VAL:CG2 | 2.47 | 0.44 |
| 1:B:151:LEU:HD12 | 1:B:151:LEU:O | 2.18 | 0.44 |
| 1:A:195:MET:CE | 1:B:195:MET:HE1 | 2.48 | 0.44 |
| 1:A:393:SER:HB3 | 1:A:396:ARG:HG3 | 1.99 | 0.44 |
| 1:B:291:GLN:O | 1:B:295:ILE:HG13 | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:300:ARG:HE | 1:B:309:PRO:CD | 2.31 | 0.44 |
| 1:B:83:VAL:HG23 | 1:B:127:MET:HE1 | 1.99 | 0.44 |
| 1:A:346:LEU:HB3 | 1:A:348:LEU:HD11 | 1.98 | 0.44 |
| 1:B:231:GLU:HG2 | 1:B:231:GLU:H | 0.94 | 0.44 |
| 1:B:90:ALA:HB1 | 1:B:95:PHE:O | 2.18 | 0.44 |
| 1:B:48:ASP:HA | 1:B:58:HIS:HE2 | 1.83 | 0.44 |
| 1:A:550:PRO:CB | 1:A:552:GLN:NE2 | 2.77 | 0.44 |
| 1:A:168:VAL:HA | 1:A:169:PRO:HD3 | 1.66 | 0.44 |
| 1:A:102:ILE:CG2 | 1:A:104:ARG:HD2 | 2.48 | 0.44 |
| 1:A:238:ILE:HA | 1:A:241:LEU:HD22 | 1.98 | 0.44 |
| 1:B:188:THR:CB | 1:B:189:PRO:HD2 | 2.47 | 0.44 |
| 1:A:447:CYS:O | 1:A:452:LEU:N | 2.49 | 0.44 |
| 1:A:151:LEU:HD12 | 1:A:151:LEU:O | 2.18 | 0.44 |
| 1:A:432:SER:HB3 | 1:A:435:ASP:HB2 | 2.00 | 0.44 |
| 1:A:180:ALA:O | 1:A:194:TRP:HE3 | 2.00 | 0.43 |
| 1:A:346:LEU:HB2 | 1:A:348:LEU:HD12 | 1.99 | 0.43 |
| 1:B:156:GLU:HG3 | 1:B:161:ARG:CZ | 2.48 | 0.43 |
| 1:A:156:GLU:HG3 | 1:A:161:ARG:CZ | 2.48 | 0.43 |
| 1:B:151:LEU:O | 1:B:155:LEU:HG | 2.17 | 0.43 |
| 1:A:195:MET:HE1 | 1:B:195:MET:CE | 2.48 | 0.43 |
| 1:A:155:LEU:HA | 1:A:155:LEU:HD23 | 1.38 | 0.43 |
| 1:B:89:LEU:HD23 | 1:B:89:LEU:HA | 1.44 | 0.43 |
| 1:B:308:VAL:HG13 | 1:B:460:VAL:O | 2.17 | 0.43 |
| 1:B:307:ASN:HB3 | 1:B:358:TYR:CE1 | 2.53 | 0.43 |
| 1:A:332:GLU:CB | 1:A:333:PRO:HD3 | 2.49 | 0.43 |
| 1:B:269:LEU:HD23 | 1:B:269:LEU:HA | 1.77 | 0.43 |
| 1:A:385:PHE:HB2 | 3:A:606:HOH:O | 2.18 | 0.43 |
| 1:A:389:THR:HB | 1:A:390:PRO:CD | 2.47 | 0.43 |
| 1:A:478:LEU:CD1 | 1:A:478:LEU:N | 2.80 | 0.43 |
| 1:B:447:CYS:O | 1:B:452:LEU:N | 2.49 | 0.43 |
| 1:A:222:ARG:HB2 | 1:A:223:PRO:CD | 2.47 | 0.43 |
| 1:A:201:GLU:O | 1:A:262:VAL:HG13 | 2.18 | 0.43 |
| 1:A:179:ASN:OD1 | 1:A:184:GLY:HA3 | 2.19 | 0.43 |
| 1:A:247:GLY:HA2 | 1:B:256:GLN:HB3 | 2.00 | 0.43 |
| 1:A:90:ALA:HB1 | 1:A:95:PHE:O | 2.18 | 0.43 |
| 1:B:25:ILE:HD12 | 1:B:25:ILE:HA | 1.74 | 0.43 |
| 1:B:179:ASN:OD1 | 1:B:184:GLY:HA3 | 2.19 | 0.43 |
| 1:B:102:ILE:CG2 | 1:B:104:ARG:HD2 | 2.48 | 0.43 |
| 1:A:307:ASN:HB3 | 1:A:358:TYR:CE1 | 2.53 | 0.43 |
| 1:A:14:PRO:HG3 | 1:A:558:TRP:CZ2 | 2.53 | 0.43 |
| 1:A:250:ILE:HD12 | 1:A:254:PHE:HE2 | 1.84 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:280:LEU:CD1 | 1:B:281:ILE:N | 2.78 | 0.43 |
| 1:B:139:TYR:CD1 | 1:B:139:TYR:C | 2.92 | 0.43 |
| 1:B:421:ALA:HA | 3:B:636:HOH:O | 2.18 | 0.43 |
| 1:A:156:GLU:CG | 1:A:161:ARG:NH2 | 2.82 | 0.43 |
| 1:A:90:ALA:HB2 | 1:A:97:LEU:HD11 | 2.01 | 0.43 |
| 1:B:14:PRO:HG3 | 1:B:558:TRP:CZ2 | 2.53 | 0.43 |
| 1:B:432:SER:HB3 | 1:B:435:ASP:HB2 | 2.00 | 0.43 |
| 1:A:48:ASP:HA | 1:A:58:HIS:HE2 | 1.83 | 0.43 |
| 1:B:506:HIS:CE1 | 1:B:507:LEU:HB2 | 2.53 | 0.43 |
| 1:B:156:GLU:CG | 1:B:161:ARG:NH2 | 2.82 | 0.43 |
| 1:B:316:LEU:HA | 1:B:316:LEU:HD12 | 1.69 | 0.43 |
| 1:A:230:PRO:HA | 1:A:233:GLN:CD | 2.39 | 0.43 |
| 1:B:540:ILE:O | 1:B:540:ILE:HG22 | 2.18 | 0.43 |
| 1:A:29:ILE:C | 1:A:31:ILE:H | 2.21 | 0.43 |
| 1:A:139:TYR:CD1 | 1:A:139:TYR:C | 2.92 | 0.43 |
| 1:A:200:MET:HE2 | 1:A:251:ASP:CB | 2.35 | 0.43 |
| 1:A:83:VAL:HG23 | 1:A:127:MET:HE1 | 2.01 | 0.43 |
| 1:A:550:PRO:HB2 | 1:A:552:GLN:CG | 2.42 | 0.43 |
| 1:B:230:PRO:HA | 1:B:233:GLN:CD | 2.39 | 0.43 |
| 1:B:121:LEU:HD12 | 1:B:121:LEU:HA | 1.44 | 0.43 |
| 1:B:29:ILE:C | 1:B:31:ILE:H | 2.21 | 0.43 |
| 1:A:299:LEU:CB | 1:A:305:LEU:HG | 2.49 | 0.43 |
| 1:B:290:LYS:HB2 | 1:B:437:MET:SD | 2.59 | 0.43 |
| 1:B:332:GLU:CB | 1:B:333:PRO:HD3 | 2.49 | 0.43 |
| 1:B:452:LEU:HD23 | 1:B:452:LEU:HA | 1.31 | 0.43 |
| 1:B:283:LEU:O | 1:B:350:ARG:N | 2.48 | 0.42 |
| 1:A:545:LYS:HE3 | 1:A:546:SER:OG | 2.19 | 0.42 |
| 1:B:368:TRP:HA | 1:B:368:TRP:CE3 | 2.54 | 0.42 |
| 1:A:361:GLU:HB2 | 1:A:364:ARG:NH2 | 2.34 | 0.42 |
| 1:B:359:GLY:HA3 | 1:B:360:PRO:HD3 | 1.79 | 0.42 |
| 1:A:316:LEU:HD11 | 1:A:413:TRP:NE1 | 2.34 | 0.42 |
| 1:B:137:GLY:O | 1:B:138:ALA:HB3 | 2.19 | 0.42 |
| 1:B:201:GLU:O | 1:B:262:VAL:HG13 | 2.19 | 0.42 |
| 1:A:370:THR:O | 1:A:374:ALA:N | 2.52 | 0.42 |
| 1:B:299:LEU:CB | 1:B:305:LEU:HG | 2.49 | 0.42 |
| 1:A:429:ALA:O | 1:A:465:MET:HB2 | 2.19 | 0.42 |
| 1:A:507:LEU:HD23 | 1:A:510:MET:CE | 2.50 | 0.42 |
| 1:B:90:ALA:HB2 | 1:B:97:LEU:HD11 | 2.01 | 0.42 |
| 1:A:36:ASN:HB3 | 1:A:76:ALA:O | 2.20 | 0.42 |
| 1:A:88:GLY:O | 1:A:92:LYS:N | 2.51 | 0.42 |
| 1:A:309:PRO:CB | 1:A:353:PHE:CE1 | 3.03 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:346:LEU:CB | 1:A:348:LEU:CD1 | 2.97 | 0.42 |
| 1:A:537:PRO:CD | 1:A:538:ASN:N | 2.82 | 0.42 |
| 1:A:549:TRP:HA | 1:A:550:PRO:HD3 | 1.75 | 0.42 |
| 1:B:361:GLU:N | 1:B:364:ARG:HH21 | 2.18 | 0.42 |
| 1:A:195:MET:HE1 | 1:B:195:MET:HE1 | 2.01 | 0.42 |
| 1:A:368:TRP:CE3 | 1:A:368:TRP:HA | 2.55 | 0.42 |
| 1:B:545:LYS:HE3 | 1:B:546:SER:OG | 2.19 | 0.42 |
| 1:B:448:GLN:HB3 | 1:B:449:GLU:H | 1.53 | 0.42 |
| 1:A:202:VAL:CG2 | 1:A:261:ILE:N | 2.83 | 0.42 |
| 1:B:370:THR:O | 1:B:374:ALA:N | 2.52 | 0.42 |
| 1:A:257:SER:CB | 1:B:248:PRO:HG3 | 2.50 | 0.42 |
| 1:B:378:ILE:HA | 1:B:379:PRO:HD2 | 1.78 | 0.42 |
| 1:A:200:MET:CE | 1:A:251:ASP:CB | 2.95 | 0.42 |
| 1:A:290:LYS:HB2 | 1:A:437:MET:SD | 2.59 | 0.42 |
| 1:A:40:ILE:CD1 | 1:A:57:THR:CG2 | 2.98 | 0.42 |
| 1:A:231:GLU:H | 1:A:231:GLU:HG2 | 0.94 | 0.42 |
| 1:B:202:VAL:CG2 | 1:B:261:ILE:N | 2.83 | 0.42 |
| 1:A:102:ILE:HB | 2:A:600:FAA:O2P | 2.19 | 0.42 |
| 1:B:102:ILE:HB | 2:B:600:FAA:O2P | 2.19 | 0.42 |
| 1:B:445:LYS:HE2 | 1:B:449:GLU:OE2 | 2.20 | 0.42 |
| 1:B:10:LEU:CD2 | 1:B:41:SER:C | 2.88 | 0.42 |
| 1:B:361:GLU:HB2 | 1:B:364:ARG:NH2 | 2.34 | 0.42 |
| 1:B:354:TYR:HD2 | 1:B:395:LEU:CD1 | 2.33 | 0.42 |
| 1:B:108:TYR:HA | 1:B:506:HIS:HA | 2.02 | 0.42 |
| 1:B:516:THR:C | 1:B:518:ASN:H | 2.23 | 0.42 |
| 1:B:282:THR:O | 1:B:283:LEU:HD23 | 2.20 | 0.42 |
| 1:A:283:LEU:O | 1:A:349:GLY:CA | 2.66 | 0.42 |
| 1:A:283:LEU:O | 1:A:350:ARG:N | 2.48 | 0.42 |
| 1:B:317:ASP:O | 1:B:320:VAL:HB | 2.20 | 0.42 |
| 1:A:10:LEU:CD2 | 1:A:41:SER:C | 2.88 | 0.42 |
| 1:B:36:ASN:HB3 | 1:B:76:ALA:O | 2.19 | 0.42 |
| 1:A:527:PHE:CE1 | 1:B:204:LEU:HD22 | 2.55 | 0.42 |
| 1:B:429:ALA:O | 1:B:465:MET:HB2 | 2.20 | 0.41 |
| 1:B:346:LEU:CB | 1:B:348:LEU:CD1 | 2.97 | 0.41 |
| 1:A:229:LYS:HB2 | 1:A:231:GLU:HG3 | 2.02 | 0.41 |
| 1:B:95:PHE:CE1 | 1:B:119:VAL:CG2 | 3.00 | 0.41 |
| 1:B:532:LYS:NZ | 1:B:541:ILE:HB | 2.35 | 0.41 |
| 1:A:327:TYR:O | 1:A:328:SER:HB2 | 2.19 | 0.41 |
| 1:B:327:TYR:O | 1:B:328:SER:HB2 | 2.19 | 0.41 |
| 1:B:102:ILE:HG22 | 1:B:104:ARG:H | 1.85 | 0.41 |
| 1:B:314:ILE:HG22 | 1:B:350:ARG:O | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:282:THR:O | 1:A:283:LEU:HD23 | 2.20 | 0.41 |
| 1:B:69:PHE:HB3 | 1:B:113:PRO:O | 2.20 | 0.41 |
| 1:B:229:LYS:HB2 | 1:B:231:GLU:HG3 | 2.02 | 0.41 |
| 1:A:532:LYS:NZ | 1:A:541:ILE:HB | 2.35 | 0.41 |
| 1:A:155:LEU:N | 1:A:155:LEU:HD23 | 2.19 | 0.41 |
| 1:A:89:LEU:HA | 1:A:89:LEU:HD23 | 1.45 | 0.41 |
| 1:B:250:ILE:HD12 | 1:B:254:PHE:HE2 | 1.84 | 0.41 |
| 1:A:172:GLY:HA3 | 1:A:408:TYR:CE1 | 2.55 | 0.41 |
| 1:A:502:GLU:CG | 1:A:503:TYR:N | 2.82 | 0.41 |
| 1:B:361:GLU:O | 1:B:365:ARG:HB2 | 2.21 | 0.41 |
| 1:A:102:ILE:HG22 | 1:A:104:ARG:H | 1.85 | 0.41 |
| 1:A:138:ALA:HA | 1:A:164:LEU:HD21 | 2.03 | 0.41 |
| 2:B:600:FAA:C9A | 2:B:600:FAA:H6P | 2.50 | 0.41 |
| 1:B:283:LEU:N | 1:B:283:LEU:HD23 | 2.35 | 0.41 |
| 1:B:278:SER:OG | 1:B:399:ASP:OD2 | 2.28 | 0.41 |
| 1:A:33:GLY:C | 1:A:35:GLU:N | 2.73 | 0.41 |
| 1:B:222:ARG:HB2 | 1:B:223:PRO:CD | 2.47 | 0.41 |
| 1:A:454:PHE:CD1 | 1:A:455:ILE:N | 2.89 | 0.41 |
| 1:B:351:TRP:HA | 1:B:351:TRP:HE3 | 1.81 | 0.41 |
| 1:A:317:ASP:O | 1:A:320:VAL:HB | 2.20 | 0.41 |
| 1:A:540:ILE:O | 1:A:540:ILE:HG22 | 2.18 | 0.41 |
| 1:A:361:GLU:N | 1:A:364:ARG:HH21 | 2.18 | 0.41 |
| 1:A:520:ASN:O | 1:A:521:ASN:CB | 2.68 | 0.41 |
| 1:A:137:GLY:O | 1:A:138:ALA:HB3 | 2.19 | 0.41 |
| 1:B:297:ARG:HG2 | 1:B:298:PRO:HD3 | 2.03 | 0.41 |
| 1:B:505:THR:CG2 | 1:B:506:HIS:N | 2.74 | 0.41 |
| 1:A:188:THR:CB | 1:A:189:PRO:HD2 | 2.47 | 0.41 |
| 1:B:316:LEU:HD11 | 1:B:413:TRP:NE1 | 2.34 | 0.41 |
| 1:B:307:ASN:N | 1:B:307:ASN:OD1 | 2.50 | 0.41 |
| 1:A:363:ILE:CD1 | 1:A:363:ILE:N | 2.80 | 0.41 |
| 1:A:370:THR:O | 1:A:374:ALA:HB2 | 2.20 | 0.41 |
| 1:A:368:TRP:NE1 | 1:A:372:LYS:HD2 | 2.36 | 0.41 |
| 1:B:309:PRO:CB | 1:B:353:PHE:CE1 | 3.03 | 0.41 |
| 1:B:200:MET:CE | 1:B:251:ASP:CB | 2.95 | 0.41 |
| 1:B:341:LYS:HA | 1:B:344:LYS:HE2 | 2.03 | 0.41 |
| 1:B:537:PRO:CD | 1:B:538:ASN:N | 2.82 | 0.41 |
| 1:A:69:PHE:HB3 | 1:A:113:PRO:O | 2.20 | 0.41 |
| 1:A:278:SER:OG | 1:A:399:ASP:OD2 | 2.28 | 0.41 |
| 1:A:311:ILE:HG12 | 1:A:353:PHE:CD1 | 2.56 | 0.41 |
| 1:B:172:GLY:HA3 | 1:B:408:TYR:CE1 | 2.55 | 0.41 |
| 1:A:132:GLU:CG | 1:A:133:VAL:N | 2.72 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:283:LEU:HA | 1:B:284:PRO:HD3 | 1.76 | 0.41 |
| 1:A:387:GLU:C | 1:A:389:THR:H | 2.24 | 0.41 |
| 2:A:600:FAA:H6P | 2:A:600:FAA:C9A | 2.50 | 0.41 |
| 1:A:112:ALA:O | 1:A:507:LEU:HD11 | 2.21 | 0.41 |
| 1:A:58:HIS:CD2 | 1:A:59:ASP:O | 2.74 | 0.41 |
| 1:B:421:ALA:O | 1:B:472:VAL:HA | 2.21 | 0.41 |
| 1:B:108:TYR:CE1 | 1:B:505:THR:CA | 3.04 | 0.41 |
| 1:A:479:ILE:HG22 | 1:A:483:LYS:HE3 | 2.02 | 0.41 |
| 1:B:342:ILE:HG21 | 1:B:342:ILE:HD13 | 1.83 | 0.41 |
| 1:A:314:ILE:HG22 | 1:A:350:ARG:O | 2.20 | 0.41 |
| 1:A:437:MET:CE | 1:A:437:MET:HA | 2.51 | 0.41 |
| 1:B:202:VAL:CG2 | 1:B:203:VAL:N | 2.84 | 0.41 |
| 1:A:272:ASN:OD1 | 1:A:273:PRO:HD2 | 2.21 | 0.41 |
| 1:B:272:ASN:OD1 | 1:B:273:PRO:HD2 | 2.21 | 0.41 |
| 1:B:217:LEU:HA | 1:B:217:LEU:HD12 | 1.33 | 0.41 |
| 1:B:166:LEU:HD23 | 1:B:269:LEU:CD2 | 2.50 | 0.41 |
| 1:B:166:LEU:HA | 1:B:166:LEU:HD23 | 1.82 | 0.41 |
| 1:B:478:LEU:HD12 | 1:B:478:LEU:N | 2.36 | 0.41 |
| 1:B:368:TRP:NE1 | 1:B:372:LYS:HD2 | 2.36 | 0.41 |
| 1:B:550:PRO:HB2 | 1:B:552:GLN:CG | 2.42 | 0.41 |
| 1:A:98:TRP:CD2 | 1:A:113:PRO:HA | 2.56 | 0.41 |
| 1:A:272:ASN:HA | 1:A:273:PRO:HD3 | 1.55 | 0.41 |
| 1:A:361:GLU:O | 1:A:365:ARG:HB2 | 2.21 | 0.41 |
| 1:A:383:PHE:N | 1:A:383:PHE:CD1 | 2.89 | 0.41 |
| 1:A:478:LEU:HD12 | 1:A:478:LEU:N | 2.36 | 0.41 |
| 1:B:520:ASN:O | 1:B:521:ASN:CB | 2.68 | 0.41 |
| 1:B:370:THR:O | 1:B:374:ALA:HB2 | 2.20 | 0.41 |
| 1:B:434:GLU:HB3 | 1:B:435:ASP:H | 1.70 | 0.41 |
| 1:A:545:LYS:C | 1:A:547:GLY:N | 2.72 | 0.41 |
| 1:A:421:ALA:O | 1:A:472:VAL:HA | 2.21 | 0.40 |
| 1:A:166:LEU:HD23 | 1:A:269:LEU:CD2 | 2.50 | 0.40 |
| 1:A:378:ILE:HA | 1:A:379:PRO:HD2 | 1.78 | 0.40 |
| 1:A:445:LYS:HE2 | 1:A:449:GLU:OE2 | 2.20 | 0.40 |
| 1:B:98:TRP:CD2 | 1:B:113:PRO:HA | 2.56 | 0.40 |
| 1:A:59:ASP:HA | 1:A:60:PRO:HD3 | 1.80 | 0.40 |
| 1:B:454:PHE:CD1 | 1:B:455:ILE:N | 2.89 | 0.40 |
| 1:B:58:HIS:HD2 | 1:B:59:ASP:O | 2.04 | 0.40 |
| 1:B:8:ARG:HA | 1:B:9:PRO:HD2 | 1.90 | 0.40 |
| 1:A:517:TYR:OH | 1:B:214:MET:CE | 2.69 | 0.40 |
| 1:B:222:ARG:HA | 1:B:223:PRO:HD3 | 1.63 | 0.40 |
| 1:B:387:GLU:C | 1:B:389:THR:H | 2.24 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:310:THR:HA | 1:B:459:THR:HA | 2.03 | 0.40 |
| 1:A:27:ASP:OD1 | 1:A:27:ASP:N | 2.54 | 0.40 |
| 1:B:27:ASP:OD1 | 1:B:27:ASP:N | 2.54 | 0.40 |
| 1:A:108:TYR:HA | 1:A:506:HIS:HA | 2.02 | 0.40 |
| 1:A:516:THR:C | 1:A:518:ASN:H | 2.23 | 0.40 |
| 1:B:112:ALA:O | 1:B:507:LEU:HD11 | 2.21 | 0.40 |
| 1:A:283:LEU:HA | 1:A:284:PRO:HD3 | 1.76 | 0.40 |
| 1:A:341:LYS:HA | 1:A:344:LYS:HE2 | 2.03 | 0.40 |
| 1:B:40:ILE:CD1 | 1:B:57:THR:CG2 | 2.98 | 0.40 |
| 1:B:10:LEU:HD21 | 1:B:42:SER:C | 2.42 | 0.40 |
| 1:B:33:GLY:C | 1:B:35:GLU:N | 2.73 | 0.40 |
| 1:A:8:ARG:H | 1:A:8:ARG:HG3 | 1.61 | 0.40 |
| 1:A:308:VAL:HA | 1:A:309:PRO:HD2 | 1.87 | 0.40 |
| 1:B:54:PRO:HD3 | 1:B:104:ARG:HH21 | 1.86 | 0.40 |
| 1:B:311:ILE:HG12 | 1:B:353:PHE:CD1 | 2.56 | 0.40 |
| 1:B:188:THR:CB | 1:B:189:PRO:CD | 2.98 | 0.40 |
| 1:B:552:GLN:N | 1:B:552:GLN:CD | 2.75 | 0.40 |
| 1:B:138:ALA:HA | 1:B:164:LEU:HD21 | 2.03 | 0.40 |
| 1:A:421:ALA:HB3 | 1:A:473:PHE:CZ | 2.57 | 0.40 |
| 1:A:108:TYR:CE1 | 1:A:505:THR:HA | 2.56 | 0.40 |
| 1:B:75:VAL:O | 1:B:77:PRO:HD2 | 2.22 | 0.40 |
| 1:B:344:LYS:HG3 | 1:B:345:GLN:N | 2.37 | 0.40 |
| 1:A:342:ILE:HG22 | 1:A:342:ILE:O | 2.22 | 0.40 |
| 1:A:156:GLU:CB | 1:A:161:ARG:HH21 | 2.27 | 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 | 553/560 (99%) | 470 (85%) | 69 (12%) | 14 (2%) | 7 18 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|-----------|-----------|----------|-------------|----|
| 1 | B | 553/560 (99%) | 470 (85%) | 69 (12%) | 14 (2%) | 7 | 18 |
| All | All | 1106/1120 (99%) | 940 (85%) | 138 (12%) | 28 (2%) | 7 | 18 |

All (28) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 44 | ASP |
| 1 | B | 44 | ASP |
| 1 | A | 30 | ARG |
| 1 | A | 46 | ILE |
| 1 | A | 328 | SER |
| 1 | B | 30 | ARG |
| 1 | B | 46 | ILE |
| 1 | B | 328 | SER |
| 1 | A | 105 | ASN |
| 1 | A | 199 | GLY |
| 1 | A | 508 | ALA |
| 1 | B | 105 | ASN |
| 1 | B | 199 | GLY |
| 1 | A | 329 | SER |
| 1 | A | 408 | TYR |
| 1 | B | 329 | SER |
| 1 | B | 408 | TYR |
| 1 | B | 508 | ALA |
| 1 | A | 388 | ASP |
| 1 | B | 388 | ASP |
| 1 | A | 248 | PRO |
| 1 | B | 248 | PRO |
| 1 | A | 390 | PRO |
| 1 | B | 390 | PRO |
| 1 | A | 60 | PRO |
| 1 | B | 60 | PRO |
| 1 | A | 223 | PRO |
| 1 | B | 223 | PRO |

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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 | 475/482 (98%) | 452 (95%) | 23 (5%) | 31 | 62 |
| 1 | B | 475/482 (98%) | 452 (95%) | 23 (5%) | 31 | 62 |
| All | All | 950/964 (98%) | 904 (95%) | 46 (5%) | 31 | 62 |

All (46) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 10 | LEU |
| 1 | A | 63 | VAL |
| 1 | A | 65 | ASP |
| 1 | A | 95 | PHE |
| 1 | A | 114 | ARG |
| 1 | A | 128 | ASN |
| 1 | A | 134 | ASN |
| 1 | A | 220 | PRO |
| 1 | A | 231 | GLU |
| 1 | A | 241 | LEU |
| 1 | A | 251 | ASP |
| 1 | A | 310 | THR |
| 1 | A | 346 | LEU |
| 1 | A | 363 | ILE |
| 1 | A | 373 | ASP |
| 1 | A | 409 | ASP |
| 1 | A | 413 | TRP |
| 1 | A | 435 | ASP |
| 1 | A | 437 | MET |
| 1 | A | 443 | THR |
| 1 | A | 466 | HIS |
| 1 | A | 478 | LEU |
| 1 | A | 552 | GLN |
| 1 | B | 10 | LEU |
| 1 | B | 63 | VAL |
| 1 | B | 65 | ASP |
| 1 | B | 95 | PHE |
| 1 | B | 114 | ARG |
| 1 | B | 128 | ASN |
| 1 | B | 134 | ASN |
| 1 | B | 220 | PRO |
| 1 | B | 231 | GLU |
| 1 | B | 241 | LEU |
| 1 | B | 251 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 310 | THR |
| 1 | B | 346 | LEU |
| 1 | B | 363 | ILE |
| 1 | B | 373 | ASP |
| 1 | B | 409 | ASP |
| 1 | B | 413 | TRP |
| 1 | B | 435 | ASP |
| 1 | B | 437 | MET |
| 1 | B | 443 | THR |
| 1 | B | 466 | HIS |
| 1 | B | 478 | LEU |
| 1 | B | 552 | GLN |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 58 | HIS |
| 1 | A | 66 | GLN |
| 1 | A | 91 | ASN |
| 1 | A | 152 | HIS |
| 1 | A | 197 | HIS |
| 1 | A | 240 | HIS |
| 1 | A | 277 | GLN |
| 1 | A | 403 | GLN |
| 1 | A | 467 | HIS |
| 1 | A | 485 | GLN |
| 1 | A | 520 | ASN |
| 1 | A | 552 | GLN |
| 1 | B | 58 | HIS |
| 1 | B | 66 | GLN |
| 1 | B | 91 | ASN |
| 1 | B | 152 | HIS |
| 1 | B | 197 | HIS |
| 1 | B | 240 | HIS |
| 1 | B | 277 | GLN |
| 1 | B | 403 | GLN |
| 1 | B | 467 | HIS |
| 1 | B | 485 | GLN |
| 1 | B | 520 | ASN |
| 1 | B | 552 | GLN |

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | # $ Z > 2$ | Counts | RMSZ | # $ Z > 2$ |
| 2 | FAA | A | 600 | 1 | 55,67,67 | 0.90 | 1 (1%) | 61,102,102 | 2.08 | 5 (8%) |
| 2 | FAA | B | 600 | 1 | 55,67,67 | 0.89 | 1 (1%) | 61,102,102 | 2.08 | 5 (8%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 2 | FAA | A | 600 | 1 | - | 0/34/54/54 | 0/7/7/7 |
| 2 | FAA | B | 600 | 1 | - | 0/34/54/54 | 0/7/7/7 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 2 | A | 600 | FAA | C4-N3 | 3.38 | 1.39 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 2 | B | 600 | FAA | C4-N3 | 3.40 | 1.39 | 1.33 |

All (10) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 2 | A | 600 | FAA | C7P-N5-C5X | -11.46 | 102.71 | 120.13 |
| 2 | B | 600 | FAA | C7P-N5-C5X | -11.46 | 102.72 | 120.13 |
| 2 | B | 600 | FAA | C4X-C4-N3 | -5.62 | 115.91 | 123.59 |
| 2 | A | 600 | FAA | C4X-C4-N3 | -5.59 | 115.94 | 123.59 |
| 2 | A | 600 | FAA | C2B-C1B-N9A | -2.78 | 110.05 | 114.29 |
| 2 | A | 600 | FAA | C4X-C10-N10 | -2.77 | 118.88 | 120.52 |
| 2 | B | 600 | FAA | C2B-C1B-N9A | -2.77 | 110.06 | 114.29 |
| 2 | B | 600 | FAA | C4X-C10-N10 | -2.75 | 118.90 | 120.52 |
| 2 | B | 600 | FAA | C4-N3-C2 | 7.44 | 121.67 | 115.25 |
| 2 | A | 600 | FAA | C4-N3-C2 | 7.48 | 121.72 | 115.25 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 26 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2 | A | 600 | FAA | 13 | 0 |
| 2 | B | 600 | FAA | 13 | 0 |

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.