# WORLDWIDE PDB

## PROTEIN DATA BANK

# Full wwPDB X-ray Structure Validation Report (i)

Aug 28, 2023 – 10:33 AM EDT

| | | |
|---|---|---|
| PDB ID | : | 3KLF |
| Title | : | Crystal structure of wild-type HIV-1 Reverse Transcriptase crosslinked to a DSDNA with a bound excision product, AZTPPPPA |
| Authors | : | Tu, X.; Das, K.; Sarafianos, S.G.; Arnold, E. |
| Deposited on | : | 2009-11-07 |
| Resolution | : | 3.15 Å(reported) |

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

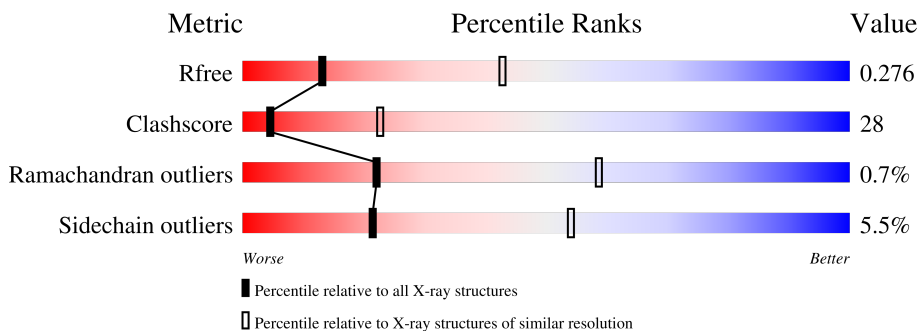| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.35 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.35 |

# 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 3.15 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.
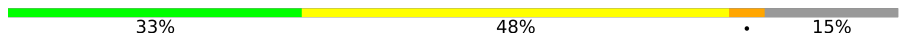
| Metric | Percentile Ranks | Value |
|--------|------------------|-------|
| Rfree | | 0.276 |
| Clashscore | | 28 |
| Ramachandran outliers | | 0.7% |
| Sidechain outliers | | 5.5% |

*Worse* — *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
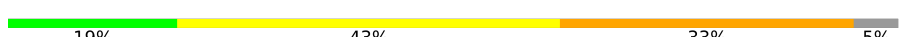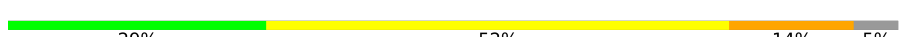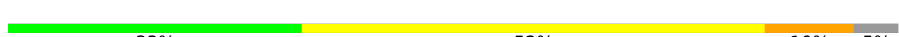
| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|--------|--------------------------|----------------------------------------------------|
| R$_{free}$ | 130704 | 1665 (3.20-3.12) |
| Clashscore | 141614 | 1804 (3.20-3.12) |
| Ramachandran outliers | 138981 | 1770 (3.20-3.12) |
| Sidechain outliers | 138945 | 1769 (3.20-3.12) |

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 557 | 48% 46% 5% · |
| 1 | E | 557 | 50% 45% · · |
| 1 | I | 557 | 50% 45% · · |
| 1 | M | 557 | 48% 47% · · |
| 2 | B | 444 | 55% 36% · 7% |
| 2 | F | 444 | 58% 32% · 7% |
| 2 | J | 444 | 57% 34% · 7% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2 | N | 444 | 55%     36%     7% |
| 3 | C | 27 | 33%     48%     15% |
| 3 | G | 27 | 30%     56%     15% |
| 3 | K | 27 | 30%     56%     15% |
| 3 | O | 27 | 30%     56%     15% |
| 4 | D | 21 | 19%     43%     33%     5% |
| 4 | H | 21 | 29%     52%     14%     5% |
| 4 | L | 21 | 33%     52%     10%     5% |
| 4 | P | 21 | 29%     57%     10%     5% |

# 2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 35440 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 Reverse transcriptase/ribonuclease H.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|-----|---------|---------|-------|
| 1 | A | 553 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4499 | 2912 | 748 | 831 | 8 | | | |
| 1 | E | 553 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4499 | 2912 | 748 | 831 | 8 | | | |
| 1 | I | 553 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4499 | 2912 | 748 | 831 | 8 | | | |
| 1 | M | 553 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4499 | 2912 | 748 | 831 | 8 | | | |

There are 16 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------|-----------|
| A | -1 | MET | - | expression tag | UNP P03366 |
| A | 0 | VAL | - | expression tag | UNP P03366 |
| A | 258 | CYS | GLN | engineered mutation | UNP P03366 |
| A | 280 | SER | CYS | engineered mutation | UNP P03366 |
| E | -1 | MET | - | expression tag | UNP P03366 |
| E | 0 | VAL | - | expression tag | UNP P03366 |
| E | 258 | CYS | GLN | engineered mutation | UNP P03366 |
| E | 280 | SER | CYS | engineered mutation | UNP P03366 |
| I | -1 | MET | - | expression tag | UNP P03366 |
| I | 0 | VAL | - | expression tag | UNP P03366 |
| I | 258 | CYS | GLN | engineered mutation | UNP P03366 |
| I | 280 | SER | CYS | engineered mutation | UNP P03366 |
| M | -1 | MET | - | expression tag | UNP P03366 |
| M | 0 | VAL | - | expression tag | UNP P03366 |
| M | 258 | CYS | GLN | engineered mutation | UNP P03366 |
| M | 280 | SER | CYS | engineered mutation | UNP P03366 |

- Molecule 2 is a protein called p51 RT.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | B | 413 | Total 3405 | C 2215 | N 564 | O 620 | S 6 | 0 | 0 | 0 |
| 2 | F | 413 | Total 3405 | C 2215 | N 564 | O 620 | S 6 | 0 | 0 | 0 |
| 2 | J | 413 | Total 3405 | C 2215 | N 564 | O 620 | S 6 | 0 | 0 | 0 |
| 2 | N | 413 | Total 3405 | C 2215 | N 564 | O 620 | S 6 | 0 | 0 | 0 |

There are 68 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| B | -15 | MET | - | expression tag | UNP P03366 |
| B | -14 | ALA | - | expression tag | UNP P03366 |
| B | -13 | HIS | - | expression tag | UNP P03366 |
| B | -12 | HIS | - | expression tag | UNP P03366 |
| B | -11 | HIS | - | expression tag | UNP P03366 |
| B | -10 | HIS | - | expression tag | UNP P03366 |
| B | -9 | HIS | - | expression tag | UNP P03366 |
| B | -8 | HIS | - | expression tag | UNP P03366 |
| B | -7 | ALA | - | expression tag | UNP P03366 |
| B | -6 | LEU | - | expression tag | UNP P03366 |
| B | -5 | GLU | - | expression tag | UNP P03366 |
| B | -4 | VAL | - | expression tag | UNP P03366 |
| B | -3 | LEU | - | expression tag | UNP P03366 |
| B | -2 | PHE | - | expression tag | UNP P03366 |
| B | -1 | GLN | - | expression tag | UNP P03366 |
| B | 0 | GLY | - | expression tag | UNP P03366 |
| B | 280 | SER | CYS | engineered mutation | UNP P03366 |
| F | -15 | MET | - | expression tag | UNP P03366 |
| F | -14 | ALA | - | expression tag | UNP P03366 |
| F | -13 | HIS | - | expression tag | UNP P03366 |
| F | -12 | HIS | - | expression tag | UNP P03366 |
| F | -11 | HIS | - | expression tag | UNP P03366 |
| F | -10 | HIS | - | expression tag | UNP P03366 |
| F | -9 | HIS | - | expression tag | UNP P03366 |
| F | -8 | HIS | - | expression tag | UNP P03366 |
| F | -7 | ALA | - | expression tag | UNP P03366 |
| F | -6 | LEU | - | expression tag | UNP P03366 |
| F | -5 | GLU | - | expression tag | UNP P03366 |
| F | -4 | VAL | - | expression tag | UNP P03366 |
| F | -3 | LEU | - | expression tag | UNP P03366 |
| F | -2 | PHE | - | expression tag | UNP P03366 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|:---:|:---:|:---:|:---:|:---:|:---:|
| F | -1 | GLN | - | expression tag | UNP P03366 |
| F | 0 | GLY | - | expression tag | UNP P03366 |
| F | 280 | SER | CYS | engineered mutation | UNP P03366 |
| J | -15 | MET | - | expression tag | UNP P03366 |
| J | -14 | ALA | - | expression tag | UNP P03366 |
| J | -13 | HIS | - | expression tag | UNP P03366 |
| J | -12 | HIS | - | expression tag | UNP P03366 |
| J | -11 | HIS | - | expression tag | UNP P03366 |
| J | -10 | HIS | - | expression tag | UNP P03366 |
| J | -9 | HIS | - | expression tag | UNP P03366 |
| J | -8 | HIS | - | expression tag | UNP P03366 |
| J | -7 | ALA | - | expression tag | UNP P03366 |
| J | -6 | LEU | - | expression tag | UNP P03366 |
| J | -5 | GLU | - | expression tag | UNP P03366 |
| J | -4 | VAL | - | expression tag | UNP P03366 |
| J | -3 | LEU | - | expression tag | UNP P03366 |
| J | -2 | PHE | - | expression tag | UNP P03366 |
| J | -1 | GLN | - | expression tag | UNP P03366 |
| J | 0 | GLY | - | expression tag | UNP P03366 |
| J | 280 | SER | CYS | engineered mutation | UNP P03366 |
| N | -15 | MET | - | expression tag | UNP P03366 |
| N | -14 | ALA | - | expression tag | UNP P03366 |
| N | -13 | HIS | - | expression tag | UNP P03366 |
| N | -12 | HIS | - | expression tag | UNP P03366 |
| N | -11 | HIS | - | expression tag | UNP P03366 |
| N | -10 | HIS | - | expression tag | UNP P03366 |
| N | -9 | HIS | - | expression tag | UNP P03366 |
| N | -8 | HIS | - | expression tag | UNP P03366 |
| N | -7 | ALA | - | expression tag | UNP P03366 |
| N | -6 | LEU | - | expression tag | UNP P03366 |
| N | -5 | GLU | - | expression tag | UNP P03366 |
| N | -4 | VAL | - | expression tag | UNP P03366 |
| N | -3 | LEU | - | expression tag | UNP P03366 |
| N | -2 | PHE | - | expression tag | UNP P03366 |
| N | -1 | GLN | - | expression tag | UNP P03366 |
| N | 0 | GLY | - | expression tag | UNP P03366 |
| N | 280 | SER | CYS | engineered mutation | UNP P03366 |

- Molecule 3 is a DNA chain called DNA (5'-D(*AP*T*GP*CP*AP*TP*GP*GP*CP*GP*C P*CP*CP*GP*AP*AP*CP*AP*GP*GP*GP*AP*CP*TP*GP*TP*G)-3').

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|---------|-------|
| 3 | C | 23 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 473 | 223 | 95 | 133 | 22 | | | |
| 3 | G | 23 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 473 | 223 | 95 | 133 | 22 | | | |
| 3 | K | 23 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 473 | 223 | 95 | 133 | 22 | | | |
| 3 | O | 23 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 473 | 223 | 95 | 133 | 22 | | | |

- Molecule 4 is a DNA chain called DNA (5'-D(*A*CP*AP*GP*TP*CP*CP*CP*TP*GP*T P*TP*CP*GP*GP*(MRG)P*CP*GP*CP*CP*(2DA))-3').

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---|---------|---------|-------|
| 4 | D | 20 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 406 | 195 | 72 | 119 | 19 | 1 | | | |
| 4 | H | 20 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 406 | 195 | 72 | 119 | 19 | 1 | | | |
| 4 | L | 20 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 406 | 195 | 72 | 119 | 19 | 1 | | | |
| 4 | P | 20 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 406 | 195 | 72 | 119 | 19 | 1 | | | |

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 5 | A | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 5 | E | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 5 | I | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 5 | M | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |

- Molecule 6 is [[[[(2R,3S,4R,5R)-5-(6-aminopurin-9-yl)-3,4-dihydroxy-oxolan-2-yl]methoxy-hydroxy-phosphoryl]oxy-hydroxy-phosphoryl]oxy-hydroxy-phosphoryl] [(2S,3S,5R)-3-azido-5-(5-methyl-2,4-dioxo-pyrimidin-1-yl)oxolan-2-yl]methyl hydrogen phosphate (three-letter code: ZP4) (formula: $C_{20}H_{28}N_{10}O_{19}P_4$).
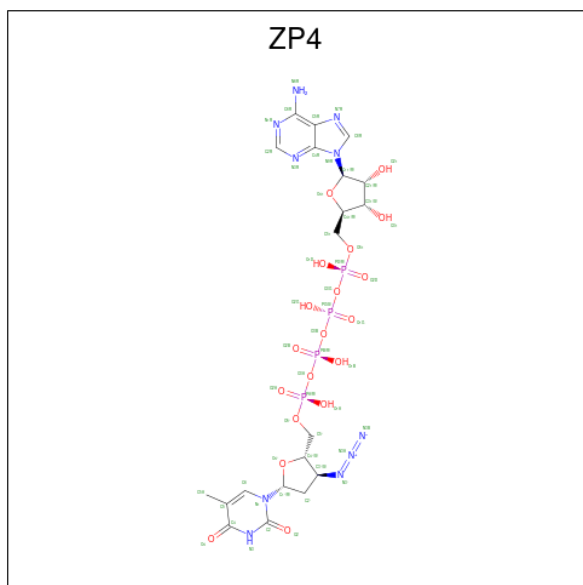
ZP4

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 6 | A | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 20 | 10 | 19 | 4 | | |
| 6 | E | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 20 | 10 | 19 | 4 | | |
| 6 | I | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 20 | 10 | 19 | 4 | | |
| 6 | M | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 20 | 10 | 19 | 4 | | |

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



GOL
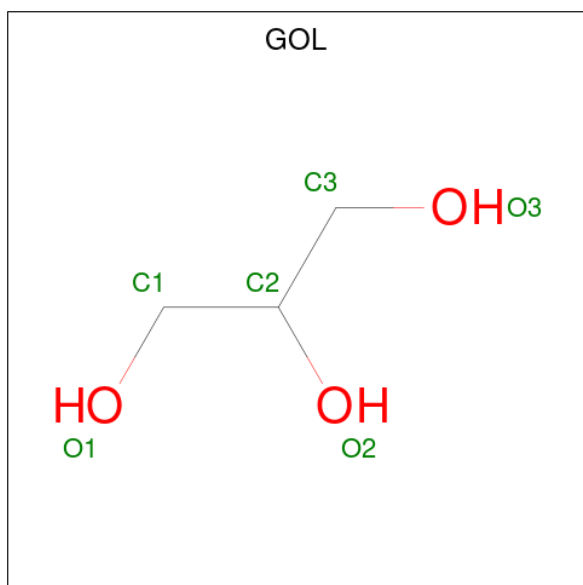
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 7 | B | 1 | Total 6 | C 3 | O 3 | 0 | 0 |
| 7 | F | 1 | Total 6 | C 3 | O 3 | 0 | 0 |

- Molecule 8 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 8 | A | 12 | Total 12 | O 12 | 0 | 0 |
| 8 | B | 9 | Total 9 | O 9 | 0 | 0 |
| 8 | E | 11 | Total 11 | O 11 | 0 | 0 |
| 8 | F | 12 | Total 12 | O 12 | 0 | 0 |
| 8 | I | 10 | Total 10 | O 10 | 0 | 0 |
| 8 | J | 5 | Total 5 | O 5 | 0 | 0 |
| 8 | M | 3 | Total 3 | O 3 | 0 | 0 |
| 8 | N | 5 | Total 5 | O 5 | 0 | 0 |
| 8 | C | 1 | Total 1 | O 1 | 0 | 0 |
| 8 | G | 3 | Total 3 | O 3 | 0 | 0 |
| 8 | K | 1 | Total 1 | O 1 | 0 | 0 |
| 8 | L | 2 | Total 2 | O 2 | 0 | 0 |
| 8 | O | 2 | Total 2 | O 2 | 0 | 0 |

# 3 Residue-property plots ⓘ

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

• Molecule 1: Reverse transcriptase/ribonuclease H

Chain A:



• Molecule 1: Reverse transcriptase/ribonuclease H

Chain E:

I244 V245 L246 P247 D250 S251 W252 T253 V254 K259 L260 L264 N265 W266 Q269 R277 Q278 L279 S280 K281 L282 L283 R284 G285 T286 K287 A288 L289 T290 E291 V292 I293 P294 L295 T296 E297 E298 A299 E302 L303 A304 E305 E312 P313 V314 H315 G316 V317 Y318 Y319 D320 P321

D324 L325 I326 A327 E328 I329 Q330 K331 Q332 G335 Q336 W337 T338 Y339 Q340 I341 E344 P345 G352 M357 R358 T362 V365 K366 Q367 L368 T369 E370 A371 V372 I375 E378 S379 I380 G384 K385 T386 P387 K388 F389 K390 L391 W398 E399 T400 W401 W402 T403 E404 Y405

W406 Q407 I411 P412 E413 W414 T419 P420 P421 L422 V423 K424 L425 W426 Y427 Q428 L429 E430 K431 E432 P433 I434 T439 F440 Y441 G444 A445 R448 E449 T450 K451 V458 T459 N460 K465 V466 Q475 K476 T477 E478 L479 Q480 Y483 S489 G490 L491 E492 V493 N494 I495

V496 T497 D498 S499 Q500 Y501 A502 I505 I506 Q509 P510 D511 K512 V518 I522 I526 K527 K528 E529 K530 V531 Y532 L533 A534 W535 V536 P537 A538 H539 K540 G541 I542 G543 G544 N545 E546 Q547 V548 V552 S553 A554 GLY

• Molecule 1: Reverse transcriptase/ribonuclease H

Chain I:    50%       45%    • •

MET VAL PRO I2 S3 P4 I5 E6 T7 V8 P9 V10 K11 L12 K13 D17 G18 P19 K20 V21 K22 Q23 W24 P25 L26 T27 E28 E29 K30 I31 K32 A33 E36 I37 K46 I50 Y56 N57 T58 P59 V60 D67 S68 T69 K70 K73 L74 V75 D76 L80 N81 K82

R83 T84 Q85 D86 F87 I94 P95 H96 K102 V108 L109 D110 V111 G112 D113 A114 Y115 S117 V118 P119 R125 K126 Y127 F130 T131 I132 P133 N137 I142 R143 Y144 Q145 Y146 N147 V148 L149 G155 S156 P157 A158 I159 F160 Q161 T165 L168 F171 N175
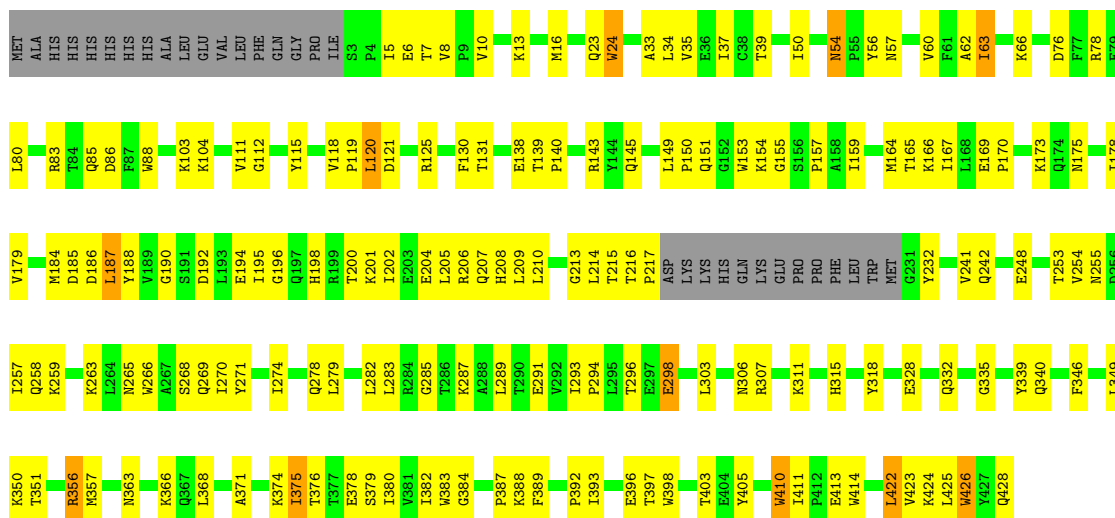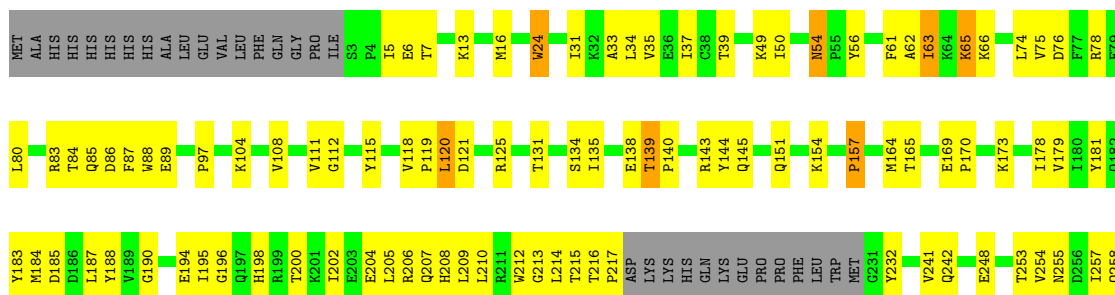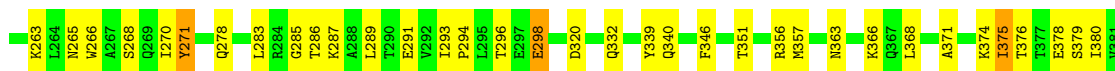
I178 Y181 Q182 Y183 M184 D185 D186 L187 Y188 E194 Q197 H198 R199 T200 K201 I202 E203 E204 L205 R206 Q207 H208 L209 L210 L214 T215 T216 K220 H221 Q222 K223 E224 P225 P226 F227 L228 W229 H235 P236 D237 K238 W239 T240 I244 V245 L246 P247 D250 S251 W252 T253

V254 N255 C258 K259 L260 L264 N265 A267 S268 Q269 Q278 L279 S280 K281 L282 L283 R284 G285 T286 K287 A288 L289 T290 E291 V292 I293 P294 L295 T296 E297 E298 A299 E300 L301 E302 L303 A304 E305 E312 P313 V314 H315 G316 V317 Y318 Y319 D320 P321 D324 L325 I326 A327 E328 I329

Q330 K331 Q332 G333 Q334 G335 Q336 W337 T338 Y339 Q340 I341 E344 P345 G352 M357 T362 K366 Q367 L368 T369 E370 A371 V372 Q373 K374 I375 S379 I380 V381 I382 W383 G384 K385 T386 P387 K388 F389 K390 L391 P392 I393 T397 W398 E399 T400 W401 W402 T403 E404 Y405 W406 Q407

W410 I411 V417 N418 T419 P420 P421 L422 V423 W426 Y427 Q428 L429 E430 K431 E432 P433 I434 E438 T439 F440 Y441 G444 A445 R448 E449 T450 K451 Y457 V458 T459 R463 Q464 K465 V466 Q475 K476 T477 E478 L479 Q480 Y483 S489 G490 L491 E492 V493 N494 I495

V496 T497 D498 S499 Q500 Y501 A502 L503 Q504 I505 I506 Q509 P510 D511 K512 S513 E514 V518 I522 I526 K527 K528 E529 K530 L533 A534 W535 V536 P537 A538 H539 K540 G541 I542 G543 G544 N545 V548 L551 V552 S553 A554 GLY

• Molecule 1: Reverse transcriptase/ribonuclease H

Chain M:    48%       47%    • •

MET VAL PRO I2 S3 P4 I5 E6 T7 V8 P9 V10 K11 L12 K13 D17 Q23 W24 P25 L26 T27 E28 E29 K30 I31 K32 A33 E36 I37 E42 K43 E44 G45 K46 K49 Y56 N57 T58 P59 V60 K65 K66 D67 S68 R72 F77 L80 N81 K82 R83

T84 Q85 D86 Q91 L92 G93 I94 P95 H96 P97 K102 V108 L109 D110 V111 Y115 F116 S117 V118 P119 R125 K126 Y127 F130 T131 I132 P133 N136 N137 E138 I142 R143 Y144 N147 V148 L149 P150 Q151 K154 S155 S156 P157 A158 I159 F160 Q161 T165 L168

F171 N175 I178 V179 I180 Y181 Q182 Y183 M184 D186 L187 Y188 E194 Q197 H198 R199 T200 K201 I202 E203 E204 L205 R206 Q207 H208 L209 L210 L214 T215 T216 P217 K220 H221 Q222 K223 E224 P225 P226 F227 L228 Y232 H235 P236 D237 K238 W239 T240 P243 I244

V245 L246 P247 D250 S251 W252 T253 V254 K259 L260 Q269 K275 V276 R277 Q278 L279 S280 K281 L282 L283 R284 G285 T286 K287 A288 L289 T290 V292 I293 P294 L295 T296 E297 E298 A299 E302 L303 A304 E305 L310 K311 E312 P313 V314 H315 G316 V317 Y318 Y319 D320 P321 D324

L325 I326 A327 E328 I329 Q330 K331 Q332 G333 Q334 G335 Q336 W337 T338 Y339 Q340 I341 Y342 Q343 E344 P345 F346 K347 N348 L349 G352 M357 H361 T362 K366 Q367 L368 T369 E370 A371 V372 I375 S379 I380 G384 K385 T386 P387 K388 F389 K390 L391 P392 I393 W398 E399 T400

W401 W402 T403 E404 Y405 W406 Q407 W410 I411 P412 E413 W414 V417 N418 T419 P420 P421 L422 V423 W426 Y427 Q428 L429 E430 K431 E432 P433 I434 V435 E438 T439 F440 F441 G444 A445 R448 E449 T450 K451 Y457 V458 T459 R463 Q464 K465 V466 Q475 K476 T477 E478 L479

Q480 Y483 S489 Q490 L491 E492 V493 N494 I495 V496 T497 D498 S499 Q500 Y501 A502 L503 G504 I506 Q509 P510 D511 K512 V518 I522 I526 K527 K528 E529 K530 L533 A534 W535 A538 G541 I542 G543 G544 V548 D549 K550 L551 V552 S553 A554 GLY

● Molecule 2: p51 RT

Chain B:

55%　　　　　　36%　　　7%

MET ALA HIS HIS HIS HIS HIS HIS ALA LEU GLU VAL LEU PHE GLN GLY PRO ILE S3 P4 I5 E6 T7 V8 P9 V10 K13 M16 Q23 W24 A33 L34 V35 E36 I37 C38 T39 I50 N54 P55 Y56 N57 V60 F61 A62 I63 K66 D76 F77 R78 E79

L80 R83 T84 Q85 D86 F87 W88 K103 K104 V111 G112 Y115 V118 P119 L120 D121 R125 F130 T131 E138 T139 P140 R143 V144 Q145 L149 P150 Q151 G152 W153 K154 G155 S156 P157 A158 I159 M164 T165 K166 I167 L168 E169 P170 K173 Q174 N175 I178

V179 M184 D185 D186 L187 Y188 V189 G190 S191 D192 L193 E194 I195 G196 Q197 H198 R199 T200 K201 I202 E203 E204 L205 R206 Q207 H208 L209 L210 G213 L214 T215 T216 P217 ASP LYS LYS HIS GLN LYS GLU PRO PRO PHE LEU TRP MET G231 Y232 V241 Q242 E248 T253 V254 N255 D256

I257 Q258 K259 K263 L264 N265 W266 A267 S268 Q269 I270 Y271 I274 Q278 L279 L282 L283 R284 G285 T286 K287 A288 L289 T290 E291 V292 I293 P294 L295 T296 E297 E298 L303 N306 R307 K311 H315 Y318 E328 Q332 G335 Y339 Q340 F346 L349

K350 T351 R356 M357 N363 K366 Q367 L368 A371 K374 I375 T376 I377 E378 S379 I380 V381 I382 W383 G384 P387 K388 F389 P392 I393 E396 T397 W398 T403 E404 Y405 W410 I411 P412 E413 W414 L422 V423 K424 L425 W426 Y427 Q428

● Molecule 2: p51 RT

Chain F:

58%　　　　　　32%　　　7%

MET ALA HIS HIS HIS HIS HIS HIS ALA LEU GLU VAL LEU PHE GLN GLY PRO ILE S3 P4 I5 E6 T7 K13 M16 W24 I31 K32 A33 L34 V35 E36 I37 C38 T39 K49 I50 N54 P55 Y56 F61 A62 I63 K64 K65 K66 L74 V75 D76 F77 R78 E79

L80 R83 T84 Q85 D86 F87 W88 E89 P97 K104 V108 V111 G112 Y115 V118 P119 L120 D121 R125 T131 S134 I135 E138 T139 P140 R143 Y144 Q145 Q151 K154 P157 M164 T165 E169 P170 K173 I178 V179 I180 Y181 Q182

Y183 M184 D185 D186 L187 Y188 V189 G190 E194 I195 G196 Q197 H198 R199 T200 K201 I202 E203 E204 L205 R206 Q207 H208 L209 L210 R211 W212 G213 L214 T215 T216 P217 ASP LYS LYS HIS GLN LYS GLU PRO PRO PHE LEU TRP MET G231 Y232 V241 Q242 E248 T253 V254 N255 D256 I257 Q258

• Molecule 2: p51 RT

Chain J:



• Molecule 2: p51 RT

Chain N:



• Molecule 3: DNA (5'-D(\*AP\*T\*GP\*CP\*AP\*TP\*GP\*GP\*CP\*GP\*CP\*CP\*CP\*GP\*AP\*AP\*
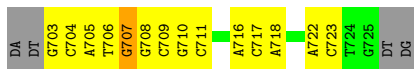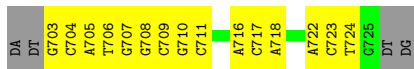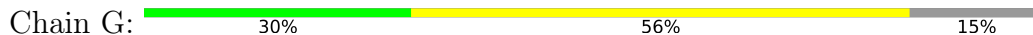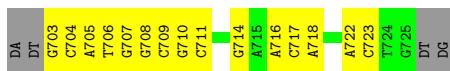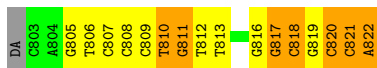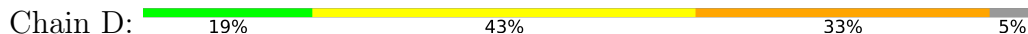CP\*AP\*GP\*GP\*GP\*AP\*CP\*TP\*GP\*TP\*G)-3')

Chain C:

• Molecule 3: DNA (5'-D(*AP*T*GP*CP*AP*TP*GP*GP*CP*GP*CP*CP*CP*GP*AP*AP*CP*AP*GP*GP*GP*AP*CP*TP*GP*TP*G)-3')

Chain G: 

• Molecule 3: DNA (5'-D(*AP*T*GP*CP*AP*TP*GP*GP*CP*GP*CP*CP*CP*GP*AP*AP*CP*AP*GP*GP*GP*AP*CP*TP*GP*TP*G)-3')

Chain K: 

• Molecule 3: DNA (5'-D(*AP*T*GP*CP*AP*TP*GP*GP*CP*GP*CP*CP*CP*GP*AP*AP*CP*AP*GP*GP*GP*AP*CP*TP*GP*TP*G)-3')

Chain O: 

• Molecule 4: DNA (5'-D(*A*CP*AP*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*GP*(MRG)P*CP*GP*CP*CP*(2DA))-3')

Chain D: 

• Molecule 4: DNA (5'-D(*A*CP*AP*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*GP*(MRG)P*CP*GP*CP*CP*(2DA))-3')

Chain H: 

• Molecule 4: DNA (5'-D(*A*CP*AP*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*GP*(MRG)P*CP*GP*CP*CP*(2DA))-3')

Chain L: 

DA C303 A804 G805 T806 C807 C808 C809 T810 G817 C818 G819 C820 C821 A822

• Molecule 4: DNA (5'-D(*A*CP*AP*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*GP*(MRG)P*CP*GP*CP*CP*(2DA))-3')

Chain P: 29% 57% 10% 5%

DA C803 A804 G805 T806 C807 C808 C809 T810 G816 G817 C818 G819 C820 C821 A822
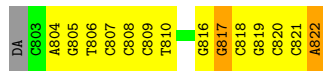
# 4 Data and refinement statistics ⓘ

| Property | Value | Source |
|---|---|---|
| Space group | P 1 21 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 78.53Å　　274.81Å　　152.37Å<br>90.00°　　90.11°　　　90.00° | Depositor |
| Resolution (Å) | 24.83　–　3.15<br>24.83　–　3.14 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 88.6 (24.83-3.15)<br>88.2 (24.83-3.14) | Depositor<br>EDS |
| $R_{merge}$ | 0.13 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 2.38 (at 3.17Å) | Xtriage |
| Refinement program | CNS 1.2 | Depositor |
| R, $R_{free}$ | 0.264　,　0.288<br>0.250　,　0.276 | Depositor<br>DCC |
| $R_{free}$ test set | 1979 reflections (2.01%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 73.3 | Xtriage |
| Anisotropy | 0.001 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.31 , 17.2 | EDS |
| L-test for twinning[2] | $< |L| > = 0.39, < L^2 > = 0.22$ | Xtriage |
| Estimated twinning fraction | 0.359 for h,-k,-l | Xtriage |
| $F_o,F_c$ correlation | 0.91 | EDS |
| Total number of atoms | 35440 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 72.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

# 5 Model quality ⓘ

## 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, ZP4, 2DA, MRG

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 | 0.60 | 0/4616 | 0.69 | 0/6271 |
| 1 | E | 0.57 | 1/4616 (0.0%) | 0.66 | 2/6271 (0.0%) |
| 1 | I | 0.44 | 0/4616 | 0.61 | 0/6271 |
| 1 | M | 0.40 | 0/4616 | 0.60 | 1/6271 (0.0%) |
| 2 | B | 0.67 | 0/3502 | 0.75 | 2/4760 (0.0%) |
| 2 | F | 0.66 | 0/3502 | 0.74 | 1/4760 (0.0%) |
| 2 | J | 0.47 | 0/3502 | 0.66 | 1/4760 (0.0%) |
| 2 | N | 0.42 | 0/3502 | 0.64 | 0/4760 |
| 3 | C | 0.78 | 0/532 | 0.79 | 0/820 |
| 3 | G | 0.78 | 0/532 | 0.78 | 0/820 |
| 3 | K | 0.49 | 0/532 | 0.72 | 0/820 |
| 3 | O | 0.46 | 0/532 | 0.74 | 0/820 |
| 4 | D | 0.91 | 0/400 | 0.97 | 1/612 (0.2%) |
| 4 | H | 0.90 | 0/400 | 0.87 | 0/612 |
| 4 | L | 0.59 | 0/400 | 0.78 | 0/612 |
| 4 | P | 0.50 | 0/400 | 0.77 | 0/612 |
| All | All | 0.55 | 1/36200 (0.0%) | 0.68 | 8/49852 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 3 | C | 0 | 1 |
| 4 | D | 0 | 5 |
| 4 | H | 0 | 2 |
| 4 | L | 0 | 1 |
| All | All | 0 | 9 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|---|-------------|----------|
| 1 | E | 378 | GLU | CG-CD | 5.04 | 1.59 | 1.51 |

All (8) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|-----|-------|-----|------|-------|---|-----------------|-------------|
| 1 | M | 286 | THR | N-CA-C | 5.71 | 126.42 | 111.00 |
| 2 | J | 65 | LYS | CB-CA-C | -5.67 | 99.06 | 110.40 |
| 4 | D | 821 | DC | O5'-P-OP1 | -5.45 | 100.80 | 105.70 |
| 2 | B | 349 | LEU | CB-CA-C | 5.36 | 120.38 | 110.20 |
| 1 | E | 284 | ARG | CB-CA-C | -5.35 | 99.71 | 110.40 |
| 2 | F | 65 | LYS | CB-CA-C | -5.14 | 100.12 | 110.40 |
| 2 | B | 187 | LEU | N-CA-C | -5.09 | 97.25 | 111.00 |
| 1 | E | 285 | GLY | N-CA-C | -5.03 | 100.53 | 113.10 |

There are no chirality outliers.

All (9) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-------|
| 3 | C | 707 | DG | Sidechain |
| 4 | D | 810 | DT | Sidechain |
| 4 | D | 811 | DG | Sidechain |
| 4 | D | 816 | DG | Sidechain |
| 4 | D | 818 | DC | Sidechain |
| 4 | D | 820 | DC | Sidechain |
| 4 | H | 811 | DG | Sidechain |
| 4 | H | 820 | DC | Sidechain |
| 4 | L | 820 | DC | Sidechain |

## 5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 4499 | 0 | 4556 | 312 | 0 |
| 1 | E | 4499 | 0 | 4556 | 310 | 0 |
| 1 | I | 4499 | 0 | 4556 | 275 | 0 |
| 1 | M | 4499 | 0 | 4556 | 308 | 0 |
| 2 | B | 3405 | 0 | 3437 | 163 | 0 |
| 2 | F | 3405 | 0 | 3437 | 156 | 0 |

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2 | J | 3405 | 0 | 3437 | 164 | 0 |
| 2 | N | 3405 | 0 | 3437 | 175 | 0 |
| 3 | C | 473 | 0 | 257 | 29 | 0 |
| 3 | G | 473 | 0 | 257 | 24 | 0 |
| 3 | K | 473 | 0 | 257 | 22 | 0 |
| 3 | O | 473 | 0 | 257 | 26 | 0 |
| 4 | D | 406 | 0 | 231 | 32 | 0 |
| 4 | H | 406 | 0 | 231 | 34 | 0 |
| 4 | L | 406 | 0 | 231 | 20 | 0 |
| 4 | P | 406 | 0 | 231 | 26 | 0 |
| 5 | A | 2 | 0 | 0 | 0 | 0 |
| 5 | E | 2 | 0 | 0 | 0 | 0 |
| 5 | I | 2 | 0 | 0 | 0 | 0 |
| 5 | M | 2 | 0 | 0 | 0 | 0 |
| 6 | A | 53 | 0 | 24 | 4 | 0 |
| 6 | E | 53 | 0 | 24 | 6 | 0 |
| 6 | I | 53 | 0 | 24 | 6 | 0 |
| 6 | M | 53 | 0 | 24 | 3 | 0 |
| 7 | B | 6 | 0 | 8 | 0 | 0 |
| 7 | F | 6 | 0 | 8 | 0 | 0 |
| 8 | A | 12 | 0 | 0 | 3 | 0 |
| 8 | B | 9 | 0 | 0 | 3 | 0 |
| 8 | C | 1 | 0 | 0 | 0 | 0 |
| 8 | E | 11 | 0 | 0 | 5 | 0 |
| 8 | F | 12 | 0 | 0 | 4 | 0 |
| 8 | G | 3 | 0 | 0 | 0 | 0 |
| 8 | I | 10 | 0 | 0 | 5 | 0 |
| 8 | J | 5 | 0 | 0 | 0 | 0 |
| 8 | K | 1 | 0 | 0 | 0 | 0 |
| 8 | L | 2 | 0 | 0 | 0 | 0 |
| 8 | M | 3 | 0 | 0 | 0 | 0 |
| 8 | N | 5 | 0 | 0 | 3 | 0 |
| 8 | O | 2 | 0 | 0 | 0 | 0 |
| All | All | 35440 | 0 | 34036 | 1972 | 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 28.

All (1972) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:511:ASP:OD1 | 1:E:512:LYS:HG2 | 1.42 | 1.19 |
| 1:M:339:TYR:CZ | 1:M:352:GLY:HA3 | 1.77 | 1.19 |
| 1:M:511:ASP:OD1 | 1:M:512:LYS:HG2 | 1.38 | 1.18 |
| 1:A:175:ASN:HB3 | 1:A:178:ILE:HD13 | 1.19 | 1.18 |
| 2:N:66:LYS:NZ | 2:N:66:LYS:HB3 | 1.40 | 1.18 |
| 1:M:108:VAL:HG22 | 1:M:221:HIS:HB2 | 1.17 | 1.14 |
| 1:A:317:VAL:HG12 | 1:A:348:ASN:O | 1.47 | 1.14 |
| 1:A:511:ASP:OD1 | 1:A:512:LYS:HG2 | 1.47 | 1.13 |
| 1:I:102:LYS:H | 1:I:102:LYS:HD2 | 1.09 | 1.12 |
| 1:E:537:PRO:HB2 | 1:E:540:LYS:HB2 | 1.33 | 1.10 |
| 1:M:102:LYS:HD2 | 1:M:102:LYS:H | 1.16 | 1.10 |
| 1:I:108:VAL:HG22 | 1:I:221:HIS:HB2 | 1.35 | 1.08 |
| 1:M:343:GLN:HG3 | 1:M:349:LEU:HD11 | 1.32 | 1.08 |
| 1:I:431:LYS:HA | 8:I:559:HOH:O | 1.53 | 1.07 |
| 1:A:102:LYS:H | 1:A:102:LYS:HD2 | 1.10 | 1.06 |
| 1:E:102:LYS:HD2 | 1:E:102:LYS:H | 1.18 | 1.06 |
| 1:E:175:ASN:HB3 | 1:E:178:ILE:HD13 | 1.31 | 1.06 |
| 1:M:286:THR:O | 1:M:286:THR:HG22 | 1.46 | 1.06 |
| 1:A:344:GLU:HB3 | 1:A:345:PRO:HD2 | 1.34 | 1.05 |
| 1:I:175:ASN:HB3 | 1:I:178:ILE:HD13 | 1.34 | 1.04 |
| 1:M:175:ASN:HB3 | 1:M:178:ILE:HD13 | 1.34 | 1.04 |
| 1:E:108:VAL:HG22 | 1:E:221:HIS:HB2 | 1.07 | 1.03 |
| 1:I:253:THR:HG22 | 1:I:292:VAL:HG22 | 1.39 | 1.03 |
| 2:J:5:ILE:CG2 | 2:J:119:PRO:HG3 | 1.87 | 1.02 |
| 1:A:108:VAL:HG22 | 1:A:221:HIS:HB2 | 1.37 | 1.02 |
| 4:P:807:DC:H2" | 4:P:808:DC:H5' | 1.42 | 1.01 |
| 2:J:5:ILE:HG23 | 2:J:119:PRO:HG3 | 1.40 | 1.00 |
| 1:M:344:GLU:HB3 | 1:M:345:PRO:HD2 | 1.43 | 1.00 |
| 1:A:344:GLU:HB3 | 1:A:345:PRO:CD | 1.91 | 0.99 |
| 2:N:66:LYS:HB3 | 2:N:66:LYS:HZ3 | 1.17 | 0.98 |
| 1:I:511:ASP:OD1 | 1:I:512:LYS:HG2 | 1.63 | 0.98 |
| 1:M:253:THR:HG22 | 1:M:292:VAL:HG22 | 1.45 | 0.97 |
| 2:N:66:LYS:NZ | 2:N:66:LYS:CB | 2.30 | 0.94 |
| 4:H:807:DC:H2" | 4:H:808:DC:H5' | 1.49 | 0.94 |
| 1:I:235:HIS:HB3 | 1:I:236:PRO:HD2 | 1.48 | 0.94 |
| 1:M:344:GLU:HB3 | 1:M:345:PRO:CD | 1.96 | 0.94 |
| 1:M:344:GLU:HB2 | 1:M:347:LYS:HB2 | 1.46 | 0.94 |
| 1:E:235:HIS:HB3 | 1:E:236:PRO:HD2 | 1.49 | 0.94 |
| 1:E:439:THR:HG21 | 2:F:289:LEU:HD13 | 1.46 | 0.94 |
| 1:E:532:TYR:HA | 8:E:564:HOH:O | 1.66 | 0.93 |
| 3:G:707:DG:H2" | 3:G:708:DG:H5' | 1.51 | 0.92 |
| 1:M:342:TYR:CD2 | 1:M:344:GLU:O | 2.23 | 0.92 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:439:THR:HG21 | 2:B:289:LEU:HD13 | 1.49 | 0.92 |
| 3:C:707:DG:H2" | 3:C:708:DG:H5' | 1.52 | 0.91 |
| 1:E:537:PRO:CB | 1:E:540:LYS:HB2 | 1.99 | 0.91 |
| 1:E:174:GLN:HB2 | 8:E:563:HOH:O | 1.70 | 0.91 |
| 1:M:434:ILE:HD12 | 1:M:530:LYS:HE2 | 1.53 | 0.90 |
| 1:A:518:VAL:O | 1:A:522:ILE:HG12 | 1.71 | 0.90 |
| 1:E:430:GLU:HG3 | 1:E:434:ILE:HD11 | 1.54 | 0.90 |
| 2:J:13:LYS:HB2 | 2:J:16:MET:HG3 | 1.52 | 0.90 |
| 1:E:108:VAL:HG22 | 1:E:221:HIS:CB | 2.00 | 0.90 |
| 2:N:66:LYS:HB3 | 2:N:66:LYS:HZ2 | 1.18 | 0.89 |
| 4:D:806:DT:H2" | 4:D:807:DC:C5' | 2.01 | 0.89 |
| 1:E:253:THR:HG22 | 1:E:292:VAL:HG22 | 1.54 | 0.89 |
| 1:A:235:HIS:HB3 | 1:A:236:PRO:HD2 | 1.53 | 0.89 |
| 1:E:317:VAL:HG22 | 1:E:318:TYR:H | 1.38 | 0.89 |
| 1:A:223:LYS:HG2 | 1:A:223:LYS:O | 1.73 | 0.88 |
| 4:D:806:DT:H2" | 4:D:807:DC:H5" | 1.55 | 0.88 |
| 1:I:430:GLU:HG3 | 1:I:434:ILE:HD11 | 1.56 | 0.88 |
| 2:N:422:LEU:HG | 2:N:426:TRP:HZ2 | 1.39 | 0.88 |
| 1:E:518:VAL:O | 1:E:522:ILE:HG12 | 1.74 | 0.87 |
| 2:J:422:LEU:HG | 2:J:426:TRP:HZ2 | 1.39 | 0.87 |
| 4:L:807:DC:H2" | 4:L:808:DC:H5' | 1.54 | 0.87 |
| 1:M:235:HIS:HB3 | 1:M:236:PRO:HD2 | 1.54 | 0.87 |
| 1:A:317:VAL:HG13 | 1:A:349:LEU:HG | 1.57 | 0.87 |
| 1:A:430:GLU:HG3 | 1:A:434:ILE:HD11 | 1.55 | 0.87 |
| 1:I:518:VAL:O | 1:I:522:ILE:HG12 | 1.74 | 0.87 |
| 2:B:422:LEU:HG | 2:B:426:TRP:HZ2 | 1.39 | 0.86 |
| 1:E:458:VAL:CG1 | 1:E:548:VAL:HG22 | 2.05 | 0.86 |
| 1:E:108:VAL:CG2 | 1:E:221:HIS:HB2 | 2.01 | 0.86 |
| 1:A:458:VAL:CG1 | 1:A:548:VAL:HG22 | 2.06 | 0.86 |
| 1:M:430:GLU:HG3 | 1:M:434:ILE:HD11 | 1.58 | 0.86 |
| 1:A:317:VAL:O | 1:A:349:LEU:HD23 | 1.75 | 0.86 |
| 3:K:707:DG:H2" | 3:K:708:DG:H5' | 1.58 | 0.86 |
| 1:M:343:GLN:HG3 | 1:M:349:LEU:CD1 | 2.04 | 0.85 |
| 2:F:169:GLU:HG3 | 2:F:173:LYS:HE2 | 1.55 | 0.85 |
| 2:B:33:ALA:O | 2:B:37:ILE:HG12 | 1.75 | 0.85 |
| 3:G:705:DA:H2" | 3:G:706:DT:H5' | 1.58 | 0.85 |
| 2:B:76:ASP:OD1 | 2:B:78:ARG:HB2 | 1.75 | 0.85 |
| 1:M:511:ASP:OD1 | 1:M:512:LYS:CG | 2.24 | 0.85 |
| 4:D:807:DC:H2" | 4:D:808:DC:H5' | 1.56 | 0.85 |
| 1:E:420:PRO:HA | 1:E:422:LEU:HD22 | 1.59 | 0.84 |
| 3:C:705:DA:H2" | 3:C:706:DT:H5' | 1.57 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:342:TYR:CD2 | 1:A:344:GLU:O | 2.30 | 0.84 |
| 3:O:707:DG:H2" | 3:O:708:DG:H5' | 1.59 | 0.84 |
| 1:M:518:VAL:O | 1:M:522:ILE:HG12 | 1.77 | 0.84 |
| 1:E:157:PRO:O | 1:E:161:GLN:HG3 | 1.77 | 0.84 |
| 2:N:76:ASP:OD1 | 2:N:78:ARG:HB2 | 1.78 | 0.84 |
| 2:F:33:ALA:O | 2:F:37:ILE:HG12 | 1.78 | 0.84 |
| 1:I:102:LYS:HD2 | 1:I:102:LYS:N | 1.90 | 0.84 |
| 3:O:705:DA:H2" | 3:O:706:DT:H5' | 1.60 | 0.84 |
| 1:E:429:LEU:HD13 | 1:E:533:LEU:HD13 | 1.59 | 0.83 |
| 2:N:33:ALA:O | 2:N:37:ILE:HG12 | 1.77 | 0.83 |
| 3:G:710:DG:H2" | 3:G:711:DC:H5' | 1.59 | 0.83 |
| 1:E:174:GLN:CB | 8:E:563:HOH:O | 2.25 | 0.83 |
| 1:E:537:PRO:HB2 | 1:E:540:LYS:CB | 2.08 | 0.83 |
| 1:M:223:LYS:O | 1:M:223:LYS:HG2 | 1.78 | 0.83 |
| 1:E:223:LYS:O | 1:E:223:LYS:HG2 | 1.79 | 0.82 |
| 2:J:33:ALA:O | 2:J:37:ILE:HG12 | 1.78 | 0.82 |
| 2:F:422:LEU:HG | 2:F:426:TRP:HZ2 | 1.44 | 0.82 |
| 1:I:31:ILE:HD12 | 1:I:133:PRO:HG2 | 1.61 | 0.82 |
| 1:A:441:TYR:CD2 | 1:A:544:GLY:HA3 | 2.14 | 0.82 |
| 1:M:108:VAL:HG22 | 1:M:221:HIS:CB | 2.06 | 0.82 |
| 1:M:286:THR:O | 1:M:286:THR:CG2 | 2.22 | 0.82 |
| 2:B:169:GLU:HG3 | 2:B:173:LYS:HE2 | 1.61 | 0.82 |
| 1:M:478:GLU:HG2 | 1:M:499:SER:HB2 | 1.60 | 0.82 |
| 1:M:501:TYR:CE1 | 1:M:505:ILE:HD11 | 2.15 | 0.81 |
| 3:K:705:DA:H2" | 3:K:706:DT:H5' | 1.61 | 0.81 |
| 1:A:344:GLU:HB2 | 1:A:347:LYS:HB2 | 1.61 | 0.81 |
| 4:H:820:DC:H2" | 4:H:821:DC:H5' | 1.61 | 0.81 |
| 2:J:76:ASP:OD1 | 2:J:78:ARG:HB2 | 1.80 | 0.81 |
| 2:N:254:VAL:HG22 | 2:N:293:ILE:HD11 | 1.62 | 0.81 |
| 3:C:708:DG:H2' | 3:C:709:DC:C6 | 2.16 | 0.81 |
| 2:N:13:LYS:HB2 | 2:N:16:MET:HG3 | 1.63 | 0.81 |
| 1:A:317:VAL:HG22 | 1:A:318:TYR:H | 1.46 | 0.81 |
| 1:M:108:VAL:HG21 | 1:M:221:HIS:HD2 | 1.45 | 0.81 |
| 1:M:65:LYS:HD3 | 6:M:823:ZP4:O2D | 1.81 | 0.80 |
| 2:N:111:VAL:HG11 | 2:N:187:LEU:HD12 | 1.64 | 0.80 |
| 2:F:151:GLN:HB3 | 2:F:185:ASP:OD2 | 1.82 | 0.80 |
| 1:I:441:TYR:CD2 | 1:I:544:GLY:HA3 | 2.16 | 0.80 |
| 2:J:6:GLU:HG3 | 2:J:6:GLU:O | 1.81 | 0.80 |
| 2:B:54:ASN:C | 2:B:54:ASN:HD22 | 1.86 | 0.80 |
| 2:F:50:ILE:HD13 | 2:F:145:GLN:HB3 | 1.63 | 0.80 |
| 4:L:819:DG:H2' | 4:L:820:DC:H6 | 1.47 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:O:708:DG:H2' | 3:O:709:DC:C6 | 2.17 | 0.80 |
| 2:B:13:LYS:HD3 | 2:B:86:ASP:HB2 | 1.64 | 0.79 |
| 1:E:215:THR:HG22 | 1:E:217:PRO:HD3 | 1.63 | 0.79 |
| 1:E:458:VAL:HG12 | 1:E:548:VAL:HG22 | 1.63 | 0.79 |
| 1:M:317:VAL:HG13 | 1:M:349:LEU:HD23 | 1.63 | 0.79 |
| 2:J:332:GLN:HG3 | 2:J:428:GLN:HG3 | 1.65 | 0.79 |
| 1:A:137:ASN:HD22 | 1:A:137:ASN:N | 1.79 | 0.79 |
| 1:E:434:ILE:HD12 | 1:E:530:LYS:HE2 | 1.63 | 0.79 |
| 1:I:253:THR:HA | 1:I:292:VAL:HA | 1.64 | 0.79 |
| 2:N:371:ALA:O | 2:N:375:ILE:HG12 | 1.83 | 0.79 |
| 1:A:429:LEU:HD13 | 1:A:533:LEU:HD13 | 1.63 | 0.79 |
| 1:M:31:ILE:HD12 | 1:M:133:PRO:HG2 | 1.63 | 0.79 |
| 1:M:293:ILE:HG13 | 1:M:294:PRO:HD2 | 1.65 | 0.79 |
| 1:E:109:LEU:CD2 | 1:E:220:LYS:HD3 | 2.13 | 0.78 |
| 1:A:253:THR:HG22 | 1:A:292:VAL:HG22 | 1.63 | 0.78 |
| 3:G:708:DG:H2' | 3:G:709:DC:C6 | 2.19 | 0.78 |
| 1:A:125:ARG:HD3 | 1:A:147:ASN:HA | 1.66 | 0.78 |
| 1:A:215:THR:HG22 | 1:A:217:PRO:HD3 | 1.66 | 0.78 |
| 1:I:157:PRO:O | 1:I:161:GLN:HG3 | 1.83 | 0.78 |
| 1:I:362:THR:HG22 | 1:I:366:LYS:HE2 | 1.66 | 0.78 |
| 2:B:332:GLN:HE22 | 2:B:425:LEU:HD13 | 1.47 | 0.78 |
| 2:J:169:GLU:HG3 | 2:J:173:LYS:HE2 | 1.64 | 0.78 |
| 2:B:194:GLU:OE2 | 2:B:195:ILE:HG22 | 1.84 | 0.78 |
| 1:A:109:LEU:N | 1:A:109:LEU:HD12 | 1.99 | 0.77 |
| 1:E:109:LEU:CD2 | 1:E:220:LYS:CD | 2.62 | 0.77 |
| 1:M:157:PRO:O | 1:M:161:GLN:HG3 | 1.84 | 0.77 |
| 2:B:13:LYS:HB2 | 2:B:16:MET:HG3 | 1.66 | 0.77 |
| 1:E:24:TRP:CZ2 | 3:G:704:DC:H5' | 2.20 | 0.77 |
| 1:I:5:ILE:HD12 | 1:I:6:GLU:N | 1.99 | 0.77 |
| 3:C:710:DG:H2" | 3:C:711:DC:H5' | 1.66 | 0.77 |
| 1:E:137:ASN:HD22 | 1:E:137:ASN:N | 1.80 | 0.77 |
| 1:I:439:THR:HG21 | 2:J:289:LEU:HD13 | 1.65 | 0.77 |
| 2:B:54:ASN:ND2 | 2:B:56:TYR:H | 1.82 | 0.77 |
| 3:G:709:DC:H2' | 3:G:710:DG:H8 | 1.50 | 0.76 |
| 4:D:806:DT:C2' | 4:D:807:DC:H5" | 2.15 | 0.76 |
| 2:J:265:ASN:O | 2:J:268:SER:HB3 | 1.84 | 0.76 |
| 3:O:710:DG:H2" | 3:O:711:DC:H5' | 1.67 | 0.76 |
| 1:A:317:VAL:HG22 | 1:A:318:TYR:N | 2.00 | 0.76 |
| 1:A:458:VAL:HG12 | 1:A:548:VAL:HG22 | 1.67 | 0.76 |
| 2:F:13:LYS:HB2 | 2:F:16:MET:HG3 | 1.68 | 0.76 |
| 2:F:332:GLN:HG3 | 2:F:428:GLN:HG3 | 1.67 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:F:368:LEU:HD11 | 2:F:392:PRO:HD2 | 1.67 | 0.76 |
| 1:E:317:VAL:HG22 | 1:E:318:TYR:N | 1.99 | 0.76 |
| 1:A:157:PRO:O | 1:A:161:GLN:HG3 | 1.86 | 0.75 |
| 1:A:7:THR:HG22 | 1:A:119:PRO:HB2 | 1.67 | 0.75 |
| 1:A:96:HIS:HE2 | 1:A:269:GLN:HE21 | 1.34 | 0.75 |
| 1:A:102:LYS:HD2 | 1:A:102:LYS:N | 1.95 | 0.75 |
| 1:M:317:VAL:HG22 | 1:M:318:TYR:H | 1.49 | 0.75 |
| 2:N:169:GLU:HG3 | 2:N:173:LYS:HE2 | 1.66 | 0.75 |
| 4:H:819:DG:H2' | 4:H:820:DC:H6 | 1.52 | 0.75 |
| 4:H:806:DT:H2" | 4:H:807:DC:C5' | 2.16 | 0.75 |
| 1:I:102:LYS:H | 1:I:102:LYS:CD | 1.96 | 0.74 |
| 1:I:434:ILE:HD12 | 1:I:530:LYS:HE2 | 1.67 | 0.74 |
| 1:M:125:ARG:HD3 | 1:M:147:ASN:HA | 1.68 | 0.74 |
| 2:N:111:VAL:HG11 | 2:N:187:LEU:CD1 | 2.17 | 0.74 |
| 2:F:76:ASP:OD1 | 2:F:78:ARG:HB2 | 1.87 | 0.74 |
| 2:N:254:VAL:HG23 | 2:N:291:GLU:O | 1.87 | 0.74 |
| 1:A:165:THR:HG21 | 2:B:140:PRO:HG2 | 1.70 | 0.74 |
| 1:E:478:GLU:HG2 | 1:E:499:SER:HB2 | 1.70 | 0.74 |
| 1:I:429:LEU:HD13 | 1:I:533:LEU:HD13 | 1.69 | 0.74 |
| 2:J:5:ILE:HG21 | 2:J:119:PRO:HG3 | 1.69 | 0.74 |
| 2:J:254:VAL:HG23 | 2:J:291:GLU:O | 1.88 | 0.74 |
| 3:O:709:DC:H2' | 3:O:710:DG:H8 | 1.53 | 0.74 |
| 2:N:378:GLU:O | 2:N:382:ILE:HG12 | 1.87 | 0.74 |
| 3:K:710:DG:H2" | 3:K:711:DC:H5' | 1.69 | 0.74 |
| 1:A:125:ARG:NH1 | 1:A:147:ASN:HB3 | 2.03 | 0.74 |
| 1:A:293:ILE:HG13 | 1:A:294:PRO:HD2 | 1.68 | 0.73 |
| 1:M:420:PRO:HA | 1:M:422:LEU:HD22 | 1.70 | 0.73 |
| 2:B:54:ASN:HD22 | 2:B:56:TYR:H | 1.34 | 0.73 |
| 3:K:708:DG:H2' | 3:K:709:DC:C6 | 2.23 | 0.73 |
| 4:L:819:DG:H2' | 4:L:820:DC:C6 | 2.24 | 0.73 |
| 2:F:371:ALA:O | 2:F:375:ILE:HG12 | 1.89 | 0.73 |
| 2:J:54:ASN:C | 2:J:54:ASN:HD22 | 1.91 | 0.73 |
| 2:J:371:ALA:O | 2:J:375:ILE:HG12 | 1.88 | 0.73 |
| 1:M:165:THR:HG22 | 1:M:182:GLN:NE2 | 2.02 | 0.73 |
| 2:B:254:VAL:HG23 | 2:B:291:GLU:O | 1.88 | 0.73 |
| 1:E:253:THR:HA | 1:E:292:VAL:HA | 1.70 | 0.73 |
| 1:E:548:VAL:O | 1:E:552:VAL:HG22 | 1.88 | 0.73 |
| 1:A:318:TYR:C | 1:A:349:LEU:HD21 | 2.09 | 0.73 |
| 1:E:475:GLN:HE21 | 4:H:809:DC:H5" | 1.53 | 0.73 |
| 2:F:54:ASN:HD22 | 2:F:54:ASN:C | 1.91 | 0.73 |
| 4:P:806:DT:H2" | 4:P:807:DC:C5' | 2.18 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:289:LEU:H | 1:I:289:LEU:HD12 | 1.53 | 0.73 |
| 1:M:137:ASN:HD22 | 1:M:137:ASN:N | 1.87 | 0.73 |
| 1:M:362:THR:HG22 | 1:M:366:LYS:HE2 | 1.69 | 0.73 |
| 1:E:109:LEU:HD23 | 1:E:220:LYS:HD3 | 1.69 | 0.73 |
| 2:J:378:GLU:O | 2:J:382:ILE:HG12 | 1.89 | 0.73 |
| 1:E:108:VAL:HG21 | 1:E:221:HIS:HD2 | 1.52 | 0.72 |
| 2:J:254:VAL:HG22 | 2:J:293:ILE:HD11 | 1.70 | 0.72 |
| 1:I:317:VAL:HG22 | 1:I:318:TYR:H | 1.54 | 0.72 |
| 1:I:165:THR:HG21 | 2:J:140:PRO:HG2 | 1.70 | 0.72 |
| 1:M:429:LEU:HD13 | 1:M:533:LEU:HD13 | 1.72 | 0.72 |
| 1:A:420:PRO:HA | 1:A:422:LEU:HD22 | 1.70 | 0.72 |
| 1:M:296:THR:HG23 | 1:M:299:ALA:H | 1.53 | 0.72 |
| 2:F:378:GLU:O | 2:F:382:ILE:HG12 | 1.90 | 0.72 |
| 1:E:296:THR:HG23 | 1:E:299:ALA:H | 1.54 | 0.71 |
| 1:I:223:LYS:HG2 | 1:I:223:LYS:O | 1.89 | 0.71 |
| 2:J:7:THR:HG22 | 2:J:119:PRO:HG2 | 1.72 | 0.71 |
| 2:F:13:LYS:HD3 | 2:F:86:ASP:HB2 | 1.71 | 0.71 |
| 2:F:254:VAL:HG22 | 2:F:293:ILE:HD11 | 1.73 | 0.71 |
| 1:M:463:ARG:HH11 | 1:M:463:ARG:HG2 | 1.55 | 0.71 |
| 2:B:332:GLN:NE2 | 2:B:425:LEU:HD13 | 2.04 | 0.71 |
| 2:J:104:LYS:O | 2:J:104:LYS:HD3 | 1.89 | 0.71 |
| 2:N:54:ASN:HD22 | 2:N:56:TYR:H | 1.38 | 0.71 |
| 1:A:327:ALA:HB2 | 1:A:341:ILE:HG13 | 1.72 | 0.71 |
| 2:F:254:VAL:O | 2:F:258:GLN:HG3 | 1.90 | 0.71 |
| 3:K:709:DC:H2' | 3:K:710:DG:H8 | 1.56 | 0.71 |
| 1:A:426:TRP:HB3 | 1:A:526:ILE:HD12 | 1.71 | 0.71 |
| 1:I:137:ASN:HD22 | 1:I:137:ASN:N | 1.88 | 0.71 |
| 2:N:265:ASN:O | 2:N:268:SER:HB3 | 1.90 | 0.71 |
| 2:N:5:ILE:CG2 | 2:N:119:PRO:HG3 | 2.21 | 0.71 |
| 1:I:125:ARG:HD3 | 1:I:147:ASN:HA | 1.72 | 0.71 |
| 2:F:7:THR:HG22 | 2:F:119:PRO:HG2 | 1.71 | 0.71 |
| 1:A:432:GLU:HG3 | 1:A:433:PRO:HD2 | 1.73 | 0.71 |
| 2:B:200:THR:O | 2:B:204:GLU:HG3 | 1.91 | 0.71 |
| 2:B:378:GLU:O | 2:B:382:ILE:HG12 | 1.90 | 0.70 |
| 2:F:194:GLU:OE2 | 2:F:195:ILE:HG22 | 1.91 | 0.70 |
| 1:A:445:ALA:N | 1:A:477:THR:HG21 | 2.06 | 0.70 |
| 1:M:108:VAL:HG21 | 1:M:221:HIS:CD2 | 2.26 | 0.70 |
| 1:A:24:TRP:CH2 | 3:C:704:DC:H5' | 2.26 | 0.70 |
| 1:I:246:LEU:HD12 | 1:I:246:LEU:H | 1.56 | 0.70 |
| 2:B:265:ASN:O | 2:B:268:SER:HB3 | 1.92 | 0.70 |
| 1:I:165:THR:HG22 | 1:I:182:GLN:NE2 | 2.05 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:N:66:LYS:HZ3 | 2:N:66:LYS:CB | 2.00 | 0.70 |
| 4:H:806:DT:H2" | 4:H:807:DC:H5" | 1.74 | 0.70 |
| 2:F:254:VAL:HG23 | 2:F:291:GLU:O | 1.91 | 0.70 |
| 1:E:165:THR:HG21 | 2:F:140:PRO:HG2 | 1.72 | 0.70 |
| 2:F:265:ASN:O | 2:F:268:SER:HB3 | 1.92 | 0.70 |
| 4:L:806:DT:H2" | 4:L:807:DC:H5' | 1.74 | 0.70 |
| 1:E:260:LEU:O | 1:E:264:LEU:HG | 1.91 | 0.69 |
| 1:E:165:THR:HG22 | 1:E:182:GLN:NE2 | 2.07 | 0.69 |
| 1:I:420:PRO:HA | 1:I:422:LEU:HD22 | 1.74 | 0.69 |
| 4:L:809:DC:H1' | 4:L:810:DT:H5' | 1.74 | 0.69 |
| 1:A:24:TRP:CZ2 | 3:C:704:DC:H5' | 2.26 | 0.69 |
| 1:M:339:TYR:CE1 | 1:M:352:GLY:HA3 | 2.26 | 0.69 |
| 1:I:181:TYR:CD2 | 2:J:138:GLU:HA | 2.27 | 0.69 |
| 2:J:60:VAL:HG12 | 2:J:75:VAL:HG22 | 1.75 | 0.69 |
| 1:E:339:TYR:CZ | 1:E:352:GLY:HA3 | 2.28 | 0.69 |
| 1:I:296:THR:HG23 | 1:I:299:ALA:H | 1.56 | 0.69 |
| 3:G:709:DC:H2' | 3:G:710:DG:C8 | 2.28 | 0.69 |
| 1:E:108:VAL:HG21 | 1:E:221:HIS:CD2 | 2.28 | 0.69 |
| 1:I:445:ALA:N | 1:I:477:THR:HG21 | 2.07 | 0.69 |
| 1:I:458:VAL:CG1 | 1:I:548:VAL:HG22 | 2.23 | 0.69 |
| 1:A:244:ILE:O | 1:A:244:ILE:HG13 | 1.92 | 0.69 |
| 1:A:289:LEU:H | 1:A:289:LEU:HD12 | 1.58 | 0.69 |
| 1:A:492:GLU:OE2 | 1:A:530:LYS:HD3 | 1.93 | 0.69 |
| 3:O:709:DC:H2' | 3:O:710:DG:C8 | 2.28 | 0.69 |
| 1:A:94:ILE:CD1 | 3:C:708:DG:H21 | 2.06 | 0.69 |
| 1:E:125:ARG:HD3 | 1:E:147:ASN:HA | 1.75 | 0.69 |
| 1:E:125:ARG:NH1 | 1:E:147:ASN:HB3 | 2.08 | 0.69 |
| 1:M:458:VAL:HG12 | 1:M:548:VAL:HG22 | 1.74 | 0.69 |
| 2:N:104:LYS:O | 2:N:104:LYS:HD3 | 1.92 | 0.69 |
| 4:L:806:DT:H2" | 4:L:807:DC:C5' | 2.23 | 0.69 |
| 1:M:240:THR:HG22 | 1:M:315:HIS:HA | 1.74 | 0.69 |
| 1:A:434:ILE:HD12 | 1:A:530:LYS:HE2 | 1.74 | 0.68 |
| 1:I:492:GLU:OE2 | 1:I:530:LYS:HD3 | 1.93 | 0.68 |
| 2:N:50:ILE:HD13 | 2:N:145:GLN:HB3 | 1.75 | 0.68 |
| 1:A:25:PRO:HD2 | 3:C:703:DG:N2 | 2.08 | 0.68 |
| 1:A:287:LYS:NZ | 1:A:293:ILE:HD12 | 2.08 | 0.68 |
| 1:E:132:ILE:HD11 | 1:E:142:ILE:CD1 | 2.24 | 0.68 |
| 1:I:7:THR:HG22 | 1:I:119:PRO:HB2 | 1.74 | 0.68 |
| 1:I:339:TYR:CZ | 1:I:352:GLY:HA3 | 2.28 | 0.68 |
| 2:N:151:GLN:HB3 | 2:N:185:ASP:OD2 | 1.93 | 0.68 |
| 3:C:709:DC:H2' | 3:C:710:DG:H8 | 1.57 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:D:806:DT:H6 | 4:D:806:DT:H5' | 1.58 | 0.68 |
| 1:A:548:VAL:O | 1:A:552:VAL:HG22 | 1.92 | 0.68 |
| 1:A:246:LEU:HD12 | 1:A:246:LEU:H | 1.58 | 0.68 |
| 1:I:206:ARG:HG3 | 1:I:216:THR:HG21 | 1.75 | 0.68 |
| 1:I:426:TRP:HB3 | 1:I:526:ILE:HD12 | 1.75 | 0.68 |
| 4:P:806:DT:H2" | 4:P:807:DC:H5" | 1.75 | 0.68 |
| 1:A:94:ILE:HD11 | 3:C:708:DG:H21 | 1.58 | 0.68 |
| 2:B:206:ARG:O | 2:B:210:LEU:HD13 | 1.93 | 0.68 |
| 2:B:151:GLN:HB3 | 2:B:185:ASP:OD2 | 1.94 | 0.68 |
| 1:A:24:TRP:CE3 | 3:C:703:DG:H1' | 2.28 | 0.67 |
| 2:B:85:GLN:HA | 2:B:88:TRP:CE2 | 2.29 | 0.67 |
| 1:M:286:THR:OG1 | 3:O:714:DG:H4' | 1.93 | 0.67 |
| 2:B:371:ALA:O | 2:B:375:ILE:HG12 | 1.94 | 0.67 |
| 1:M:56:TYR:O | 1:M:143:ARG:NH2 | 2.27 | 0.67 |
| 3:C:706:DT:H2' | 3:C:707:DG:C8 | 2.29 | 0.67 |
| 1:E:108:VAL:CG2 | 1:E:108:VAL:O | 2.43 | 0.67 |
| 2:F:332:GLN:HE22 | 2:F:425:LEU:HD13 | 1.59 | 0.67 |
| 1:I:207:GLN:HA | 1:I:210:LEU:HD12 | 1.76 | 0.67 |
| 1:E:439:THR:HG21 | 2:F:289:LEU:CD1 | 2.24 | 0.67 |
| 2:B:209:LEU:HD22 | 2:B:214:LEU:HD12 | 1.77 | 0.67 |
| 2:F:54:ASN:HD22 | 2:F:56:TYR:H | 1.43 | 0.67 |
| 1:I:96:HIS:HE2 | 1:I:269:GLN:HE21 | 1.43 | 0.67 |
| 1:M:445:ALA:N | 1:M:477:THR:HG21 | 2.10 | 0.67 |
| 1:E:493:VAL:HG12 | 1:E:494:ASN:N | 2.10 | 0.67 |
| 2:N:254:VAL:O | 2:N:258:GLN:HG3 | 1.95 | 0.67 |
| 4:H:819:DG:H2' | 4:H:820:DC:C6 | 2.29 | 0.67 |
| 2:N:215:THR:HG22 | 2:N:217:PRO:HD3 | 1.77 | 0.66 |
| 4:D:806:DT:H2" | 4:D:807:DC:H5' | 1.74 | 0.66 |
| 4:D:818:DC:H2" | 4:D:819:DG:H5' | 1.77 | 0.66 |
| 2:F:108:VAL:N | 2:F:232:TYR:OH | 2.28 | 0.66 |
| 1:M:207:GLN:HA | 1:M:210:LEU:HD12 | 1.77 | 0.66 |
| 1:M:246:LEU:H | 1:M:246:LEU:HD12 | 1.60 | 0.66 |
| 1:A:25:PRO:HD2 | 3:C:703:DG:C2 | 2.30 | 0.66 |
| 2:B:318:TYR:HB3 | 8:B:438:HOH:O | 1.95 | 0.66 |
| 1:I:115:TYR:CD2 | 6:I:823:ZP4:H2'A | 2.30 | 0.66 |
| 1:E:102:LYS:H | 1:E:102:LYS:CD | 2.00 | 0.66 |
| 2:F:54:ASN:ND2 | 2:F:56:TYR:H | 1.94 | 0.66 |
| 4:P:807:DC:H2" | 4:P:808:DC:C5' | 2.23 | 0.66 |
| 1:M:492:GLU:OE2 | 1:M:530:LYS:HD3 | 1.95 | 0.66 |
| 4:P:820:DC:H2" | 4:P:821:DC:H5' | 1.78 | 0.66 |
| 1:A:326:ILE:HG21 | 1:A:390:LYS:HE2 | 1.77 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:317:VAL:HG13 | 1:M:349:LEU:CD2 | 2.26 | 0.66 |
| 2:N:54:ASN:HD22 | 2:N:54:ASN:C | 1.98 | 0.66 |
| 2:B:263:LYS:HB2 | 2:B:423:VAL:HG11 | 1.77 | 0.66 |
| 2:N:332:GLN:HG3 | 2:N:428:GLN:HG3 | 1.76 | 0.66 |
| 1:A:296:THR:HG23 | 1:A:299:ALA:H | 1.58 | 0.66 |
| 1:A:357:MET:HG2 | 1:A:367:GLN:NE2 | 2.11 | 0.66 |
| 2:J:170:PRO:HG2 | 2:J:208:HIS:CE1 | 2.31 | 0.66 |
| 1:M:253:THR:HA | 1:M:292:VAL:HA | 1.76 | 0.66 |
| 1:E:439:THR:CG2 | 2:F:289:LEU:HD13 | 2.24 | 0.66 |
| 3:K:709:DC:H2' | 3:K:710:DG:C8 | 2.31 | 0.66 |
| 1:A:108:VAL:CG2 | 1:A:108:VAL:O | 2.44 | 0.66 |
| 1:A:406:TRP:HD1 | 1:A:407:GLN:HE21 | 1.45 | 0.66 |
| 1:E:246:LEU:H | 1:E:246:LEU:HD12 | 1.59 | 0.66 |
| 2:F:206:ARG:O | 2:F:210:LEU:HD13 | 1.96 | 0.66 |
| 1:I:228:LEU:HD12 | 6:I:823:ZP4:N1R | 2.10 | 0.66 |
| 2:J:54:ASN:HD22 | 2:J:56:TYR:H | 1.44 | 0.66 |
| 1:A:541:GLY:O | 1:A:542:ILE:O | 2.13 | 0.65 |
| 1:I:229:TRP:HA | 8:I:563:HOH:O | 1.95 | 0.65 |
| 1:M:317:VAL:HG22 | 1:M:318:TYR:N | 2.10 | 0.65 |
| 2:B:254:VAL:HG22 | 2:B:293:ILE:HD11 | 1.77 | 0.65 |
| 1:A:181:TYR:CD2 | 2:B:138:GLU:HA | 2.32 | 0.65 |
| 1:E:432:GLU:HG3 | 1:E:433:PRO:HD2 | 1.79 | 0.65 |
| 2:J:254:VAL:O | 2:J:258:GLN:HG3 | 1.97 | 0.65 |
| 2:J:423:VAL:HB | 2:J:426:TRP:CD1 | 2.31 | 0.65 |
| 1:A:12:LEU:HD11 | 1:A:127:TYR:CZ | 2.32 | 0.65 |
| 1:M:94:ILE:CD1 | 3:O:708:DG:H21 | 2.09 | 0.65 |
| 1:I:501:TYR:CE1 | 1:I:505:ILE:HD11 | 2.32 | 0.65 |
| 1:M:125:ARG:NH1 | 1:M:147:ASN:HB3 | 2.11 | 0.65 |
| 2:B:63:ILE:H | 2:B:63:ILE:HD13 | 1.60 | 0.65 |
| 1:E:7:THR:HG22 | 1:E:119:PRO:HB2 | 1.79 | 0.65 |
| 2:F:154:LYS:O | 2:F:157:PRO:HD2 | 1.97 | 0.65 |
| 2:F:215:THR:HG22 | 2:F:217:PRO:HD3 | 1.77 | 0.65 |
| 1:I:115:TYR:CE2 | 6:I:823:ZP4:H2'A | 2.32 | 0.65 |
| 2:J:257:ILE:HG23 | 2:J:283:LEU:HD21 | 1.78 | 0.65 |
| 1:M:17:ASP:O | 1:M:83:ARG:HD3 | 1.96 | 0.65 |
| 2:N:206:ARG:O | 2:N:210:LEU:HD13 | 1.95 | 0.65 |
| 4:P:818:DC:H2'' | 4:P:819:DG:H5' | 1.78 | 0.65 |
| 2:J:13:LYS:CB | 2:J:16:MET:HG3 | 2.25 | 0.65 |
| 2:J:215:THR:HG22 | 2:J:217:PRO:HD3 | 1.78 | 0.65 |
| 2:J:423:VAL:HB | 2:J:426:TRP:NE1 | 2.12 | 0.65 |
| 1:E:501:TYR:CE1 | 1:E:505:ILE:HD11 | 2.32 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:F:423:VAL:HB | 2:F:426:TRP:NE1 | 2.12 | 0.65 |
| 1:M:206:ARG:HG3 | 1:M:216:THR:HG21 | 1.79 | 0.65 |
| 3:C:709:DC:H2' | 3:C:710:DG:C8 | 2.32 | 0.64 |
| 3:K:716:DA:H1' | 3:K:717:DC:H5' | 1.79 | 0.64 |
| 1:A:5:ILE:HD12 | 1:A:6:GLU:N | 2.13 | 0.64 |
| 1:A:102:LYS:H | 1:A:102:LYS:CD | 1.92 | 0.64 |
| 2:B:340:GLN:HG3 | 2:B:351:THR:HG22 | 1.78 | 0.64 |
| 1:E:109:LEU:CD2 | 1:E:220:LYS:CG | 2.75 | 0.64 |
| 1:E:108:VAL:O | 1:E:108:VAL:HG23 | 1.97 | 0.64 |
| 2:F:332:GLN:NE2 | 2:F:425:LEU:HD13 | 2.11 | 0.64 |
| 2:J:340:GLN:HG3 | 2:J:351:THR:HG22 | 1.79 | 0.64 |
| 1:M:5:ILE:HD12 | 1:M:6:GLU:N | 2.13 | 0.64 |
| 2:N:54:ASN:ND2 | 2:N:56:TYR:H | 1.95 | 0.64 |
| 1:M:335:GLY:HA2 | 1:M:367:GLN:HE22 | 1.62 | 0.64 |
| 2:N:209:LEU:HD22 | 2:N:214:LEU:HD12 | 1.80 | 0.64 |
| 1:A:498:ASP:HB2 | 1:A:538:ALA:HA | 1.79 | 0.64 |
| 1:A:500:GLN:NE2 | 2:B:422:LEU:HD13 | 2.12 | 0.64 |
| 1:E:289:LEU:H | 1:E:289:LEU:HD12 | 1.63 | 0.64 |
| 1:I:209:LEU:HB3 | 1:I:214:LEU:HB2 | 1.80 | 0.64 |
| 3:K:706:DT:H2' | 3:K:707:DG:C8 | 2.33 | 0.64 |
| 2:F:85:GLN:HA | 2:F:88:TRP:CE2 | 2.32 | 0.64 |
| 1:I:458:VAL:HG12 | 1:I:548:VAL:HG22 | 1.79 | 0.64 |
| 1:E:244:ILE:HG23 | 1:E:244:ILE:O | 1.96 | 0.64 |
| 1:I:252:TRP:NE1 | 1:I:295:LEU:HD22 | 2.12 | 0.64 |
| 2:J:54:ASN:ND2 | 2:J:56:TYR:H | 1.95 | 0.64 |
| 2:J:375:ILE:HB | 2:J:389:PHE:HZ | 1.63 | 0.64 |
| 3:G:716:DA:H1' | 3:G:717:DC:H5' | 1.79 | 0.64 |
| 1:E:24:TRP:CE3 | 3:G:703:DG:H1' | 2.32 | 0.64 |
| 1:E:132:ILE:HG13 | 1:E:142:ILE:HG13 | 1.79 | 0.64 |
| 1:E:132:ILE:CG1 | 1:E:142:ILE:HG13 | 2.27 | 0.64 |
| 2:F:423:VAL:HB | 2:F:426:TRP:CD1 | 2.33 | 0.64 |
| 1:A:444:GLY:HA3 | 1:A:477:THR:HG22 | 1.80 | 0.63 |
| 2:B:368:LEU:HD11 | 2:B:392:PRO:HD2 | 1.80 | 0.63 |
| 1:E:199:ARG:O | 1:E:202:ILE:HG22 | 1.99 | 0.63 |
| 1:M:441:TYR:CD2 | 1:M:544:GLY:HA3 | 2.33 | 0.63 |
| 3:O:706:DT:H2' | 3:O:707:DG:C8 | 2.33 | 0.63 |
| 4:P:806:DT:C2' | 4:P:807:DC:H5" | 2.28 | 0.63 |
| 1:A:325:LEU:HD13 | 1:A:385:LYS:HE2 | 1.80 | 0.63 |
| 1:E:109:LEU:HD22 | 1:E:220:LYS:HG2 | 1.79 | 0.63 |
| 1:E:209:LEU:HB3 | 1:E:214:LEU:HB2 | 1.80 | 0.63 |
| 1:E:529:GLU:O | 1:E:530:LYS:HG3 | 1.98 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:J:206:ARG:O | 2:J:210:LEU:HD13 | 1.98 | 0.63 |
| 1:M:108:VAL:CG2 | 1:M:108:VAL:O | 2.46 | 0.63 |
| 1:M:501:TYR:HE1 | 1:M:505:ILE:HD11 | 1.62 | 0.63 |
| 2:N:375:ILE:HB | 2:N:389:PHE:HZ | 1.63 | 0.63 |
| 4:H:806:DT:C2' | 4:H:807:DC:H5" | 2.28 | 0.63 |
| 1:A:26:LEU:HB2 | 1:A:31:ILE:CD1 | 2.28 | 0.63 |
| 1:A:458:VAL:HG11 | 1:A:548:VAL:HG22 | 1.79 | 0.63 |
| 1:M:326:ILE:HG21 | 1:M:390:LYS:HE2 | 1.80 | 0.63 |
| 2:N:131:THR:OG1 | 2:N:143:ARG:HD2 | 1.98 | 0.63 |
| 3:C:706:DT:H2' | 3:C:707:DG:H8 | 1.63 | 0.63 |
| 1:A:31:ILE:O | 1:A:35:VAL:HG22 | 1.99 | 0.63 |
| 1:A:207:GLN:HA | 1:A:210:LEU:HD12 | 1.79 | 0.63 |
| 2:B:104:LYS:O | 2:B:104:LYS:HD3 | 1.98 | 0.63 |
| 1:A:253:THR:HA | 1:A:292:VAL:HA | 1.80 | 0.63 |
| 1:E:25:PRO:HD2 | 3:G:703:DG:C2 | 2.33 | 0.63 |
| 1:M:94:ILE:HD11 | 3:O:708:DG:H21 | 1.61 | 0.63 |
| 1:A:331:LYS:HE3 | 8:A:564:HOH:O | 1.98 | 0.63 |
| 2:F:393:ILE:HD13 | 2:F:398:TRP:HB2 | 1.81 | 0.63 |
| 1:E:102:LYS:HD2 | 1:E:102:LYS:N | 2.02 | 0.63 |
| 1:I:491:LEU:HD12 | 1:I:491:LEU:N | 2.14 | 0.63 |
| 1:M:199:ARG:O | 1:M:202:ILE:HG22 | 1.99 | 0.63 |
| 1:A:199:ARG:O | 1:A:202:ILE:HG22 | 1.99 | 0.63 |
| 2:B:278:GLN:HG2 | 2:B:298:GLU:O | 1.98 | 0.63 |
| 1:M:209:LEU:HB3 | 1:M:214:LEU:HB2 | 1.81 | 0.63 |
| 1:M:215:THR:HG22 | 1:M:217:PRO:HD3 | 1.81 | 0.63 |
| 2:N:13:LYS:O | 2:N:16:MET:HB2 | 1.99 | 0.63 |
| 1:A:26:LEU:HB2 | 1:A:31:ILE:HD11 | 1.81 | 0.62 |
| 1:A:178:ILE:HD12 | 1:A:178:ILE:N | 2.14 | 0.62 |
| 1:E:206:ARG:HG3 | 1:E:216:THR:HG21 | 1.80 | 0.62 |
| 1:E:335:GLY:HA2 | 1:E:367:GLN:HE22 | 1.64 | 0.62 |
| 2:N:7:THR:HG22 | 2:N:119:PRO:HG2 | 1.80 | 0.62 |
| 2:F:170:PRO:HG2 | 2:F:208:HIS:CE1 | 2.33 | 0.62 |
| 2:N:374:LYS:O | 2:N:378:GLU:HG3 | 1.99 | 0.62 |
| 2:N:376:THR:O | 2:N:380:ILE:HG13 | 1.98 | 0.62 |
| 1:A:132:ILE:HD11 | 1:A:142:ILE:CD1 | 2.29 | 0.62 |
| 2:B:170:PRO:HG2 | 2:B:208:HIS:CE1 | 2.33 | 0.62 |
| 2:N:332:GLN:HE22 | 2:N:425:LEU:HD13 | 1.65 | 0.62 |
| 1:A:137:ASN:HD22 | 1:A:137:ASN:H | 1.48 | 0.62 |
| 1:I:155:GLY:O | 1:I:159:ILE:HG12 | 1.99 | 0.62 |
| 1:I:238:LYS:HD2 | 1:I:315:HIS:ND1 | 2.15 | 0.62 |
| 1:I:439:THR:CG2 | 2:J:289:LEU:HD13 | 2.29 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:427:TYR:OH | 1:M:509:GLN:HA | 2.00 | 0.62 |
| 1:M:498:ASP:HB2 | 1:M:538:ALA:HA | 1.80 | 0.62 |
| 2:B:423:VAL:HB | 2:B:426:TRP:NE1 | 2.14 | 0.62 |
| 1:E:181:TYR:CD2 | 2:F:138:GLU:HA | 2.34 | 0.62 |
| 2:J:151:GLN:HB3 | 2:J:185:ASP:OD2 | 1.99 | 0.62 |
| 1:A:317:VAL:O | 1:A:349:LEU:CD2 | 2.46 | 0.62 |
| 2:B:376:THR:O | 2:B:380:ILE:HG13 | 2.00 | 0.62 |
| 1:E:235:HIS:HB3 | 1:E:236:PRO:CD | 2.27 | 0.62 |
| 1:I:8:VAL:O | 1:I:10:VAL:HG23 | 2.00 | 0.62 |
| 1:I:317:VAL:HG22 | 1:I:318:TYR:N | 2.13 | 0.62 |
| 1:E:498:ASP:HB2 | 1:E:538:ALA:HA | 1.81 | 0.62 |
| 1:E:542:ILE:HB | 1:E:545:ASN:HB3 | 1.82 | 0.62 |
| 1:I:178:ILE:N | 1:I:178:ILE:HD12 | 2.15 | 0.62 |
| 2:J:376:THR:O | 2:J:380:ILE:HG13 | 1.99 | 0.62 |
| 2:N:278:GLN:HG2 | 2:N:298:GLU:O | 1.99 | 0.62 |
| 2:N:66:LYS:CB | 2:N:66:LYS:HZ2 | 2.01 | 0.62 |
| 1:E:207:GLN:HA | 1:E:210:LEU:HD12 | 1.81 | 0.61 |
| 2:B:154:LYS:O | 2:B:157:PRO:HD2 | 2.00 | 0.61 |
| 2:F:209:LEU:HD22 | 2:F:214:LEU:HD12 | 1.83 | 0.61 |
| 1:M:111:VAL:HB | 1:M:185:ASP:HB2 | 1.82 | 0.61 |
| 3:C:716:DA:H1' | 3:C:717:DC:H5' | 1.82 | 0.61 |
| 2:B:263:LYS:CA | 2:B:423:VAL:HG11 | 2.30 | 0.61 |
| 1:E:80:LEU:HD12 | 1:E:80:LEU:O | 2.01 | 0.61 |
| 1:E:252:TRP:NE1 | 1:E:295:LEU:HD22 | 2.16 | 0.61 |
| 2:F:278:GLN:HG2 | 2:F:298:GLU:O | 2.00 | 0.61 |
| 1:I:33:ALA:O | 1:I:37:ILE:HG12 | 2.00 | 0.61 |
| 1:I:59:PRO:HG2 | 1:I:76:ASP:HB3 | 1.81 | 0.61 |
| 1:I:80:LEU:O | 1:I:84:THR:HG22 | 1.99 | 0.61 |
| 2:J:85:GLN:HA | 2:J:88:TRP:CE2 | 2.35 | 0.61 |
| 1:M:102:LYS:H | 1:M:102:LYS:CD | 2.00 | 0.61 |
| 1:M:57:ASN:ND2 | 1:M:131:THR:OG1 | 2.33 | 0.61 |
| 1:M:252:TRP:NE1 | 1:M:295:LEU:HD22 | 2.16 | 0.61 |
| 4:L:806:DT:H1' | 4:L:807:DC:H5" | 1.83 | 0.61 |
| 2:B:379:SER:OG | 2:B:387:PRO:HD3 | 2.01 | 0.61 |
| 2:N:60:VAL:HG12 | 2:N:75:VAL:HG22 | 1.83 | 0.61 |
| 1:A:501:TYR:CE1 | 1:A:505:ILE:HD11 | 2.36 | 0.61 |
| 1:E:24:TRP:CH2 | 3:G:704:DC:H5' | 2.34 | 0.61 |
| 1:M:155:GLY:O | 1:M:159:ILE:HG12 | 2.00 | 0.61 |
| 2:N:88:TRP:CZ2 | 2:N:154:LYS:HD3 | 2.35 | 0.61 |
| 2:N:170:PRO:HG2 | 2:N:208:HIS:CE1 | 2.36 | 0.61 |
| 4:D:818:DC:H2' | 4:D:819:DG:H8 | 1.65 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:N:108:VAL:HG22 | 2:N:188:TYR:CD2 | 2.36 | 0.61 |
| 3:K:706:DT:H2' | 3:K:707:DG:H8 | 1.66 | 0.61 |
| 1:E:111:VAL:HB | 1:E:185:ASP:HB2 | 1.82 | 0.61 |
| 1:A:342:TYR:HB2 | 1:A:347:LYS:O | 2.00 | 0.61 |
| 1:A:441:TYR:CE2 | 1:A:544:GLY:HA3 | 2.35 | 0.61 |
| 1:E:327:ALA:HB2 | 1:E:341:ILE:HG13 | 1.83 | 0.61 |
| 1:I:366:LYS:O | 1:I:370:GLU:HG3 | 2.01 | 0.61 |
| 1:A:137:ASN:N | 1:A:137:ASN:ND2 | 2.49 | 0.60 |
| 2:B:241:VAL:HG13 | 2:B:351:THR:H | 1.66 | 0.60 |
| 2:B:254:VAL:O | 2:B:258:GLN:HG3 | 2.01 | 0.60 |
| 2:B:423:VAL:HB | 2:B:426:TRP:CD1 | 2.36 | 0.60 |
| 1:M:439:THR:HG21 | 2:N:289:LEU:HD13 | 1.83 | 0.60 |
| 1:E:65:LYS:HD3 | 6:E:823:ZP4:O2D | 2.01 | 0.60 |
| 1:A:235:HIS:HB3 | 1:A:236:PRO:CD | 2.29 | 0.60 |
| 1:E:137:ASN:HD22 | 1:E:137:ASN:H | 1.50 | 0.60 |
| 1:M:478:GLU:CG | 1:M:499:SER:HB2 | 2.30 | 0.60 |
| 1:M:96:HIS:HE2 | 1:M:269:GLN:HE21 | 1.48 | 0.60 |
| 1:A:206:ARG:HG3 | 1:A:216:THR:HG21 | 1.82 | 0.60 |
| 1:E:109:LEU:HD23 | 1:E:220:LYS:CD | 2.29 | 0.60 |
| 1:I:228:LEU:HB2 | 6:I:823:ZP4:H2R | 1.82 | 0.60 |
| 2:J:209:LEU:HD22 | 2:J:214:LEU:HD12 | 1.83 | 0.60 |
| 1:M:3:SER:HB2 | 1:M:119:PRO:HD3 | 1.82 | 0.60 |
| 1:M:287:LYS:NZ | 1:M:293:ILE:HD12 | 2.17 | 0.60 |
| 1:M:289:LEU:H | 1:M:289:LEU:HD12 | 1.65 | 0.60 |
| 1:I:108:VAL:O | 1:I:108:VAL:CG2 | 2.49 | 0.60 |
| 1:E:109:LEU:HD21 | 1:E:220:LYS:CE | 2.32 | 0.60 |
| 1:E:137:ASN:N | 1:E:137:ASN:ND2 | 2.50 | 0.60 |
| 1:I:125:ARG:NH1 | 1:I:147:ASN:HB3 | 2.15 | 0.60 |
| 3:G:722:DA:H1' | 3:G:723:DC:H5' | 1.83 | 0.60 |
| 2:F:340:GLN:HG3 | 2:F:351:THR:HG22 | 1.84 | 0.60 |
| 1:I:17:ASP:O | 1:I:83:ARG:HD3 | 2.02 | 0.60 |
| 1:I:285:GLY:N | 3:K:714:DG:OP1 | 2.35 | 0.60 |
| 2:N:423:VAL:HB | 2:N:426:TRP:CD1 | 2.36 | 0.60 |
| 4:D:818:DC:H2' | 4:D:819:DG:C8 | 2.36 | 0.60 |
| 1:E:372:VAL:HG13 | 1:E:389:PHE:CZ | 2.37 | 0.60 |
| 2:F:206:ARG:CB | 2:F:206:ARG:HH11 | 2.15 | 0.60 |
| 1:I:254:VAL:HG23 | 1:I:291:GLU:O | 2.00 | 0.59 |
| 1:I:379:SER:OG | 1:I:387:PRO:HD3 | 2.02 | 0.59 |
| 1:I:441:TYR:CE2 | 1:I:544:GLY:HA3 | 2.36 | 0.59 |
| 2:J:278:GLN:HG2 | 2:J:298:GLU:O | 2.01 | 0.59 |
| 2:N:332:GLN:NE2 | 2:N:425:LEU:HD13 | 2.16 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:115:TYR:CE1 | 1:E:184:MET:HE1 | 2.37 | 0.59 |
| 2:F:425:LEU:CA | 8:F:438:HOH:O | 2.51 | 0.59 |
| 1:I:335:GLY:HA2 | 1:I:367:GLN:HE22 | 1.67 | 0.59 |
| 1:I:439:THR:HG21 | 2:J:289:LEU:CD1 | 2.32 | 0.59 |
| 1:M:26:LEU:HB2 | 1:M:31:ILE:HD11 | 1.83 | 0.59 |
| 1:E:109:LEU:CD2 | 1:E:220:LYS:HG2 | 2.32 | 0.59 |
| 1:I:498:ASP:HB2 | 1:I:538:ALA:HA | 1.84 | 0.59 |
| 1:A:379:SER:OG | 1:A:387:PRO:HD3 | 2.02 | 0.59 |
| 3:G:706:DT:H2' | 3:G:707:DG:C8 | 2.37 | 0.59 |
| 1:A:398:TRP:CZ2 | 1:A:411:ILE:HG12 | 2.37 | 0.59 |
| 1:A:493:VAL:HG12 | 1:A:494:ASN:N | 2.16 | 0.59 |
| 1:E:151:GLN:NE2 | 6:E:823:ZP4:N3B | 2.50 | 0.59 |
| 1:I:199:ARG:O | 1:I:202:ILE:HG22 | 2.02 | 0.59 |
| 1:M:286:THR:OG1 | 3:O:714:DG:C5' | 2.50 | 0.59 |
| 1:M:366:LYS:O | 1:M:370:GLU:HG3 | 2.03 | 0.59 |
| 1:M:438:GLU:CD | 1:M:463:ARG:HD2 | 2.23 | 0.59 |
| 1:M:339:TYR:CG | 1:M:375:ILE:HD11 | 2.37 | 0.59 |
| 3:O:716:DA:H1' | 3:O:717:DC:H5' | 1.85 | 0.59 |
| 1:A:529:GLU:O | 1:A:530:LYS:HG3 | 2.03 | 0.59 |
| 1:E:25:PRO:HD2 | 3:G:703:DG:N2 | 2.17 | 0.59 |
| 1:E:222:GLN:O | 1:E:224:GLU:HG3 | 2.02 | 0.59 |
| 1:E:406:TRP:HD1 | 1:E:407:GLN:HE21 | 1.50 | 0.59 |
| 2:F:13:LYS:HE3 | 2:F:86:ASP:H | 1.67 | 0.59 |
| 1:M:108:VAL:O | 1:M:108:VAL:HG23 | 2.02 | 0.59 |
| 1:M:400:THR:O | 1:M:404:GLU:HG2 | 2.02 | 0.59 |
| 2:N:257:ILE:HG23 | 2:N:283:LEU:HD21 | 1.84 | 0.59 |
| 3:C:722:DA:H1' | 3:C:723:DC:H5' | 1.84 | 0.59 |
| 1:A:29:GLU:O | 1:A:32:LYS:HB3 | 2.02 | 0.59 |
| 1:E:5:ILE:HD12 | 1:E:6:GLU:N | 2.17 | 0.59 |
| 1:I:478:GLU:CD | 1:I:499:SER:HB2 | 2.23 | 0.59 |
| 2:N:340:GLN:HG3 | 2:N:351:THR:HG22 | 1.84 | 0.59 |
| 1:A:351:THR:HB | 8:A:556:HOH:O | 2.03 | 0.59 |
| 1:A:372:VAL:HG13 | 1:A:389:PHE:CZ | 2.38 | 0.59 |
| 1:E:429:LEU:HD13 | 1:E:533:LEU:CD1 | 2.32 | 0.59 |
| 1:I:94:ILE:CD1 | 3:K:708:DG:H21 | 2.15 | 0.59 |
| 1:E:183:TYR:O | 1:E:184:MET:HB2 | 2.03 | 0.58 |
| 2:F:425:LEU:HB3 | 8:F:438:HOH:O | 2.02 | 0.58 |
| 1:I:237:ASP:C | 1:I:238:LYS:HG2 | 2.22 | 0.58 |
| 1:E:178:ILE:HD12 | 1:E:178:ILE:N | 2.18 | 0.58 |
| 1:M:491:LEU:HD12 | 1:M:491:LEU:N | 2.19 | 0.58 |
| 1:M:33:ALA:O | 1:M:37:ILE:HG12 | 2.03 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:O:706:DT:H2' | 3:O:707:DG:H8 | 1.68 | 0.58 |
| 1:A:445:ALA:H | 1:A:477:THR:HG21 | 1.68 | 0.58 |
| 1:A:24:TRP:HE3 | 3:C:703:DG:H1' | 1.69 | 0.58 |
| 1:A:31:ILE:HD12 | 1:A:133:PRO:HG2 | 1.84 | 0.58 |
| 1:A:439:THR:CG2 | 2:B:289:LEU:HD13 | 2.29 | 0.58 |
| 2:B:215:THR:HG22 | 2:B:217:PRO:HD3 | 1.85 | 0.58 |
| 1:E:33:ALA:O | 1:E:37:ILE:HG12 | 2.04 | 0.58 |
| 2:F:368:LEU:HD22 | 2:F:398:TRP:CZ3 | 2.38 | 0.58 |
| 2:F:374:LYS:O | 2:F:378:GLU:HG3 | 2.04 | 0.58 |
| 1:M:8:VAL:O | 1:M:10:VAL:HG23 | 2.04 | 0.58 |
| 1:M:281:LYS:HG3 | 1:M:284:ARG:NH1 | 2.19 | 0.58 |
| 2:N:85:GLN:HA | 2:N:88:TRP:CE2 | 2.38 | 0.58 |
| 1:A:165:THR:HG21 | 2:B:140:PRO:CG | 2.32 | 0.58 |
| 1:A:183:TYR:O | 1:A:184:MET:HB2 | 2.02 | 0.58 |
| 2:B:263:LYS:CB | 2:B:423:VAL:HG11 | 2.34 | 0.58 |
| 2:B:13:LYS:O | 2:B:16:MET:HB2 | 2.02 | 0.58 |
| 2:J:131:THR:OG1 | 2:J:143:ARG:HD2 | 2.04 | 0.58 |
| 2:J:194:GLU:OE2 | 2:J:195:ILE:HG22 | 2.03 | 0.58 |
| 2:J:200:THR:O | 2:J:204:GLU:HG3 | 2.03 | 0.58 |
| 1:E:13:LYS:HE3 | 1:E:84:THR:O | 2.03 | 0.58 |
| 1:E:535:TRP:O | 1:E:536:VAL:CG1 | 2.52 | 0.58 |
| 2:F:263:LYS:HB2 | 2:F:423:VAL:HG11 | 1.86 | 0.58 |
| 1:I:327:ALA:HB2 | 1:I:341:ILE:HG13 | 1.85 | 0.58 |
| 1:I:235:HIS:HB3 | 1:I:236:PRO:CD | 2.28 | 0.58 |
| 2:J:206:ARG:CB | 2:J:206:ARG:HH11 | 2.17 | 0.58 |
| 2:N:169:GLU:N | 2:N:170:PRO:HD2 | 2.19 | 0.58 |
| 3:O:722:DA:H1' | 3:O:723:DC:H5' | 1.86 | 0.58 |
| 1:A:27:THR:O | 1:A:31:ILE:HG12 | 2.04 | 0.58 |
| 2:B:374:LYS:O | 2:B:378:GLU:HG3 | 2.04 | 0.58 |
| 1:E:26:LEU:HB2 | 1:E:31:ILE:HD11 | 1.86 | 0.58 |
| 1:E:221:HIS:CE1 | 6:E:823:ZP4:HN6A | 2.21 | 0.58 |
| 2:F:206:ARG:HB3 | 2:F:206:ARG:NH1 | 2.19 | 0.58 |
| 1:I:429:LEU:N | 1:I:429:LEU:HD23 | 2.18 | 0.58 |
| 1:M:426:TRP:HB3 | 1:M:526:ILE:HD12 | 1.85 | 0.58 |
| 1:A:439:THR:HG21 | 2:B:289:LEU:CD1 | 2.28 | 0.57 |
| 1:E:109:LEU:HD21 | 1:E:220:LYS:CD | 2.34 | 0.57 |
| 2:F:104:LYS:O | 2:F:104:LYS:HD3 | 2.04 | 0.57 |
| 1:M:23:GLN:HG3 | 1:M:131:THR:O | 2.04 | 0.57 |
| 1:A:33:ALA:O | 1:A:37:ILE:HG12 | 2.05 | 0.57 |
| 2:B:376:THR:HG21 | 2:B:410:TRP:CZ3 | 2.39 | 0.57 |
| 1:E:326:ILE:HG21 | 1:E:390:LYS:HE2 | 1.86 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------|--------|--------------------------|-------------------|
| 1:E:422:LEU:HD22 | 1:E:422:LEU:N | 2.19 | 0.57 |
| 1:I:252:TRP:CD1 | 1:I:295:LEU:HD22 | 2.40 | 0.57 |
| 1:I:326:ILE:HG21 | 1:I:390:LYS:HE2 | 1.85 | 0.57 |
| 1:I:444:GLY:HA3 | 1:I:477:THR:HG22 | 1.86 | 0.57 |
| 4:H:808:DC:H1' | 4:H:809:DC:H5' | 1.85 | 0.57 |
| 1:E:109:LEU:HD23 | 1:E:220:LYS:CG | 2.34 | 0.57 |
| 1:I:260:LEU:O | 1:I:264:LEU:CD1 | 2.52 | 0.57 |
| 1:M:108:VAL:CG2 | 1:M:221:HIS:CD2 | 2.86 | 0.57 |
| 2:N:114:ALA:HB2 | 2:N:214:LEU:HD13 | 1.86 | 0.57 |
| 1:A:132:ILE:CG1 | 1:A:142:ILE:HG13 | 2.35 | 0.57 |
| 2:B:332:GLN:HG3 | 2:B:428:GLN:HG3 | 1.86 | 0.57 |
| 1:M:429:LEU:HD23 | 1:M:429:LEU:N | 2.19 | 0.57 |
| 1:A:44:GLU:OE1 | 1:A:46:LYS:HE2 | 2.04 | 0.57 |
| 2:B:131:THR:OG1 | 2:B:143:ARG:HD2 | 2.04 | 0.57 |
| 2:J:66:LYS:HB3 | 2:J:66:LYS:NZ | 2.19 | 0.57 |
| 2:J:108:VAL:N | 2:J:232:TYR:OH | 2.38 | 0.57 |
| 1:M:344:GLU:CB | 1:M:345:PRO:CD | 2.73 | 0.57 |
| 1:M:529:GLU:O | 1:M:530:LYS:HG3 | 2.04 | 0.57 |
| 1:E:12:LEU:HD11 | 1:E:127:TYR:CZ | 2.39 | 0.57 |
| 1:E:27:THR:O | 1:E:31:ILE:HG12 | 2.04 | 0.57 |
| 1:E:379:SER:OG | 1:E:387:PRO:HD3 | 2.04 | 0.57 |
| 1:E:444:GLY:HA3 | 1:E:477:THR:HG22 | 1.84 | 0.57 |
| 1:I:438:GLU:CD | 1:I:463:ARG:HD2 | 2.25 | 0.57 |
| 2:J:169:GLU:N | 2:J:170:PRO:HD2 | 2.19 | 0.57 |
| 1:M:60:VAL:HG11 | 1:M:130:PHE:CD2 | 2.40 | 0.57 |
| 1:M:244:ILE:C | 1:M:244:ILE:HD13 | 2.24 | 0.57 |
| 1:M:317:VAL:CG1 | 1:M:349:LEU:HD23 | 2.33 | 0.57 |
| 1:M:465:LYS:HG3 | 1:M:466:VAL:N | 2.20 | 0.57 |
| 4:H:806:DT:H2" | 4:H:807:DC:H5' | 1.87 | 0.57 |
| 1:E:109:LEU:HD21 | 1:E:220:LYS:HD3 | 1.86 | 0.57 |
| 2:N:278:GLN:CG | 2:N:298:GLU:HB3 | 2.35 | 0.57 |
| 1:A:209:LEU:HB3 | 1:A:214:LEU:HB2 | 1.87 | 0.57 |
| 1:E:252:TRP:CD1 | 1:E:295:LEU:HD22 | 2.40 | 0.57 |
| 1:A:503:LEU:HD22 | 1:A:535:TRP:HB2 | 1.85 | 0.57 |
| 1:E:492:GLU:OE2 | 1:E:530:LYS:HD3 | 2.05 | 0.57 |
| 1:I:389:PHE:HB3 | 1:I:391:LEU:HD21 | 1.87 | 0.57 |
| 1:M:12:LEU:HD11 | 1:M:127:TYR:CZ | 2.40 | 0.57 |
| 2:N:423:VAL:HB | 2:N:426:TRP:NE1 | 2.20 | 0.57 |
| 1:A:221:HIS:HB3 | 1:A:227:PHE:CD1 | 2.40 | 0.56 |
| 2:B:422:LEU:HG | 2:B:426:TRP:CZ2 | 2.31 | 0.56 |
| 1:E:50:ILE:HG13 | 1:E:143:ARG:CB | 2.34 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:260:LEU:HD23 | 1:E:279:LEU:HD22 | 1.87 | 0.56 |
| 1:I:3:SER:HB3 | 1:I:5:ILE:HG22 | 1.87 | 0.56 |
| 1:M:444:GLY:HA3 | 1:M:477:THR:HG22 | 1.86 | 0.56 |
| 1:M:463:ARG:HG2 | 1:M:463:ARG:NH1 | 2.19 | 0.56 |
| 2:B:7:THR:HG22 | 2:B:119:PRO:HG2 | 1.87 | 0.56 |
| 1:I:337:TRP:CZ3 | 1:I:368:LEU:HD13 | 2.40 | 0.56 |
| 2:J:13:LYS:O | 2:J:16:MET:HB2 | 2.06 | 0.56 |
| 2:J:357:MET:HE3 | 2:J:360:ALA:HB2 | 1.85 | 0.56 |
| 1:A:362:THR:HG22 | 1:A:366:LYS:HE2 | 1.87 | 0.56 |
| 1:I:344:GLU:HB3 | 1:I:345:PRO:CD | 2.34 | 0.56 |
| 2:J:285:GLY:O | 2:J:287:LYS:HG3 | 2.06 | 0.56 |
| 1:M:165:THR:HA | 1:M:182:GLN:HE22 | 1.69 | 0.56 |
| 1:M:168:LEU:HD11 | 1:M:187:LEU:HD21 | 1.87 | 0.56 |
| 1:M:337:TRP:CZ3 | 1:M:368:LEU:HD13 | 2.41 | 0.56 |
| 2:N:360:ALA:HB1 | 8:N:430:HOH:O | 2.04 | 0.56 |
| 1:A:108:VAL:O | 1:A:108:VAL:HG23 | 2.05 | 0.56 |
| 2:B:63:ILE:HD13 | 2:B:63:ILE:N | 2.20 | 0.56 |
| 1:M:118:VAL:O | 1:M:148:VAL:HG23 | 2.06 | 0.56 |
| 2:N:263:LYS:N | 2:N:423:VAL:HG11 | 2.20 | 0.56 |
| 3:C:707:DG:C2' | 3:C:708:DG:H5' | 2.33 | 0.56 |
| 1:E:81:ASN:HA | 1:E:84:THR:HG22 | 1.87 | 0.56 |
| 1:E:116:PHE:HA | 1:E:148:VAL:HG21 | 1.88 | 0.56 |
| 1:I:432:GLU:HG3 | 1:I:433:PRO:HD2 | 1.87 | 0.56 |
| 2:J:63:ILE:H | 2:J:63:ILE:HD13 | 1.70 | 0.56 |
| 1:A:287:LYS:HZ3 | 1:A:293:ILE:HD12 | 1.70 | 0.56 |
| 1:E:362:THR:HG22 | 1:E:366:LYS:HE2 | 1.86 | 0.56 |
| 1:E:475:GLN:NE2 | 4:H:809:DC:C5' | 2.69 | 0.56 |
| 1:I:137:ASN:HD22 | 1:I:137:ASN:H | 1.53 | 0.56 |
| 1:M:183:TYR:O | 1:M:184:MET:HB2 | 2.05 | 0.56 |
| 2:N:263:LYS:CA | 2:N:423:VAL:HG11 | 2.36 | 0.56 |
| 1:A:491:LEU:N | 1:A:491:LEU:HD12 | 2.20 | 0.56 |
| 1:M:108:VAL:CG2 | 1:M:221:HIS:HD2 | 2.17 | 0.56 |
| 1:M:438:GLU:OE2 | 1:M:463:ARG:HD2 | 2.05 | 0.56 |
| 1:A:199:ARG:O | 1:A:203:GLU:HG3 | 2.06 | 0.56 |
| 2:B:206:ARG:CB | 2:B:206:ARG:HH11 | 2.18 | 0.56 |
| 2:B:215:THR:O | 2:B:217:PRO:HD3 | 2.06 | 0.56 |
| 1:E:96:HIS:HE2 | 1:E:269:GLN:HE21 | 1.51 | 0.56 |
| 1:E:326:ILE:HD12 | 1:E:326:ILE:N | 2.21 | 0.56 |
| 2:J:206:ARG:NH1 | 2:J:206:ARG:HB3 | 2.20 | 0.56 |
| 1:M:181:TYR:CD2 | 2:N:138:GLU:HA | 2.41 | 0.56 |
| 1:M:503:LEU:HD22 | 1:M:535:TRP:HB2 | 1.88 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:475:GLN:HE22 | 4:D:808:DC:C4' | 2.18 | 0.56 |
| 2:B:375:ILE:HB | 2:B:389:PHE:HZ | 1.71 | 0.56 |
| 1:E:344:GLU:HB3 | 1:E:345:PRO:CD | 2.35 | 0.56 |
| 2:F:263:LYS:CA | 2:F:423:VAL:HG11 | 2.35 | 0.56 |
| 2:J:278:GLN:CG | 2:J:298:GLU:HB3 | 2.36 | 0.56 |
| 1:M:29:GLU:O | 1:M:32:LYS:HB3 | 2.06 | 0.56 |
| 1:A:165:THR:HA | 1:A:182:GLN:HE22 | 1.70 | 0.56 |
| 1:E:337:TRP:CZ3 | 1:E:368:LEU:HD13 | 2.41 | 0.56 |
| 1:E:429:LEU:HD23 | 1:E:429:LEU:N | 2.20 | 0.56 |
| 2:F:339:TYR:C | 2:F:340:GLN:NE2 | 2.59 | 0.56 |
| 1:I:24:TRP:CE3 | 3:K:703:DG:H1' | 2.40 | 0.56 |
| 1:I:260:LEU:HD23 | 1:I:279:LEU:HD22 | 1.88 | 0.56 |
| 1:M:3:SER:HB3 | 1:M:5:ILE:HG22 | 1.87 | 0.56 |
| 1:M:13:LYS:HE2 | 1:M:86:ASP:OD1 | 2.06 | 0.56 |
| 1:M:341:ILE:N | 1:M:341:ILE:HD12 | 2.20 | 0.56 |
| 2:F:131:THR:OG1 | 2:F:143:ARG:HD2 | 2.06 | 0.55 |
| 1:I:183:TYR:O | 1:I:184:MET:HB2 | 2.06 | 0.55 |
| 1:M:81:ASN:HA | 1:M:84:THR:HG22 | 1.87 | 0.55 |
| 2:J:422:LEU:HD23 | 2:J:422:LEU:H | 1.71 | 0.55 |
| 1:M:67:ASP:O | 1:M:68:SER:HB2 | 2.06 | 0.55 |
| 2:F:215:THR:O | 2:F:217:PRO:HD3 | 2.06 | 0.55 |
| 2:F:257:ILE:CG2 | 2:F:283:LEU:HD21 | 2.36 | 0.55 |
| 1:I:3:SER:HB2 | 1:I:119:PRO:HD3 | 1.88 | 0.55 |
| 1:M:178:ILE:HD12 | 1:M:178:ILE:N | 2.21 | 0.55 |
| 1:E:116:PHE:C | 1:E:148:VAL:HG21 | 2.26 | 0.55 |
| 2:J:213:GLY:C | 2:J:214:LEU:HD23 | 2.27 | 0.55 |
| 2:J:213:GLY:O | 2:J:214:LEU:HD23 | 2.07 | 0.55 |
| 1:M:137:ASN:HD22 | 1:M:137:ASN:H | 1.53 | 0.55 |
| 1:A:32:LYS:O | 1:A:36:GLU:HG3 | 2.07 | 0.55 |
| 1:M:197:GLN:O | 1:M:200:THR:HB | 2.06 | 0.55 |
| 1:M:225:PRO:HB2 | 1:M:226:PRO:HD3 | 1.87 | 0.55 |
| 1:E:317:VAL:CG2 | 1:E:318:TYR:H | 2.16 | 0.55 |
| 1:I:181:TYR:CE2 | 2:J:138:GLU:HA | 2.41 | 0.55 |
| 1:A:115:TYR:O | 1:A:148:VAL:HG22 | 2.07 | 0.55 |
| 1:A:284:ARG:HH11 | 1:A:284:ARG:HG3 | 1.71 | 0.55 |
| 1:E:50:ILE:HG13 | 1:E:143:ARG:HB2 | 1.87 | 0.55 |
| 1:E:165:THR:HA | 1:E:182:GLN:HE22 | 1.72 | 0.55 |
| 1:A:12:LEU:HD11 | 1:A:127:TYR:CE2 | 2.41 | 0.55 |
| 2:B:206:ARG:NH1 | 2:B:206:ARG:HB3 | 2.21 | 0.55 |
| 2:B:213:GLY:C | 2:B:214:LEU:HD23 | 2.27 | 0.55 |
| 1:E:174:GLN:HB3 | 8:E:563:HOH:O | 2.00 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:426:TRP:HB3 | 1:E:526:ILE:HD12 | 1.89 | 0.55 |
| 1:E:445:ALA:H | 1:E:477:THR:HG21 | 1.72 | 0.55 |
| 1:I:490:GLY:O | 1:I:528:LYS:HD2 | 2.07 | 0.55 |
| 2:J:354:TYR:OH | 2:J:357:MET:HB2 | 2.05 | 0.55 |
| 1:M:379:SER:OG | 1:M:387:PRO:HD3 | 2.06 | 0.55 |
| 2:N:368:LEU:HD11 | 2:N:392:PRO:HD2 | 1.89 | 0.55 |
| 4:H:809:DC:H1' | 4:H:810:DT:H5" | 1.89 | 0.55 |
| 4:L:820:DC:H2" | 4:L:821:DC:H5' | 1.88 | 0.55 |
| 4:P:806:DT:H2" | 4:P:807:DC:H5' | 1.88 | 0.55 |
| 2:B:54:ASN:HD21 | 2:B:56:TYR:HB2 | 1.72 | 0.55 |
| 1:E:108:VAL:CG2 | 1:E:221:HIS:CD2 | 2.90 | 0.55 |
| 1:E:284:ARG:HG3 | 1:E:284:ARG:HH11 | 1.72 | 0.55 |
| 2:N:200:THR:O | 2:N:204:GLU:HG3 | 2.06 | 0.55 |
| 2:B:35:VAL:O | 2:B:39:THR:HG23 | 2.06 | 0.55 |
| 2:J:375:ILE:HB | 2:J:389:PHE:CZ | 2.41 | 0.55 |
| 1:A:8:VAL:O | 1:A:10:VAL:HG23 | 2.07 | 0.54 |
| 2:B:5:ILE:HG22 | 2:B:6:GLU:N | 2.22 | 0.54 |
| 1:E:412:PRO:HB2 | 8:E:557:HOH:O | 2.07 | 0.54 |
| 1:I:67:ASP:O | 1:I:68:SER:HB2 | 2.06 | 0.54 |
| 1:M:46:LYS:O | 1:M:147:ASN:HB2 | 2.07 | 0.54 |
| 2:N:206:ARG:CB | 2:N:206:ARG:HH11 | 2.20 | 0.54 |
| 1:E:57:ASN:OD1 | 1:E:58:THR:N | 2.41 | 0.54 |
| 1:E:115:TYR:CE2 | 6:E:823:ZP4:H2'A | 2.43 | 0.54 |
| 1:E:427:TYR:OH | 1:E:509:GLN:HA | 2.07 | 0.54 |
| 2:F:255:ASN:O | 2:F:258:GLN:HB2 | 2.07 | 0.54 |
| 1:I:293:ILE:HG13 | 1:I:294:PRO:HD2 | 1.89 | 0.54 |
| 2:N:215:THR:O | 2:N:217:PRO:HD3 | 2.06 | 0.54 |
| 1:A:151:GLN:NE2 | 6:A:823:ZP4:N3B | 2.56 | 0.54 |
| 1:A:204:GLU:HG2 | 2:N:4:PRO:HG3 | 1.90 | 0.54 |
| 2:B:393:ILE:HD13 | 2:B:398:TRP:HB2 | 1.89 | 0.54 |
| 1:I:503:LEU:HD22 | 1:I:535:TRP:HB2 | 1.89 | 0.54 |
| 2:J:257:ILE:CG2 | 2:J:283:LEU:HD21 | 2.37 | 0.54 |
| 2:J:279:LEU:HA | 2:J:282:LEU:HD13 | 1.89 | 0.54 |
| 1:M:91:GLN:HG3 | 1:M:161:GLN:HE22 | 1.72 | 0.54 |
| 1:M:252:TRP:CD1 | 1:M:295:LEU:HD22 | 2.43 | 0.54 |
| 1:M:361:HIS:CD2 | 1:M:505:ILE:HG23 | 2.42 | 0.54 |
| 3:K:722:DA:H1' | 3:K:723:DC:H5' | 1.89 | 0.54 |
| 1:E:138:GLU:N | 1:E:138:GLU:OE2 | 2.40 | 0.54 |
| 2:F:206:ARG:CB | 2:F:206:ARG:NH1 | 2.71 | 0.54 |
| 1:I:56:TYR:O | 1:I:143:ARG:NH2 | 2.40 | 0.54 |
| 1:I:137:ASN:N | 1:I:137:ASN:ND2 | 2.55 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:26:LEU:HB2 | 1:M:31:ILE:CD1 | 2.37 | 0.54 |
| 4:L:808:DC:H1' | 4:L:809:DC:H5' | 1.90 | 0.54 |
| 1:A:400:THR:O | 1:A:404:GLU:HG2 | 2.07 | 0.54 |
| 2:F:241:VAL:HG13 | 2:F:351:THR:H | 1.73 | 0.54 |
| 2:F:257:ILE:HG23 | 2:F:283:LEU:HD21 | 1.89 | 0.54 |
| 1:M:23:GLN:HG2 | 1:M:59:PRO:HA | 1.90 | 0.54 |
| 1:A:148:VAL:O | 1:A:150:PRO:HD3 | 2.08 | 0.54 |
| 1:M:318:TYR:O | 1:M:349:LEU:HD21 | 2.07 | 0.54 |
| 2:N:285:GLY:O | 2:N:287:LYS:HG3 | 2.08 | 0.54 |
| 1:A:94:ILE:HD11 | 3:C:708:DG:N2 | 2.22 | 0.54 |
| 1:E:278:GLN:HB2 | 1:E:302:GLU:CD | 2.27 | 0.54 |
| 2:F:376:THR:O | 2:F:380:ILE:HG13 | 2.07 | 0.54 |
| 1:A:252:TRP:CD1 | 1:A:295:LEU:HD22 | 2.43 | 0.54 |
| 1:A:303:LEU:O | 1:A:303:LEU:HD22 | 2.08 | 0.54 |
| 1:A:429:LEU:N | 1:A:429:LEU:HD23 | 2.22 | 0.54 |
| 2:B:257:ILE:HG23 | 2:B:283:LEU:HD21 | 1.90 | 0.54 |
| 1:E:399:GLU:HA | 1:E:402:TRP:CD1 | 2.43 | 0.54 |
| 1:I:406:TRP:CD1 | 1:I:407:GLN:HG2 | 2.43 | 0.54 |
| 1:M:57:ASN:HD21 | 1:M:131:THR:CB | 2.21 | 0.54 |
| 1:M:493:VAL:HG12 | 1:M:494:ASN:N | 2.22 | 0.54 |
| 1:A:441:TYR:HA | 1:A:496:VAL:HG22 | 1.90 | 0.54 |
| 1:I:287:LYS:NZ | 1:I:293:ILE:HD12 | 2.23 | 0.54 |
| 1:I:542:ILE:HB | 1:I:545:ASN:HB3 | 1.90 | 0.54 |
| 1:I:548:VAL:O | 1:I:552:VAL:HG22 | 2.08 | 0.54 |
| 2:J:379:SER:OG | 2:J:387:PRO:HD3 | 2.08 | 0.54 |
| 1:M:235:HIS:HB3 | 1:M:236:PRO:CD | 2.32 | 0.54 |
| 1:A:109:LEU:N | 1:A:109:LEU:CD1 | 2.71 | 0.53 |
| 2:F:206:ARG:HH11 | 2:F:206:ARG:HB2 | 1.73 | 0.53 |
| 2:F:278:GLN:CG | 2:F:298:GLU:HB3 | 2.39 | 0.53 |
| 1:I:21:VAL:HG23 | 1:I:59:PRO:HD3 | 1.91 | 0.53 |
| 1:M:32:LYS:O | 1:M:36:GLU:HG3 | 2.07 | 0.53 |
| 2:N:65:LYS:HG2 | 2:N:66:LYS:H | 1.73 | 0.53 |
| 4:P:818:DC:H2' | 4:P:819:DG:H8 | 1.72 | 0.53 |
| 1:A:132:ILE:HD11 | 1:A:142:ILE:HD11 | 1.89 | 0.53 |
| 1:A:339:TYR:CG | 1:A:375:ILE:HD11 | 2.43 | 0.53 |
| 1:E:118:VAL:O | 1:E:148:VAL:HG23 | 2.08 | 0.53 |
| 1:E:197:GLN:O | 1:E:200:THR:HB | 2.08 | 0.53 |
| 1:I:450:THR:O | 1:I:451:LYS:HB2 | 2.08 | 0.53 |
| 1:M:24:TRP:CZ2 | 3:O:704:DC:H5' | 2.43 | 0.53 |
| 1:M:450:THR:O | 1:M:451:LYS:HB2 | 2.08 | 0.53 |
| 2:N:213:GLY:O | 2:N:214:LEU:HD23 | 2.09 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:N:422:LEU:HG | 2:N:426:TRP:CZ2 | 2.31 | 0.53 |
| 1:A:252:TRP:NE1 | 1:A:295:LEU:HD22 | 2.24 | 0.53 |
| 2:B:13:LYS:HE3 | 2:B:86:ASP:H | 1.73 | 0.53 |
| 1:E:475:GLN:HE21 | 4:H:809:DC:C5' | 2.19 | 0.53 |
| 1:M:95:PRO:HA | 2:N:136:ASN:O | 2.07 | 0.53 |
| 1:M:222:GLN:O | 1:M:224:GLU:HG3 | 2.09 | 0.53 |
| 1:M:254:VAL:HG23 | 1:M:291:GLU:O | 2.09 | 0.53 |
| 1:M:344:GLU:OE1 | 1:M:347:LYS:HG3 | 2.09 | 0.53 |
| 2:B:34:LEU:HD13 | 2:B:62:ALA:HB2 | 1.89 | 0.53 |
| 2:F:66:LYS:NZ | 2:F:66:LYS:HB3 | 2.24 | 0.53 |
| 1:I:445:ALA:H | 1:I:477:THR:HG21 | 1.72 | 0.53 |
| 1:M:339:TYR:OH | 1:M:352:GLY:HA3 | 2.04 | 0.53 |
| 1:M:548:VAL:O | 1:M:552:VAL:HG22 | 2.08 | 0.53 |
| 2:N:206:ARG:HB3 | 2:N:206:ARG:NH1 | 2.23 | 0.53 |
| 4:H:810:DT:H2" | 4:H:811:DG:C8 | 2.44 | 0.53 |
| 1:A:222:GLN:O | 1:A:224:GLU:HG3 | 2.09 | 0.53 |
| 1:A:326:ILE:N | 1:A:326:ILE:HD12 | 2.24 | 0.53 |
| 2:B:397:THR:HG21 | 8:B:432:HOH:O | 2.09 | 0.53 |
| 1:I:165:THR:HA | 1:I:182:GLN:HE22 | 1.72 | 0.53 |
| 1:M:342:TYR:HD2 | 1:M:344:GLU:O | 1.86 | 0.53 |
| 1:M:438:GLU:OE1 | 1:M:463:ARG:HD2 | 2.09 | 0.53 |
| 1:E:8:VAL:O | 1:E:10:VAL:HG23 | 2.09 | 0.53 |
| 1:E:441:TYR:HA | 1:E:496:VAL:HG22 | 1.91 | 0.53 |
| 2:F:34:LEU:HD13 | 2:F:62:ALA:HB2 | 1.91 | 0.53 |
| 1:M:42:GLU:OE1 | 1:M:49:LYS:HG3 | 2.09 | 0.53 |
| 1:M:342:TYR:CE2 | 1:M:344:GLU:O | 2.62 | 0.53 |
| 2:N:375:ILE:HB | 2:N:389:PHE:CZ | 2.44 | 0.53 |
| 1:A:389:PHE:HB3 | 1:A:391:LEU:HD21 | 1.91 | 0.53 |
| 1:E:168:LEU:HD11 | 1:E:187:LEU:HD21 | 1.90 | 0.53 |
| 1:E:358:ARG:HH12 | 2:F:396:GLU:CD | 2.12 | 0.53 |
| 1:I:5:ILE:HD12 | 1:I:6:GLU:H | 1.71 | 0.53 |
| 2:J:115:TYR:OH | 2:J:157:PRO:HB3 | 2.08 | 0.53 |
| 1:M:406:TRP:HD1 | 1:M:407:GLN:HE21 | 1.56 | 0.53 |
| 2:N:213:GLY:C | 2:N:214:LEU:HD23 | 2.29 | 0.53 |
| 1:I:58:THR:CG2 | 1:I:59:PRO:HD2 | 2.38 | 0.53 |
| 4:H:806:DT:H1' | 4:H:807:DC:H5" | 1.90 | 0.53 |
| 2:B:196:GLY:O | 2:B:200:THR:HG23 | 2.09 | 0.53 |
| 1:E:155:GLY:O | 1:E:159:ILE:HG12 | 2.09 | 0.53 |
| 1:I:357:MET:HG2 | 1:I:367:GLN:OE1 | 2.09 | 0.53 |
| 2:J:380:ILE:O | 2:J:384:GLY:HA2 | 2.09 | 0.53 |
| 4:P:819:DG:H2' | 4:P:820:DC:C6 | 2.43 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:50:ILE:HD13 | 2:B:145:GLN:HB3 | 1.90 | 0.53 |
| 1:I:32:LYS:O | 1:I:36:GLU:HG3 | 2.09 | 0.53 |
| 1:I:260:LEU:HD21 | 1:I:303:LEU:HD23 | 1.90 | 0.53 |
| 3:C:705:DA:H2" | 3:C:706:DT:C5' | 2.35 | 0.53 |
| 1:E:115:TYR:CD2 | 6:E:823:ZP4:H2'A | 2.43 | 0.52 |
| 1:E:293:ILE:HG13 | 1:E:294:PRO:HD2 | 1.89 | 0.52 |
| 2:J:3:SER:OG | 2:J:4:PRO:HD2 | 2.09 | 0.52 |
| 1:M:137:ASN:N | 1:M:137:ASN:ND2 | 2.56 | 0.52 |
| 2:N:393:ILE:HD13 | 2:N:398:TRP:HB2 | 1.91 | 0.52 |
| 1:I:94:ILE:HD11 | 3:K:708:DG:H21 | 1.72 | 0.52 |
| 1:I:393:ILE:HB | 1:I:423:VAL:HB | 1.89 | 0.52 |
| 1:M:84:THR:CG2 | 1:M:154:LYS:HD3 | 2.39 | 0.52 |
| 1:M:342:TYR:HB3 | 1:M:348:ASN:HA | 1.91 | 0.52 |
| 3:K:717:DC:H2" | 3:K:718:DA:OP2 | 2.09 | 0.52 |
| 1:A:545:ASN:O | 1:A:546:GLU:C | 2.48 | 0.52 |
| 1:E:132:ILE:HD11 | 1:E:144:TYR:HE2 | 1.74 | 0.52 |
| 1:I:27:THR:O | 1:I:31:ILE:HG12 | 2.09 | 0.52 |
| 1:I:441:TYR:HA | 1:I:496:VAL:HG22 | 1.90 | 0.52 |
| 1:M:102:LYS:HD2 | 1:M:102:LYS:N | 2.01 | 0.52 |
| 1:M:399:GLU:HA | 1:M:402:TRP:CD1 | 2.44 | 0.52 |
| 1:A:282:LEU:HD21 | 1:A:296:THR:HG22 | 1.92 | 0.52 |
| 2:F:425:LEU:C | 8:F:438:HOH:O | 2.48 | 0.52 |
| 1:I:197:GLN:O | 1:I:200:THR:HB | 2.09 | 0.52 |
| 1:M:25:PRO:HD2 | 3:O:703:DG:C2 | 2.45 | 0.52 |
| 1:M:156:SER:HB2 | 1:M:157:PRO:CD | 2.39 | 0.52 |
| 2:N:194:GLU:OE2 | 2:N:195:ILE:HG22 | 2.08 | 0.52 |
| 3:G:707:DG:H2" | 3:G:708:DG:C5' | 2.34 | 0.52 |
| 1:A:115:TYR:CE2 | 6:A:823:ZP4:H2'A | 2.45 | 0.52 |
| 1:M:285:GLY:N | 3:O:714:DG:OP1 | 2.42 | 0.52 |
| 2:N:72:ARG:NH2 | 2:N:151:GLN:NE2 | 2.58 | 0.52 |
| 2:N:73:LYS:NZ | 2:N:146:TYR:OH | 2.37 | 0.52 |
| 2:N:115:TYR:OH | 2:N:157:PRO:HB3 | 2.09 | 0.52 |
| 2:N:257:ILE:CG2 | 2:N:283:LEU:HD21 | 2.40 | 0.52 |
| 2:N:422:LEU:HD23 | 2:N:422:LEU:H | 1.73 | 0.52 |
| 4:D:819:DG:H2' | 4:D:820:DC:H6 | 1.74 | 0.52 |
| 1:A:48:SER:O | 1:A:144:TYR:HA | 2.10 | 0.52 |
| 1:A:197:GLN:O | 1:A:200:THR:HB | 2.10 | 0.52 |
| 1:A:198:HIS:O | 1:A:200:THR:N | 2.43 | 0.52 |
| 2:B:278:GLN:CG | 2:B:298:GLU:HB3 | 2.40 | 0.52 |
| 1:E:475:GLN:NE2 | 4:H:809:DC:H5" | 2.24 | 0.52 |
| 2:F:375:ILE:HB | 2:F:389:PHE:HZ | 1.74 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:F:410:TRP:O | 2:F:411:ILE:HD13 | 2.10 | 0.52 |
| 2:J:8:VAL:HG23 | 2:J:8:VAL:O | 2.09 | 0.52 |
| 2:B:13:LYS:CD | 2:B:86:ASP:HB2 | 2.38 | 0.52 |
| 1:E:94:ILE:CD1 | 3:G:708:DG:H21 | 2.23 | 0.52 |
| 1:E:148:VAL:HG22 | 1:E:149:LEU:N | 2.25 | 0.52 |
| 1:E:215:THR:HG22 | 1:E:216:THR:N | 2.25 | 0.52 |
| 1:E:491:LEU:HD12 | 1:E:491:LEU:N | 2.25 | 0.52 |
| 1:I:493:VAL:HG12 | 1:I:494:ASN:N | 2.24 | 0.52 |
| 2:J:66:LYS:HB3 | 2:J:66:LYS:HZ2 | 1.75 | 0.52 |
| 1:M:109:LEU:HD23 | 1:M:216:THR:HG21 | 1.91 | 0.52 |
| 2:N:13:LYS:HB2 | 2:N:16:MET:CG | 2.37 | 0.52 |
| 1:A:221:HIS:HB3 | 1:A:227:PHE:HD1 | 1.73 | 0.52 |
| 2:B:257:ILE:CG2 | 2:B:283:LEU:HD21 | 2.40 | 0.52 |
| 2:J:374:LYS:O | 2:J:378:GLU:HG3 | 2.09 | 0.52 |
| 1:M:254:VAL:HB | 1:M:288:ALA:O | 2.10 | 0.52 |
| 1:M:333:GLY:H | 1:M:336:GLN:HB2 | 1.74 | 0.52 |
| 1:A:155:GLY:O | 1:A:159:ILE:HG12 | 2.09 | 0.52 |
| 2:B:422:LEU:HD23 | 2:B:422:LEU:H | 1.75 | 0.52 |
| 2:F:97:PRO:HD2 | 2:F:181:TYR:CD1 | 2.45 | 0.52 |
| 1:I:29:GLU:O | 1:I:32:LYS:HB3 | 2.10 | 0.52 |
| 1:I:57:ASN:ND2 | 1:I:131:THR:OG1 | 2.43 | 0.52 |
| 1:I:240:THR:HG22 | 1:I:315:HIS:HA | 1.91 | 0.52 |
| 4:H:821:DC:H2' | 4:H:822:2DA:H8 | 1.91 | 0.52 |
| 1:E:389:PHE:HB3 | 1:E:391:LEU:HD21 | 1.92 | 0.52 |
| 2:F:293:ILE:HG23 | 2:F:294:PRO:HD2 | 1.92 | 0.52 |
| 1:I:31:ILE:CD1 | 1:I:133:PRO:HG2 | 2.36 | 0.52 |
| 1:I:225:PRO:HB2 | 1:I:226:PRO:HD3 | 1.91 | 0.52 |
| 2:J:88:TRP:CZ2 | 2:J:154:LYS:HD3 | 2.45 | 0.52 |
| 2:J:170:PRO:HG2 | 2:J:208:HIS:NE2 | 2.25 | 0.52 |
| 2:N:266:TRP:CD1 | 2:N:269:GLN:NE2 | 2.78 | 0.52 |
| 2:N:400:THR:HG22 | 2:N:401:TRP:CD2 | 2.45 | 0.52 |
| 1:A:317:VAL:HG12 | 1:A:348:ASN:C | 2.26 | 0.51 |
| 1:A:427:TYR:OH | 1:A:509:GLN:HA | 2.10 | 0.51 |
| 2:B:88:TRP:CZ2 | 2:B:154:LYS:HD3 | 2.45 | 0.51 |
| 1:E:420:PRO:HA | 1:E:422:LEU:CD2 | 2.36 | 0.51 |
| 2:F:13:LYS:O | 2:F:16:MET:HB2 | 2.09 | 0.51 |
| 1:I:168:LEU:HD11 | 1:I:187:LEU:HD21 | 1.92 | 0.51 |
| 2:J:293:ILE:HG23 | 2:J:294:PRO:HD2 | 1.92 | 0.51 |
| 3:G:706:DT:H2' | 3:G:707:DG:H8 | 1.75 | 0.51 |
| 1:A:317:VAL:CG2 | 1:A:318:TYR:H | 2.19 | 0.51 |
| 2:B:285:GLY:O | 2:B:287:LYS:HG3 | 2.10 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:260:LEU:HD21 | 1:E:303:LEU:HD23 | 1.93 | 0.51 |
| 1:I:246:LEU:HD12 | 1:I:246:LEU:N | 2.23 | 0.51 |
| 1:I:260:LEU:O | 1:I:264:LEU:HD13 | 2.10 | 0.51 |
| 1:I:406:TRP:HD1 | 1:I:407:GLN:HE21 | 1.57 | 0.51 |
| 1:A:109:LEU:HD12 | 1:A:109:LEU:H | 1.74 | 0.51 |
| 1:E:535:TRP:C | 1:E:536:VAL:HG13 | 2.30 | 0.51 |
| 2:F:202:ILE:O | 2:F:206:ARG:HG3 | 2.09 | 0.51 |
| 1:I:81:ASN:HA | 1:I:84:THR:HG22 | 1.92 | 0.51 |
| 1:M:445:ALA:H | 1:M:477:THR:HG21 | 1.74 | 0.51 |
| 2:N:88:TRP:CE2 | 2:N:154:LYS:HD3 | 2.45 | 0.51 |
| 3:K:707:DG:H2" | 3:K:708:DG:C5' | 2.36 | 0.51 |
| 4:L:806:DT:C2' | 4:L:807:DC:H5" | 2.40 | 0.51 |
| 1:A:165:THR:HG22 | 1:A:182:GLN:NE2 | 2.26 | 0.51 |
| 1:A:298:GLU:OE1 | 1:A:298:GLU:N | 2.43 | 0.51 |
| 2:B:356:ARG:NE | 8:B:436:HOH:O | 2.43 | 0.51 |
| 2:B:410:TRP:O | 2:B:411:ILE:HD13 | 2.11 | 0.51 |
| 1:E:281:LYS:HG3 | 1:E:284:ARG:NH1 | 2.26 | 0.51 |
| 1:E:298:GLU:OE1 | 1:E:298:GLU:N | 2.43 | 0.51 |
| 2:F:376:THR:HG21 | 2:F:410:TRP:CZ3 | 2.45 | 0.51 |
| 1:I:480:GLN:O | 1:I:483:TYR:HB3 | 2.10 | 0.51 |
| 2:J:278:GLN:HG3 | 2:J:298:GLU:HB3 | 1.93 | 0.51 |
| 1:M:72:ARG:HG3 | 1:M:151:GLN:HE22 | 1.74 | 0.51 |
| 1:M:81:ASN:HA | 1:M:84:THR:CG2 | 2.40 | 0.51 |
| 1:M:108:VAL:CG2 | 1:M:221:HIS:HB2 | 2.11 | 0.51 |
| 2:N:54:ASN:HD21 | 2:N:56:TYR:HB2 | 1.75 | 0.51 |
| 4:H:821:DC:H2" | 4:H:822:2DA:H5' | 1.92 | 0.51 |
| 4:P:806:DT:H5' | 4:P:806:DT:H6 | 1.75 | 0.51 |
| 1:A:116:PHE:HA | 1:A:148:VAL:HG21 | 1.91 | 0.51 |
| 1:E:287:LYS:NZ | 1:E:293:ILE:HD12 | 2.25 | 0.51 |
| 1:I:116:PHE:C | 1:I:148:VAL:HG21 | 2.31 | 0.51 |
| 1:I:198:HIS:O | 1:I:201:LYS:N | 2.44 | 0.51 |
| 1:M:490:GLY:O | 1:M:528:LYS:HD2 | 2.11 | 0.51 |
| 1:A:419:THR:HG23 | 1:A:419:THR:O | 2.10 | 0.51 |
| 2:B:213:GLY:O | 2:B:214:LEU:HD23 | 2.10 | 0.51 |
| 1:E:536:VAL:O | 1:E:537:PRO:C | 2.48 | 0.51 |
| 2:F:63:ILE:HD13 | 2:F:63:ILE:H | 1.75 | 0.51 |
| 1:I:399:GLU:HA | 1:I:402:TRP:CD1 | 2.45 | 0.51 |
| 1:I:400:THR:O | 1:I:404:GLU:HG2 | 2.10 | 0.51 |
| 1:M:184:MET:HG3 | 4:P:822:2DA:H1' | 1.93 | 0.51 |
| 1:A:250:ASP:OD1 | 1:A:250:ASP:N | 2.43 | 0.51 |
| 1:A:318:TYR:CA | 1:A:349:LEU:HD21 | 2.41 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:399:GLU:HA | 1:A:402:TRP:CD1 | 2.46 | 0.51 |
| 1:E:445:ALA:N | 1:E:477:THR:HG21 | 2.25 | 0.51 |
| 1:I:465:LYS:HG3 | 1:I:466:VAL:N | 2.26 | 0.51 |
| 2:F:88:TRP:CZ2 | 2:F:154:LYS:HD3 | 2.45 | 0.51 |
| 1:I:223:LYS:O | 1:I:225:PRO:HD3 | 2.11 | 0.51 |
| 2:J:97:PRO:HD2 | 2:J:181:TYR:CD1 | 2.46 | 0.51 |
| 2:N:368:LEU:HD22 | 2:N:398:TRP:CZ3 | 2.45 | 0.51 |
| 2:B:66:LYS:HB3 | 2:B:66:LYS:NZ | 2.26 | 0.51 |
| 2:B:242:GLN:NE2 | 2:B:242:GLN:O | 2.44 | 0.51 |
| 1:I:220:LYS:HD2 | 1:I:220:LYS:O | 2.11 | 0.51 |
| 1:I:438:GLU:OE2 | 1:I:463:ARG:HD2 | 2.11 | 0.51 |
| 2:N:202:ILE:O | 2:N:206:ARG:HG3 | 2.11 | 0.51 |
| 1:E:165:THR:HG21 | 2:F:140:PRO:CG | 2.41 | 0.51 |
| 1:E:400:THR:O | 1:E:404:GLU:HG2 | 2.11 | 0.51 |
| 1:E:537:PRO:CB | 1:E:540:LYS:CB | 2.77 | 0.51 |
| 1:M:341:ILE:N | 1:M:341:ILE:CD1 | 2.74 | 0.51 |
| 1:M:432:GLU:HG3 | 1:M:433:PRO:HD2 | 1.92 | 0.51 |
| 4:L:807:DC:C4 | 4:L:808:DC:N4 | 2.79 | 0.51 |
| 2:F:285:GLY:O | 2:F:287:LYS:HG3 | 2.11 | 0.50 |
| 2:J:5:ILE:O | 2:J:7:THR:HG23 | 2.11 | 0.50 |
| 2:J:120:LEU:HD23 | 2:J:121:ASP:H | 1.77 | 0.50 |
| 2:J:422:LEU:HG | 2:J:426:TRP:CZ2 | 2.31 | 0.50 |
| 1:M:24:TRP:CH2 | 3:O:704:DC:H5' | 2.46 | 0.50 |
| 1:M:303:LEU:O | 1:M:303:LEU:HD22 | 2.11 | 0.50 |
| 4:D:817:MRG:H2" | 4:D:818:DC:C6 | 2.45 | 0.50 |
| 1:E:537:PRO:HG2 | 1:E:542:ILE:HD11 | 1.91 | 0.50 |
| 1:M:91:GLN:HG3 | 1:M:161:GLN:NE2 | 2.26 | 0.50 |
| 1:A:450:THR:O | 1:A:451:LYS:HB2 | 2.11 | 0.50 |
| 2:J:215:THR:O | 2:J:217:PRO:HD3 | 2.10 | 0.50 |
| 1:M:44:GLU:HB3 | 1:M:46:LYS:HE2 | 1.92 | 0.50 |
| 1:M:459:THR:CG2 | 1:M:463:ARG:HB2 | 2.42 | 0.50 |
| 1:M:489:SER:HB2 | 1:M:493:VAL:HG22 | 1.92 | 0.50 |
| 1:A:109:LEU:HD11 | 1:A:202:ILE:HD11 | 1.94 | 0.50 |
| 1:A:367:GLN:NE2 | 1:A:512:LYS:HE3 | 2.25 | 0.50 |
| 2:B:120:LEU:HD23 | 2:B:121:ASP:H | 1.76 | 0.50 |
| 2:F:88:TRP:CZ3 | 2:F:89:GLU:HB2 | 2.46 | 0.50 |
| 2:J:206:ARG:CB | 2:J:206:ARG:NH1 | 2.74 | 0.50 |
| 2:N:54:ASN:O | 2:N:143:ARG:NH2 | 2.44 | 0.50 |
| 4:H:809:DC:H2" | 4:H:810:DT:OP2 | 2.11 | 0.50 |
| 1:A:65:LYS:HD3 | 6:A:823:ZP4:O2D | 2.11 | 0.50 |
| 1:A:168:LEU:HD11 | 1:A:187:LEU:HD21 | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:198:HIS:O | 1:A:201:LYS:N | 2.44 | 0.50 |
| 1:E:156:SER:O | 1:E:157:PRO:C | 2.47 | 0.50 |
| 2:F:422:LEU:HG | 2:F:426:TRP:CZ2 | 2.35 | 0.50 |
| 1:I:326:ILE:O | 1:I:341:ILE:HA | 2.11 | 0.50 |
| 1:M:337:TRP:HE1 | 1:M:367:GLN:NE2 | 2.10 | 0.50 |
| 1:M:410:TRP:CE2 | 2:N:363:ASN:ND2 | 2.80 | 0.50 |
| 2:N:380:ILE:O | 2:N:384:GLY:HA2 | 2.11 | 0.50 |
| 1:E:458:VAL:HG11 | 1:E:548:VAL:HG22 | 1.87 | 0.50 |
| 1:E:535:TRP:O | 1:E:536:VAL:HG12 | 2.11 | 0.50 |
| 2:F:213:GLY:C | 2:F:214:LEU:HD23 | 2.32 | 0.50 |
| 2:F:270:ILE:HD13 | 2:F:346:PHE:HB3 | 1.94 | 0.50 |
| 1:I:108:VAL:O | 1:I:108:VAL:HG23 | 2.10 | 0.50 |
| 4:H:810:DT:H2” | 4:H:811:DG:H8 | 1.75 | 0.50 |
| 1:A:281:LYS:HG3 | 1:A:284:ARG:NH1 | 2.26 | 0.50 |
| 1:A:358:ARG:HH12 | 2:B:396:GLU:CD | 2.14 | 0.50 |
| 2:B:115:TYR:OH | 2:B:184:MET:O | 2.29 | 0.50 |
| 2:B:263:LYS:HB2 | 2:B:423:VAL:CG1 | 2.41 | 0.50 |
| 1:E:225:PRO:HB2 | 1:E:226:PRO:HD3 | 1.93 | 0.50 |
| 2:F:108:VAL:O | 2:F:232:TYR:OH | 2.25 | 0.50 |
| 2:F:169:GLU:N | 2:F:170:PRO:HD2 | 2.27 | 0.50 |
| 2:N:206:ARG:CB | 2:N:206:ARG:NH1 | 2.75 | 0.50 |
| 1:A:17:ASP:O | 1:A:83:ARG:HD3 | 2.12 | 0.50 |
| 1:A:108:VAL:HG21 | 1:A:221:HIS:HD2 | 1.75 | 0.50 |
| 1:A:489:SER:HB2 | 1:A:493:VAL:HG22 | 1.93 | 0.50 |
| 1:I:115:TYR:CE1 | 1:I:184:MET:HE3 | 2.47 | 0.50 |
| 1:I:282:LEU:HD21 | 1:I:296:THR:CG2 | 2.42 | 0.50 |
| 1:A:237:ASP:O | 1:A:238:LYS:HD3 | 2.12 | 0.50 |
| 1:A:541:GLY:O | 1:A:542:ILE:C | 2.50 | 0.50 |
| 1:A:542:ILE:HG22 | 1:A:543:GLY:N | 2.27 | 0.50 |
| 1:E:344:GLU:CB | 1:E:345:PRO:CD | 2.90 | 0.50 |
| 1:E:489:SER:HB2 | 1:E:493:VAL:HG22 | 1.93 | 0.50 |
| 2:F:425:LEU:CB | 8:F:438:HOH:O | 2.59 | 0.50 |
| 1:I:458:VAL:HG13 | 1:I:458:VAL:O | 2.11 | 0.50 |
| 2:N:6:GLU:HG3 | 2:N:6:GLU:O | 2.12 | 0.50 |
| 2:N:8:VAL:HG21 | 2:N:159:ILE:HG12 | 1.94 | 0.50 |
| 2:N:278:GLN:HG3 | 2:N:298:GLU:HB3 | 1.94 | 0.50 |
| 1:A:246:LEU:HD12 | 1:A:246:LEU:N | 2.26 | 0.49 |
| 1:E:132:ILE:HD11 | 1:E:142:ILE:HD11 | 1.94 | 0.49 |
| 1:I:132:ILE:HD11 | 1:I:142:ILE:CD1 | 2.41 | 0.49 |
| 1:A:138:GLU:N | 1:A:138:GLU:OE2 | 2.44 | 0.49 |
| 1:E:26:LEU:HB2 | 1:E:31:ILE:CD1 | 2.42 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:366:LYS:O | 1:E:370:GLU:HG3 | 2.12 | 0.49 |
| 1:I:29:GLU:HG3 | 1:I:30:LYS:N | 2.27 | 0.49 |
| 2:N:13:LYS:CB | 2:N:16:MET:HG3 | 2.39 | 0.49 |
| 3:O:707:DG:H2" | 3:O:708:DG:C5' | 2.38 | 0.49 |
| 1:A:110:ASP:C | 1:A:110:ASP:OD1 | 2.50 | 0.49 |
| 1:A:115:TYR:CD2 | 6:A:823:ZP4:H2'A | 2.47 | 0.49 |
| 1:E:94:ILE:HD11 | 3:G:708:DG:H21 | 1.77 | 0.49 |
| 1:I:427:TYR:OH | 1:I:509:GLN:HA | 2.12 | 0.49 |
| 2:N:5:ILE:HG23 | 2:N:119:PRO:HG3 | 1.94 | 0.49 |
| 2:N:366:LYS:HA | 2:N:405:TYR:CD2 | 2.47 | 0.49 |
| 4:P:818:DC:H2" | 4:P:819:DG:C5' | 2.42 | 0.49 |
| 1:A:175:ASN:HB3 | 1:A:178:ILE:CD1 | 2.14 | 0.49 |
| 2:B:54:ASN:C | 2:B:54:ASN:ND2 | 2.59 | 0.49 |
| 2:B:169:GLU:O | 2:B:173:LYS:HG3 | 2.11 | 0.49 |
| 2:B:241:VAL:HG22 | 2:B:350:LYS:HG3 | 1.94 | 0.49 |
| 1:E:338:THR:HG22 | 1:E:339:TYR:N | 2.28 | 0.49 |
| 2:J:50:ILE:HD13 | 2:J:145:GLN:HB3 | 1.93 | 0.49 |
| 2:J:263:LYS:N | 2:J:423:VAL:HG11 | 2.27 | 0.49 |
| 2:N:207:GLN:O | 2:N:210:LEU:HB2 | 2.13 | 0.49 |
| 1:A:50:ILE:HG13 | 1:A:143:ARG:CB | 2.42 | 0.49 |
| 2:B:207:GLN:O | 2:B:210:LEU:HB2 | 2.12 | 0.49 |
| 1:E:194:GLU:HB2 | 1:E:197:GLN:HG3 | 1.94 | 0.49 |
| 1:I:81:ASN:HA | 1:I:84:THR:CG2 | 2.42 | 0.49 |
| 2:J:24:TRP:CH2 | 2:J:403:THR:HG21 | 2.48 | 0.49 |
| 1:M:459:THR:OG1 | 1:M:463:ARG:HB2 | 2.12 | 0.49 |
| 2:N:134:SER:CB | 2:N:139:THR:HG23 | 2.42 | 0.49 |
| 4:P:818:DC:H2' | 4:P:819:DG:C8 | 2.47 | 0.49 |
| 2:B:335:GLY:HA3 | 2:B:356:ARG:HG2 | 1.94 | 0.49 |
| 1:E:326:ILE:O | 1:E:341:ILE:HA | 2.13 | 0.49 |
| 1:I:58:THR:HG23 | 1:I:59:PRO:HD2 | 1.94 | 0.49 |
| 1:I:132:ILE:CG1 | 1:I:142:ILE:HG13 | 2.43 | 0.49 |
| 1:I:282:LEU:HD21 | 1:I:296:THR:HG22 | 1.95 | 0.49 |
| 1:I:373:GLN:NE2 | 2:J:397:THR:HG23 | 2.27 | 0.49 |
| 1:I:478:GLU:CG | 1:I:499:SER:HB2 | 2.42 | 0.49 |
| 1:I:529:GLU:HG2 | 1:I:530:LYS:HG3 | 1.94 | 0.49 |
| 2:J:54:ASN:C | 2:J:54:ASN:ND2 | 2.64 | 0.49 |
| 2:J:255:ASN:O | 2:J:258:GLN:HB2 | 2.12 | 0.49 |
| 1:M:298:GLU:N | 1:M:298:GLU:OE1 | 2.45 | 0.49 |
| 1:M:326:ILE:HD12 | 1:M:326:ILE:N | 2.27 | 0.49 |
| 4:P:806:DT:H1' | 4:P:807:DC:H5" | 1.93 | 0.49 |
| 1:A:270:ILE:HD12 | 1:A:270:ILE:O | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:317:VAL:CG2 | 1:A:318:TYR:N | 2.71 | 0.49 |
| 1:A:341:ILE:HD12 | 1:A:341:ILE:N | 2.28 | 0.49 |
| 1:E:493:VAL:HG12 | 1:E:494:ASN:H | 1.77 | 0.49 |
| 2:F:13:LYS:CD | 2:F:86:ASP:HB2 | 2.40 | 0.49 |
| 1:I:344:GLU:CB | 1:I:345:PRO:CD | 2.90 | 0.49 |
| 2:J:207:GLN:O | 2:J:210:LEU:HB2 | 2.13 | 0.49 |
| 1:M:343:GLN:CG | 1:M:349:LEU:HD11 | 2.24 | 0.49 |
| 2:N:281:LYS:CE | 8:N:432:HOH:O | 2.60 | 0.49 |
| 1:E:48:SER:O | 1:E:144:TYR:HA | 2.13 | 0.49 |
| 1:E:339:TYR:CD1 | 1:E:375:ILE:HD11 | 2.48 | 0.49 |
| 2:F:118:VAL:HG12 | 2:F:119:PRO:O | 2.13 | 0.49 |
| 1:I:372:VAL:HG13 | 1:I:389:PHE:CZ | 2.47 | 0.49 |
| 1:M:199:ARG:O | 1:M:203:GLU:HG3 | 2.13 | 0.49 |
| 1:M:406:TRP:CD1 | 1:M:407:GLN:HG2 | 2.47 | 0.49 |
| 1:A:325:LEU:C | 1:A:326:ILE:HD12 | 2.33 | 0.49 |
| 1:A:366:LYS:O | 1:A:370:GLU:HG3 | 2.12 | 0.49 |
| 2:B:380:ILE:O | 2:B:384:GLY:HA2 | 2.13 | 0.49 |
| 1:E:3:SER:HB3 | 1:E:5:ILE:HG22 | 1.95 | 0.49 |
| 1:E:250:ASP:OD1 | 1:E:250:ASP:N | 2.45 | 0.49 |
| 1:E:357:MET:HG2 | 1:E:367:GLN:OE1 | 2.13 | 0.49 |
| 2:F:65:LYS:HA | 2:F:407:GLN:OE1 | 2.12 | 0.49 |
| 2:J:205:LEU:HD23 | 2:J:205:LEU:O | 2.11 | 0.49 |
| 2:J:266:TRP:CD1 | 2:J:269:GLN:NE2 | 2.81 | 0.49 |
| 1:M:457:TYR:CE2 | 1:M:465:LYS:HB3 | 2.47 | 0.49 |
| 4:L:806:DT:C1' | 4:L:807:DC:H5" | 2.43 | 0.49 |
| 4:P:821:DC:H2' | 4:P:822:2DA:H8 | 1.95 | 0.49 |
| 1:E:536:VAL:O | 1:E:537:PRO:O | 2.30 | 0.49 |
| 2:F:207:GLN:O | 2:F:210:LEU:HB2 | 2.13 | 0.49 |
| 2:F:213:GLY:O | 2:F:214:LEU:HD23 | 2.12 | 0.49 |
| 1:I:108:VAL:HG21 | 1:I:221:HIS:HD2 | 1.78 | 0.49 |
| 1:I:132:ILE:HD11 | 1:I:142:ILE:HD11 | 1.94 | 0.49 |
| 1:I:339:TYR:CG | 1:I:375:ILE:HD11 | 2.48 | 0.49 |
| 1:M:96:HIS:N | 2:N:136:ASN:OD1 | 2.46 | 0.49 |
| 1:M:151:GLN:OE1 | 6:M:823:ZP4:N3B | 2.46 | 0.49 |
| 1:A:184:MET:HG3 | 4:D:822:2DA:H1' | 1.94 | 0.48 |
| 1:A:337:TRP:CZ3 | 1:A:368:LEU:HD13 | 2.48 | 0.48 |
| 1:E:198:HIS:O | 1:E:200:THR:N | 2.46 | 0.48 |
| 1:E:533:LEU:HD12 | 1:E:533:LEU:N | 2.28 | 0.48 |
| 2:F:54:ASN:C | 2:F:54:ASN:ND2 | 2.64 | 0.48 |
| 1:I:199:ARG:O | 1:I:203:GLU:HG3 | 2.13 | 0.48 |
| 1:M:24:TRP:CE3 | 3:O:703:DG:H1' | 2.47 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:480:GLN:O | 1:M:483:TYR:HB3 | 2.13 | 0.48 |
| 1:A:114:ALA:HB1 | 1:A:160:PHE:CZ | 2.48 | 0.48 |
| 1:A:272:PRO:HA | 8:A:556:HOH:O | 2.13 | 0.48 |
| 2:B:24:TRP:CH2 | 2:B:403:THR:HG21 | 2.47 | 0.48 |
| 1:M:339:TYR:CZ | 1:M:352:GLY:CA | 2.72 | 0.48 |
| 4:P:805:DG:C2' | 4:P:806:DT:H71 | 2.43 | 0.48 |
| 1:A:458:VAL:HG13 | 1:A:458:VAL:O | 2.13 | 0.48 |
| 1:E:283:LEU:CD1 | 4:H:817:MRG:H231 | 2.42 | 0.48 |
| 2:F:263:LYS:CB | 2:F:423:VAL:HG11 | 2.43 | 0.48 |
| 1:I:489:SER:HB2 | 1:I:493:VAL:HG22 | 1.94 | 0.48 |
| 4:L:804:DA:H2" | 4:L:805:DG:OP2 | 2.13 | 0.48 |
| 2:B:169:GLU:N | 2:B:170:PRO:HD2 | 2.29 | 0.48 |
| 1:E:425:LEU:HD22 | 1:E:509:GLN:NE2 | 2.28 | 0.48 |
| 1:I:326:ILE:N | 1:I:326:ILE:HD12 | 2.28 | 0.48 |
| 1:I:344:GLU:HB3 | 1:I:345:PRO:HD2 | 1.93 | 0.48 |
| 2:J:88:TRP:CE2 | 2:J:154:LYS:HD3 | 2.48 | 0.48 |
| 1:M:502:ALA:O | 1:M:506:ILE:HG12 | 2.13 | 0.48 |
| 3:O:717:DC:H2" | 3:O:718:DA:OP2 | 2.13 | 0.48 |
| 1:A:480:GLN:O | 1:A:483:TYR:HB3 | 2.13 | 0.48 |
| 1:E:480:GLN:O | 1:E:483:TYR:HB3 | 2.14 | 0.48 |
| 1:I:198:HIS:O | 1:I:200:THR:N | 2.46 | 0.48 |
| 2:J:42:GLU:OE2 | 2:J:49:LYS:HG3 | 2.13 | 0.48 |
| 1:M:2:ILE:HD13 | 1:M:2:ILE:C | 2.33 | 0.48 |
| 1:M:198:HIS:O | 1:M:201:LYS:N | 2.46 | 0.48 |
| 1:M:286:THR:OG1 | 3:O:714:DG:C4' | 2.62 | 0.48 |
| 1:M:357:MET:HG2 | 1:M:367:GLN:OE1 | 2.13 | 0.48 |
| 2:B:255:ASN:O | 2:B:258:GLN:HB2 | 2.14 | 0.48 |
| 1:E:242:GLN:O | 1:E:243:PRO:C | 2.51 | 0.48 |
| 1:E:460:ASN:HB3 | 2:F:287:LYS:O | 2.13 | 0.48 |
| 2:F:125:ARG:HB3 | 2:F:145:GLN:HE21 | 1.77 | 0.48 |
| 1:I:148:VAL:HG22 | 1:I:149:LEU:N | 2.28 | 0.48 |
| 1:I:156:SER:O | 1:I:157:PRO:C | 2.52 | 0.48 |
| 1:I:380:ILE:O | 1:I:384:GLY:HA2 | 2.13 | 0.48 |
| 1:A:50:ILE:HG13 | 1:A:143:ARG:HB2 | 1.95 | 0.48 |
| 1:A:174:GLN:OE1 | 2:N:3:SER:O | 2.32 | 0.48 |
| 2:B:206:ARG:CB | 2:B:206:ARG:NH1 | 2.75 | 0.48 |
| 2:B:340:GLN:CG | 2:B:351:THR:HG22 | 2.44 | 0.48 |
| 1:E:67:ASP:O | 1:E:68:SER:HB2 | 2.14 | 0.48 |
| 2:F:196:GLY:O | 2:F:200:THR:HG23 | 2.13 | 0.48 |
| 1:I:24:TRP:CZ2 | 3:K:704:DC:H5' | 2.48 | 0.48 |
| 2:J:85:GLN:HA | 2:J:88:TRP:NE1 | 2.28 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:27:THR:O | 1:M:31:ILE:HG12 | 2.14 | 0.48 |
| 1:A:223:LYS:O | 1:A:225:PRO:HD3 | 2.14 | 0.48 |
| 1:E:31:ILE:O | 1:E:35:VAL:HG22 | 2.14 | 0.48 |
| 1:E:478:GLU:CG | 1:E:499:SER:HB2 | 2.42 | 0.48 |
| 1:I:264:LEU:O | 1:I:267:ALA:HB3 | 2.14 | 0.48 |
| 1:I:325:LEU:C | 1:I:326:ILE:HD12 | 2.33 | 0.48 |
| 2:J:111:VAL:HG11 | 2:J:187:LEU:HD12 | 1.96 | 0.48 |
| 1:M:286:THR:OG1 | 3:O:714:DG:H5" | 2.12 | 0.48 |
| 1:M:287:LYS:HZ3 | 1:M:293:ILE:HD12 | 1.79 | 0.48 |
| 2:N:8:VAL:HG23 | 2:N:8:VAL:O | 2.14 | 0.48 |
| 2:N:417:VAL:HG22 | 2:N:419:THR:HG23 | 1.95 | 0.48 |
| 1:A:156:SER:O | 1:A:157:PRO:C | 2.50 | 0.48 |
| 1:A:339:TYR:CD1 | 1:A:375:ILE:HD11 | 2.48 | 0.48 |
| 2:B:332:GLN:HE22 | 2:B:425:LEU:CD1 | 2.20 | 0.48 |
| 2:F:115:TYR:OH | 2:F:157:PRO:HB3 | 2.13 | 0.48 |
| 1:I:13:LYS:HE3 | 1:I:84:THR:O | 2.13 | 0.48 |
| 1:I:333:GLY:H | 1:I:336:GLN:HB2 | 1.79 | 0.48 |
| 1:I:501:TYR:HE1 | 1:I:505:ILE:HD11 | 1.78 | 0.48 |
| 1:M:115:TYR:O | 1:M:148:VAL:HG22 | 2.14 | 0.48 |
| 4:D:805:DG:H2" | 4:D:806:DT:H71 | 1.95 | 0.48 |
| 4:D:809:DC:H2" | 4:D:810:DT:H5' | 1.94 | 0.48 |
| 3:K:705:DA:H2" | 3:K:706:DT:C5' | 2.40 | 0.48 |
| 1:A:221:HIS:NE2 | 1:A:228:LEU:HB2 | 2.29 | 0.48 |
| 1:E:188:TYR:CD1 | 1:E:188:TYR:C | 2.87 | 0.48 |
| 2:F:157:PRO:HG3 | 2:F:184:MET:HA | 1.94 | 0.48 |
| 1:I:156:SER:HB2 | 1:I:157:PRO:CD | 2.44 | 0.48 |
| 1:I:238:LYS:HD2 | 1:I:315:HIS:CE1 | 2.48 | 0.48 |
| 1:I:529:GLU:O | 1:I:530:LYS:HG3 | 2.13 | 0.48 |
| 2:J:332:GLN:NE2 | 2:J:425:LEU:HD13 | 2.29 | 0.48 |
| 1:M:31:ILE:CD1 | 1:M:133:PRO:HG2 | 2.40 | 0.48 |
| 2:N:125:ARG:HB3 | 2:N:145:GLN:HE21 | 1.78 | 0.48 |
| 1:A:205:LEU:O | 1:A:208:HIS:N | 2.38 | 0.47 |
| 2:B:103:LYS:HG3 | 2:B:192:ASP:OD2 | 2.13 | 0.47 |
| 1:E:325:LEU:C | 1:E:326:ILE:HD12 | 2.34 | 0.47 |
| 1:E:420:PRO:HA | 1:E:421:PRO:C | 2.34 | 0.47 |
| 1:E:500:GLN:NE2 | 2:F:422:LEU:HD13 | 2.29 | 0.47 |
| 1:I:260:LEU:O | 1:I:264:LEU:HD12 | 2.13 | 0.47 |
| 2:J:125:ARG:HB3 | 2:J:145:GLN:HE21 | 1.78 | 0.47 |
| 2:J:303:LEU:HD23 | 2:J:303:LEU:O | 2.14 | 0.47 |
| 4:H:809:DC:H1' | 4:H:810:DT:C5' | 2.44 | 0.47 |
| 1:A:132:ILE:HD11 | 1:A:144:TYR:HE2 | 1.79 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:5:ILE:CG2 | 2:B:6:GLU:N | 2.77 | 0.47 |
| 1:I:444:GLY:HA3 | 1:I:477:THR:CG2 | 2.44 | 0.47 |
| 1:I:502:ALA:O | 1:I:506:ILE:HG12 | 2.14 | 0.47 |
| 1:M:336:GLN:C | 1:M:337:TRP:CD1 | 2.88 | 0.47 |
| 2:N:206:ARG:HH11 | 2:N:206:ARG:HB2 | 1.78 | 0.47 |
| 1:A:420:PRO:HA | 1:A:421:PRO:C | 2.35 | 0.47 |
| 1:E:109:LEU:HD23 | 1:E:220:LYS:HB2 | 1.95 | 0.47 |
| 2:J:202:ILE:O | 2:J:206:ARG:HG3 | 2.15 | 0.47 |
| 1:M:156:SER:O | 1:M:157:PRO:C | 2.53 | 0.47 |
| 1:M:198:HIS:O | 1:M:200:THR:N | 2.47 | 0.47 |
| 4:H:804:DA:H2" | 4:H:805:DG:OP2 | 2.14 | 0.47 |
| 4:P:809:DC:H1' | 4:P:810:DT:H5' | 1.97 | 0.47 |
| 1:A:332:GLN:OE1 | 1:A:332:GLN:HA | 2.15 | 0.47 |
| 1:A:393:ILE:HB | 1:A:423:VAL:HB | 1.96 | 0.47 |
| 1:A:475:GLN:HE22 | 4:D:808:DC:H4' | 1.80 | 0.47 |
| 1:E:148:VAL:HG22 | 1:E:149:LEU:H | 1.78 | 0.47 |
| 2:F:74:LEU:HD12 | 2:F:75:VAL:N | 2.29 | 0.47 |
| 2:F:242:GLN:O | 2:F:242:GLN:NE2 | 2.47 | 0.47 |
| 2:F:382:ILE:HB | 2:F:383:TRP:CE3 | 2.50 | 0.47 |
| 1:M:246:LEU:HD12 | 1:M:246:LEU:N | 2.27 | 0.47 |
| 2:N:205:LEU:O | 2:N:205:LEU:HD23 | 2.13 | 0.47 |
| 4:D:806:DT:H5' | 4:D:806:DT:C6 | 2.44 | 0.47 |
| 1:E:246:LEU:HD12 | 1:E:246:LEU:N | 2.29 | 0.47 |
| 1:E:490:GLY:O | 1:E:528:LYS:HD2 | 2.14 | 0.47 |
| 2:F:380:ILE:O | 2:F:384:GLY:HA2 | 2.15 | 0.47 |
| 1:A:13:LYS:HE3 | 1:A:84:THR:O | 2.14 | 0.47 |
| 1:A:278:GLN:HB2 | 1:A:302:GLU:OE1 | 2.13 | 0.47 |
| 1:A:338:THR:HG22 | 1:A:339:TYR:N | 2.30 | 0.47 |
| 1:E:529:GLU:HG2 | 1:E:530:LYS:HG3 | 1.97 | 0.47 |
| 2:F:340:GLN:HG3 | 2:F:351:THR:CG2 | 2.44 | 0.47 |
| 1:M:57:ASN:HD21 | 1:M:131:THR:HB | 1.78 | 0.47 |
| 1:A:125:ARG:NH1 | 1:A:147:ASN:CB | 2.76 | 0.47 |
| 1:A:157:PRO:HG3 | 3:C:707:DG:O4' | 2.14 | 0.47 |
| 1:A:318:TYR:O | 1:A:349:LEU:HD11 | 2.15 | 0.47 |
| 1:A:475:GLN:NE2 | 4:D:808:DC:O3' | 2.48 | 0.47 |
| 1:A:502:ALA:O | 1:A:506:ILE:HG12 | 2.15 | 0.47 |
| 2:B:382:ILE:HB | 2:B:383:TRP:CE3 | 2.50 | 0.47 |
| 2:F:13:LYS:CB | 2:F:16:MET:HG3 | 2.42 | 0.47 |
| 1:I:410:TRP:CE2 | 2:J:363:ASN:ND2 | 2.83 | 0.47 |
| 2:J:72:ARG:NH2 | 2:J:151:GLN:NE2 | 2.63 | 0.47 |
| 2:J:206:ARG:HH11 | 2:J:206:ARG:HB2 | 1.79 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:J:263:LYS:CA | 2:J:423:VAL:HG11 | 2.45 | 0.47 |
| 2:J:382:ILE:HB | 2:J:383:TRP:CE3 | 2.50 | 0.47 |
| 1:M:3:SER:HB2 | 1:M:119:PRO:CD | 2.43 | 0.47 |
| 1:M:77:PHE:CD1 | 1:M:80:LEU:HD23 | 2.50 | 0.47 |
| 1:M:444:GLY:HA3 | 1:M:477:THR:CG2 | 2.45 | 0.47 |
| 4:D:810:DT:H2" | 4:D:811:DG:H8 | 1.80 | 0.47 |
| 1:E:450:THR:O | 1:E:451:LYS:HB2 | 2.15 | 0.47 |
| 1:I:116:PHE:HA | 1:I:148:VAL:HG21 | 1.96 | 0.47 |
| 2:J:422:LEU:HD23 | 2:J:422:LEU:N | 2.29 | 0.47 |
| 1:M:433:PRO:HB3 | 2:N:289:LEU:HD23 | 1.95 | 0.47 |
| 2:N:157:PRO:HG3 | 2:N:184:MET:HA | 1.97 | 0.47 |
| 1:A:96:HIS:ND1 | 1:A:97:PRO:HD2 | 2.30 | 0.47 |
| 1:A:242:GLN:O | 1:A:243:PRO:C | 2.52 | 0.47 |
| 1:A:320:ASP:HA | 1:A:321:PRO:HD3 | 1.70 | 0.47 |
| 2:B:422:LEU:O | 2:B:424:LYS:O | 2.33 | 0.47 |
| 2:F:54:ASN:HD21 | 2:F:56:TYR:HB2 | 1.79 | 0.47 |
| 2:J:332:GLN:HE22 | 2:J:425:LEU:HD13 | 1.80 | 0.47 |
| 2:J:368:LEU:HD22 | 2:J:398:TRP:CZ3 | 2.49 | 0.47 |
| 1:A:260:LEU:HD23 | 1:A:279:LEU:HD22 | 1.97 | 0.47 |
| 1:E:81:ASN:HA | 1:E:84:THR:CG2 | 2.44 | 0.47 |
| 1:I:132:ILE:HD11 | 1:I:144:TYR:HE2 | 1.80 | 0.47 |
| 1:I:281:LYS:HG3 | 1:I:284:ARG:NH1 | 2.30 | 0.47 |
| 2:N:76:ASP:C | 2:N:78:ARG:H | 2.18 | 0.47 |
| 4:D:817:MRG:H2" | 4:D:818:DC:H6 | 1.80 | 0.47 |
| 1:A:3:SER:HB3 | 1:A:5:ILE:HG22 | 1.97 | 0.46 |
| 1:A:270:ILE:HG13 | 1:A:314:VAL:CG2 | 2.44 | 0.46 |
| 1:A:500:GLN:HE22 | 2:B:422:LEU:HD13 | 1.79 | 0.46 |
| 2:B:274:ILE:HA | 2:B:306:ASN:OD1 | 2.15 | 0.46 |
| 1:E:49:LYS:HG2 | 1:E:144:TYR:CE1 | 2.50 | 0.46 |
| 2:F:120:LEU:HD23 | 2:F:121:ASP:H | 1.80 | 0.46 |
| 2:F:164:MET:O | 2:F:165:THR:C | 2.52 | 0.46 |
| 2:N:363:ASN:ND2 | 2:N:405:TYR:OH | 2.48 | 0.46 |
| 2:B:8:VAL:HG21 | 2:B:159:ILE:HG12 | 1.97 | 0.46 |
| 2:B:205:LEU:HD23 | 2:B:205:LEU:O | 2.15 | 0.46 |
| 1:E:109:LEU:HD23 | 1:E:220:LYS:CB | 2.46 | 0.46 |
| 1:E:303:LEU:O | 1:E:303:LEU:HD22 | 2.15 | 0.46 |
| 1:E:448:ARG:HG2 | 1:E:448:ARG:NH1 | 2.31 | 0.46 |
| 1:E:535:TRP:C | 1:E:536:VAL:CG1 | 2.84 | 0.46 |
| 2:F:340:GLN:CG | 2:F:351:THR:HG22 | 2.45 | 0.46 |
| 1:I:188:TYR:C | 1:I:188:TYR:CD1 | 2.88 | 0.46 |
| 1:I:325:LEU:HD12 | 1:I:325:LEU:N | 2.30 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:244:ILE:HD12 | 1:M:310:LEU:HD23 | 1.97 | 0.46 |
| 1:M:372:VAL:HG13 | 1:M:389:PHE:CZ | 2.50 | 0.46 |
| 2:N:340:GLN:CG | 2:N:351:THR:HG22 | 2.44 | 0.46 |
| 2:N:410:TRP:O | 2:N:411:ILE:HD13 | 2.15 | 0.46 |
| 4:D:806:DT:C1' | 4:D:807:DC:H5" | 2.46 | 0.46 |
| 2:F:379:SER:OG | 2:F:387:PRO:HD3 | 2.16 | 0.46 |
| 1:I:27:THR:HG22 | 1:I:28:GLU:N | 2.31 | 0.46 |
| 1:I:339:TYR:CD1 | 1:I:375:ILE:HD11 | 2.50 | 0.46 |
| 2:J:154:LYS:O | 2:J:157:PRO:HD2 | 2.14 | 0.46 |
| 1:M:389:PHE:HB3 | 1:M:391:LEU:HD21 | 1.97 | 0.46 |
| 3:G:717:DC:H2" | 3:G:718:DA:OP2 | 2.15 | 0.46 |
| 4:H:820:DC:C2' | 4:H:821:DC:H5' | 2.40 | 0.46 |
| 1:A:97:PRO:HG3 | 1:A:232:TYR:CD1 | 2.50 | 0.46 |
| 1:A:324:ASP:OD2 | 1:A:388:LYS:NZ | 2.44 | 0.46 |
| 1:A:372:VAL:HG13 | 1:A:389:PHE:CE1 | 2.51 | 0.46 |
| 2:B:266:TRP:CD1 | 2:B:269:GLN:NE2 | 2.84 | 0.46 |
| 2:B:307:ARG:HG2 | 2:B:311:LYS:NZ | 2.30 | 0.46 |
| 1:E:171:PHE:CD2 | 1:E:205:LEU:HD23 | 2.51 | 0.46 |
| 2:F:417:VAL:O | 2:F:417:VAL:HG13 | 2.15 | 0.46 |
| 4:H:806:DT:C1' | 4:H:807:DC:H5" | 2.46 | 0.46 |
| 4:H:807:DC:H2" | 4:H:808:DC:C5' | 2.32 | 0.46 |
| 1:A:132:ILE:HG13 | 1:A:142:ILE:HG13 | 1.97 | 0.46 |
| 1:A:215:THR:HG22 | 1:A:216:THR:N | 2.31 | 0.46 |
| 1:A:282:LEU:HD21 | 1:A:296:THR:CG2 | 2.45 | 0.46 |
| 1:E:198:HIS:O | 1:E:201:LYS:N | 2.48 | 0.46 |
| 1:E:398:TRP:CZ2 | 1:E:411:ILE:HG12 | 2.51 | 0.46 |
| 2:F:200:THR:O | 2:F:204:GLU:HG3 | 2.15 | 0.46 |
| 2:J:242:GLN:NE2 | 2:J:242:GLN:O | 2.49 | 0.46 |
| 1:M:199:ARG:NH2 | 1:M:222:GLN:NE2 | 2.63 | 0.46 |
| 1:M:398:TRP:CZ2 | 1:M:411:ILE:HG12 | 2.50 | 0.46 |
| 1:A:3:SER:HB3 | 1:A:5:ILE:CG2 | 2.45 | 0.46 |
| 1:A:63:ILE:HG21 | 1:A:74:LEU:HD11 | 1.97 | 0.46 |
| 1:A:490:GLY:O | 1:A:528:LYS:HD2 | 2.15 | 0.46 |
| 1:E:406:TRP:CD1 | 1:E:407:GLN:HG2 | 2.51 | 0.46 |
| 1:E:441:TYR:O | 1:E:548:VAL:HG21 | 2.15 | 0.46 |
| 1:I:171:PHE:CD2 | 1:I:205:LEU:HD23 | 2.51 | 0.46 |
| 1:I:398:TRP:CZ2 | 1:I:411:ILE:HG12 | 2.51 | 0.46 |
| 2:J:169:GLU:O | 2:J:173:LYS:HG3 | 2.16 | 0.46 |
| 1:M:44:GLU:HB2 | 1:M:46:LYS:HD3 | 1.98 | 0.46 |
| 1:M:94:ILE:HD11 | 3:O:708:DG:N2 | 2.30 | 0.46 |
| 1:M:115:TYR:HB3 | 1:M:149:LEU:O | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:148:VAL:HG22 | 1:M:149:LEU:N | 2.31 | 0.46 |
| 1:M:327:ALA:HB2 | 1:M:341:ILE:HG13 | 1.97 | 0.46 |
| 1:M:533:LEU:HD12 | 1:M:533:LEU:N | 2.31 | 0.46 |
| 1:M:548:VAL:O | 1:M:551:LEU:HB2 | 2.15 | 0.46 |
| 2:N:48:SER:HB2 | 2:N:147:ASN:OD1 | 2.15 | 0.46 |
| 2:N:111:VAL:HG11 | 2:N:187:LEU:HD13 | 1.96 | 0.46 |
| 1:A:24:TRP:CH2 | 3:C:704:DC:C5' | 2.96 | 0.46 |
| 2:B:118:VAL:HB | 2:B:149:LEU:HG | 1.97 | 0.46 |
| 2:B:178:ILE:HG23 | 2:B:190:GLY:O | 2.16 | 0.46 |
| 1:E:116:PHE:CA | 1:E:148:VAL:HG21 | 2.45 | 0.46 |
| 1:E:536:VAL:HB | 1:E:537:PRO:HD2 | 1.98 | 0.46 |
| 1:M:57:ASN:OD1 | 1:M:58:THR:N | 2.48 | 0.46 |
| 1:M:171:PHE:CD2 | 1:M:205:LEU:HD23 | 2.51 | 0.46 |
| 1:M:223:LYS:O | 1:M:225:PRO:HD3 | 2.15 | 0.46 |
| 1:E:223:LYS:O | 1:E:225:PRO:HD3 | 2.16 | 0.46 |
| 2:F:332:GLN:HE22 | 2:F:425:LEU:CD1 | 2.28 | 0.46 |
| 2:J:303:LEU:HD23 | 2:J:303:LEU:C | 2.36 | 0.46 |
| 1:M:439:THR:HG21 | 2:N:289:LEU:CD1 | 2.46 | 0.46 |
| 1:A:259:LYS:HG2 | 1:A:259:LYS:O | 2.16 | 0.46 |
| 2:B:388:LYS:HG3 | 2:B:413:GLU:O | 2.16 | 0.46 |
| 2:F:366:LYS:HA | 2:F:405:TYR:CD2 | 2.51 | 0.46 |
| 1:I:188:TYR:O | 1:I:188:TYR:HD1 | 1.99 | 0.46 |
| 1:I:250:ASP:OD1 | 1:I:250:ASP:N | 2.45 | 0.46 |
| 1:I:438:GLU:OE1 | 1:I:463:ARG:HD2 | 2.15 | 0.46 |
| 2:N:120:LEU:HD23 | 2:N:121:ASP:H | 1.80 | 0.46 |
| 4:P:805:DG:H2" | 4:P:806:DT:H71 | 1.98 | 0.46 |
| 4:P:821:DC:H2" | 4:P:822:2DA:H5' | 1.98 | 0.46 |
| 1:A:478:GLU:HG2 | 1:A:499:SER:HB2 | 1.97 | 0.46 |
| 1:E:132:ILE:CD1 | 1:E:144:TYR:HE2 | 2.29 | 0.46 |
| 1:E:215:THR:CG2 | 1:E:216:THR:N | 2.78 | 0.46 |
| 1:I:26:LEU:HB2 | 1:I:31:ILE:HD11 | 1.96 | 0.46 |
| 1:I:298:GLU:OE1 | 1:I:298:GLU:N | 2.49 | 0.46 |
| 2:B:85:GLN:HA | 2:B:88:TRP:NE1 | 2.31 | 0.45 |
| 1:E:31:ILE:HD12 | 1:E:133:PRO:HG2 | 1.97 | 0.45 |
| 1:E:118:VAL:HB | 1:E:149:LEU:HD22 | 1.98 | 0.45 |
| 1:E:475:GLN:NE2 | 4:H:809:DC:H5' | 2.30 | 0.45 |
| 1:E:510:PRO:HG2 | 1:E:522:ILE:CD1 | 2.46 | 0.45 |
| 1:M:46:LYS:HD2 | 1:M:46:LYS:N | 2.30 | 0.45 |
| 2:B:154:LYS:C | 2:B:157:PRO:HD2 | 2.37 | 0.45 |
| 2:F:422:LEU:HD23 | 2:F:422:LEU:H | 1.81 | 0.45 |
| 1:I:26:LEU:HB2 | 1:I:31:ILE:CD1 | 2.46 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:11:LYS:O | 1:M:85:GLN:HB3 | 2.16 | 0.45 |
| 1:M:325:LEU:HD13 | 1:M:385:LYS:HE2 | 1.97 | 0.45 |
| 2:N:46:LYS:O | 2:N:147:ASN:HB2 | 2.17 | 0.45 |
| 2:N:255:ASN:O | 2:N:258:GLN:HB2 | 2.16 | 0.45 |
| 1:A:107:THR:OG1 | 1:A:202:ILE:CD1 | 2.65 | 0.45 |
| 1:A:148:VAL:HG22 | 1:A:149:LEU:H | 1.81 | 0.45 |
| 1:A:349:LEU:O | 1:A:350:LYS:HB2 | 2.17 | 0.45 |
| 2:B:112:GLY:C | 2:B:151:GLN:HE21 | 2.19 | 0.45 |
| 2:B:413:GLU:OE1 | 2:B:413:GLU:HA | 2.16 | 0.45 |
| 2:F:212:TRP:N | 2:F:212:TRP:CD1 | 2.84 | 0.45 |
| 1:I:111:VAL:HB | 1:I:185:ASP:HB2 | 1.99 | 0.45 |
| 1:I:475:GLN:HB3 | 1:I:501:TYR:CE2 | 2.52 | 0.45 |
| 2:J:6:GLU:O | 2:J:6:GLU:CG | 2.54 | 0.45 |
| 2:J:88:TRP:CZ3 | 2:J:89:GLU:HB2 | 2.51 | 0.45 |
| 1:M:80:LEU:O | 1:M:84:THR:HG22 | 2.16 | 0.45 |
| 1:M:148:VAL:HG22 | 1:M:149:LEU:H | 1.81 | 0.45 |
| 1:M:529:GLU:HG2 | 1:M:530:LYS:HG3 | 1.98 | 0.45 |
| 1:A:125:ARG:O | 1:A:128:THR:OG1 | 2.28 | 0.45 |
| 1:A:344:GLU:OE1 | 1:A:347:LYS:HG3 | 2.15 | 0.45 |
| 1:A:465:LYS:HG3 | 1:A:466:VAL:N | 2.31 | 0.45 |
| 1:A:546:GLU:O | 1:A:549:ASP:HB3 | 2.15 | 0.45 |
| 1:E:44:GLU:HB2 | 1:E:46:LYS:HD3 | 1.98 | 0.45 |
| 1:E:247:PRO:HB3 | 1:E:259:LYS:CE | 2.47 | 0.45 |
| 2:F:24:TRP:CH2 | 2:F:61:PHE:HB3 | 2.51 | 0.45 |
| 1:I:148:VAL:HG22 | 1:I:149:LEU:H | 1.81 | 0.45 |
| 4:L:821:DC:H2' | 4:L:822:2DA:H8 | 1.99 | 0.45 |
| 1:E:365:VAL:HG11 | 1:E:401:TRP:CD1 | 2.52 | 0.45 |
| 1:I:491:LEU:N | 1:I:491:LEU:CD1 | 2.79 | 0.45 |
| 2:J:120:LEU:HD23 | 2:J:121:ASP:N | 2.32 | 0.45 |
| 2:N:215:THR:C | 2:N:217:PRO:HD3 | 2.36 | 0.45 |
| 1:A:87:PHE:N | 1:A:87:PHE:CD1 | 2.84 | 0.45 |
| 1:A:406:TRP:CD1 | 1:A:407:GLN:HG2 | 2.52 | 0.45 |
| 1:A:475:GLN:HB3 | 1:A:501:TYR:CD2 | 2.51 | 0.45 |
| 2:B:422:LEU:HD23 | 2:B:422:LEU:N | 2.32 | 0.45 |
| 1:E:171:PHE:CG | 1:E:205:LEU:HD23 | 2.52 | 0.45 |
| 1:I:13:LYS:HE2 | 1:I:86:ASP:OD1 | 2.16 | 0.45 |
| 2:J:266:TRP:C | 2:J:268:SER:H | 2.20 | 0.45 |
| 1:M:132:ILE:HD11 | 1:M:142:ILE:CD1 | 2.46 | 0.45 |
| 1:M:325:LEU:C | 1:M:326:ILE:HD12 | 2.36 | 0.45 |
| 1:M:393:ILE:HB | 1:M:423:VAL:HB | 1.97 | 0.45 |
| 2:N:350:LYS:HG2 | 2:N:351:THR:N | 2.32 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:340:GLN:HG3 | 2:B:351:THR:CG2 | 2.47 | 0.45 |
| 1:I:3:SER:HB3 | 1:I:5:ILE:CG2 | 2.46 | 0.45 |
| 1:I:382:ILE:O | 2:J:136:ASN:HB2 | 2.16 | 0.45 |
| 2:J:387:PRO:HG2 | 2:J:389:PHE:CE1 | 2.52 | 0.45 |
| 1:M:441:TYR:CE2 | 1:M:544:GLY:HA3 | 2.51 | 0.45 |
| 1:M:459:THR:OG1 | 1:M:463:ARG:N | 2.49 | 0.45 |
| 2:N:103:LYS:HG3 | 2:N:192:ASP:OD2 | 2.17 | 0.45 |
| 1:A:96:HIS:CG | 1:A:97:PRO:HD2 | 2.51 | 0.45 |
| 1:A:202:ILE:HD12 | 1:A:202:ILE:HA | 1.83 | 0.45 |
| 1:A:232:TYR:CE1 | 1:A:269:GLN:NE2 | 2.85 | 0.45 |
| 1:A:278:GLN:HB2 | 1:A:302:GLU:CD | 2.36 | 0.45 |
| 1:E:493:VAL:CG1 | 1:E:494:ASN:N | 2.79 | 0.45 |
| 2:F:376:THR:HB | 2:F:410:TRP:CH2 | 2.52 | 0.45 |
| 1:I:284:ARG:HH11 | 1:I:284:ARG:HG3 | 1.81 | 0.45 |
| 2:J:234:LEU:HD21 | 2:J:377:THR:CG2 | 2.47 | 0.45 |
| 1:M:92:LEU:CD1 | 2:N:133:PRO:HA | 2.47 | 0.45 |
| 2:N:164:MET:O | 2:N:165:THR:C | 2.55 | 0.45 |
| 2:N:169:GLU:O | 2:N:173:LYS:HG3 | 2.16 | 0.45 |
| 3:K:707:DG:H2' | 3:K:708:DG:H8 | 1.82 | 0.45 |
| 1:A:148:VAL:HG22 | 1:A:149:LEU:N | 2.32 | 0.45 |
| 1:A:397:THR:O | 1:A:400:THR:HB | 2.17 | 0.45 |
| 2:B:88:TRP:CE2 | 2:B:154:LYS:HD3 | 2.52 | 0.45 |
| 1:E:29:GLU:O | 1:E:32:LYS:HB3 | 2.16 | 0.45 |
| 1:E:312:GLU:HA | 1:E:313:PRO:HD2 | 1.76 | 0.45 |
| 2:F:215:THR:C | 2:F:217:PRO:HD3 | 2.38 | 0.45 |
| 2:F:271:TYR:CD1 | 2:F:271:TYR:N | 2.85 | 0.45 |
| 1:I:287:LYS:HZ3 | 1:I:293:ILE:HD12 | 1.81 | 0.45 |
| 1:I:402:TRP:CE3 | 2:J:364:ASP:OD2 | 2.70 | 0.45 |
| 2:J:34:LEU:HD13 | 2:J:62:ALA:HB2 | 1.99 | 0.45 |
| 1:M:544:GLY:HA2 | 2:N:286:THR:HG22 | 1.99 | 0.45 |
| 3:G:705:DA:H2" | 3:G:706:DT:C5' | 2.39 | 0.45 |
| 4:L:803:DC:H2" | 4:L:804:DA:C8 | 2.51 | 0.45 |
| 1:A:380:ILE:O | 1:A:384:GLY:HA2 | 2.17 | 0.45 |
| 2:B:293:ILE:HG23 | 2:B:294:PRO:HD2 | 1.99 | 0.45 |
| 1:E:75:VAL:HG11 | 1:E:77:PHE:CE2 | 2.52 | 0.45 |
| 1:E:188:TYR:O | 1:E:188:TYR:HD1 | 2.00 | 0.45 |
| 1:E:320:ASP:HA | 1:E:321:PRO:HD3 | 1.71 | 0.45 |
| 1:E:448:ARG:HG2 | 1:E:448:ARG:HH11 | 1.81 | 0.45 |
| 1:M:221:HIS:HB3 | 1:M:227:PHE:CD1 | 2.52 | 0.45 |
| 2:N:422:LEU:O | 2:N:424:LYS:O | 2.35 | 0.45 |
| 4:D:806:DT:H1' | 4:D:807:DC:H5" | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:L:807:DC:H2" | 4:L:808:DC:C5' | 2.38 | 0.45 |
| 1:A:56:TYR:O | 1:A:143:ARG:NH2 | 2.50 | 0.44 |
| 1:A:180:ILE:CG2 | 1:A:187:LEU:HD22 | 2.46 | 0.44 |
| 2:B:10:VAL:HG21 | 2:B:153:TRP:HH2 | 1.82 | 0.44 |
| 2:B:175:ASN:ND2 | 2:B:201:LYS:HE2 | 2.32 | 0.44 |
| 1:E:240:THR:HG22 | 1:E:315:HIS:HA | 1.98 | 0.44 |
| 1:M:171:PHE:CE2 | 1:M:205:LEU:HD23 | 2.52 | 0.44 |
| 2:N:196:GLY:O | 2:N:200:THR:HG23 | 2.17 | 0.44 |
| 2:N:375:ILE:HG12 | 2:N:375:ILE:H | 1.60 | 0.44 |
| 1:E:23:GLN:HG2 | 1:E:59:PRO:HA | 1.99 | 0.44 |
| 2:F:5:ILE:HG13 | 2:F:6:GLU:N | 2.31 | 0.44 |
| 2:F:88:TRP:CE2 | 2:F:154:LYS:HD3 | 2.53 | 0.44 |
| 1:I:12:LEU:HD11 | 1:I:127:TYR:CZ | 2.52 | 0.44 |
| 1:I:448:ARG:NH1 | 1:I:448:ARG:HG2 | 2.32 | 0.44 |
| 2:J:13:LYS:HB2 | 2:J:16:MET:CG | 2.36 | 0.44 |
| 2:N:340:GLN:HG3 | 2:N:351:THR:CG2 | 2.47 | 0.44 |
| 1:A:232:TYR:HE1 | 1:A:269:GLN:NE2 | 2.15 | 0.44 |
| 1:A:422:LEU:HD22 | 1:A:422:LEU:N | 2.33 | 0.44 |
| 2:B:278:GLN:HG3 | 2:B:298:GLU:HB3 | 1.99 | 0.44 |
| 1:E:24:TRP:CH2 | 3:G:704:DC:C5' | 3.00 | 0.44 |
| 2:F:278:GLN:HG3 | 2:F:298:GLU:HB3 | 2.00 | 0.44 |
| 1:I:397:THR:O | 1:I:400:THR:HB | 2.17 | 0.44 |
| 2:J:164:MET:O | 2:J:165:THR:C | 2.54 | 0.44 |
| 1:M:207:GLN:NE2 | 1:M:210:LEU:HD13 | 2.31 | 0.44 |
| 1:M:244:ILE:HD13 | 1:M:244:ILE:O | 2.17 | 0.44 |
| 1:M:541:GLY:O | 1:M:542:ILE:C | 2.56 | 0.44 |
| 2:N:266:TRP:O | 2:N:269:GLN:HG3 | 2.17 | 0.44 |
| 1:A:358:ARG:HE | 1:A:358:ARG:HB2 | 1.65 | 0.44 |
| 1:E:132:ILE:HD11 | 1:E:142:ILE:HD12 | 1.99 | 0.44 |
| 1:E:181:TYR:CE2 | 2:F:138:GLU:HA | 2.52 | 0.44 |
| 1:E:502:ALA:O | 1:E:506:ILE:HG12 | 2.17 | 0.44 |
| 1:I:320:ASP:HA | 1:I:321:PRO:HD3 | 1.73 | 0.44 |
| 1:I:344:GLU:O | 1:I:345:PRO:C | 2.55 | 0.44 |
| 1:I:448:ARG:HG2 | 1:I:448:ARG:HH11 | 1.83 | 0.44 |
| 2:J:46:LYS:HD2 | 2:J:116:PHE:HB3 | 1.99 | 0.44 |
| 1:M:278:GLN:HB2 | 1:M:302:GLU:CD | 2.37 | 0.44 |
| 1:M:380:ILE:O | 1:M:384:GLY:HA2 | 2.17 | 0.44 |
| 1:A:333:GLY:H | 1:A:336:GLN:HB2 | 1.82 | 0.44 |
| 2:B:350:LYS:HG2 | 2:B:351:THR:N | 2.31 | 0.44 |
| 2:B:363:ASN:ND2 | 2:B:405:TYR:OH | 2.50 | 0.44 |
| 1:E:63:ILE:HG12 | 1:E:64:LYS:N | 2.32 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:F:417:VAL:HG22 | 2:F:419:THR:HG23 | 1.98 | 0.44 |
| 1:I:206:ARG:HG3 | 1:I:216:THR:CG2 | 2.47 | 0.44 |
| 1:M:188:TYR:CD1 | 1:M:188:TYR:C | 2.90 | 0.44 |
| 1:M:238:LYS:HD2 | 1:M:315:HIS:ND1 | 2.32 | 0.44 |
| 2:N:332:GLN:HE22 | 2:N:425:LEU:CD1 | 2.29 | 0.44 |
| 1:A:77:PHE:CD1 | 1:A:80:LEU:HD23 | 2.52 | 0.44 |
| 1:A:91:GLN:HG2 | 1:A:161:GLN:NE2 | 2.33 | 0.44 |
| 2:B:157:PRO:HG3 | 2:B:184:MET:HA | 1.98 | 0.44 |
| 2:F:31:ILE:HD12 | 2:F:135:ILE:HG12 | 2.00 | 0.44 |
| 1:I:24:TRP:CH2 | 3:K:704:DC:H5' | 2.53 | 0.44 |
| 1:I:25:PRO:HD2 | 3:K:703:DG:C2 | 2.53 | 0.44 |
| 1:I:463:ARG:HG2 | 1:I:463:ARG:NH1 | 2.32 | 0.44 |
| 2:J:11:LYS:H | 2:J:11:LYS:HG2 | 1.57 | 0.44 |
| 2:J:266:TRP:C | 2:J:268:SER:N | 2.71 | 0.44 |
| 1:M:317:VAL:HG12 | 1:M:348:ASN:O | 2.17 | 0.44 |
| 1:M:320:ASP:HA | 1:M:321:PRO:HD3 | 1.73 | 0.44 |
| 1:A:98:ALA:O | 1:A:349:LEU:HD22 | 2.18 | 0.44 |
| 1:A:281:LYS:CG | 1:A:284:ARG:NH1 | 2.80 | 0.44 |
| 1:A:444:GLY:HA3 | 1:A:477:THR:CG2 | 2.45 | 0.44 |
| 2:B:258:GLN:O | 2:B:259:LYS:C | 2.56 | 0.44 |
| 1:E:56:TYR:O | 1:E:143:ARG:NH2 | 2.50 | 0.44 |
| 1:E:254:VAL:HG23 | 1:E:291:GLU:O | 2.17 | 0.44 |
| 2:F:266:TRP:C | 2:F:268:SER:H | 2.21 | 0.44 |
| 1:I:113:ASP:HA | 6:I:823:ZP4:N3B | 2.33 | 0.44 |
| 1:I:289:LEU:H | 1:I:289:LEU:CD1 | 2.28 | 0.44 |
| 1:M:278:GLN:HB2 | 1:M:302:GLU:OE1 | 2.18 | 0.44 |
| 4:D:812:DT:H2'' | 4:D:813:DT:OP2 | 2.17 | 0.44 |
| 4:D:819:DG:H2' | 4:D:820:DC:C6 | 2.51 | 0.44 |
| 1:A:3:SER:HB2 | 1:A:119:PRO:HD3 | 1.99 | 0.44 |
| 1:A:339:TYR:O | 1:A:352:GLY:N | 2.51 | 0.44 |
| 1:A:448:ARG:NH1 | 1:A:448:ARG:HG2 | 2.32 | 0.44 |
| 1:A:511:ASP:OD1 | 1:A:511:ASP:C | 2.56 | 0.44 |
| 1:I:57:ASN:HD21 | 1:I:131:THR:HB | 1.83 | 0.44 |
| 1:I:254:VAL:HB | 1:I:288:ALA:O | 2.18 | 0.44 |
| 1:I:458:VAL:HG11 | 1:I:548:VAL:HG22 | 2.00 | 0.44 |
| 1:M:2:ILE:O | 1:M:2:ILE:HG23 | 2.18 | 0.44 |
| 1:M:510:PRO:HG2 | 1:M:522:ILE:CD1 | 2.48 | 0.44 |
| 1:A:458:VAL:HG12 | 1:A:548:VAL:CG2 | 2.44 | 0.44 |
| 1:A:475:GLN:HB3 | 1:A:501:TYR:CE2 | 2.52 | 0.44 |
| 1:A:513:SER:OG | 1:A:514:GLU:N | 2.51 | 0.44 |
| 2:B:57:ASN:OD1 | 2:B:143:ARG:NH1 | 2.50 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:205:LEU:O | 1:E:208:HIS:N | 2.34 | 0.44 |
| 1:E:221:HIS:NE2 | 6:E:823:ZP4:N1R | 2.66 | 0.44 |
| 1:E:412:PRO:O | 1:E:414:TRP:HD1 | 2.01 | 0.44 |
| 2:F:115:TYR:OH | 2:F:184:MET:O | 2.34 | 0.44 |
| 2:J:63:ILE:HD13 | 2:J:63:ILE:N | 2.32 | 0.44 |
| 1:M:94:ILE:HA | 1:M:95:PRO:HD3 | 1.87 | 0.44 |
| 1:M:132:ILE:CG1 | 1:M:142:ILE:HG13 | 2.48 | 0.44 |
| 1:M:287:LYS:HZ2 | 1:M:293:ILE:HD12 | 1.83 | 0.44 |
| 2:N:62:ALA:O | 2:N:63:ILE:HG22 | 2.17 | 0.44 |
| 2:N:379:SER:OG | 2:N:387:PRO:HD3 | 2.18 | 0.44 |
| 4:P:806:DT:C1' | 4:P:807:DC:H5" | 2.48 | 0.44 |
| 1:A:91:GLN:CG | 1:A:161:GLN:NE2 | 2.81 | 0.43 |
| 1:A:188:TYR:CD1 | 1:A:188:TYR:C | 2.92 | 0.43 |
| 1:A:457:TYR:CE2 | 1:A:465:LYS:HB3 | 2.53 | 0.43 |
| 1:E:109:LEU:CD2 | 1:E:220:LYS:CE | 2.94 | 0.43 |
| 1:E:440:PHE:N | 1:E:494:ASN:O | 2.45 | 0.43 |
| 2:F:198:HIS:O | 2:F:202:ILE:HG12 | 2.18 | 0.43 |
| 2:J:422:LEU:O | 2:J:424:LYS:O | 2.36 | 0.43 |
| 1:M:194:GLU:HB2 | 1:M:197:GLN:HG3 | 1.98 | 0.43 |
| 4:D:820:DC:H2" | 4:D:821:DC:H5' | 1.99 | 0.43 |
| 3:G:707:DG:C2' | 3:G:708:DG:H5' | 2.35 | 0.43 |
| 4:P:807:DC:H5' | 4:P:807:DC:H6 | 1.83 | 0.43 |
| 1:A:111:VAL:HG13 | 1:A:215:THR:O | 2.18 | 0.43 |
| 1:A:169:GLU:HB3 | 1:A:170:PRO:HD3 | 1.98 | 0.43 |
| 1:E:42:GLU:OE1 | 1:E:49:LYS:HG3 | 2.19 | 0.43 |
| 1:E:50:ILE:HG13 | 1:E:143:ARG:HB3 | 2.00 | 0.43 |
| 1:E:96:HIS:ND1 | 1:E:97:PRO:HD2 | 2.34 | 0.43 |
| 2:J:57:ASN:OD1 | 2:J:143:ARG:NH1 | 2.51 | 0.43 |
| 1:M:312:GLU:HA | 1:M:313:PRO:HD2 | 1.79 | 0.43 |
| 1:M:317:VAL:CG2 | 1:M:318:TYR:H | 2.25 | 0.43 |
| 1:A:27:THR:HG22 | 1:A:28:GLU:N | 2.33 | 0.43 |
| 1:A:529:GLU:HG2 | 1:A:530:LYS:HG3 | 2.00 | 0.43 |
| 1:E:325:LEU:N | 1:E:325:LEU:HD12 | 2.33 | 0.43 |
| 1:E:427:TYR:HE2 | 1:E:429:LEU:HD21 | 1.84 | 0.43 |
| 1:E:475:GLN:NE2 | 4:H:808:DC:O3' | 2.52 | 0.43 |
| 2:J:368:LEU:HD11 | 2:J:392:PRO:HD2 | 1.99 | 0.43 |
| 1:M:325:LEU:HB2 | 1:M:387:PRO:HB3 | 2.00 | 0.43 |
| 1:M:412:PRO:O | 1:M:414:TRP:HD1 | 2.02 | 0.43 |
| 1:M:448:ARG:HG2 | 1:M:448:ARG:NH1 | 2.33 | 0.43 |
| 2:N:88:TRP:CZ3 | 2:N:89:GLU:HB2 | 2.53 | 0.43 |
| 2:N:125:ARG:HB3 | 2:N:145:GLN:NE2 | 2.34 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------|--------|:---:|:---:|
| 2:N:180:ILE:HG23 | 2:N:187:LEU:HD21 | 1.99 | 0.43 |
| 3:C:707:DG:H2" | 3:C:708:DG:C5' | 2.36 | 0.43 |
| 1:A:207:GLN:NE2 | 1:A:210:LEU:HD13 | 2.33 | 0.43 |
| 1:A:342:TYR:HD2 | 1:A:344:GLU:O | 1.96 | 0.43 |
| 2:B:339:TYR:C | 2:B:340:GLN:NE2 | 2.72 | 0.43 |
| 2:B:368:LEU:HD23 | 2:B:368:LEU:C | 2.38 | 0.43 |
| 1:I:50:ILE:HG13 | 1:I:143:ARG:HB2 | 2.01 | 0.43 |
| 1:I:165:THR:HG21 | 2:J:140:PRO:CG | 2.42 | 0.43 |
| 1:I:440:PHE:N | 1:I:494:ASN:O | 2.46 | 0.43 |
| 1:M:260:LEU:HD21 | 1:M:303:LEU:HD23 | 1.99 | 0.43 |
| 1:M:339:TYR:CE2 | 1:M:352:GLY:HA3 | 2.42 | 0.43 |
| 2:N:108:VAL:O | 2:N:232:TYR:OH | 2.27 | 0.43 |
| 2:N:422:LEU:HD23 | 2:N:422:LEU:N | 2.32 | 0.43 |
| 4:L:805:DG:H2" | 4:L:806:DT:H71 | 2.00 | 0.43 |
| 2:B:23:GLN:HG3 | 2:B:24:TRP:N | 2.32 | 0.43 |
| 1:E:44:GLU:HB3 | 1:E:46:LYS:HE2 | 2.00 | 0.43 |
| 1:E:125:ARG:NH1 | 1:E:147:ASN:CB | 2.81 | 0.43 |
| 1:E:505:ILE:H | 1:E:505:ILE:HG12 | 1.53 | 0.43 |
| 1:I:434:ILE:HG21 | 1:I:492:GLU:HB3 | 2.00 | 0.43 |
| 1:I:457:TYR:CE2 | 1:I:465:LYS:HB3 | 2.54 | 0.43 |
| 2:J:31:ILE:HD12 | 2:J:135:ILE:HG12 | 2.00 | 0.43 |
| 2:J:366:LYS:HA | 2:J:405:TYR:CD2 | 2.54 | 0.43 |
| 4:H:817:MRG:H2" | 4:H:818:DC:H6 | 1.83 | 0.43 |
| 4:L:807:DC:H5' | 4:L:807:DC:H6 | 1.84 | 0.43 |
| 1:A:178:ILE:N | 1:A:178:ILE:CD1 | 2.82 | 0.43 |
| 1:A:441:TYR:CD2 | 1:A:544:GLY:CA | 2.95 | 0.43 |
| 1:E:171:PHE:CE2 | 1:E:205:LEU:HD23 | 2.54 | 0.43 |
| 1:E:380:ILE:O | 1:E:384:GLY:HA2 | 2.18 | 0.43 |
| 2:J:54:ASN:HD21 | 2:J:56:TYR:HB2 | 1.84 | 0.43 |
| 2:J:76:ASP:C | 2:J:78:ARG:H | 2.20 | 0.43 |
| 2:J:104:LYS:HD3 | 2:J:104:LYS:C | 2.38 | 0.43 |
| 2:J:125:ARG:HD3 | 2:J:147:ASN:HD22 | 1.83 | 0.43 |
| 2:J:196:GLY:O | 2:J:200:THR:HG23 | 2.18 | 0.43 |
| 2:N:57:ASN:OD1 | 2:N:143:ARG:NH1 | 2.51 | 0.43 |
| 2:N:169:GLU:N | 2:N:170:PRO:CD | 2.82 | 0.43 |
| 2:N:366:LYS:HD3 | 8:N:430:HOH:O | 2.17 | 0.43 |
| 4:D:807:DC:C2' | 4:D:808:DC:H5' | 2.40 | 0.43 |
| 4:H:806:DT:H6 | 4:H:806:DT:H5' | 1.82 | 0.43 |
| 1:A:118:VAL:HA | 1:A:119:PRO:HD3 | 1.85 | 0.43 |
| 1:A:171:PHE:CD2 | 1:A:205:LEU:HD23 | 2.54 | 0.43 |
| 2:B:279:LEU:HA | 2:B:282:LEU:HD13 | 2.01 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:375:ILE:HB | 2:B:389:PHE:CZ | 2.52 | 0.43 |
| 1:E:180:ILE:CG2 | 1:E:187:LEU:HD22 | 2.49 | 0.43 |
| 1:E:277:ARG:HG2 | 1:E:277:ARG:HH11 | 1.84 | 0.43 |
| 1:E:325:LEU:HB2 | 1:E:387:PRO:HB3 | 2.01 | 0.43 |
| 1:I:118:VAL:HB | 1:I:149:LEU:HD22 | 2.00 | 0.43 |
| 1:I:171:PHE:CG | 1:I:205:LEU:HD23 | 2.53 | 0.43 |
| 2:J:340:GLN:CG | 2:J:351:THR:HG22 | 2.47 | 0.43 |
| 1:M:325:LEU:N | 1:M:325:LEU:HD12 | 2.34 | 0.43 |
| 4:D:821:DC:H2" | 4:D:822:2DA:H5' | 1.99 | 0.43 |
| 2:B:206:ARG:HH11 | 2:B:206:ARG:HB2 | 1.82 | 0.43 |
| 2:F:188:TYR:N | 2:F:188:TYR:CD1 | 2.87 | 0.43 |
| 1:I:73:LYS:HD2 | 1:I:146:TYR:OH | 2.19 | 0.43 |
| 2:J:410:TRP:O | 2:J:411:ILE:HD13 | 2.19 | 0.43 |
| 1:M:332:GLN:HA | 1:M:332:GLN:OE1 | 2.19 | 0.43 |
| 1:A:475:GLN:HE21 | 4:D:809:DC:H5" | 1.84 | 0.43 |
| 2:B:202:ILE:O | 2:B:206:ARG:HG3 | 2.19 | 0.43 |
| 1:E:46:LYS:O | 1:E:147:ASN:HB2 | 2.18 | 0.43 |
| 1:E:208:HIS:HA | 1:E:211:ARG:CZ | 2.48 | 0.43 |
| 1:E:332:GLN:OE1 | 1:E:332:GLN:HA | 2.18 | 0.43 |
| 2:F:35:VAL:O | 2:F:39:THR:HG23 | 2.18 | 0.43 |
| 1:I:247:PRO:HB3 | 1:I:259:LYS:CE | 2.49 | 0.43 |
| 1:I:537:PRO:HB2 | 1:I:540:LYS:HB2 | 2.01 | 0.43 |
| 2:J:254:VAL:HG22 | 2:J:293:ILE:CD1 | 2.44 | 0.43 |
| 1:M:448:ARG:HG2 | 1:M:448:ARG:HH11 | 1.84 | 0.43 |
| 2:N:303:LEU:C | 2:N:303:LEU:HD23 | 2.39 | 0.43 |
| 4:L:805:DG:C2' | 4:L:806:DT:H71 | 2.49 | 0.43 |
| 4:P:816:DG:C6 | 4:P:817:MRG:C6 | 3.02 | 0.43 |
| 1:A:23:GLN:HG2 | 1:A:59:PRO:HA | 2.00 | 0.43 |
| 1:A:198:HIS:C | 1:A:200:THR:N | 2.72 | 0.43 |
| 1:E:115:TYR:C | 1:E:117:SER:H | 2.21 | 0.43 |
| 1:E:458:VAL:O | 1:E:458:VAL:HG13 | 2.18 | 0.43 |
| 2:F:112:GLY:C | 2:F:151:GLN:HE21 | 2.22 | 0.43 |
| 2:F:154:LYS:C | 2:F:157:PRO:HD2 | 2.39 | 0.43 |
| 1:I:95:PRO:HB2 | 1:I:229:TRP:CH2 | 2.54 | 0.43 |
| 1:I:332:GLN:OE1 | 1:I:332:GLN:HA | 2.18 | 0.43 |
| 1:M:5:ILE:HD12 | 1:M:6:GLU:H | 1.82 | 0.43 |
| 2:N:54:ASN:C | 2:N:54:ASN:ND2 | 2.71 | 0.43 |
| 1:A:26:LEU:HB2 | 1:A:31:ILE:HD13 | 2.01 | 0.42 |
| 1:A:417:VAL:HG13 | 1:A:417:VAL:O | 2.19 | 0.42 |
| 1:A:448:ARG:HG2 | 1:A:448:ARG:HH11 | 1.84 | 0.42 |
| 1:E:77:PHE:CD1 | 1:E:80:LEU:HD23 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:F:178:ILE:HG23 | 2:F:190:GLY:O | 2.19 | 0.42 |
| 2:F:375:ILE:HB | 2:F:389:PHE:CZ | 2.53 | 0.42 |
| 1:I:3:SER:OG | 1:I:117:SER:O | 2.33 | 0.42 |
| 1:I:420:PRO:HA | 1:I:421:PRO:C | 2.38 | 0.42 |
| 1:M:289:LEU:HD12 | 1:M:289:LEU:N | 2.32 | 0.42 |
| 1:M:435:VAL:HG22 | 2:N:290:THR:HG21 | 2.01 | 0.42 |
| 2:N:108:VAL:N | 2:N:232:TYR:OH | 2.52 | 0.42 |
| 2:F:63:ILE:HD13 | 2:F:63:ILE:N | 2.33 | 0.42 |
| 2:F:320:ASP:C | 2:F:320:ASP:OD1 | 2.58 | 0.42 |
| 2:F:389:PHE:HB3 | 2:F:391:LEU:CD2 | 2.49 | 0.42 |
| 1:I:46:LYS:N | 1:I:46:LYS:HD2 | 2.34 | 0.42 |
| 1:I:171:PHE:CD1 | 1:I:205:LEU:HD23 | 2.54 | 0.42 |
| 1:I:303:LEU:O | 1:I:303:LEU:HD22 | 2.19 | 0.42 |
| 1:M:27:THR:HG22 | 1:M:28:GLU:N | 2.35 | 0.42 |
| 1:M:132:ILE:HD11 | 1:M:142:ILE:HD11 | 2.01 | 0.42 |
| 2:N:266:TRP:C | 2:N:268:SER:H | 2.23 | 0.42 |
| 1:A:179:VAL:O | 1:A:179:VAL:HG23 | 2.19 | 0.42 |
| 2:B:425:LEU:HD23 | 2:B:425:LEU:HA | 1.76 | 0.42 |
| 1:E:171:PHE:CD1 | 1:E:205:LEU:HD23 | 2.53 | 0.42 |
| 1:E:179:VAL:O | 1:E:179:VAL:HG23 | 2.18 | 0.42 |
| 1:E:260:LEU:HD23 | 1:E:279:LEU:CD2 | 2.49 | 0.42 |
| 2:F:425:LEU:HD23 | 2:F:425:LEU:HA | 1.78 | 0.42 |
| 1:I:266:TRP:CE2 | 4:L:820:DC:H4' | 2.55 | 0.42 |
| 1:I:312:GLU:HA | 1:I:313:PRO:HD2 | 1.82 | 0.42 |
| 2:J:258:GLN:O | 2:J:259:LYS:C | 2.58 | 0.42 |
| 1:M:250:ASP:OD1 | 1:M:250:ASP:N | 2.46 | 0.42 |
| 1:M:511:ASP:OD1 | 1:M:511:ASP:C | 2.57 | 0.42 |
| 2:N:104:LYS:HD3 | 2:N:104:LYS:C | 2.38 | 0.42 |
| 3:C:717:DC:H2" | 3:C:718:DA:OP2 | 2.19 | 0.42 |
| 4:D:805:DG:H2" | 4:D:806:DT:OP2 | 2.19 | 0.42 |
| 4:D:805:DG:C2' | 4:D:806:DT:H71 | 2.48 | 0.42 |
| 1:E:244:ILE:O | 1:E:244:ILE:CG2 | 2.65 | 0.42 |
| 1:E:422:LEU:N | 1:E:422:LEU:CD2 | 2.82 | 0.42 |
| 2:F:363:ASN:HB3 | 2:F:366:LYS:HB3 | 2.00 | 0.42 |
| 1:I:57:ASN:OD1 | 1:I:58:THR:N | 2.52 | 0.42 |
| 1:I:417:VAL:HG13 | 1:I:417:VAL:O | 2.19 | 0.42 |
| 1:M:215:THR:HG22 | 1:M:216:THR:N | 2.34 | 0.42 |
| 1:M:439:THR:CG2 | 2:N:289:LEU:HD13 | 2.48 | 0.42 |
| 2:N:70:LYS:HD3 | 2:N:70:LYS:HA | 1.80 | 0.42 |
| 1:A:94:ILE:HD12 | 3:C:709:DC:H1' | 2.00 | 0.42 |
| 1:A:302:GLU:O | 1:A:303:LEU:C | 2.58 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:111:VAL:HG11 | 2:B:187:LEU:HD12 | 2.02 | 0.42 |
| 1:E:156:SER:HB2 | 1:E:157:PRO:CD | 2.49 | 0.42 |
| 1:E:465:LYS:HG3 | 1:E:466:VAL:N | 2.34 | 0.42 |
| 1:I:57:ASN:HD21 | 1:I:131:THR:CB | 2.31 | 0.42 |
| 1:I:87:PHE:N | 1:I:87:PHE:CD1 | 2.87 | 0.42 |
| 1:I:118:VAL:O | 1:I:148:VAL:HG23 | 2.20 | 0.42 |
| 1:I:171:PHE:CE2 | 1:I:205:LEU:HD23 | 2.54 | 0.42 |
| 2:J:363:ASN:ND2 | 2:J:405:TYR:OH | 2.52 | 0.42 |
| 1:M:171:PHE:CG | 1:M:205:LEU:HD23 | 2.54 | 0.42 |
| 2:N:386:THR:HG23 | 2:N:387:PRO:HD2 | 2.00 | 0.42 |
| 1:A:463:ARG:HG2 | 1:A:463:ARG:NH1 | 2.34 | 0.42 |
| 2:B:76:ASP:C | 2:B:78:ARG:H | 2.23 | 0.42 |
| 2:B:270:ILE:CD1 | 2:B:346:PHE:HD1 | 2.33 | 0.42 |
| 1:I:419:THR:HG23 | 1:I:419:THR:O | 2.20 | 0.42 |
| 1:I:548:VAL:O | 1:I:551:LEU:HB2 | 2.20 | 0.42 |
| 1:M:44:GLU:OE1 | 1:M:46:LYS:HE2 | 2.20 | 0.42 |
| 1:M:459:THR:HG21 | 1:M:463:ARG:HB2 | 2.01 | 0.42 |
| 2:N:59:PRO:HG2 | 2:N:76:ASP:HB3 | 2.02 | 0.42 |
| 2:N:183:TYR:CD2 | 2:N:380:ILE:HD13 | 2.54 | 0.42 |
| 2:N:368:LEU:HD23 | 2:N:368:LEU:C | 2.40 | 0.42 |
| 1:A:25:PRO:CD | 3:C:703:DG:N2 | 2.81 | 0.42 |
| 1:A:287:LYS:HZ2 | 1:A:293:ILE:HD12 | 1.81 | 0.42 |
| 1:A:327:ALA:CB | 1:A:341:ILE:HG13 | 2.47 | 0.42 |
| 2:F:422:LEU:O | 2:F:424:LYS:O | 2.38 | 0.42 |
| 1:I:222:GLN:O | 1:I:224:GLU:HG3 | 2.20 | 0.42 |
| 1:I:341:ILE:HD12 | 1:I:341:ILE:N | 2.34 | 0.42 |
| 2:J:111:VAL:HG11 | 2:J:187:LEU:CD1 | 2.49 | 0.42 |
| 1:M:254:VAL:HG21 | 1:M:287:LYS:HB2 | 2.02 | 0.42 |
| 2:N:62:ALA:C | 2:N:63:ILE:CG2 | 2.87 | 0.42 |
| 1:A:57:ASN:OD1 | 1:A:58:THR:N | 2.53 | 0.42 |
| 1:A:165:THR:CG2 | 2:B:140:PRO:CG | 2.97 | 0.42 |
| 1:E:529:GLU:O | 1:E:530:LYS:CG | 2.67 | 0.42 |
| 2:J:215:THR:C | 2:J:217:PRO:HD3 | 2.40 | 0.42 |
| 1:M:92:LEU:HD12 | 2:N:133:PRO:HA | 2.01 | 0.42 |
| 1:M:275:LYS:HB2 | 1:M:275:LYS:HE3 | 1.88 | 0.42 |
| 2:N:17:ASP:O | 2:N:83:ARG:NH1 | 2.53 | 0.42 |
| 4:P:819:DG:H2' | 4:P:820:DC:H6 | 1.84 | 0.42 |
| 1:A:67:ASP:O | 1:A:68:SER:HB2 | 2.19 | 0.42 |
| 2:B:80:LEU:O | 2:B:80:LEU:HD22 | 2.20 | 0.42 |
| 1:E:182:GLN:HG3 | 1:E:182:GLN:O | 2.20 | 0.42 |
| 1:E:424:LYS:NZ | 1:E:426:TRP:CZ3 | 2.87 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:529:GLU:C | 1:E:530:LYS:HG3 | 2.39 | 0.42 |
| 1:I:60:VAL:HG12 | 1:I:75:VAL:HG13 | 2.02 | 0.42 |
| 1:I:94:ILE:HD13 | 3:K:708:DG:H21 | 1.84 | 0.42 |
| 1:I:459:THR:CG2 | 1:I:463:ARG:HB2 | 2.50 | 0.42 |
| 1:I:497:THR:OG1 | 1:I:499:SER:HB3 | 2.20 | 0.42 |
| 2:J:169:GLU:N | 2:J:170:PRO:CD | 2.83 | 0.42 |
| 2:J:301:LEU:O | 2:J:305:GLU:HB2 | 2.20 | 0.42 |
| 1:M:29:GLU:HG3 | 1:M:30:LYS:N | 2.35 | 0.42 |
| 1:M:97:PRO:HG3 | 1:M:232:TYR:CD1 | 2.54 | 0.42 |
| 1:M:444:GLY:HA2 | 1:M:552:VAL:HG11 | 2.01 | 0.42 |
| 1:M:458:VAL:CG1 | 1:M:548:VAL:HG22 | 2.47 | 0.42 |
| 2:N:339:TYR:C | 2:N:340:GLN:NE2 | 2.72 | 0.42 |
| 4:H:817:MRG:H2" | 4:H:818:DC:C6 | 2.55 | 0.42 |
| 1:A:552:VAL:HG22 | 1:A:552:VAL:H | 1.65 | 0.42 |
| 2:B:118:VAL:HG12 | 2:B:119:PRO:O | 2.20 | 0.42 |
| 2:B:166:LYS:O | 2:B:167:ILE:C | 2.57 | 0.42 |
| 2:N:242:GLN:O | 2:N:242:GLN:NE2 | 2.53 | 0.42 |
| 2:N:376:THR:HB | 2:N:410:TRP:CH2 | 2.55 | 0.42 |
| 1:A:247:PRO:HB3 | 1:A:259:LYS:CE | 2.50 | 0.41 |
| 1:A:438:GLU:CD | 1:A:463:ARG:HD2 | 2.39 | 0.41 |
| 1:I:80:LEU:O | 1:I:80:LEU:HD12 | 2.20 | 0.41 |
| 1:I:194:GLU:HB2 | 1:I:197:GLN:HG3 | 2.01 | 0.41 |
| 1:I:221:HIS:NE2 | 1:I:228:LEU:HB2 | 2.35 | 0.41 |
| 1:I:422:LEU:HD22 | 1:I:422:LEU:N | 2.35 | 0.41 |
| 2:N:258:GLN:O | 2:N:259:LYS:C | 2.59 | 0.41 |
| 2:N:382:ILE:HB | 2:N:383:TRP:CE3 | 2.55 | 0.41 |
| 2:B:366:LYS:HA | 2:B:405:TYR:CD2 | 2.55 | 0.41 |
| 2:B:376:THR:HB | 2:B:410:TRP:CH2 | 2.55 | 0.41 |
| 1:E:32:LYS:O | 1:E:35:VAL:CG2 | 2.69 | 0.41 |
| 2:F:216:THR:HG22 | 2:F:216:THR:O | 2.18 | 0.41 |
| 2:F:339:TYR:O | 2:F:340:GLN:NE2 | 2.53 | 0.41 |
| 2:J:49:LYS:HG2 | 2:J:144:TYR:CE1 | 2.54 | 0.41 |
| 1:M:188:TYR:O | 1:M:188:TYR:HD1 | 2.02 | 0.41 |
| 1:M:277:ARG:HB2 | 1:M:336:GLN:CD | 2.41 | 0.41 |
| 2:N:125:ARG:HD3 | 2:N:147:ASN:HD22 | 1.84 | 0.41 |
| 4:P:808:DC:H1' | 4:P:809:DC:H5' | 2.02 | 0.41 |
| 2:B:266:TRP:C | 2:B:268:SER:H | 2.24 | 0.41 |
| 1:E:87:PHE:CD1 | 1:E:87:PHE:N | 2.87 | 0.41 |
| 1:E:537:PRO:HB3 | 1:E:540:LYS:HB2 | 1.92 | 0.41 |
| 2:F:170:PRO:HG2 | 2:F:208:HIS:NE2 | 2.35 | 0.41 |
| 1:I:182:GLN:O | 1:I:182:GLN:HG3 | 2.19 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:J:339:TYR:C | 2:J:340:GLN:NE2 | 2.73 | 0.41 |
| 2:J:363:ASN:HB3 | 2:J:366:LYS:HB3 | 2.01 | 0.41 |
| 1:M:260:LEU:HD23 | 1:M:279:LEU:HD22 | 2.02 | 0.41 |
| 1:M:422:LEU:HD22 | 1:M:422:LEU:N | 2.35 | 0.41 |
| 1:M:441:TYR:HA | 1:M:496:VAL:HG22 | 2.01 | 0.41 |
| 2:N:254:VAL:HG22 | 2:N:293:ILE:CD1 | 2.41 | 0.41 |
| 4:D:810:DT:H2" | 4:D:811:DG:C8 | 2.54 | 0.41 |
| 4:P:804:DA:H2" | 4:P:805:DG:OP2 | 2.20 | 0.41 |
| 1:A:31:ILE:HG12 | 1:A:31:ILE:H | 1.65 | 0.41 |
| 1:A:217:PRO:C | 1:A:219:LYS:H | 2.23 | 0.41 |
| 1:A:270:ILE:HG13 | 1:A:314:VAL:HG21 | 2.02 | 0.41 |
| 2:B:178:ILE:HG22 | 2:B:179:VAL:N | 2.35 | 0.41 |
| 2:B:184:MET:HB3 | 2:B:185:ASP:H | 1.47 | 0.41 |
| 2:B:198:HIS:O | 2:B:202:ILE:HG12 | 2.20 | 0.41 |
| 2:B:328:GLU:O | 2:B:339:TYR:HA | 2.21 | 0.41 |
| 1:E:75:VAL:HG11 | 1:E:77:PHE:CZ | 2.55 | 0.41 |
| 1:E:188:TYR:CD1 | 1:E:188:TYR:O | 2.73 | 0.41 |
| 2:F:13:LYS:HE3 | 2:F:86:ASP:N | 2.33 | 0.41 |
| 2:F:386:THR:HG23 | 2:F:387:PRO:HD2 | 2.02 | 0.41 |
| 2:J:302:GLU:HA | 2:J:305:GLU:CB | 2.49 | 0.41 |
| 1:M:115:TYR:CZ | 6:M:823:ZP4:H2'A | 2.56 | 0.41 |
| 2:N:170:PRO:HG2 | 2:N:208:HIS:NE2 | 2.35 | 0.41 |
| 1:A:215:THR:CG2 | 1:A:216:THR:N | 2.83 | 0.41 |
| 2:B:13:LYS:HB2 | 2:B:16:MET:CG | 2.45 | 0.41 |
| 2:B:186:ASP:HB3 | 2:B:188:TYR:CE1 | 2.55 | 0.41 |
| 1:E:17:ASP:O | 1:E:83:ARG:HD3 | 2.20 | 0.41 |
| 1:E:344:GLU:HB3 | 1:E:345:PRO:HD3 | 2.02 | 0.41 |
| 2:F:111:VAL:HG11 | 2:F:187:LEU:HD12 | 2.03 | 0.41 |
| 2:F:422:LEU:HD23 | 2:F:422:LEU:N | 2.35 | 0.41 |
| 1:I:255:ASN:HB3 | 8:I:558:HOH:O | 2.20 | 0.41 |
| 6:I:823:ZP4:O21 | 8:I:564:HOH:O | 2.22 | 0.41 |
| 2:J:59:PRO:HG2 | 2:J:76:ASP:HB3 | 2.03 | 0.41 |
| 2:J:198:HIS:O | 2:J:202:ILE:HG12 | 2.20 | 0.41 |
| 3:O:708:DG:H2' | 3:O:709:DC:H6 | 1.81 | 0.41 |
| 1:A:505:ILE:H | 1:A:505:ILE:HG12 | 1.56 | 0.41 |
| 2:B:125:ARG:HB3 | 2:B:145:GLN:HE21 | 1.86 | 0.41 |
| 2:B:270:ILE:HD11 | 2:B:346:PHE:HD1 | 1.84 | 0.41 |
| 1:E:419:THR:O | 1:E:419:THR:HG23 | 2.21 | 0.41 |
| 2:F:118:VAL:HG12 | 2:F:119:PRO:N | 2.35 | 0.41 |
| 2:F:178:ILE:HG22 | 2:F:179:VAL:N | 2.35 | 0.41 |
| 2:F:205:LEU:HD23 | 2:F:205:LEU:O | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:115:TYR:C | 1:M:117:SER:H | 2.23 | 0.41 |
| 2:N:302:GLU:HA | 2:N:305:GLU:HB3 | 2.02 | 0.41 |
| 3:C:705:DA:C2' | 3:C:706:DT:H5' | 2.40 | 0.41 |
| 1:A:81:ASN:HA | 1:A:84:THR:HG22 | 2.02 | 0.41 |
| 1:A:529:GLU:C | 1:A:530:LYS:HG3 | 2.40 | 0.41 |
| 2:B:164:MET:O | 2:B:165:THR:C | 2.57 | 0.41 |
| 1:E:116:PHE:HA | 1:E:148:VAL:CG2 | 2.50 | 0.41 |
| 1:E:221:HIS:NE2 | 1:E:228:LEU:HB2 | 2.36 | 0.41 |
| 1:E:278:GLN:HB2 | 1:E:302:GLU:OE1 | 2.20 | 0.41 |
| 1:E:451:LYS:HD3 | 1:E:451:LYS:HA | 1.85 | 0.41 |
| 2:F:80:LEU:O | 2:F:80:LEU:HD13 | 2.20 | 0.41 |
| 2:F:183:TYR:CD2 | 2:F:380:ILE:HD13 | 2.56 | 0.41 |
| 1:I:23:GLN:HG2 | 1:I:59:PRO:HA | 2.02 | 0.41 |
| 2:J:302:GLU:HA | 2:J:305:GLU:HB3 | 2.02 | 0.41 |
| 2:J:393:ILE:HD13 | 2:J:398:TRP:HB2 | 2.02 | 0.41 |
| 4:H:821:DC:H2" | 4:H:822:2DA:C5' | 2.50 | 0.41 |
| 1:A:171:PHE:CE2 | 1:A:205:LEU:HD23 | 2.55 | 0.41 |
| 2:B:8:VAL:O | 2:B:8:VAL:HG23 | 2.20 | 0.41 |
| 2:B:13:LYS:HE3 | 2:B:86:ASP:N | 2.36 | 0.41 |
| 1:E:543:GLY:O | 1:E:547:GLN:NE2 | 2.53 | 0.41 |
| 2:F:49:LYS:HG2 | 2:F:144:TYR:CE1 | 2.55 | 0.41 |
| 2:F:266:TRP:C | 2:F:268:SER:N | 2.73 | 0.41 |
| 1:I:202:ILE:HD12 | 1:I:202:ILE:HA | 1.66 | 0.41 |
| 1:I:255:ASN:HB2 | 1:I:289:LEU:HB3 | 2.03 | 0.41 |
| 1:I:478:GLU:HG2 | 1:I:499:SER:HB2 | 2.01 | 0.41 |
| 1:M:180:ILE:CG2 | 1:M:187:LEU:HD22 | 2.51 | 0.41 |
| 1:M:330:GLN:HE21 | 1:M:330:GLN:HB2 | 1.74 | 0.41 |
| 1:M:417:VAL:O | 1:M:417:VAL:HG13 | 2.20 | 0.41 |
| 1:M:529:GLU:C | 1:M:530:LYS:HG3 | 2.40 | 0.41 |
| 2:N:11:LYS:H | 2:N:11:LYS:HG2 | 1.61 | 0.41 |
| 2:N:257:ILE:O | 2:N:261:VAL:HG23 | 2.21 | 0.41 |
| 2:N:307:ARG:HG2 | 2:N:311:LYS:NZ | 2.36 | 0.41 |
| 4:D:808:DC:H1' | 4:D:809:DC:H5' | 2.03 | 0.41 |
| 1:A:130:PHE:N | 1:A:130:PHE:CD1 | 2.89 | 0.41 |
| 1:A:188:TYR:O | 1:A:188:TYR:HD1 | 2.04 | 0.41 |
| 1:A:493:VAL:CG1 | 1:A:494:ASN:N | 2.84 | 0.41 |
| 2:B:216:THR:O | 2:B:216:THR:HG22 | 2.21 | 0.41 |
| 2:B:303:LEU:HD23 | 2:B:303:LEU:C | 2.41 | 0.41 |
| 1:E:198:HIS:C | 1:E:200:THR:N | 2.74 | 0.41 |
| 2:F:84:THR:O | 2:F:87:PHE:HB3 | 2.21 | 0.41 |
| 1:I:178:ILE:N | 1:I:178:ILE:CD1 | 2.83 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:302:GLU:O | 1:I:303:LEU:C | 2.59 | 0.41 |
| 1:I:511:ASP:OD1 | 1:I:511:ASP:C | 2.59 | 0.41 |
| 1:I:513:SER:OG | 1:I:514:GLU:N | 2.54 | 0.41 |
| 2:J:16:MET:SD | 2:J:83:ARG:HB3 | 2.61 | 0.41 |
| 1:M:91:GLN:CG | 1:M:161:GLN:NE2 | 2.84 | 0.41 |
| 1:M:132:ILE:HD11 | 1:M:144:TYR:HE2 | 1.86 | 0.41 |
| 1:M:136:ASN:OD1 | 1:M:138:GLU:HB3 | 2.20 | 0.41 |
| 1:M:171:PHE:CZ | 1:M:205:LEU:HD23 | 2.56 | 0.41 |
| 1:M:281:LYS:CG | 1:M:284:ARG:NH1 | 2.84 | 0.41 |
| 1:M:286:THR:HG1 | 3:O:714:DG:H4' | 1.84 | 0.41 |
| 1:M:510:PRO:O | 1:M:522:ILE:HD12 | 2.20 | 0.41 |
| 2:N:62:ALA:O | 2:N:63:ILE:CG2 | 2.68 | 0.41 |
| 2:N:266:TRP:C | 2:N:268:SER:N | 2.74 | 0.41 |
| 3:G:723:DC:H2" | 3:G:724:DT:OP2 | 2.19 | 0.41 |
| 1:A:310:LEU:N | 1:A:310:LEU:HD12 | 2.36 | 0.41 |
| 2:B:60:VAL:HG11 | 2:B:130:PHE:CD2 | 2.55 | 0.41 |
| 1:E:344:GLU:O | 1:E:345:PRO:C | 2.59 | 0.41 |
| 2:F:134:SER:CB | 2:F:139:THR:HG23 | 2.51 | 0.41 |
| 1:I:278:GLN:HB2 | 1:I:302:GLU:CD | 2.42 | 0.41 |
| 8:I:562:HOH:O | 2:J:50:ILE:C | 2.58 | 0.41 |
| 2:J:212:TRP:CD1 | 2:J:212:TRP:N | 2.89 | 0.41 |
| 2:J:266:TRP:O | 2:J:269:GLN:HG3 | 2.21 | 0.41 |
| 2:J:350:LYS:HG2 | 2:J:351:THR:N | 2.36 | 0.41 |
| 2:N:198:HIS:O | 2:N:202:ILE:HG12 | 2.21 | 0.41 |
| 2:N:274:ILE:HD11 | 2:N:309:ILE:HB | 2.03 | 0.41 |
| 2:B:266:TRP:C | 2:B:268:SER:N | 2.73 | 0.40 |
| 1:E:358:ARG:NH1 | 2:F:396:GLU:OE2 | 2.55 | 0.40 |
| 1:E:427:TYR:CE2 | 1:E:429:LEU:HD21 | 2.56 | 0.40 |
| 1:I:221:HIS:HB3 | 1:I:227:PHE:CD1 | 2.56 | 0.40 |
| 1:I:522:ILE:HG12 | 1:I:522:ILE:H | 1.76 | 0.40 |
| 2:J:125:ARG:HB3 | 2:J:145:GLN:NE2 | 2.35 | 0.40 |
| 1:M:221:HIS:HB3 | 1:M:227:PHE:HD1 | 1.86 | 0.40 |
| 1:M:247:PRO:HB3 | 1:M:259:LYS:CE | 2.51 | 0.40 |
| 2:N:96:HIS:HA | 2:N:97:PRO:HD2 | 1.98 | 0.40 |
| 2:N:187:LEU:HD23 | 2:N:187:LEU:C | 2.42 | 0.40 |
| 2:N:293:ILE:HG23 | 2:N:294:PRO:HD2 | 2.03 | 0.40 |
| 1:A:132:ILE:CD1 | 1:A:144:TYR:HE2 | 2.34 | 0.40 |
| 2:B:263:LYS:HA | 2:B:423:VAL:HG11 | 2.00 | 0.40 |
| 1:E:56:TYR:O | 1:E:57:ASN:HB2 | 2.21 | 0.40 |
| 2:F:254:VAL:HG22 | 2:F:293:ILE:CD1 | 2.45 | 0.40 |
| 1:I:130:PHE:CE1 | 1:I:144:TYR:HB2 | 2.56 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:198:HIS:C | 1:I:200:THR:N | 2.73 | 0.40 |
| 2:J:283:LEU:O | 2:J:284:ARG:C | 2.60 | 0.40 |
| 1:M:282:LEU:HD21 | 1:M:296:THR:HG22 | 2.04 | 0.40 |
| 2:N:363:ASN:HB3 | 2:N:366:LYS:HB3 | 2.02 | 0.40 |
| 3:G:705:DA:C2' | 3:G:706:DT:H5' | 2.40 | 0.40 |
| 1:A:194:GLU:HB2 | 1:A:197:GLN:HG3 | 2.04 | 0.40 |
| 1:A:533:LEU:N | 1:A:533:LEU:HD12 | 2.36 | 0.40 |
| 2:B:215:THR:C | 2:B:217:PRO:HD3 | 2.42 | 0.40 |
| 1:E:171:PHE:CE1 | 1:E:205:LEU:HD23 | 2.56 | 0.40 |
| 1:E:202:ILE:HA | 1:E:202:ILE:HD12 | 1.81 | 0.40 |
| 1:M:171:PHE:CD1 | 1:M:205:LEU:HD23 | 2.56 | 0.40 |
| 1:M:420:PRO:HA | 1:M:421:PRO:C | 2.41 | 0.40 |
| 1:M:491:LEU:N | 1:M:491:LEU:CD1 | 2.83 | 0.40 |
| 2:B:155:GLY:C | 2:B:157:PRO:HD2 | 2.42 | 0.40 |
| 1:I:19:PRO:HD3 | 1:I:80:LEU:HD13 | 2.03 | 0.40 |
| 1:I:278:GLN:HB2 | 1:I:302:GLU:OE1 | 2.21 | 0.40 |
| 1:I:317:VAL:CG2 | 1:I:318:TYR:H | 2.28 | 0.40 |
| 1:I:463:ARG:HG2 | 1:I:463:ARG:HH11 | 1.86 | 0.40 |
| 2:J:54:ASN:O | 2:J:143:ARG:NH2 | 2.54 | 0.40 |
| 2:J:154:LYS:C | 2:J:157:PRO:HD2 | 2.41 | 0.40 |
| 2:J:368:LEU:HD23 | 2:J:368:LEU:C | 2.41 | 0.40 |
| 2:J:417:VAL:HG22 | 2:J:419:THR:HG23 | 2.03 | 0.40 |
| 1:M:72:ARG:CG | 1:M:151:GLN:HE22 | 2.34 | 0.40 |
| 1:M:165:THR:HG21 | 2:N:140:PRO:HG2 | 2.03 | 0.40 |
| 2:N:62:ALA:C | 2:N:63:ILE:HG23 | 2.40 | 0.40 |
| 1:A:25:PRO:CG | 3:C:703:DG:H22 | 2.35 | 0.40 |
| 1:A:118:VAL:O | 1:A:148:VAL:HG23 | 2.21 | 0.40 |
| 1:A:173:LYS:O | 1:A:176:PRO:HD3 | 2.22 | 0.40 |
| 1:A:247:PRO:O | 1:A:252:TRP:HH2 | 2.04 | 0.40 |
| 1:A:427:TYR:HE2 | 1:A:429:LEU:HD21 | 1.87 | 0.40 |
| 1:A:432:GLU:CG | 1:A:433:PRO:HD2 | 2.49 | 0.40 |
| 2:B:34:LEU:HD12 | 2:B:34:LEU:HA | 1.94 | 0.40 |
| 1:E:115:TYR:HE1 | 1:E:184:MET:HE1 | 1.85 | 0.40 |
| 1:E:173:LYS:O | 1:E:176:PRO:HD3 | 2.22 | 0.40 |
| 1:E:199:ARG:O | 1:E:203:GLU:HG3 | 2.22 | 0.40 |
| 1:E:266:TRP:CE2 | 4:H:820:DC:H4' | 2.56 | 0.40 |
| 1:E:317:VAL:CG2 | 1:E:318:TYR:N | 2.71 | 0.40 |
| 1:E:325:LEU:HD13 | 1:E:385:LYS:HE2 | 2.03 | 0.40 |
| 1:I:459:THR:OG1 | 1:I:463:ARG:HB2 | 2.20 | 0.40 |
| 2:J:134:SER:CB | 2:J:139:THR:HG23 | 2.52 | 0.40 |
| 2:J:263:LYS:HE3 | 2:J:263:LYS:HB2 | 1.86 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:202:ILE:HA | 1:M:202:ILE:HD12 | 1.87 | 0.40 |
| 1:M:221:HIS:NE2 | 1:M:228:LEU:HB2 | 2.37 | 0.40 |
| 4:H:818:DC:H2' | 4:H:819:DG:C8 | 2.56 | 0.40 |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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 | 551/557 (99%) | 487 (88%) | 55 (10%) | 9 (2%) | 9 | 40 |
| 1 | E | 551/557 (99%) | 491 (89%) | 56 (10%) | 4 (1%) | 22 | 59 |
| 1 | I | 551/557 (99%) | 486 (88%) | 60 (11%) | 5 (1%) | 17 | 53 |
| 1 | M | 551/557 (99%) | 494 (90%) | 51 (9%) | 6 (1%) | 14 | 48 |
| 2 | B | 409/444 (92%) | 367 (90%) | 42 (10%) | 0 | 100 | 100 |
| 2 | F | 409/444 (92%) | 363 (89%) | 45 (11%) | 1 (0%) | 47 | 78 |
| 2 | J | 409/444 (92%) | 366 (90%) | 42 (10%) | 1 (0%) | 47 | 78 |
| 2 | N | 409/444 (92%) | 364 (89%) | 43 (10%) | 2 (0%) | 29 | 65 |
| All | All | 3840/4004 (96%) | 3418 (89%) | 394 (10%) | 28 (1%) | 22 | 59 |

All (28) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 542 | ILE |
| 1 | A | 199 | ARG |
| 1 | E | 199 | ARG |
| 1 | E | 537 | PRO |
| 2 | J | 6 | GLU |
| 1 | M | 199 | ARG |
| 1 | I | 199 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | N | 4 | PRO |
| 1 | A | 546 | GLU |
| 1 | I | 463 | ARG |
| 1 | M | 345 | PRO |
| 1 | A | 345 | PRO |
| 1 | A | 350 | LYS |
| 1 | A | 458 | VAL |
| 1 | I | 458 | VAL |
| 1 | M | 243 | PRO |
| 1 | M | 549 | ASP |
| 1 | A | 284 | ARG |
| 1 | A | 463 | ARG |
| 1 | E | 458 | VAL |
| 2 | F | 286 | THR |
| 1 | I | 285 | GLY |
| 2 | N | 18 | GLY |
| 1 | E | 243 | PRO |
| 1 | I | 505 | ILE |
| 1 | A | 243 | PRO |
| 1 | M | 505 | ILE |
| 1 | M | 542 | ILE |

### 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 | 494/497 (99%) | 467 (94%) | 27 (6%) | 21 | 54 |
| 1 | E | 494/497 (99%) | 466 (94%) | 28 (6%) | 20 | 53 |
| 1 | I | 494/497 (99%) | 462 (94%) | 32 (6%) | 17 | 48 |
| 1 | M | 494/497 (99%) | 466 (94%) | 28 (6%) | 20 | 53 |
| 2 | B | 375/403 (93%) | 354 (94%) | 21 (6%) | 21 | 53 |
| 2 | F | 375/403 (93%) | 355 (95%) | 20 (5%) | 22 | 55 |
| 2 | J | 375/403 (93%) | 358 (96%) | 17 (4%) | 27 | 61 |
| 2 | N | 375/403 (93%) | 356 (95%) | 19 (5%) | 24 | 56 |

*Continued on next page...*

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|-----|-------|----------|-----------|----------|-------------|
| All | All | 3476/3600 (97%) | 3284 (94%) | 192 (6%) | 21 54 |

All (192) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 2 | ILE |
| 1 | A | 5 | ILE |
| 1 | A | 23 | GLN |
| 1 | A | 102 | LYS |
| 1 | A | 108 | VAL |
| 1 | A | 109 | LEU |
| 1 | A | 110 | ASP |
| 1 | A | 137 | ASN |
| 1 | A | 149 | LEU |
| 1 | A | 188 | TYR |
| 1 | A | 220 | LYS |
| 1 | A | 225 | PRO |
| 1 | A | 279 | LEU |
| 1 | A | 305 | GLU |
| 1 | A | 324 | ASP |
| 1 | A | 329 | ILE |
| 1 | A | 330 | GLN |
| 1 | A | 332 | GLN |
| 1 | A | 349 | LEU |
| 1 | A | 386 | THR |
| 1 | A | 387 | PRO |
| 1 | A | 419 | THR |
| 1 | A | 432 | GLU |
| 1 | A | 448 | ARG |
| 1 | A | 475 | GLN |
| 1 | A | 505 | ILE |
| 1 | A | 548 | VAL |
| 2 | B | 24 | TRP |
| 2 | B | 54 | ASN |
| 2 | B | 63 | ILE |
| 2 | B | 83 | ARG |
| 2 | B | 120 | LEU |
| 2 | B | 139 | THR |
| 2 | B | 150 | PRO |
| 2 | B | 232 | TYR |
| 2 | B | 248 | GLU |
| 2 | B | 253 | THR |

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 271 | TYR |
| 2 | B | 296 | THR |
| 2 | B | 298 | GLU |
| 2 | B | 315 | HIS |
| 2 | B | 356 | ARG |
| 2 | B | 357 | MET |
| 2 | B | 375 | ILE |
| 2 | B | 410 | TRP |
| 2 | B | 414 | TRP |
| 2 | B | 422 | LEU |
| 2 | B | 426 | TRP |
| 1 | E | 2 | ILE |
| 1 | E | 5 | ILE |
| 1 | E | 23 | GLN |
| 1 | E | 67 | ASP |
| 1 | E | 86 | ASP |
| 1 | E | 102 | LYS |
| 1 | E | 108 | VAL |
| 1 | E | 137 | ASN |
| 1 | E | 142 | ILE |
| 1 | E | 149 | LEU |
| 1 | E | 220 | LYS |
| 1 | E | 225 | PRO |
| 1 | E | 238 | LYS |
| 1 | E | 279 | LEU |
| 1 | E | 305 | GLU |
| 1 | E | 324 | ASP |
| 1 | E | 325 | LEU |
| 1 | E | 329 | ILE |
| 1 | E | 330 | GLN |
| 1 | E | 332 | GLN |
| 1 | E | 386 | THR |
| 1 | E | 387 | PRO |
| 1 | E | 419 | THR |
| 1 | E | 432 | GLU |
| 1 | E | 448 | ARG |
| 1 | E | 475 | GLN |
| 1 | E | 505 | ILE |
| 1 | E | 548 | VAL |
| 2 | F | 24 | TRP |
| 2 | F | 54 | ASN |
| 2 | F | 63 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | F | 83 | ARG |
| 2 | F | 120 | LEU |
| 2 | F | 139 | THR |
| 2 | F | 157 | PRO |
| 2 | F | 248 | GLU |
| 2 | F | 253 | THR |
| 2 | F | 271 | TYR |
| 2 | F | 296 | THR |
| 2 | F | 298 | GLU |
| 2 | F | 356 | ARG |
| 2 | F | 357 | MET |
| 2 | F | 375 | ILE |
| 2 | F | 392 | PRO |
| 2 | F | 410 | TRP |
| 2 | F | 414 | TRP |
| 2 | F | 422 | LEU |
| 2 | F | 426 | TRP |
| 1 | I | 5 | ILE |
| 1 | I | 23 | GLN |
| 1 | I | 67 | ASP |
| 1 | I | 70 | LYS |
| 1 | I | 86 | ASP |
| 1 | I | 102 | LYS |
| 1 | I | 108 | VAL |
| 1 | I | 110 | ASP |
| 1 | I | 137 | ASN |
| 1 | I | 149 | LEU |
| 1 | I | 188 | TYR |
| 1 | I | 202 | ILE |
| 1 | I | 215 | THR |
| 1 | I | 220 | LYS |
| 1 | I | 238 | LYS |
| 1 | I | 244 | ILE |
| 1 | I | 258 | CYS |
| 1 | I | 301 | LEU |
| 1 | I | 305 | GLU |
| 1 | I | 324 | ASP |
| 1 | I | 329 | ILE |
| 1 | I | 330 | GLN |
| 1 | I | 332 | GLN |
| 1 | I | 379 | SER |
| 1 | I | 386 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | I | 387 | PRO |
| 1 | I | 419 | THR |
| 1 | I | 432 | GLU |
| 1 | I | 448 | ARG |
| 1 | I | 475 | GLN |
| 1 | I | 505 | ILE |
| 1 | I | 548 | VAL |
| 2 | J | 5 | ILE |
| 2 | J | 24 | TRP |
| 2 | J | 54 | ASN |
| 2 | J | 63 | ILE |
| 2 | J | 83 | ARG |
| 2 | J | 120 | LEU |
| 2 | J | 139 | THR |
| 2 | J | 248 | GLU |
| 2 | J | 271 | TYR |
| 2 | J | 296 | THR |
| 2 | J | 298 | GLU |
| 2 | J | 315 | HIS |
| 2 | J | 356 | ARG |
| 2 | J | 410 | TRP |
| 2 | J | 414 | TRP |
| 2 | J | 422 | LEU |
| 2 | J | 426 | TRP |
| 1 | M | 2 | ILE |
| 1 | M | 5 | ILE |
| 1 | M | 23 | GLN |
| 1 | M | 67 | ASP |
| 1 | M | 102 | LYS |
| 1 | M | 108 | VAL |
| 1 | M | 110 | ASP |
| 1 | M | 137 | ASN |
| 1 | M | 149 | LEU |
| 1 | M | 188 | TYR |
| 1 | M | 220 | LYS |
| 1 | M | 225 | PRO |
| 1 | M | 244 | ILE |
| 1 | M | 279 | LEU |
| 1 | M | 284 | ARG |
| 1 | M | 305 | GLU |
| 1 | M | 324 | ASP |
| 1 | M | 329 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | M | 330 | GLN |
| 1 | M | 332 | GLN |
| 1 | M | 386 | THR |
| 1 | M | 419 | THR |
| 1 | M | 432 | GLU |
| 1 | M | 448 | ARG |
| 1 | M | 475 | GLN |
| 1 | M | 505 | ILE |
| 1 | M | 512 | LYS |
| 1 | M | 548 | VAL |
| 2 | N | 24 | TRP |
| 2 | N | 54 | ASN |
| 2 | N | 63 | ILE |
| 2 | N | 64 | LYS |
| 2 | N | 66 | LYS |
| 2 | N | 83 | ARG |
| 2 | N | 120 | LEU |
| 2 | N | 139 | THR |
| 2 | N | 248 | GLU |
| 2 | N | 253 | THR |
| 2 | N | 271 | TYR |
| 2 | N | 296 | THR |
| 2 | N | 298 | GLU |
| 2 | N | 356 | ARG |
| 2 | N | 357 | MET |
| 2 | N | 410 | TRP |
| 2 | N | 414 | TRP |
| 2 | N | 422 | LEU |
| 2 | N | 426 | TRP |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (115) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 23 | GLN |
| 1 | A | 57 | ASN |
| 1 | A | 91 | GLN |
| 1 | A | 137 | ASN |
| 1 | A | 161 | GLN |
| 1 | A | 174 | GLN |
| 1 | A | 182 | GLN |
| 1 | A | 207 | GLN |
| 1 | A | 222 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 330 | GLN |
| 1 | A | 373 | GLN |
| 1 | A | 407 | GLN |
| 1 | A | 428 | GLN |
| 1 | A | 447 | ASN |
| 1 | A | 475 | GLN |
| 1 | A | 500 | GLN |
| 1 | A | 509 | GLN |
| 1 | A | 524 | GLN |
| 2 | B | 54 | ASN |
| 2 | B | 147 | ASN |
| 2 | B | 151 | GLN |
| 2 | B | 161 | GLN |
| 2 | B | 175 | ASN |
| 2 | B | 182 | GLN |
| 2 | B | 207 | GLN |
| 2 | B | 242 | GLN |
| 2 | B | 269 | GLN |
| 2 | B | 332 | GLN |
| 2 | B | 336 | GLN |
| 2 | B | 363 | ASN |
| 1 | E | 23 | GLN |
| 1 | E | 57 | ASN |
| 1 | E | 91 | GLN |
| 1 | E | 137 | ASN |
| 1 | E | 161 | GLN |
| 1 | E | 182 | GLN |
| 1 | E | 207 | GLN |
| 1 | E | 222 | GLN |
| 1 | E | 330 | GLN |
| 1 | E | 367 | GLN |
| 1 | E | 407 | GLN |
| 1 | E | 428 | GLN |
| 1 | E | 447 | ASN |
| 1 | E | 475 | GLN |
| 1 | E | 500 | GLN |
| 1 | E | 509 | GLN |
| 1 | E | 520 | GLN |
| 1 | E | 524 | GLN |
| 1 | E | 547 | GLN |
| 2 | F | 54 | ASN |
| 2 | F | 147 | ASN |

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | F | 151 | GLN |
| 2 | F | 161 | GLN |
| 2 | F | 175 | ASN |
| 2 | F | 182 | GLN |
| 2 | F | 207 | GLN |
| 2 | F | 242 | GLN |
| 2 | F | 269 | GLN |
| 2 | F | 332 | GLN |
| 2 | F | 336 | GLN |
| 2 | F | 363 | ASN |
| 1 | I | 57 | ASN |
| 1 | I | 91 | GLN |
| 1 | I | 137 | ASN |
| 1 | I | 151 | GLN |
| 1 | I | 182 | GLN |
| 1 | I | 207 | GLN |
| 1 | I | 222 | GLN |
| 1 | I | 269 | GLN |
| 1 | I | 330 | GLN |
| 1 | I | 367 | GLN |
| 1 | I | 373 | GLN |
| 1 | I | 407 | GLN |
| 1 | I | 428 | GLN |
| 1 | I | 447 | ASN |
| 1 | I | 475 | GLN |
| 1 | I | 500 | GLN |
| 1 | I | 509 | GLN |
| 2 | J | 54 | ASN |
| 2 | J | 151 | GLN |
| 2 | J | 161 | GLN |
| 2 | J | 175 | ASN |
| 2 | J | 182 | GLN |
| 2 | J | 207 | GLN |
| 2 | J | 242 | GLN |
| 2 | J | 332 | GLN |
| 2 | J | 336 | GLN |
| 2 | J | 363 | ASN |
| 1 | M | 57 | ASN |
| 1 | M | 91 | GLN |
| 1 | M | 137 | ASN |
| 1 | M | 151 | GLN |
| 1 | M | 161 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | M | 182 | GLN |
| 1 | M | 207 | GLN |
| 1 | M | 222 | GLN |
| 1 | M | 330 | GLN |
| 1 | M | 367 | GLN |
| 1 | M | 373 | GLN |
| 1 | M | 407 | GLN |
| 1 | M | 428 | GLN |
| 1 | M | 447 | ASN |
| 1 | M | 475 | GLN |
| 1 | M | 509 | GLN |
| 1 | M | 520 | GLN |
| 1 | M | 524 | GLN |
| 2 | N | 54 | ASN |
| 2 | N | 151 | GLN |
| 2 | N | 161 | GLN |
| 2 | N | 175 | ASN |
| 2 | N | 207 | GLN |
| 2 | N | 242 | GLN |
| 2 | N | 332 | GLN |
| 2 | N | 336 | GLN |
| 2 | N | 363 | ASN |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues 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 | #$|Z| > 2$ |
| 4 | 2DA | H | 822 | 4,3 | 17,22,23 | 0.81 | 0 | 13,31,34 | 1.12 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------|------|----------|--------|------|----------|
| | | | | | Counts | RMSZ | #\|Z\| > 2 | Counts | RMSZ | #\|Z\| > 2 |
| 4 | 2DA | L | 822 | 4,3 | 17,22,23 | 0.69 | 0 | 13,31,34 | 1.12 | 2 (15%) |
| 4 | MRG | P | 817 | 4,1,3 | 21,28,29 | 1.54 | 3 (14%) | 19,39,42 | 3.25 | 4 (21%) |
| 4 | MRG | D | 817 | 4,1,3 | 21,28,29 | 1.91 | 4 (19%) | 19,39,42 | 3.21 | 4 (21%) |
| 4 | MRG | L | 817 | 4,1,3 | 21,28,29 | 1.63 | 3 (14%) | 19,39,42 | 3.24 | 5 (26%) |
| 4 | 2DA | D | 822 | 4,3 | 17,22,23 | 0.80 | 0 | 13,31,34 | 0.97 | 1 (7%) |
| 4 | MRG | H | 817 | 4,1,3 | 21,28,29 | 1.68 | 4 (19%) | 19,39,42 | 3.46 | 5 (26%) |
| 4 | 2DA | P | 822 | 4,3 | 17,22,23 | 0.61 | 0 | 13,31,34 | 1.10 | 1 (7%) |

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 |
|-----|------|-------|-----|------|---------|----------|-------|
| 4 | 2DA | H | 822 | 4,3 | - | 0/3/18/19 | 0/3/3/3 |
| 4 | 2DA | L | 822 | 4,3 | - | 0/3/18/19 | 0/3/3/3 |
| 4 | MRG | P | 817 | 4,1,3 | - | 3/8/26/27 | 0/3/3/3 |
| 4 | MRG | D | 817 | 4,1,3 | - | 3/8/26/27 | 0/3/3/3 |
| 4 | MRG | L | 817 | 4,1,3 | - | 2/8/26/27 | 0/3/3/3 |
| 4 | 2DA | D | 822 | 4,3 | - | 0/3/18/19 | 0/3/3/3 |
| 4 | MRG | H | 817 | 4,1,3 | - | 3/8/26/27 | 0/3/3/3 |
| 4 | 2DA | P | 822 | 4,3 | - | 0/3/18/19 | 0/3/3/3 |

All (14) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 4 | D | 817 | MRG | C21-N2 | -5.70 | 1.33 | 1.46 |
| 4 | L | 817 | MRG | C21-N2 | -5.32 | 1.34 | 1.46 |
| 4 | H | 817 | MRG | C21-N2 | -4.97 | 1.34 | 1.46 |
| 4 | P | 817 | MRG | C21-N2 | -4.93 | 1.34 | 1.46 |
| 4 | D | 817 | MRG | C5-C6 | -4.50 | 1.38 | 1.47 |
| 4 | H | 817 | MRG | C5-C6 | -3.68 | 1.39 | 1.47 |
| 4 | L | 817 | MRG | C5-C6 | -3.34 | 1.40 | 1.47 |
| 4 | P | 817 | MRG | C5-C6 | -3.18 | 1.40 | 1.47 |
| 4 | D | 817 | MRG | C8-N7 | -2.79 | 1.30 | 1.35 |
| 4 | H | 817 | MRG | C8-N7 | -2.72 | 1.30 | 1.35 |
| 4 | L | 817 | MRG | C8-N7 | -2.71 | 1.30 | 1.35 |
| 4 | P | 817 | MRG | C8-N7 | -2.47 | 1.30 | 1.35 |
| 4 | D | 817 | MRG | C5-C4 | -2.19 | 1.37 | 1.43 |
| 4 | H | 817 | MRG | C5-C4 | -2.09 | 1.37 | 1.43 |

All (22) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|-----|-------|-----|------|-------|---|----------------|-------------|
| 4 | H | 817 | MRG | C21-N2-C2 | -13.17 | 98.74 | 123.41 |
| 4 | P | 817 | MRG | C21-N2-C2 | -12.61 | 99.79 | 123.41 |
| 4 | L | 817 | MRG | C21-N2-C2 | -12.40 | 100.18 | 123.41 |
| 4 | D | 817 | MRG | C21-N2-C2 | -12.09 | 100.76 | 123.41 |
| 4 | D | 817 | MRG | C23-C22-C21 | -4.38 | 98.59 | 112.65 |
| 4 | H | 817 | MRG | C23-C22-C21 | -4.23 | 99.07 | 112.65 |
| 4 | P | 817 | MRG | C23-C22-C21 | -4.16 | 99.28 | 112.65 |
| 4 | L | 817 | MRG | C23-C22-C21 | -4.16 | 99.28 | 112.65 |
| 4 | H | 817 | MRG | C2'-C1'-N9 | -3.69 | 105.76 | 114.27 |
| 4 | D | 817 | MRG | C2'-C1'-N9 | -3.36 | 106.52 | 114.27 |
| 4 | L | 817 | MRG | C2'-C1'-N9 | -2.81 | 107.79 | 114.27 |
| 4 | P | 817 | MRG | C2'-C1'-N9 | -2.59 | 108.30 | 114.27 |
| 4 | P | 822 | 2DA | C5-C6-N6 | 2.54 | 124.21 | 120.35 |
| 4 | D | 822 | 2DA | C5-C6-N6 | 2.29 | 123.83 | 120.35 |
| 4 | H | 817 | MRG | C22-C23-S24 | 2.24 | 120.14 | 112.96 |
| 4 | L | 822 | 2DA | C5-C6-N6 | 2.21 | 123.72 | 120.35 |
| 4 | L | 817 | MRG | C22-C23-S24 | 2.19 | 119.99 | 112.96 |
| 4 | P | 817 | MRG | C22-C23-S24 | 2.12 | 119.78 | 112.96 |
| 4 | D | 817 | MRG | O6-C6-C5 | 2.12 | 128.52 | 124.37 |
| 4 | H | 817 | MRG | C22-C21-N2 | 2.05 | 118.07 | 112.21 |
| 4 | L | 822 | 2DA | C2'-C1'-N9 | 2.02 | 116.29 | 112.48 |
| 4 | L | 817 | MRG | O6-C6-C5 | 2.01 | 128.30 | 124.37 |

There are no chirality outliers.

All (11) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------|
| 4 | D | 817 | MRG | N2-C21-C22-C23 |
| 4 | H | 817 | MRG | N1-C2-N2-C21 |
| 4 | H | 817 | MRG | N2-C21-C22-C23 |
| 4 | L | 817 | MRG | N3-C2-N2-C21 |
| 4 | L | 817 | MRG | N1-C2-N2-C21 |
| 4 | P | 817 | MRG | N1-C2-N2-C21 |
| 4 | P | 817 | MRG | N2-C21-C22-C23 |
| 4 | D | 817 | MRG | C21-C22-C23-S24 |
| 4 | P | 817 | MRG | N3-C2-N2-C21 |
| 4 | H | 817 | MRG | N3-C2-N2-C21 |
| 4 | D | 817 | MRG | C3'-C4'-C5'-O5' |

There are no ring outliers.

7 monomers are involved in 15 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4 | H | 822 | 2DA | 3 | 0 |
| 4 | L | 822 | 2DA | 1 | 0 |
| 4 | P | 817 | MRG | 1 | 0 |
| 4 | D | 817 | MRG | 2 | 0 |
| 4 | D | 822 | 2DA | 2 | 0 |
| 4 | H | 817 | MRG | 3 | 0 |
| 4 | P | 822 | 2DA | 3 | 0 |

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 for Mogul analysis.

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 | $\#|Z| > 2$ |
| 6 | ZP4 | E | 823 | 5 | 47,57,57 | 1.26 | 5 (10%) | 58,88,88 | 1.15 | 5 (8%) |
| 6 | ZP4 | A | 823 | 5 | 47,57,57 | 1.22 | 5 (10%) | 58,88,88 | 1.18 | 5 (8%) |
| 7 | GOL | F | 429 | - | 5,5,5 | 0.77 | 0 | 5,5,5 | 0.76 | 0 |
| 6 | ZP4 | M | 823 | 5 | 47,57,57 | 1.19 | 4 (8%) | 58,88,88 | 1.14 | 6 (10%) |
| 7 | GOL | B | 429 | - | 5,5,5 | 0.71 | 0 | 5,5,5 | 0.56 | 0 |
| 6 | ZP4 | I | 823 | 5 | 47,57,57 | 1.22 | 5 (10%) | 58,88,88 | 1.22 | 7 (12%) |

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 |
|-----|------|-------|-----|------|---------|----------|-------|
| 6 | ZP4 | E | 823 | 5 | - | 11/37/69/69 | 0/5/5/5 |
| 6 | ZP4 | A | 823 | 5 | - | 5/37/69/69 | 0/5/5/5 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 7 | GOL | F | 429 | - | - | 4/4/4/4 | - |
| 6 | ZP4 | M | 823 | 5 | - | 7/37/69/69 | 0/5/5/5 |
| 7 | GOL | B | 429 | - | - | 2/4/4/4 | - |
| 6 | ZP4 | I | 823 | 5 | - | 9/37/69/69 | 0/5/5/5 |

All (19) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|---|-------------|----------|
| 6 | I | 823 | ZP4 | O41-C11 | 4.37 | 1.47 | 1.41 |
| 6 | M | 823 | ZP4 | O41-C11 | 3.83 | 1.46 | 1.41 |
| 6 | A | 823 | ZP4 | C5R-C4R | 3.66 | 1.50 | 1.40 |
| 6 | E | 823 | ZP4 | O41-C11 | 3.64 | 1.46 | 1.41 |
| 6 | M | 823 | ZP4 | C5R-C4R | 3.57 | 1.50 | 1.40 |
| 6 | A | 823 | ZP4 | O41-C11 | 3.51 | 1.46 | 1.41 |
| 6 | I | 823 | ZP4 | C5R-C4R | 3.50 | 1.50 | 1.40 |
| 6 | E | 823 | ZP4 | C5R-C4R | 3.42 | 1.50 | 1.40 |
| 6 | E | 823 | ZP4 | C4R-N3R | 3.24 | 1.40 | 1.35 |
| 6 | E | 823 | ZP4 | C2R-N3R | 3.18 | 1.37 | 1.32 |
| 6 | M | 823 | ZP4 | C2R-N3R | 3.03 | 1.37 | 1.32 |
| 6 | A | 823 | ZP4 | C2R-N3R | 3.00 | 1.36 | 1.32 |
| 6 | I | 823 | ZP4 | C2R-N3R | 2.81 | 1.36 | 1.32 |
| 6 | M | 823 | ZP4 | C4R-N3R | 2.26 | 1.38 | 1.35 |
| 6 | A | 823 | ZP4 | C6R-C5R | 2.20 | 1.51 | 1.43 |
| 6 | E | 823 | ZP4 | C2R-N1R | 2.18 | 1.38 | 1.33 |
| 6 | I | 823 | ZP4 | C6R-C5R | 2.15 | 1.51 | 1.43 |
| 6 | I | 823 | ZP4 | C4R-N3R | 2.10 | 1.38 | 1.35 |
| 6 | A | 823 | ZP4 | C4R-N3R | 2.06 | 1.38 | 1.35 |

All (23) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------|---|-------------|----------|
| 6 | E | 823 | ZP4 | N3R-C2R-N1R | -4.38 | 121.83 | 128.68 |
| 6 | M | 823 | ZP4 | N3R-C2R-N1R | -4.04 | 122.36 | 128.68 |
| 6 | A | 823 | ZP4 | N3R-C2R-N1R | -4.03 | 122.37 | 128.68 |
| 6 | I | 823 | ZP4 | N3R-C2R-N1R | -4.00 | 122.43 | 128.68 |
| 6 | A | 823 | ZP4 | C31-C21-C11 | 3.13 | 105.68 | 100.98 |
| 6 | I | 823 | ZP4 | C2'-C1'-N1 | 3.05 | 120.81 | 113.77 |
| 6 | I | 823 | ZP4 | C31-C21-C11 | 3.03 | 105.54 | 100.98 |
| 6 | M | 823 | ZP4 | C31-C21-C11 | 2.97 | 105.46 | 100.98 |
| 6 | E | 823 | ZP4 | C31-C21-C11 | 2.94 | 105.40 | 100.98 |
| 6 | I | 823 | ZP4 | C4R-C5R-N7R | -2.41 | 106.89 | 109.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|-----|-------|-----|------|-------|---|----------------|-------------|
| 6 | E | 823 | ZP4 | C2R-N1R-C6R | 2.31 | 122.70 | 118.75 |
| 6 | I | 823 | ZP4 | PG-O3B-PB | -2.30 | 124.92 | 132.83 |
| 6 | A | 823 | ZP4 | C4R-C5R-N7R | -2.30 | 107.00 | 109.40 |
| 6 | I | 823 | ZP4 | C2R-N1R-C6R | 2.25 | 122.59 | 118.75 |
| 6 | I | 823 | ZP4 | O21-C21-C11 | 2.24 | 119.14 | 110.85 |
| 6 | A | 823 | ZP4 | C2R-N1R-C6R | 2.20 | 122.52 | 118.75 |
| 6 | E | 823 | ZP4 | C4R-C5R-N7R | -2.14 | 107.16 | 109.40 |
| 6 | M | 823 | ZP4 | C2R-N1R-C6R | 2.12 | 122.39 | 118.75 |
| 6 | M | 823 | ZP4 | C4R-C5R-N7R | -2.11 | 107.20 | 109.40 |
| 6 | M | 823 | ZP4 | O21-C21-C11 | 2.08 | 118.54 | 110.85 |
| 6 | E | 823 | ZP4 | O31-C31-C41 | -2.07 | 105.05 | 111.05 |
| 6 | M | 823 | ZP4 | O31-C31-C41 | -2.06 | 105.10 | 111.05 |
| 6 | A | 823 | ZP4 | O21-C21-C11 | 2.05 | 118.42 | 110.85 |

There are no chirality outliers.

All (38) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------|
| 6 | A | 823 | ZP4 | C5'-O5'-PA-O1A |
| 6 | E | 823 | ZP4 | C5'-O5'-PA-O1A |
| 6 | E | 823 | ZP4 | C51-O51-PD-O2D |
| 6 | E | 823 | ZP4 | C31-C41-C51-O51 |
| 6 | I | 823 | ZP4 | C5'-O5'-PA-O1A |
| 6 | M | 823 | ZP4 | C5'-O5'-PA-O1A |
| 7 | F | 429 | GOL | O2-C2-C3-O3 |
| 7 | F | 429 | GOL | O1-C1-C2-C3 |
| 7 | F | 429 | GOL | C1-C2-C3-O3 |
| 7 | F | 429 | GOL | O1-C1-C2-O2 |
| 6 | I | 823 | ZP4 | C4'-C3'-N3'-N3A |
| 6 | E | 823 | ZP4 | O41-C41-C51-O51 |
| 6 | E | 823 | ZP4 | C41-C51-O51-PD |
| 6 | A | 823 | ZP4 | C5'-O5'-PA-O3A |
| 6 | E | 823 | ZP4 | C5'-O5'-PA-O3A |
| 6 | E | 823 | ZP4 | C51-O51-PD-O3G |
| 6 | I | 823 | ZP4 | C5'-O5'-PA-O3A |
| 6 | M | 823 | ZP4 | C5'-O5'-PA-O3A |
| 7 | B | 429 | GOL | C1-C2-C3-O3 |
| 6 | A | 823 | ZP4 | C5'-O5'-PA-O2A |
| 6 | E | 823 | ZP4 | C5'-O5'-PA-O2A |
| 6 | E | 823 | ZP4 | C51-O51-PD-O1D |
| 6 | I | 823 | ZP4 | C5'-O5'-PA-O2A |
| 6 | M | 823 | ZP4 | C5'-O5'-PA-O2A |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------|
| 6 | A | 823 | ZP4 | C31-C41-C51-O51 |
| 6 | A | 823 | ZP4 | PD-O3G-PG-O2G |
| 6 | E | 823 | ZP4 | PD-O3G-PG-O2G |
| 6 | M | 823 | ZP4 | PD-O3G-PG-O2G |
| 6 | M | 823 | ZP4 | C2'-C1'-N1-C2 |
| 6 | I | 823 | ZP4 | PA-O3A-PB-O2B |
| 6 | I | 823 | ZP4 | PD-O3G-PG-O1G |
| 6 | M | 823 | ZP4 | PA-O3A-PB-O2B |
| 6 | I | 823 | ZP4 | C2'-C3'-N3'-N3A |
| 6 | I | 823 | ZP4 | PG-O3B-PB-O3A |
| 6 | E | 823 | ZP4 | PG-O3B-PB-O1B |
| 6 | I | 823 | ZP4 | PD-O3G-PG-O2G |
| 6 | M | 823 | ZP4 | PG-O3B-PB-O1B |
| 7 | B | 429 | GOL | O1-C1-C2-C3 |

There are no ring outliers.

4 monomers are involved in 19 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 6 | E | 823 | ZP4 | 6 | 0 |
| 6 | A | 823 | ZP4 | 4 | 0 |
| 6 | M | 823 | ZP4 | 3 | 0 |
| 6 | I | 823 | ZP4 | 6 | 0 |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

## Ligand ZP4 E 823


Bond lengths


Bond angles


Torsions


Rings

## Ligand ZP4 A 823


Bond lengths


Bond angles


Torsions


Rings

**Ligand ZP4 M 823**

Bond lengths

Bond angles

Torsions

Rings

**Ligand ZP4 I 823**

Bond lengths

Bond angles

Torsions

Rings
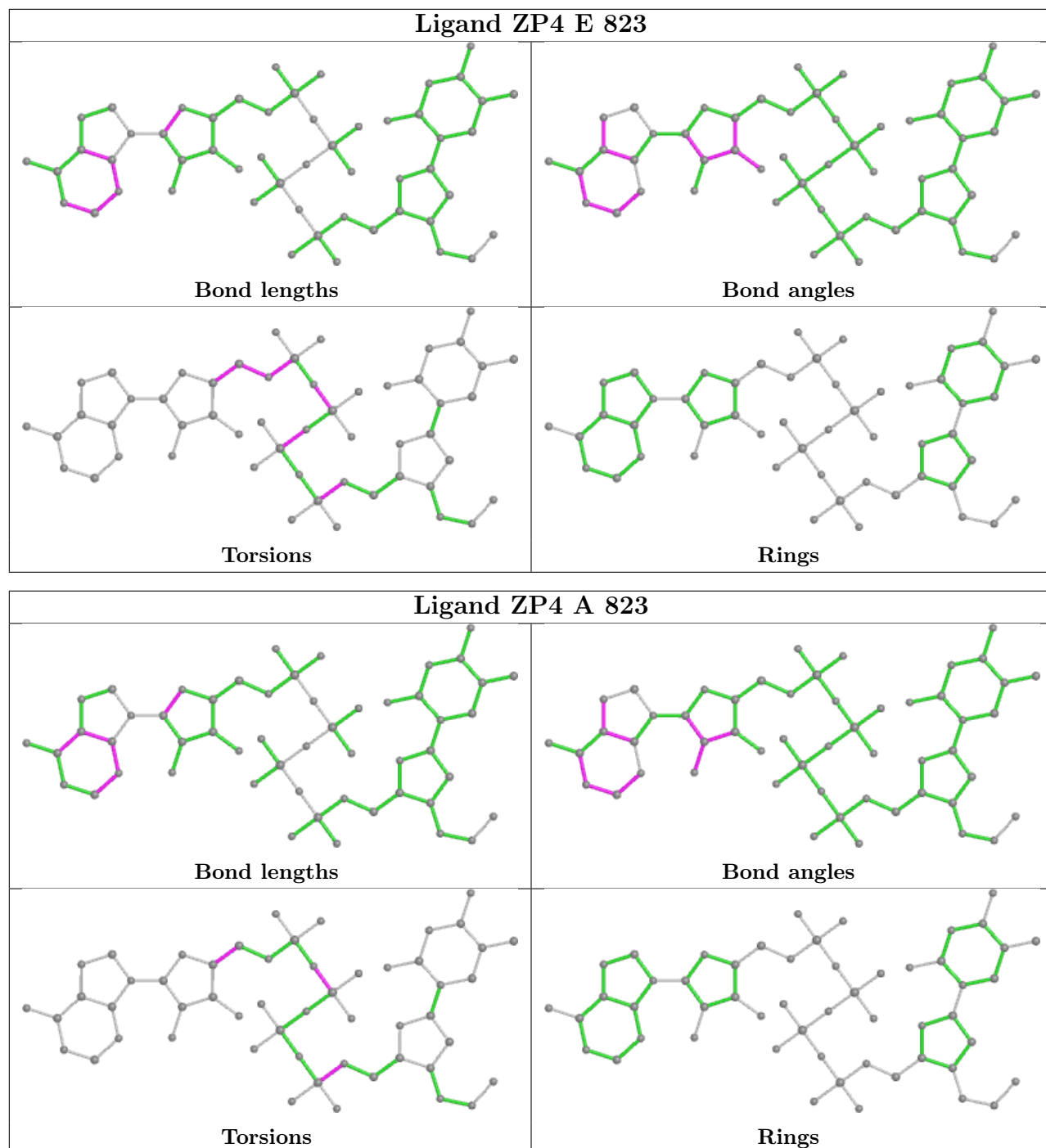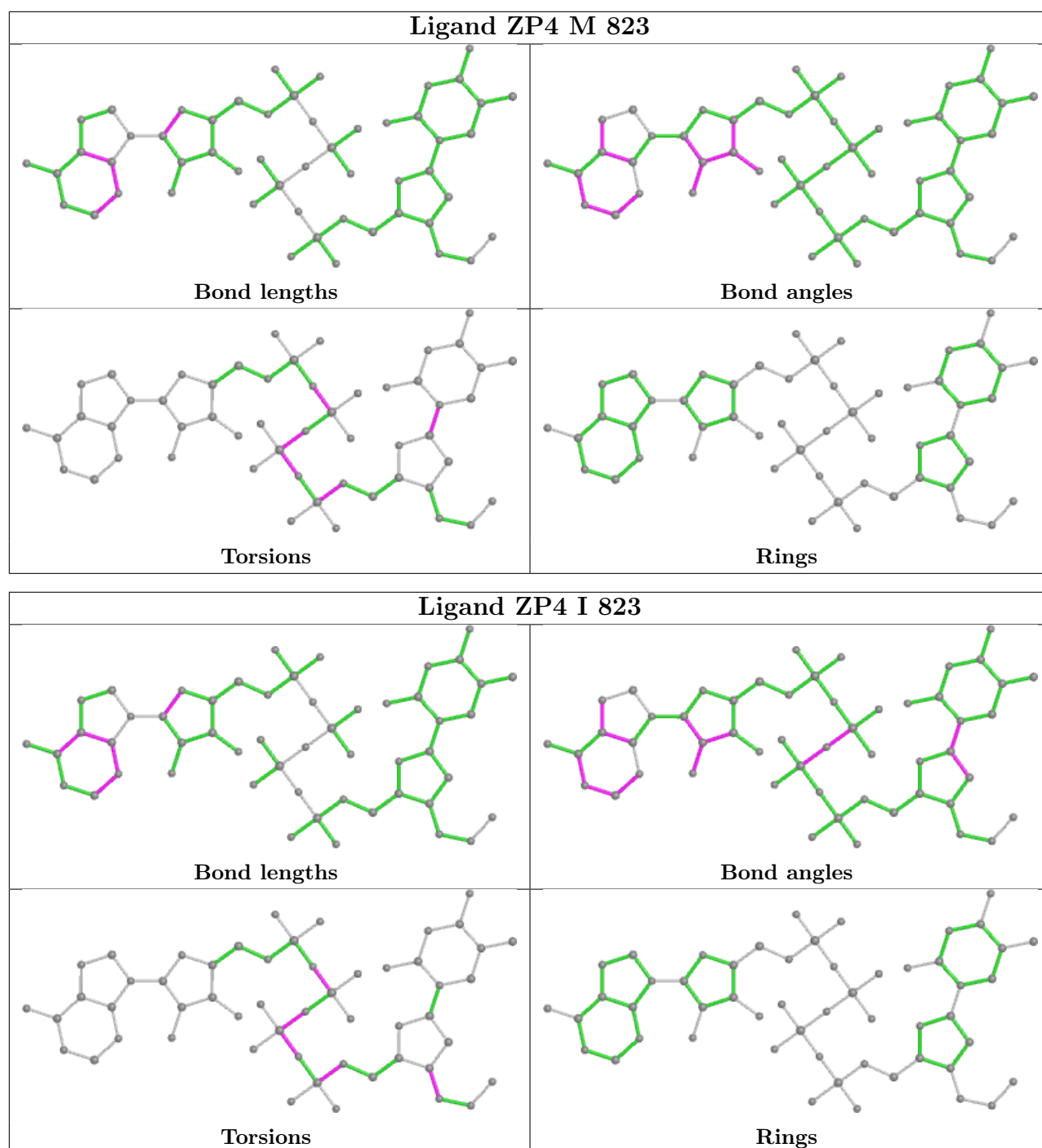
## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

# 6 Fit of model and data ⓘ

## 6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

## 6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

## 6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.
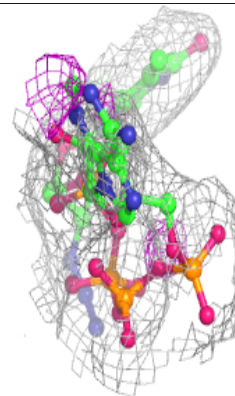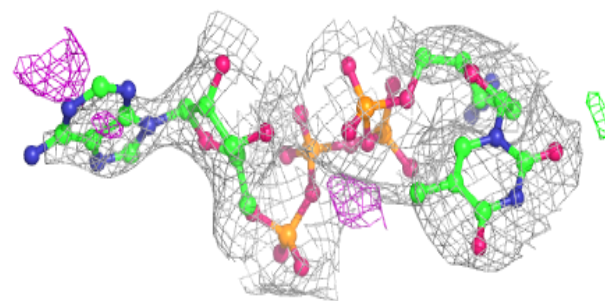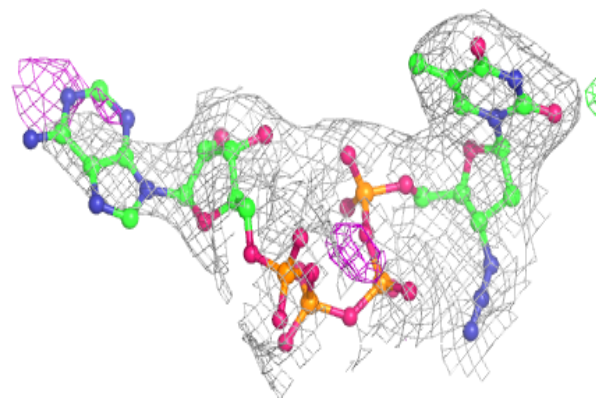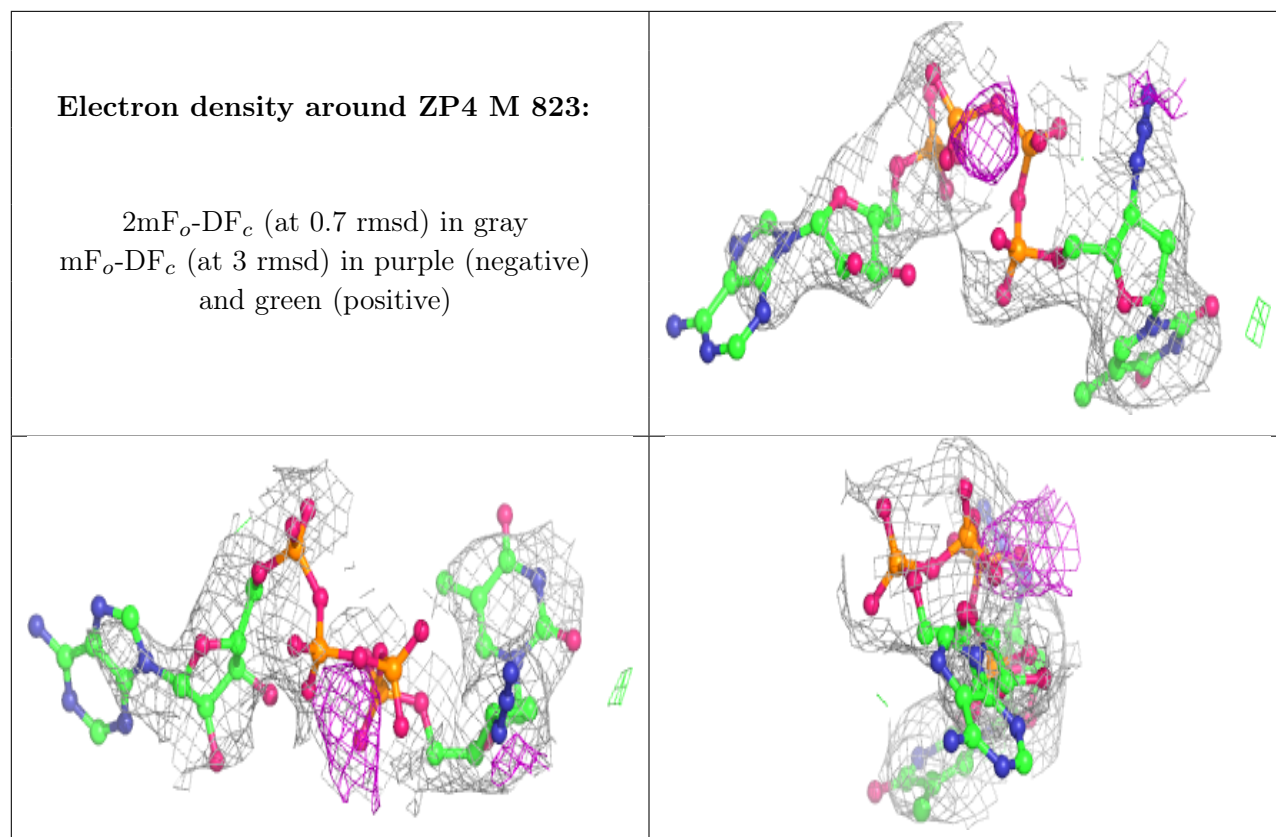


**Electron density around ZP4 A 823:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
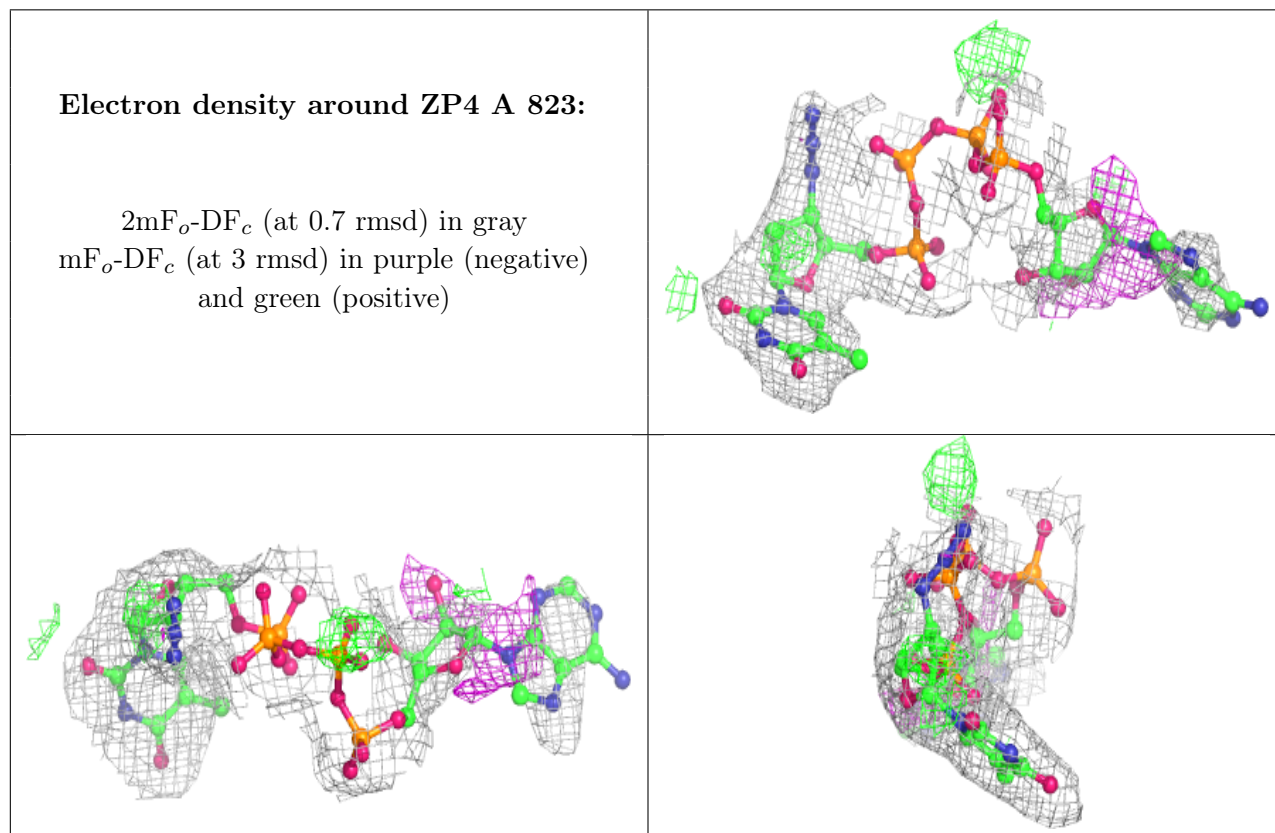
**Electron density around ZP4 E 823:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
$mF_o-DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
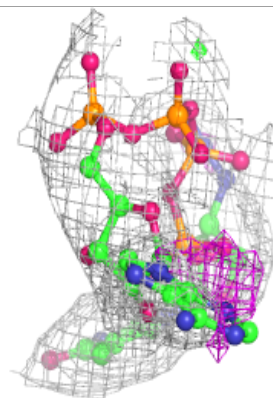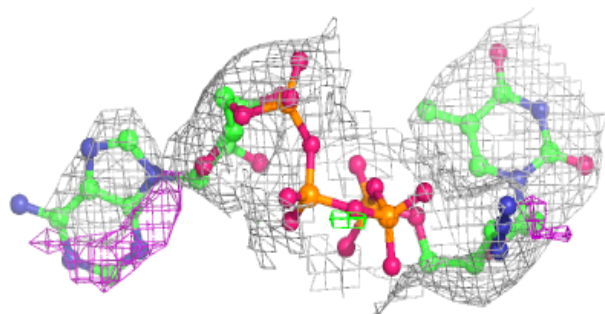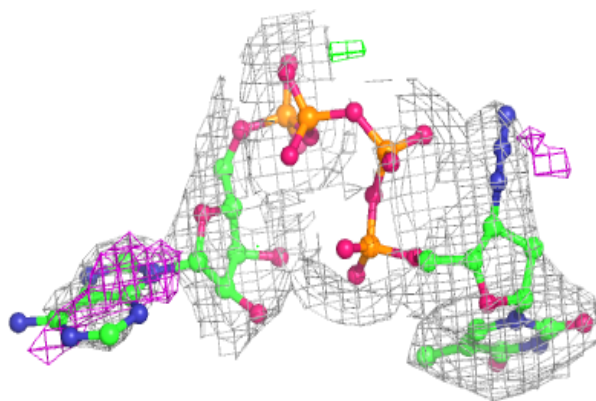


**Electron density around ZP4 I 823:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
$mF_o-DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around ZP4 M 823:**

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



## 6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.