



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 05:25 am GMT

PDB ID : 1S0V
Title : Structural basis for substrate selection by T7 RNA polymerase
Authors : Temiakov, D.; Patlan, V.; Anikin, M.; McAllister, W.T.; Yokoyama, S.; Vassilyev, D.G.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2004-01-05
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

| | | |
|--------------------------------|---|--|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.7.2 (RC1), CSD as538be (2017) |
| Xtriage (Phenix) | : | 1.9-1692 |
| EDS | : | trunk28620 |
| Percentile statistics | : | 20161228.v01 (using entries in the PDB archive December 28th 2016) |
| Refmac | : | 5.8.0135 |
| CCP4 | : | 6.5.0 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | recalc28949 |

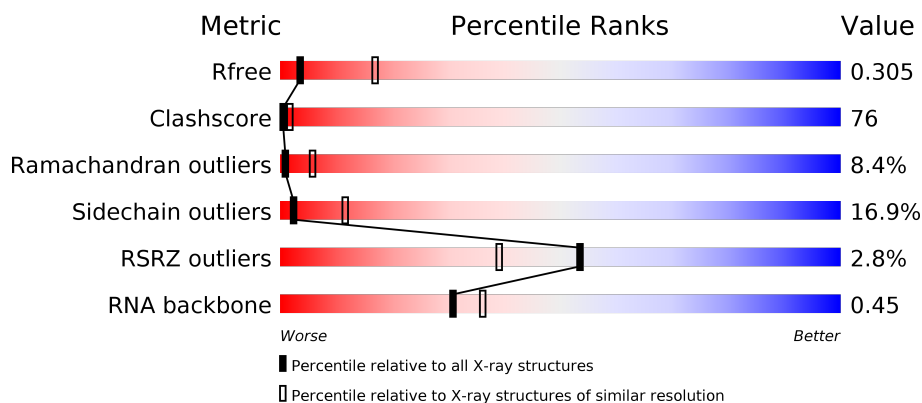
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 100719 | 1015 (3.22-3.18) |
| Clashscore | 112137 | 1009 (3.20-3.20) |
| Ramachandran outliers | 110173 | 1118 (3.22-3.18) |
| Sidechain outliers | 110143 | 1117 (3.22-3.18) |
| RSRZ outliers | 101464 | 1020 (3.22-3.18) |
| RNA backbone | 2435 | 1045 (3.60-2.80) |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | E | 18 | <div> <div>11%</div> <div>39%</div> <div>11%</div> <div>33%</div> <div>6%</div> </div> |
| 1 | H | 18 | <div> <div>6%</div> <div>17%</div> <div>28%</div> <div>22%</div> <div>28%</div> <div>6%</div> </div> |
| 1 | K | 18 | <div> <div>56%</div> <div>11%</div> <div>28%</div> <div>6%</div> </div> |
| 1 | N | 18 | <div> <div>6%</div> <div>56%</div> <div>22%</div> <div>11%</div> <div>6%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2 | F | 12 | |
| 2 | I | 12 | |
| 2 | L | 12 | |
| 2 | O | 12 | |
| 3 | G | 10 | |
| 3 | J | 10 | |
| 3 | M | 10 | |
| 3 | P | 10 | |
| 4 | A | 883 | |
| 4 | B | 883 | |
| 4 | C | 883 | |
| 4 | D | 883 | |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 6 | APC | A | 2000 | - | - | X | - |
| 6 | APC | B | 2001 | - | - | X | - |
| 6 | APC | C | 2002 | - | - | X | - |

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 30899 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 DNA chain called 5'-D(*G*GP*GP*AP*AP*TP*CP*GP*AP*TP*AP*TP*CP*GP*CP*CP*GP*C)-3'.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|---------|-------|
| 1 | E | 17 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 346 | 165 | 66 | 99 | 16 | | | |
| 1 | H | 17 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 346 | 165 | 66 | 99 | 16 | | | |
| 1 | K | 17 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 346 | 165 | 66 | 99 | 16 | | | |
| 1 | N | 17 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 346 | 165 | 66 | 99 | 16 | | | |

- Molecule 2 is a RNA chain called 5'-R(*AP*AP*CP*U*GP*CP*GP*GP*CP*GP*AP*U)-3'.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 2 | F | 8 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 171 | 77 | 33 | 54 | 7 | | | |
| 2 | I | 8 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 171 | 77 | 33 | 54 | 7 | | | |
| 2 | L | 8 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 171 | 77 | 33 | 54 | 7 | | | |
| 2 | O | 8 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 171 | 77 | 33 | 54 | 7 | | | |

- Molecule 3 is a DNA chain called 5'-D(*GP*TP*CP*GP*AP*TP*TP*CP*CP*C)-3'.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 3 | G | 9 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 179 | 87 | 30 | 54 | 8 | | | |
| 3 | J | 9 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 179 | 87 | 30 | 54 | 8 | | | |
| 3 | M | 9 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 179 | 87 | 30 | 54 | 8 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 3 | P | 9 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 179 | 87 | 30 | 54 | 8 | | | |

- Molecule 4 is a protein called DNA-directed RNA polymerase.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 4 | A | 857 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 6746 | 4296 | 1173 | 1242 | 35 | | | |
| 4 | B | 857 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 6746 | 4296 | 1173 | 1242 | 35 | | | |
| 4 | C | 857 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 6746 | 4296 | 1173 | 1242 | 35 | | | |
| 4 | D | 857 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 6746 | 4296 | 1173 | 1242 | 35 | | | |

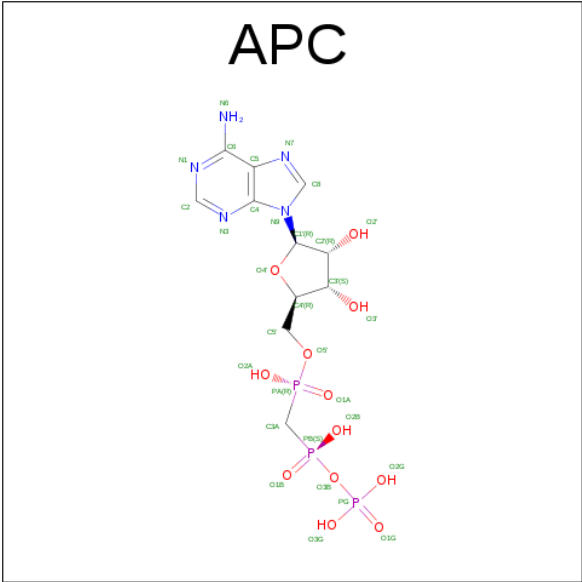
There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------|------------|
| A | 497 | LEU | - | INSERTION | UNP P00573 |
| B | 497 | LEU | - | INSERTION | UNP P00573 |
| C | 497 | LEU | - | INSERTION | UNP P00573 |
| D | 497 | LEU | - | INSERTION | UNP P00573 |

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

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 5 | B | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 5 | A | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 5 | D | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 5 | C | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 5 | F | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 6 is DIPHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (three-letter code: APC) (formula: C₁₁H₁₈N₅O₁₂P₃).



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 6 | A | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 31 | 11 | 5 | 12 | 3 | | |
| 6 | B | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 31 | 11 | 5 | 12 | 3 | | |
| 6 | C | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 31 | 11 | 5 | 12 | 3 | | |
| 6 | D | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 31 | 11 | 5 | 12 | 3 | | |

- Molecule 7 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 7 | A | 237 | Total | O | 0 | 0 |
| | | | 237 | 237 | | |
| 7 | B | 212 | Total | O | 0 | 0 |
| | | | 212 | 212 | | |
| 7 | C | 201 | Total | O | 0 | 0 |
| | | | 201 | 201 | | |
| 7 | D | 173 | Total | O | 0 | 0 |
| | | | 173 | 173 | | |
| 7 | E | 39 | Total | O | 0 | 0 |
| | | | 39 | 39 | | |
| 7 | F | 9 | Total | O | 0 | 0 |
| | | | 9 | 9 | | |
| 7 | G | 9 | Total | O | 0 | 0 |
| | | | 9 | 9 | | |
| 7 | H | 19 | Total | O | 0 | 0 |
| | | | 19 | 19 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 7 | I | 14 | Total 14 | O 14 | 0 | 0 |
| 7 | J | 13 | Total 13 | O 13 | 0 | 0 |
| 7 | K | 20 | Total 20 | O 20 | 0 | 0 |
| 7 | L | 8 | Total 8 | O 8 | 0 | 0 |
| 7 | M | 10 | Total 10 | O 10 | 0 | 0 |
| 7 | N | 14 | Total 14 | O 14 | 0 | 0 |
| 7 | O | 15 | Total 15 | O 15 | 0 | 0 |
| 7 | P | 6 | Total 6 | O 6 | 0 | 0 |

3 Residue-property plots [i](#)

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

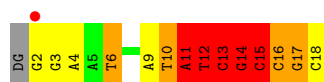
- Molecule 1: 5'-D(*G*GP*GP*AP*AP*TP*CP*GP*AP*TP*AP*TP*CP*GP*CP*CP*GP*C)-3'

Chain E: 




- Molecule 1: 5'-D(*G*GP*GP*AP*AP*TP*CP*GP*AP*TP*AP*TP*CP*GP*CP*CP*GP*C)-3'

Chain H: 



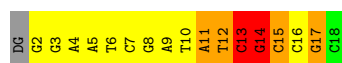
- Molecule 1: 5'-D(*G*GP*GP*AP*AP*TP*CP*GP*AP*TP*AP*TP*CP*GP*CP*CP*GP*C)-3'

Chain K: 



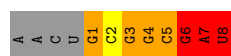
- Molecule 1: 5'-D(*G*GP*GP*AP*AP*TP*CP*GP*AP*TP*AP*TP*CP*GP*CP*CP*GP*C)-3'

Chain N: 



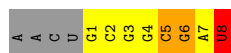
- Molecule 2: 5'-R(*AP*AP*CP*U*GP*CP*GP*GP*CP*GP*AP*U)-3'

Chain F: 



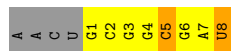
- Molecule 2: 5'-R(*AP*AP*CP*U*GP*CP*GP*GP*CP*GP*AP*U)-3'

Chain I: 



- Molecule 2: 5'-R(*AP*AP*CP*U*GP*CP*GP*GP*CP*GP*AP*U)-3'

Chain L: 




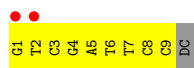
- Molecule 2: 5'-R(*AP*AP*CP*U*GP*CP*GP*GP*CP*GP*AP*U)-3'

Chain O: 

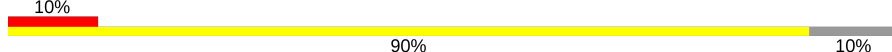


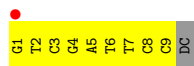
- Molecule 3: 5'-D(*GP*TP*CP*GP*AP*TP*TP*CP*CP*C)-3'

Chain G: 




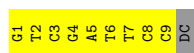
- Molecule 3: 5'-D(*GP*TP*CP*GP*AP*TP*TP*CP*CP*C)-3'

Chain J: 




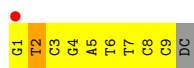
- Molecule 3: 5'-D(*GP*TP*CP*GP*AP*TP*TP*CP*CP*C)-3'

Chain M: 



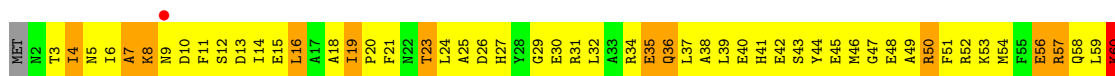
- Molecule 3: 5'-D(*GP*TP*CP*GP*AP*TP*TP*CP*CP*C)-3'

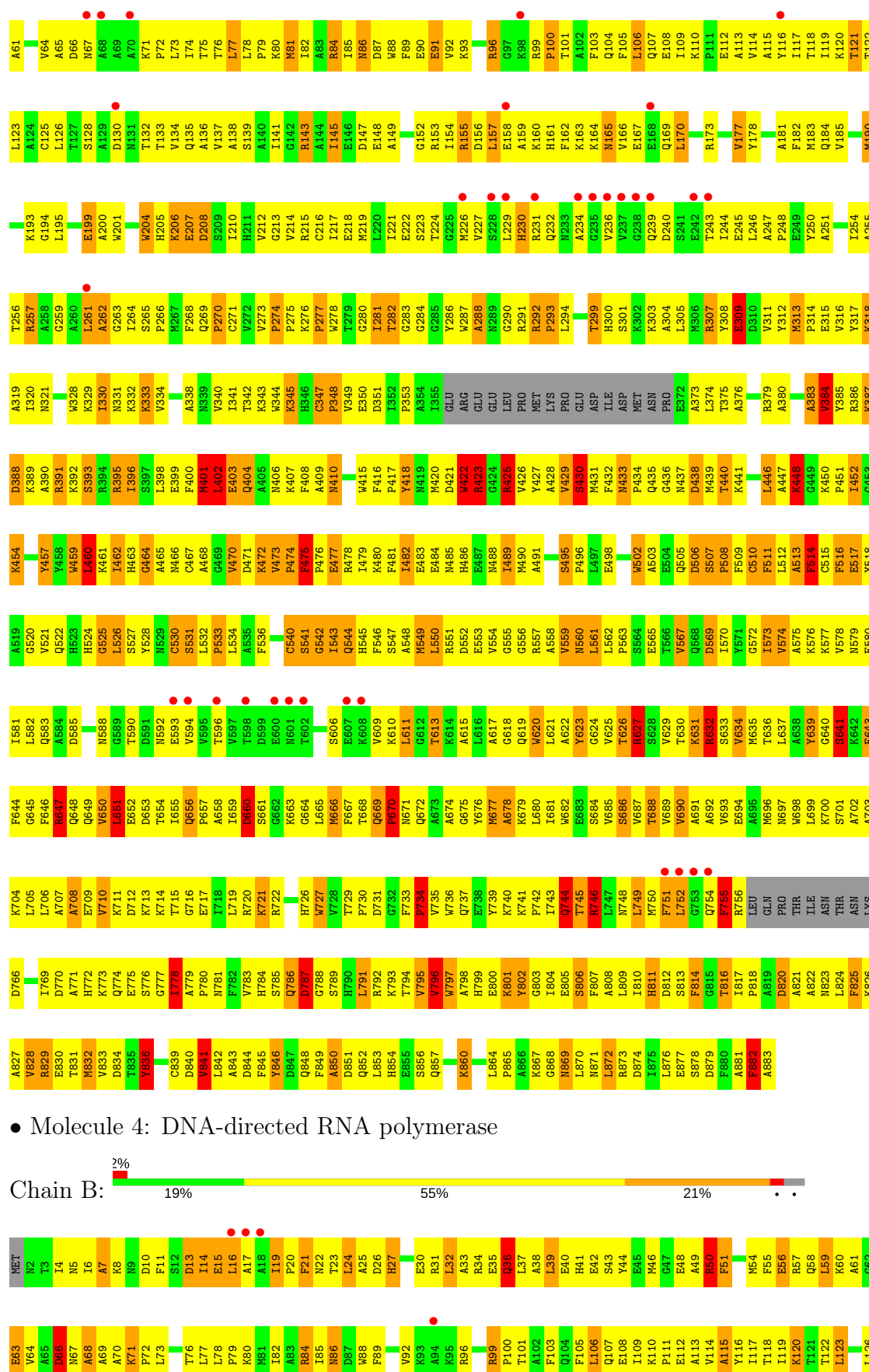
Chain P: 

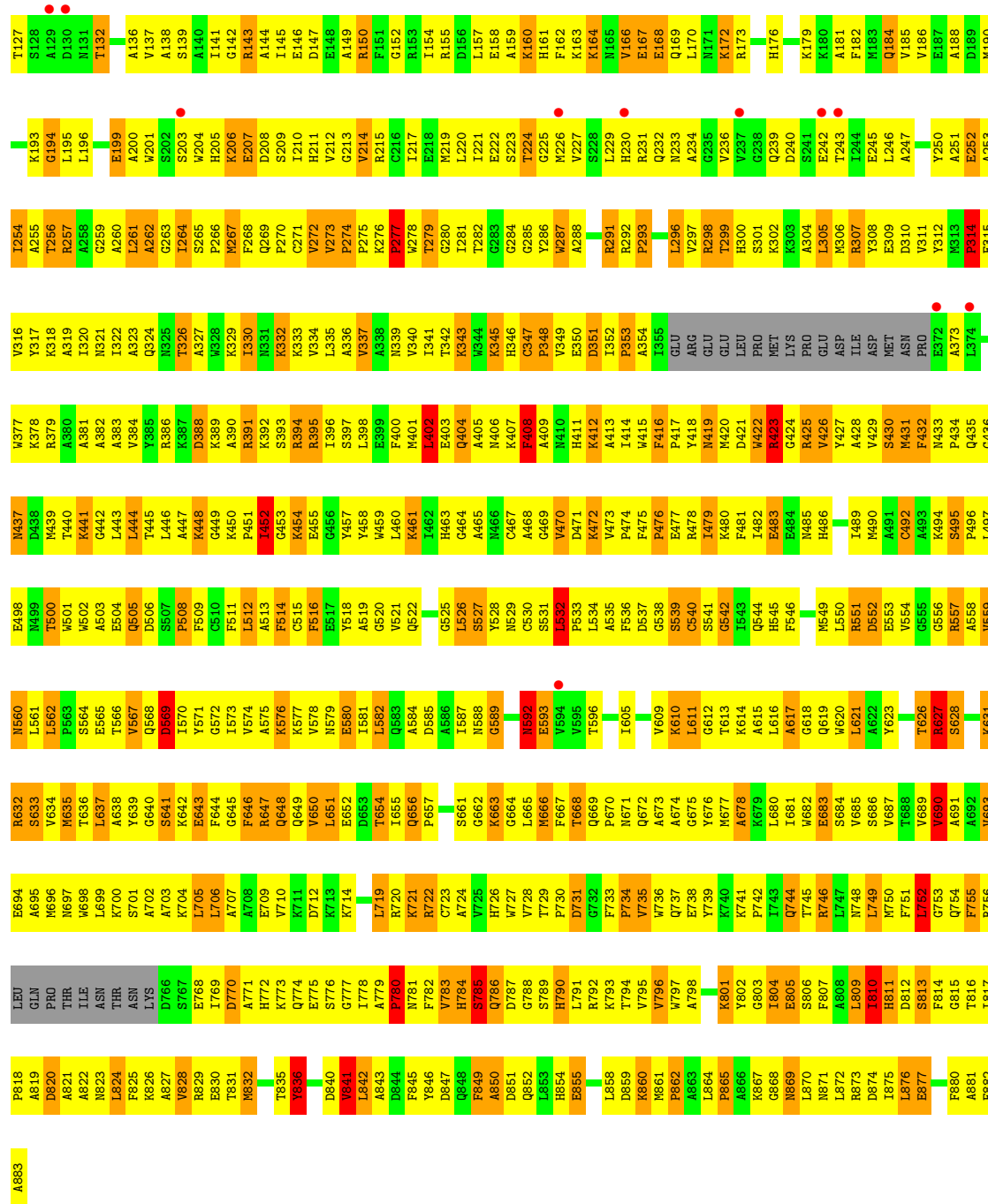


- Molecule 4: DNA-directed RNA polymerase

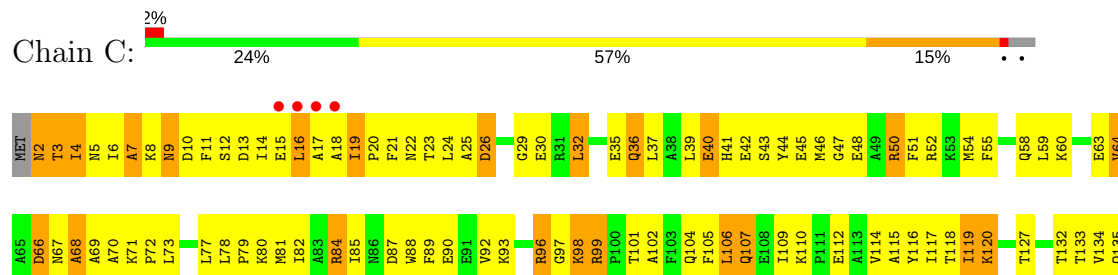
Chain A: 

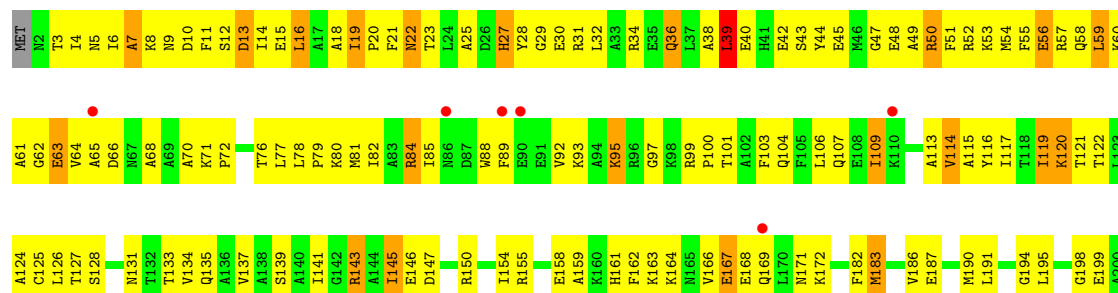






• Molecule 4: DNA-directed RNA polymerase





| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| A843 | Y846 | Q848 | F849 | A850 | D851 | Q852 | L853 | H854 | E855 | S856 | Q857 | L858 | D859 | K860 | M861 | P862 | A863 | L864 | P865 | G868 | N869 | L870 | N871 | L872 | R873 | D874 | I875 | L876 | E877 | S878 | D879 | F880 | A881 | F882 | A883 | | | | | | | | | | | | | | | | | | | | | | | | |
| 1778 | A779 | P780 | N781 | F782 | V783 | H784 | S785 | Q786 | D787 | G788 | S789 | H790 | L791 | R792 | K793 | T794 | V795 | V796 | W797 | K801 | Y802 | G803 | I804 | E805 | S806 | L809 | I810 | H811 | D812 | S813 | F814 | L749 | M750 | F751 | L752 | P818 | A819 | D820 | N823 | L824 | F825 | K826 | A827 | V828 | R829 | E830 | T831 | M832 | V833 | T835 | Y836 | E837 | D840 | L842 | | | | | |
| G716 | E717 | I718 | L719 | R720 | K721 | R722 | C723 | A724 | V725 | H726 | W727 | V728 | T729 | P730 | D731 | G732 | F733 | P734 | V735 | W736 | Q737 | E738 | Y739 | K740 | K741 | I743 | Q744 | T745 | R746 | L747 | N748 | L749 | M750 | F751 | L752 | G753 | Q754 | F755 | R756 | LEU | GLN | PRO | THR | ILE | ASN | THR | ASN | LYS | D766 | L769 | H772 | K773 | Q774 | E775 | S776 | G777 | | | |
| Q649 | V650 | L651 | E652 | D653 | T654 | L655 | Q656 | P657 | D660 | S661 | G662 | K663 | G664 | L665 | M666 | F667 | T668 | Q669 | Q672 | Y676 | M677 | A678 | K679 | L680 | I681 | G682 | T683 | K684 | V685 | S686 | G687 | T688 | V689 | L690 | A691 | G692 | V693 | M696 | N697 | W698 | L699 | K700 | S701 | S633 | A702 | A703 | K704 | L705 | L706 | E709 | V710 | K711 | D712 | T715 | | | | | |
| A575 | K576 | K577 | V578 | N579 | E580 | I581 | L582 | Q583 | D585 | N588 | G589 | T590 | Y528 | N592 | F593 | V594 | M601 | T602 | G603 | S606 | V609 | K610 | L611 | G612 | T613 | K614 | A615 | L616 | Q619 | V620 | L621 | A622 | Y623 | G624 | V625 | V629 | T630 | K631 | R632 | N633 | S634 | L662 | P663 | S664 | V667 | Q668 | K642 | E643 | F646 | R647 | Q648 | | | | | | | | |
| A513 | F514 | C515 | F516 | E517 | Y518 | A519 | G520 | L521 | H522 | H523 | H524 | G525 | L526 | S527 | Y528 | N529 | C530 | S531 | L532 | P533 | A535 | F536 | D537 | G538 | S539 | K540 | L541 | G542 | I543 | Q544 | F546 | N549 | L550 | R551 | D552 | E553 | V554 | G555 | G556 | R557 | A558 | V559 | N560 | L561 | P562 | S563 | S564 | V567 | Q568 | D569 | I570 | Y571 | G572 | L573 | V574 | | | | |
| L452 | G453 | K454 | E455 | G456 | Y457 | Y458 | W459 | L460 | K461 | I462 | A465 | N466 | C467 | A468 | G469 | V470 | D471 | K472 | V473 | F475 | P476 | E477 | R478 | I479 | K480 | F481 | I482 | E483 | E484 | N485 | H486 | E487 | I489 | M490 | A491 | C492 | A493 | N494 | S495 | P496 | L497 | E498 | N499 | T500 | V501 | W502 | A503 | E504 | Q505 | D506 | S507 | P508 | F509 | C510 | F511 | L512 | | | |
| A390 | R391 | R394 | R395 | I396 | S397 | L398 | E399 | F400 | W401 | L402 | E403 | Q404 | A405 | N406 | K407 | F408 | A409 | K412 | A413 | I414 | W415 | F416 | F417 | I418 | N419 | W420 | I355 | GLU | ARG | N233 | GLU | LEU | PRO | MET | LYS | PRO | GLU | ASP | ILE | ASP | MET | ASN | PRO | E372 | A373 | L374 | W377 | K378 | T379 | A380 | A381 | V384 | G449 | K450 | P451 | | | | |
| N325 | T326 | A327 | W328 | K329 | H206 | I330 | N331 | K332 | K333 | V334 | L335 | F400 | W401 | L402 | E403 | Q404 | A405 | N406 | K407 | F408 | A409 | K412 | A413 | I414 | W415 | F416 | F417 | I418 | N419 | W420 | I355 | GLU | ARG | N233 | GLU | LEU | PRO | MET | LYS | PRO | GLU | ASP | ILE | ASP | MET | ASN | PRO | E372 | A373 | L374 | W377 | K378 | T379 | A380 | A381 | V384 | G449 | K450 | P451 |
| N261 | S202 | S203 | W204 | K205 | H206 | I207 | D208 | S209 | I210 | H211 | V212 | G213 | V214 | R215 | C216 | I217 | E218 | M219 | L220 | I221 | E222 | S223 | T224 | G225 | M226 | V227 | S228 | L229 | H230 | R231 | Q232 | N233 | A234 | G235 | V236 | T237 | G238 | Q239 | D240 | S241 | E242 | L243 | E245 | P248 | E249 | Y250 | A251 | A253 | L254 | A255 | T256 | R257 | A258 | G259 | A260 | | | | |
| L261 | A262 | G263 | I264 | S265 | P266 | M267 | F268 | Q269 | C270 | K271 | V272 | G273 | P274 | P275 | K276 | P277 | W278 | L281 | T282 | G283 | Y286 | W287 | A288 | N289 | G290 | R291 | R292 | A293 | L294 | A295 | L296 | V297 | T298 | R299 | H300 | S301 | K302 | K303 | A304 | L305 | K306 | R307 | Y308 | E309 | D310 | V311 | Y312 | K313 | P314 | E315 | V316 | Y317 | N321 | I322 | A323 | Q324 | | | |

4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 81.13Å 87.70Å 206.53Å 91.93° 91.02° 110.66° | Depositor |
| Resolution (Å) | 40.00 – 3.20 39.88 – 3.00 | Depositor EDS |
| % Data completeness (in resolution range) | (Not available) (40.00-3.20) 82.3 (39.88-3.00) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 2.42 (at 3.01Å) | Xtriage |
| Refinement program | CNS | Depositor |
| R, R_{free} | 0.255 , 0.307 0.255 , 0.305 | Depositor DCC |
| R_{free} test set | 3685 reflections (5.04%) | DCC |
| Wilson B-factor (Å ²) | 59.0 | Xtriage |
| Anisotropy | 0.201 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.26 , 107.2 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$ | Xtriage |
| Estimated twinning fraction | 0.014 for -h,-k,l | Xtriage |
| F_o, F_c correlation | 0.89 | EDS |
| Total number of atoms | 30899 | wwPDB-VP |
| Average B, all atoms (Å ²) | 89.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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 | E | 1.74 | 9/388 (2.3%) | 1.60 | 9/597 (1.5%) |
| 1 | H | 1.62 | 7/388 (1.8%) | 1.47 | 6/597 (1.0%) |
| 1 | K | 1.59 | 7/388 (1.8%) | 1.31 | 1/597 (0.2%) |
| 1 | N | 1.26 | 3/388 (0.8%) | 1.27 | 4/597 (0.7%) |
| 2 | F | 2.39 | 9/191 (4.7%) | 2.00 | 11/297 (3.7%) |
| 2 | I | 2.25 | 7/191 (3.7%) | 1.68 | 2/297 (0.7%) |
| 2 | L | 1.65 | 1/191 (0.5%) | 1.36 | 0/297 |
| 2 | O | 1.47 | 0/191 | 1.38 | 0/297 |
| 3 | G | 0.82 | 0/199 | 0.92 | 0/305 |
| 3 | J | 0.78 | 0/199 | 0.93 | 0/305 |
| 3 | M | 0.88 | 0/199 | 0.86 | 0/305 |
| 3 | P | 0.94 | 0/199 | 1.07 | 0/305 |
| 4 | A | 1.20 | 22/6897 (0.3%) | 1.14 | 24/9329 (0.3%) |
| 4 | B | 1.21 | 24/6897 (0.3%) | 1.14 | 24/9329 (0.3%) |
| 4 | C | 0.97 | 5/6897 (0.1%) | 0.97 | 7/9329 (0.1%) |
| 4 | D | 0.92 | 3/6897 (0.0%) | 0.91 | 4/9329 (0.0%) |
| All | All | 1.14 | 97/30700 (0.3%) | 1.09 | 92/42112 (0.2%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | E | 0 | 6 |
| 1 | H | 0 | 9 |
| 1 | K | 0 | 6 |
| 1 | N | 0 | 4 |
| 2 | F | 0 | 4 |
| 2 | I | 0 | 2 |
| 2 | L | 0 | 1 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2 | O | 0 | 3 |
| 3 | P | 0 | 1 |
| 4 | A | 0 | 1 |
| 4 | B | 0 | 1 |
| 4 | D | 0 | 1 |
| All | All | 0 | 39 |

All (97) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 4 | A | 502 | TRP | CB-CG | -13.18 | 1.26 | 1.50 |
| 1 | K | 14 | DG | C5-C6 | -11.28 | 1.31 | 1.42 |
| 4 | A | 467 | CYS | CB-SG | -10.63 | 1.64 | 1.82 |
| 2 | I | 8 | U | N1-C6 | -9.75 | 1.29 | 1.38 |
| 2 | I | 7 | A | C5-C6 | -8.93 | 1.33 | 1.41 |
| 4 | A | 271 | CYS | CB-SG | -8.70 | 1.67 | 1.82 |
| 2 | F | 7 | A | C5-C6 | -8.57 | 1.33 | 1.41 |
| 1 | E | 11 | DA | C5-C6 | -8.44 | 1.33 | 1.41 |
| 2 | I | 8 | U | N1-C2 | -8.39 | 1.30 | 1.38 |
| 4 | B | 310 | ASP | CB-CG | 8.28 | 1.69 | 1.51 |
| 1 | H | 12 | DT | C2-O2 | 8.07 | 1.28 | 1.22 |
| 4 | B | 805 | GLU | CG-CD | 7.74 | 1.63 | 1.51 |
| 2 | I | 8 | U | C4-C5 | -7.73 | 1.36 | 1.43 |
| 2 | F | 5 | C | N1-C2 | -7.63 | 1.32 | 1.40 |
| 4 | A | 482 | ILE | CA-CB | -7.61 | 1.37 | 1.54 |
| 1 | H | 11 | DA | N3-C4 | -7.16 | 1.30 | 1.34 |
| 2 | F | 6 | G | C5-C6 | 7.14 | 1.49 | 1.42 |
| 1 | K | 14 | DG | C2-N3 | -7.13 | 1.27 | 1.32 |
| 2 | F | 6 | G | C6-N1 | -7.09 | 1.34 | 1.39 |
| 4 | B | 63 | GLU | CG-CD | 7.08 | 1.62 | 1.51 |
| 1 | H | 14 | DG | C5-C6 | -7.06 | 1.35 | 1.42 |
| 4 | B | 330 | ILE | CA-CB | -7.02 | 1.38 | 1.54 |
| 4 | B | 416 | PHE | CB-CG | -6.93 | 1.39 | 1.51 |
| 2 | L | 5 | C | C4-C5 | -6.88 | 1.37 | 1.43 |
| 1 | K | 11 | DA | C5-C6 | -6.86 | 1.34 | 1.41 |
| 1 | E | 11 | DA | N9-C4 | -6.77 | 1.33 | 1.37 |
| 1 | K | 16 | DC | N1-C2 | -6.72 | 1.33 | 1.40 |
| 1 | E | 12 | DT | N1-C2 | -6.68 | 1.32 | 1.38 |
| 4 | C | 807 | PHE | CB-CG | -6.60 | 1.40 | 1.51 |
| 4 | B | 498 | GLU | CG-CD | 6.55 | 1.61 | 1.51 |
| 4 | B | 683 | GLU | CG-CD | 6.46 | 1.61 | 1.51 |
| 1 | K | 14 | DG | C2-N2 | -6.40 | 1.28 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4 | C | 30 | GLU | CG-CD | 6.34 | 1.61 | 1.51 |
| 4 | A | 384 | VAL | CA-CB | -6.24 | 1.41 | 1.54 |
| 1 | N | 11 | DA | C5-C6 | -6.15 | 1.35 | 1.41 |
| 4 | A | 448 | LYS | CD-CE | 6.12 | 1.66 | 1.51 |
| 4 | B | 516 | PHE | CB-CG | -6.06 | 1.41 | 1.51 |
| 4 | A | 727 | TRP | CB-CG | 6.05 | 1.61 | 1.50 |
| 2 | F | 1 | G | C5-C6 | 6.01 | 1.48 | 1.42 |
| 2 | F | 7 | A | N3-C4 | -5.89 | 1.31 | 1.34 |
| 4 | B | 635 | MET | CG-SD | 5.88 | 1.96 | 1.81 |
| 4 | A | 35 | GLU | CG-CD | 5.84 | 1.60 | 1.51 |
| 4 | C | 30 | GLU | CB-CG | 5.82 | 1.63 | 1.52 |
| 1 | K | 13 | DC | N1-C2 | -5.82 | 1.34 | 1.40 |
| 4 | D | 797 | TRP | CB-CG | -5.79 | 1.39 | 1.50 |
| 1 | E | 13 | DC | C4-N4 | -5.76 | 1.28 | 1.33 |
| 4 | A | 347 | CYS | CB-SG | -5.76 | 1.72 | 1.81 |
| 4 | A | 775 | GLU | CG-CD | 5.75 | 1.60 | 1.51 |
| 2 | I | 7 | A | C5'-C4' | -5.74 | 1.44 | 1.51 |
| 4 | D | 504 | GLU | CG-CD | 5.73 | 1.60 | 1.51 |
| 4 | D | 504 | GLU | CB-CG | 5.71 | 1.63 | 1.52 |
| 1 | H | 11 | DA | C5-C4 | -5.68 | 1.34 | 1.38 |
| 2 | F | 8 | U | C2-O2 | -5.66 | 1.17 | 1.22 |
| 4 | B | 51 | PHE | CB-CG | -5.66 | 1.41 | 1.51 |
| 4 | C | 802 | TYR | CB-CG | -5.64 | 1.43 | 1.51 |
| 1 | E | 10 | DT | N1-C2 | -5.63 | 1.33 | 1.38 |
| 1 | E | 12 | DT | C4-C5 | -5.62 | 1.39 | 1.45 |
| 4 | B | 66 | ASP | CB-CG | 5.60 | 1.63 | 1.51 |
| 1 | N | 14 | DG | C5-C6 | -5.57 | 1.36 | 1.42 |
| 2 | I | 7 | A | N1-C2 | -5.54 | 1.29 | 1.34 |
| 4 | A | 459 | TRP | CB-CG | 5.50 | 1.60 | 1.50 |
| 4 | A | 477 | GLU | CG-CD | 5.47 | 1.60 | 1.51 |
| 1 | H | 12 | DT | C3'-O3' | -5.47 | 1.36 | 1.44 |
| 4 | B | 271 | CYS | CB-SG | -5.45 | 1.73 | 1.81 |
| 4 | B | 63 | GLU | CB-CG | 5.44 | 1.62 | 1.52 |
| 4 | A | 514 | PHE | CB-CG | -5.43 | 1.42 | 1.51 |
| 2 | F | 7 | A | C8-N7 | 5.41 | 1.35 | 1.31 |
| 4 | B | 559 | VAL | CB-CG2 | -5.36 | 1.41 | 1.52 |
| 4 | B | 432 | PHE | CE2-CZ | -5.34 | 1.27 | 1.37 |
| 4 | C | 347 | CYS | CB-SG | 5.33 | 1.91 | 1.82 |
| 4 | B | 416 | PHE | CE2-CZ | 5.33 | 1.47 | 1.37 |
| 2 | F | 8 | U | C2-N3 | -5.30 | 1.34 | 1.37 |
| 4 | A | 805 | GLU | CG-CD | 5.29 | 1.59 | 1.51 |
| 4 | B | 287 | TRP | CB-CG | -5.26 | 1.40 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4 | B | 820 | ASP | CB-CG | 5.25 | 1.62 | 1.51 |
| 4 | B | 326 | THR | CA-CB | 5.23 | 1.67 | 1.53 |
| 4 | B | 836 | TYR | CD1-CE1 | 5.23 | 1.47 | 1.39 |
| 4 | A | 91 | GLU | CB-CG | 5.22 | 1.62 | 1.52 |
| 1 | E | 14 | DG | N3-C4 | -5.20 | 1.31 | 1.35 |
| 1 | H | 14 | DG | N9-C4 | -5.19 | 1.33 | 1.38 |
| 4 | B | 408 | PHE | CB-CG | -5.17 | 1.42 | 1.51 |
| 4 | A | 639 | TYR | CG-CD1 | -5.15 | 1.32 | 1.39 |
| 1 | E | 12 | DT | C3'-O3' | -5.15 | 1.37 | 1.44 |
| 1 | N | 13 | DC | C3'-O3' | -5.14 | 1.37 | 1.44 |
| 4 | A | 808 | ALA | CA-CB | -5.11 | 1.41 | 1.52 |
| 1 | H | 12 | DT | C5-C6 | -5.10 | 1.30 | 1.34 |
| 4 | B | 408 | PHE | CD2-CE2 | -5.10 | 1.29 | 1.39 |
| 4 | B | 855 | GLU | CG-CD | 5.10 | 1.59 | 1.51 |
| 4 | A | 530 | CYS | CB-SG | -5.08 | 1.73 | 1.81 |
| 4 | B | 805 | GLU | CB-CG | 5.03 | 1.61 | 1.52 |
| 4 | A | 422 | TRP | CZ3-CH2 | 5.03 | 1.48 | 1.40 |
| 4 | A | 795 | VAL | CB-CG2 | -5.02 | 1.42 | 1.52 |
| 1 | E | 11 | DA | C3'-O3' | -5.02 | 1.37 | 1.44 |
| 1 | K | 15 | DC | N1-C2 | -5.02 | 1.35 | 1.40 |
| 4 | A | 623 | TYR | CD2-CE2 | 5.01 | 1.46 | 1.39 |
| 4 | A | 483 | GLU | CG-CD | 5.01 | 1.59 | 1.51 |
| 2 | I | 8 | U | C3'-O3' | 5.00 | 1.49 | 1.42 |

All (92) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 4 | A | 460 | LEU | CB-CG-CD1 | -10.01 | 93.98 | 111.00 |
| 1 | E | 14 | DG | O5'-P-OP1 | -9.17 | 97.45 | 105.70 |
| 4 | A | 460 | LEU | CB-CG-CD2 | 9.03 | 126.35 | 111.00 |
| 4 | D | 791 | LEU | CA-CB-CG | 8.79 | 135.52 | 115.30 |
| 4 | A | 425 | ARG | NE-CZ-NH1 | -8.45 | 116.07 | 120.30 |
| 1 | E | 13 | DC | C5'-C4'-O4' | -8.23 | 93.67 | 109.30 |
| 4 | B | 425 | ARG | NE-CZ-NH2 | -8.00 | 116.30 | 120.30 |
| 4 | B | 444 | LEU | CA-CB-CG | -7.97 | 96.96 | 115.30 |
| 2 | F | 4 | G | O4'-C4'-C3' | -7.96 | 96.04 | 104.00 |
| 4 | B | 635 | MET | CA-CB-CG | 7.91 | 126.75 | 113.30 |
| 4 | A | 627 | ARG | NE-CZ-NH1 | 7.66 | 124.13 | 120.30 |
| 2 | F | 8 | U | N1-C1'-C2' | -7.58 | 103.66 | 112.00 |
| 4 | A | 507 | SER | C-N-CD | -7.58 | 103.93 | 120.60 |
| 1 | H | 13 | DC | OP2-P-O3' | 7.03 | 120.66 | 105.20 |
| 4 | A | 448 | LYS | CD-CE-NZ | 6.95 | 127.68 | 111.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1 | H | 13 | DC | N1-C1'-C2' | -6.88 | 99.52 | 112.60 |
| 4 | B | 423 | ARG | NE-CZ-NH1 | 6.77 | 123.69 | 120.30 |
| 4 | A | 778 | ILE | CG1-CB-CG2 | -6.74 | 96.58 | 111.40 |
| 2 | I | 8 | U | C2'-C3'-O3' | 6.72 | 124.46 | 113.70 |
| 1 | H | 14 | DG | O5'-P-OP2 | -6.66 | 99.71 | 105.70 |
| 2 | F | 8 | U | C4'-C3'-O3' | 6.65 | 126.30 | 113.00 |
| 2 | F | 5 | C | N1-C2-O2 | -6.63 | 114.92 | 118.90 |
| 4 | D | 492 | CYS | CA-CB-SG | -6.50 | 102.29 | 114.00 |
| 1 | H | 15 | DC | N1-C1'-C2' | -6.49 | 100.26 | 112.60 |
| 1 | K | 12 | DT | OP1-P-O3' | 6.48 | 119.46 | 105.20 |
| 4 | A | 423 | ARG | NE-CZ-NH1 | -6.45 | 117.08 | 120.30 |
| 4 | B | 569 | ASP | CB-CG-OD1 | 6.42 | 124.08 | 118.30 |
| 4 | C | 534 | LEU | CA-CB-CG | 6.36 | 129.94 | 115.30 |
| 1 | H | 14 | DG | N9-C1'-C2' | -6.36 | 100.52 | 112.60 |
| 4 | B | 330 | ILE | CB-CA-C | -6.30 | 99.01 | 111.60 |
| 2 | F | 6 | G | O4'-C4'-C3' | -6.29 | 97.71 | 104.00 |
| 4 | A | 441 | LYS | CD-CE-NZ | -6.26 | 97.30 | 111.70 |
| 4 | B | 16 | LEU | CA-CB-CG | 6.24 | 129.65 | 115.30 |
| 4 | A | 569 | ASP | CB-CG-OD1 | -6.23 | 112.69 | 118.30 |
| 4 | B | 425 | ARG | NE-CZ-NH1 | 6.21 | 123.40 | 120.30 |
| 4 | D | 39 | LEU | CA-CB-CG | 6.17 | 129.50 | 115.30 |
| 4 | A | 387 | LYS | CD-CE-NZ | 6.06 | 125.64 | 111.70 |
| 4 | B | 296 | LEU | CA-CB-CG | -6.04 | 101.40 | 115.30 |
| 2 | I | 8 | U | O4'-C4'-C3' | -6.04 | 97.96 | 104.00 |
| 4 | C | 632 | ARG | NE-CZ-NH1 | 6.01 | 123.30 | 120.30 |
| 4 | B | 347 | CYS | CA-CB-SG | -6.00 | 103.19 | 114.00 |
| 4 | A | 660 | ASP | CB-CG-OD1 | 5.99 | 123.69 | 118.30 |
| 2 | F | 7 | A | C5'-C4'-C3' | -5.96 | 106.46 | 116.00 |
| 4 | B | 810 | ILE | CG1-CB-CG2 | -5.95 | 98.30 | 111.40 |
| 1 | E | 17 | DG | C5'-C4'-C3' | -5.93 | 103.43 | 114.10 |
| 4 | D | 792 | ARG | NE-CZ-NH1 | 5.92 | 123.26 | 120.30 |
| 1 | N | 11 | DA | N9-C1'-C2' | -5.90 | 101.39 | 112.60 |
| 4 | C | 307 | ARG | NE-CZ-NH1 | 5.78 | 123.19 | 120.30 |
| 4 | B | 637 | LEU | CA-CB-CG | -5.73 | 102.11 | 115.30 |
| 4 | C | 296 | LEU | CA-CB-CG | -5.71 | 102.17 | 115.30 |
| 1 | E | 18 | DC | C2'-C3'-O3' | -5.70 | 93.81 | 112.60 |
| 2 | F | 6 | G | OP1-P-O3' | -5.69 | 92.69 | 105.20 |
| 4 | A | 450 | LYS | C-N-CA | -5.68 | 98.14 | 122.00 |
| 1 | N | 12 | DT | O5'-P-OP2 | -5.67 | 100.60 | 105.70 |
| 1 | H | 15 | DC | OP2-P-O3' | 5.65 | 117.64 | 105.20 |
| 4 | B | 532 | LEU | CA-CB-CG | -5.65 | 102.31 | 115.30 |
| 4 | A | 651 | LEU | CA-CB-CG | 5.59 | 128.17 | 115.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4 | A | 470 | VAL | CB-CA-C | -5.54 | 100.88 | 111.40 |
| 4 | B | 562 | LEU | CA-CB-CG | 5.53 | 128.02 | 115.30 |
| 1 | E | 16 | DC | N1-C1'-C2' | -5.52 | 102.11 | 112.60 |
| 4 | B | 345 | LYS | CD-CE-NZ | 5.52 | 124.39 | 111.70 |
| 4 | C | 444 | LEU | CB-CG-CD1 | -5.44 | 101.75 | 111.00 |
| 2 | F | 5 | C | N3-C2-O2 | 5.42 | 125.69 | 121.90 |
| 2 | F | 8 | U | C1'-C2'-O2' | 5.42 | 126.85 | 110.60 |
| 4 | B | 332 | LYS | CD-CE-NZ | 5.42 | 124.16 | 111.70 |
| 4 | A | 396 | ILE | CG1-CB-CG2 | -5.42 | 99.49 | 111.40 |
| 4 | B | 632 | ARG | NE-CZ-NH1 | 5.41 | 123.00 | 120.30 |
| 1 | E | 11 | DA | O5'-P-OP2 | -5.41 | 100.83 | 105.70 |
| 4 | A | 475 | PHE | C-N-CD | 5.36 | 139.66 | 128.40 |
| 2 | F | 8 | U | O5'-P-OP1 | 5.35 | 117.12 | 110.70 |
| 1 | E | 14 | DG | O5'-P-OP2 | 5.31 | 117.08 | 110.70 |
| 4 | B | 426 | VAL | CB-CA-C | -5.29 | 101.34 | 111.40 |
| 4 | A | 836 | TYR | CA-CB-CG | -5.24 | 103.45 | 113.40 |
| 4 | B | 402 | LEU | CA-CB-CG | -5.23 | 103.27 | 115.30 |
| 4 | A | 318 | LYS | CD-CE-NZ | 5.22 | 123.71 | 111.70 |
| 4 | C | 471 | ASP | CB-CG-OD1 | 5.20 | 122.98 | 118.30 |
| 1 | N | 11 | DA | O4'-C1'-N9 | 5.19 | 111.63 | 108.00 |
| 4 | B | 448 | LYS | CD-CE-NZ | 5.17 | 123.59 | 111.70 |
| 4 | B | 59 | LEU | CA-CB-CG | -5.17 | 103.41 | 115.30 |
| 1 | N | 13 | DC | N1-C1'-C2' | -5.16 | 102.80 | 112.60 |
| 4 | C | 627 | ARG | NE-CZ-NH1 | 5.14 | 122.87 | 120.30 |
| 4 | A | 513 | ALA | O-C-N | 5.12 | 130.89 | 122.70 |
| 1 | E | 12 | DT | C6-N1-C1' | 5.09 | 128.03 | 120.40 |
| 4 | A | 489 | ILE | CB-CA-C | -5.09 | 101.43 | 111.60 |
| 4 | A | 514 | PHE | CB-CG-CD2 | -5.08 | 117.25 | 120.80 |
| 4 | B | 719 | LEU | CA-CB-CG | -5.07 | 103.64 | 115.30 |
| 2 | F | 6 | G | N1-C2-N3 | 5.04 | 126.93 | 123.90 |
| 4 | A | 787 | ASP | CB-CG-OD1 | 5.04 | 122.84 | 118.30 |
| 1 | E | 15 | DC | N1-C1'-C2' | -5.03 | 103.04 | 112.60 |
| 4 | A | 446 | LEU | CB-CG-CD2 | -5.03 | 102.45 | 111.00 |
| 4 | B | 650 | VAL | CB-CA-C | -5.02 | 101.85 | 111.40 |
| 4 | B | 576 | LYS | CD-CE-NZ | 5.02 | 123.24 | 111.70 |

There are no chirality outliers.

All (39) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 4 | A | 836 | TYR | Sidechain |
| 4 | B | 836 | TYR | Sidechain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 4 | D | 518 | TYR | Sidechain |
| 1 | E | 11 | DA | Sidechain |
| 1 | E | 12 | DT | Sidechain |
| 1 | E | 13 | DC | Sidechain |
| 1 | E | 14 | DG | Sidechain |
| 1 | E | 16 | DC | Sidechain |
| 1 | E | 17 | DG | Sidechain |
| 2 | F | 3 | G | Sidechain |
| 2 | F | 6 | G | Sidechain |
| 2 | F | 7 | A | Sidechain |
| 2 | F | 8 | U | Sidechain |
| 1 | H | 10 | DT | Sidechain |
| 1 | H | 11 | DA | Sidechain |
| 1 | H | 12 | DT | Sidechain |
| 1 | H | 13 | DC | Sidechain |
| 1 | H | 14 | DG | Sidechain |
| 1 | H | 15 | DC | Sidechain |
| 1 | H | 16 | DC | Sidechain |
| 1 | H | 17 | DG | Sidechain |
| 1 | H | 6 | DT | Sidechain |
| 2 | I | 5 | C | Sidechain |
| 2 | I | 6 | G | Sidechain |
| 1 | K | 11 | DA | Sidechain |
| 1 | K | 13 | DC | Sidechain |
| 1 | K | 14 | DG | Sidechain |
| 1 | K | 15 | DC | Sidechain |
| 1 | K | 16 | DC | Sidechain |
| 1 | K | 17 | DG | Sidechain |
| 2 | L | 8 | U | Sidechain |
| 1 | N | 13 | DC | Sidechain |
| 1 | N | 14 | DG | Sidechain |
| 1 | N | 15 | DC | Sidechain |
| 1 | N | 17 | DG | Sidechain |
| 2 | O | 4 | G | Sidechain |
| 2 | O | 6 | G | Sidechain |
| 2 | O | 8 | U | Sidechain |
| 3 | P | 2 | DT | Sidechain |

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | E | 346 | 0 | 190 | 28 | 0 |
| 1 | H | 346 | 0 | 192 | 66 | 0 |
| 1 | K | 346 | 0 | 190 | 57 | 0 |
| 1 | N | 346 | 0 | 192 | 38 | 0 |
| 2 | F | 171 | 0 | 89 | 10 | 0 |
| 2 | I | 171 | 0 | 89 | 11 | 0 |
| 2 | L | 171 | 0 | 89 | 14 | 0 |
| 2 | O | 171 | 0 | 89 | 5 | 0 |
| 3 | G | 179 | 0 | 104 | 13 | 0 |
| 3 | J | 179 | 0 | 104 | 17 | 0 |
| 3 | M | 179 | 0 | 104 | 13 | 0 |
| 3 | P | 179 | 0 | 104 | 8 | 0 |
| 4 | A | 6746 | 0 | 6708 | 1151 | 0 |
| 4 | B | 6746 | 0 | 6708 | 1190 | 0 |
| 4 | C | 6746 | 0 | 6708 | 1007 | 0 |
| 4 | D | 6746 | 0 | 6708 | 899 | 0 |
| 5 | A | 1 | 0 | 0 | 0 | 0 |
| 5 | B | 2 | 0 | 0 | 0 | 0 |
| 5 | C | 2 | 0 | 0 | 0 | 0 |
| 5 | D | 2 | 0 | 0 | 0 | 0 |
| 5 | F | 1 | 0 | 0 | 0 | 0 |
| 6 | A | 31 | 0 | 13 | 16 | 0 |
| 6 | B | 31 | 0 | 13 | 9 | 0 |
| 6 | C | 31 | 0 | 14 | 16 | 0 |
| 6 | D | 31 | 0 | 13 | 7 | 0 |
| 7 | A | 237 | 0 | 0 | 82 | 0 |
| 7 | B | 212 | 0 | 0 | 68 | 0 |
| 7 | C | 201 | 0 | 0 | 70 | 0 |
| 7 | D | 173 | 0 | 0 | 53 | 0 |
| 7 | E | 39 | 0 | 0 | 1 | 0 |
| 7 | F | 9 | 0 | 0 | 1 | 0 |
| 7 | G | 9 | 0 | 0 | 1 | 0 |
| 7 | H | 19 | 0 | 0 | 9 | 0 |
| 7 | I | 14 | 0 | 0 | 4 | 0 |
| 7 | J | 13 | 0 | 0 | 0 | 0 |
| 7 | K | 20 | 0 | 0 | 7 | 0 |
| 7 | L | 8 | 0 | 0 | 0 | 0 |
| 7 | M | 10 | 0 | 0 | 2 | 0 |
| 7 | N | 14 | 0 | 0 | 3 | 0 |
| 7 | O | 15 | 0 | 0 | 2 | 0 |
| 7 | P | 6 | 0 | 0 | 2 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| All | All | 30899 | 0 | 28421 | 4458 | 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 76.

All (4458) 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) |
|------------------|-------------------|--------------------------|-------------------|
| 4:A:313:MET:SD | 4:A:313:MET:CE | 2.05 | 1.44 |
| 4:C:631:LYS:NZ | 6:C:2002:APC:H3A2 | 1.52 | 1.22 |
| 2:F:1:G:H5'' | 7:F:3008:HOH:O | 1.40 | 1.19 |
| 4:A:631:LYS:NZ | 6:A:2000:APC:H3A2 | 1.58 | 1.18 |
| 4:A:546:PHE:CE1 | 4:A:783:VAL:HG22 | 1.78 | 1.16 |
| 4:A:631:LYS:HZ1 | 6:A:2000:APC:H3A2 | 0.97 | 1.13 |
| 4:B:452:ILE:HG23 | 4:B:453:GLY:N | 1.57 | 1.13 |
| 4:A:281:ILE:HG22 | 4:A:282:THR:HG23 | 1.20 | 1.13 |
| 4:D:720:ARG:HH11 | 4:D:720:ARG:HG2 | 0.95 | 1.12 |
| 4:B:59:LEU:HD23 | 4:B:64:VAL:HG22 | 1.17 | 1.12 |
| 4:A:109:ILE:HD13 | 4:A:145:ILE:HG22 | 1.31 | 1.11 |
| 4:A:471:ASP:OD1 | 4:A:472:LYS:HD2 | 1.47 | 1.11 |
| 4:C:281:ILE:HG22 | 4:C:282:THR:HG22 | 1.18 | 1.11 |
| 4:A:722:ARG:HB2 | 4:A:769:ILE:HD13 | 1.27 | 1.11 |
| 1:K:12:DT:H2'' | 1:K:13:DC:H5' | 1.16 | 1.11 |
| 4:A:804:ILE:HG12 | 4:A:820:ASP:HB3 | 1.33 | 1.10 |
| 4:B:452:ILE:CG2 | 4:B:453:GLY:H | 1.64 | 1.10 |
| 1:N:12:DT:H2'' | 1:N:13:DC:H5' | 1.33 | 1.10 |
| 4:A:647:ARG:HD2 | 4:A:675:GLY:HA2 | 1.34 | 1.10 |
| 4:B:816:THR:HG22 | 4:B:817:ILE:H | 1.09 | 1.09 |
| 4:A:560:ASN:O | 4:A:881:ALA:HB2 | 1.50 | 1.09 |
| 4:D:36:GLN:OE1 | 4:D:273:VAL:HG22 | 1.52 | 1.09 |
| 4:C:158:GLU:HG2 | 4:C:195:LEU:HD22 | 1.10 | 1.08 |
| 4:A:871:ASN:HD21 | 4:A:873:ARG:HB2 | 1.08 | 1.08 |
| 4:D:718:ILE:H | 4:D:718:ILE:HD12 | 1.11 | 1.08 |
| 4:C:556:GLY:HA2 | 4:C:561:LEU:HD22 | 1.35 | 1.08 |
| 4:B:435:GLN:HG2 | 4:B:810:ILE:HG23 | 1.36 | 1.07 |
| 4:C:19:ILE:HG12 | 4:C:20:PRO:HD2 | 1.30 | 1.07 |
| 1:E:12:DT:H2'' | 1:E:13:DC:H5' | 1.37 | 1.06 |
| 4:B:720:ARG:HH11 | 4:B:720:ARG:HG2 | 1.19 | 1.06 |
| 4:B:706:LEU:HD21 | 4:B:849:PHE:HB2 | 1.33 | 1.06 |
| 4:B:433:ASN:HB2 | 4:B:434:PRO:HD3 | 1.34 | 1.06 |
| 4:B:433:ASN:HB2 | 4:B:434:PRO:CD | 1.87 | 1.05 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:13:DC:H2'' | 1:H:14:DG:H5' | 1.32 | 1.05 |
| 4:D:512:LEU:HA | 4:D:515:CYS:SG | 1.97 | 1.05 |
| 4:C:333:LYS:HB3 | 4:C:516:PHE:CE2 | 1.91 | 1.05 |
| 4:C:536:PHE:HB3 | 4:C:882:PHE:HB3 | 1.35 | 1.05 |
| 4:B:473:VAL:HG13 | 4:B:474:PRO:HD2 | 1.36 | 1.04 |
| 1:H:9:DA:H5'' | 7:H:484:HOH:O | 1.57 | 1.04 |
| 4:A:281:ILE:HG22 | 4:A:282:THR:CG2 | 1.86 | 1.03 |
| 4:B:829:ARG:HH22 | 4:B:882:PHE:HA | 1.16 | 1.03 |
| 4:D:120:LYS:HG3 | 4:D:752:LEU:HD21 | 1.38 | 1.03 |
| 4:C:158:GLU:HG2 | 4:C:195:LEU:CD2 | 1.89 | 1.03 |
| 4:A:16:LEU:HD13 | 4:A:38:ALA:HB2 | 1.41 | 1.02 |
| 4:B:268:PHE:HB3 | 4:B:286:TYR:OH | 1.59 | 1.02 |
| 4:B:829:ARG:NH2 | 4:B:882:PHE:HA | 1.73 | 1.02 |
| 4:C:792:ARG:O | 4:C:796:VAL:HG23 | 1.59 | 1.02 |
| 4:C:54:MET:O | 4:C:58:GLN:HG2 | 1.58 | 1.01 |
| 4:D:737:GLN:HE22 | 4:D:778:ILE:HA | 1.23 | 1.01 |
| 4:A:794:THR:OG1 | 4:A:831:THR:HG21 | 1.58 | 1.01 |
| 4:A:829:ARG:HH11 | 4:A:829:ARG:HG3 | 1.18 | 1.01 |
| 4:B:751:PHE:HB3 | 4:B:752:LEU:HD12 | 1.36 | 1.01 |
| 1:E:12:DT:H2'' | 1:E:13:DC:C5' | 1.90 | 1.01 |
| 4:A:688:THR:HG22 | 4:A:689:VAL:HG13 | 1.41 | 1.01 |
| 4:C:342:THR:HG22 | 4:C:348:PRO:HG2 | 1.40 | 1.00 |
| 4:D:560:ASN:O | 4:D:881:ALA:HB2 | 1.60 | 1.00 |
| 4:D:794:THR:OG1 | 4:D:831:THR:HG21 | 1.58 | 1.00 |
| 4:A:304:ALA:O | 4:A:307:ARG:HG3 | 1.62 | 1.00 |
| 4:C:437:ASN:H | 4:C:437:ASN:HD22 | 1.10 | 1.00 |
| 4:C:457:TYR:CD1 | 4:C:521:VAL:HG11 | 1.97 | 1.00 |
| 4:B:418:TYR:HE2 | 4:B:428:ALA:HB2 | 1.27 | 1.00 |
| 4:C:651:LEU:O | 4:C:651:LEU:HD13 | 1.61 | 1.00 |
| 4:A:690:VAL:HG23 | 7:A:3200:HOH:O | 1.61 | 0.99 |
| 4:A:687:VAL:HG23 | 7:A:3114:HOH:O | 1.61 | 0.99 |
| 4:A:786:GLN:HE21 | 4:A:786:GLN:HA | 1.27 | 0.99 |
| 4:D:198:GLY:HA3 | 7:D:3152:HOH:O | 1.61 | 0.99 |
| 4:A:841:VAL:HG12 | 7:A:3070:HOH:O | 1.60 | 0.99 |
| 4:C:84:ARG:HH12 | 4:C:87:ASP:HB2 | 1.27 | 0.99 |
| 4:B:669:GLN:HG2 | 4:B:672:GLN:HG3 | 1.45 | 0.98 |
| 4:D:790:HIS:HE1 | 4:D:831:THR:HG23 | 1.28 | 0.98 |
| 4:A:463:HIS:HA | 4:A:466:ASN:HD22 | 1.27 | 0.98 |
| 4:C:281:ILE:HG22 | 4:C:282:THR:CG2 | 1.92 | 0.98 |
| 4:D:32:LEU:HD12 | 4:D:32:LEU:H | 1.29 | 0.97 |
| 4:A:280:GLY:HA2 | 4:A:317:TYR:OH | 1.62 | 0.97 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:B:11:PHE:HB3 | 4:B:41:HIS:HE1 | 1.28 | 0.97 |
| 4:A:169:GLN:O | 4:A:173:ARG:HG2 | 1.65 | 0.97 |
| 4:B:14:ILE:HD12 | 4:B:14:ILE:H | 1.28 | 0.97 |
| 4:C:423:ARG:HB2 | 4:C:423:ARG:HH11 | 1.26 | 0.97 |
| 4:C:551:ARG:NE | 4:C:872:LEU:HD21 | 1.80 | 0.96 |
| 4:B:84:ARG:HD2 | 4:B:219:MET:HG2 | 1.47 | 0.96 |
| 4:B:407:LYS:HG2 | 4:B:408:PHE:CE2 | 2.00 | 0.96 |
| 4:A:562:LEU:HD21 | 4:A:870:LEU:CD1 | 1.94 | 0.96 |
| 4:A:80:LYS:HE2 | 4:A:223:SER:O | 1.66 | 0.95 |
| 4:B:59:LEU:HD23 | 4:B:64:VAL:CG2 | 1.95 | 0.95 |
| 4:C:631:LYS:HZ1 | 6:C:2002:APC:H3A2 | 1.29 | 0.95 |
| 4:A:308:TYR:HE2 | 4:A:734:PRO:HG2 | 1.29 | 0.95 |
| 4:A:379:ARG:HD3 | 4:A:660:ASP:OD2 | 1.66 | 0.95 |
| 1:K:15:DC:H2'' | 1:K:16:DC:O5' | 1.64 | 0.95 |
| 4:C:338:ALA:HB2 | 4:C:509:PHE:HE1 | 1.28 | 0.95 |
| 4:C:92:VAL:HG12 | 4:C:99:ARG:HG3 | 1.44 | 0.95 |
| 4:A:404:GLN:HA | 4:A:404:GLN:HE21 | 1.30 | 0.95 |
| 4:C:706:LEU:HD22 | 4:C:725:VAL:HG13 | 1.49 | 0.94 |
| 4:A:546:PHE:HE1 | 4:A:783:VAL:HG22 | 1.28 | 0.94 |
| 4:C:341:ILE:HD12 | 4:C:348:PRO:HB3 | 1.49 | 0.94 |
| 4:B:505:GLN:N | 4:B:505:GLN:NE2 | 2.14 | 0.94 |
| 1:K:12:DT:H2'' | 1:K:13:DC:C5' | 1.96 | 0.94 |
| 4:A:544:GLN:HG2 | 4:A:559:VAL:HG21 | 1.47 | 0.94 |
| 4:C:133:THR:HA | 4:C:243:THR:HG22 | 1.49 | 0.94 |
| 4:D:16:LEU:HD13 | 4:D:38:ALA:HB2 | 1.50 | 0.94 |
| 4:C:629:VAL:HG22 | 4:C:654:THR:HG21 | 1.50 | 0.93 |
| 4:B:490:MET:SD | 4:B:522:GLN:HG3 | 2.07 | 0.93 |
| 4:C:236:VAL:HB | 4:C:239:GLN:HB2 | 1.49 | 0.93 |
| 4:A:421:ASP:OD2 | 4:A:425:ARG:HB2 | 1.67 | 0.93 |
| 1:H:15:DC:H2'' | 1:H:16:DC:O5' | 1.66 | 0.93 |
| 4:A:105:PHE:HB3 | 4:A:204:TRP:HZ2 | 1.34 | 0.93 |
| 4:C:404:GLN:HG2 | 4:C:432:PHE:CG | 2.04 | 0.93 |
| 4:C:632:ARG:HH22 | 6:C:2002:APC:H5'1 | 1.31 | 0.93 |
| 4:B:116:TYR:OH | 4:B:752:LEU:HD22 | 1.69 | 0.93 |
| 4:B:492:CYS:O | 4:B:496:PRO:HD3 | 1.68 | 0.93 |
| 2:I:4:G:H2' | 2:I:5:C:H6 | 1.33 | 0.93 |
| 4:A:154:ILE:HG23 | 4:A:190:MET:CE | 1.99 | 0.92 |
| 4:A:457:TYR:CZ | 4:A:461:LYS:HD3 | 2.05 | 0.92 |
| 4:A:457:TYR:CE2 | 4:A:461:LYS:HD3 | 2.03 | 0.92 |
| 4:C:457:TYR:CE1 | 4:C:521:VAL:HG11 | 2.04 | 0.92 |
| 4:D:380:ALA:O | 4:D:384:VAL:HG23 | 1.69 | 0.92 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:C:281:ILE:CG2 | 4:C:282:THR:HG22 | 2.00 | 0.92 |
| 4:D:264:ILE:HG23 | 4:D:292:ARG:HB2 | 1.52 | 0.92 |
| 4:B:163:LYS:HZ3 | 4:B:166:VAL:HB | 1.35 | 0.92 |
| 4:D:718:ILE:HD12 | 4:D:718:ILE:N | 1.85 | 0.92 |
| 1:H:13:DC:H2'' | 1:H:14:DG:C5' | 1.99 | 0.92 |
| 4:A:85:ILE:HG12 | 4:A:219:MET:SD | 2.10 | 0.92 |
| 4:C:778:ILE:HG23 | 4:C:779:ALA:N | 1.83 | 0.92 |
| 4:C:334:VAL:HG21 | 4:C:513:ALA:HB2 | 1.49 | 0.92 |
| 4:A:5:ASN:HD21 | 4:A:7:ALA:HB3 | 1.34 | 0.91 |
| 4:A:871:ASN:HD21 | 4:A:873:ARG:CB | 1.83 | 0.91 |
| 4:C:333:LYS:HD3 | 4:C:516:PHE:HD2 | 1.34 | 0.91 |
| 4:D:810:ILE:HB | 4:D:813:SER:OG | 1.70 | 0.91 |
| 4:A:828:VAL:HG23 | 4:A:829:ARG:H | 1.33 | 0.91 |
| 4:B:11:PHE:HB3 | 4:B:41:HIS:CE1 | 2.05 | 0.91 |
| 4:C:556:GLY:CA | 4:C:561:LEU:HD22 | 2.00 | 0.91 |
| 4:A:280:GLY:O | 4:A:282:THR:N | 2.04 | 0.91 |
| 4:B:706:LEU:HD11 | 4:B:849:PHE:CD2 | 2.05 | 0.91 |
| 4:C:560:ASN:O | 4:C:881:ALA:HB2 | 1.70 | 0.91 |
| 4:A:341:ILE:HD12 | 4:A:348:PRO:HB3 | 1.49 | 0.91 |
| 4:C:249:GLU:CD | 4:C:249:GLU:H | 1.73 | 0.91 |
| 4:A:502:TRP:CD2 | 4:A:512:LEU:HD13 | 2.06 | 0.91 |
| 4:B:646:PHE:O | 4:B:650:VAL:HG23 | 1.69 | 0.91 |
| 4:D:718:ILE:H | 4:D:718:ILE:CD1 | 1.84 | 0.91 |
| 4:A:825:PHE:CE1 | 4:A:829:ARG:NH1 | 2.39 | 0.91 |
| 4:D:552:ASP:HB2 | 4:D:691:ALA:HB2 | 1.53 | 0.91 |
| 4:D:720:ARG:NH1 | 4:D:720:ARG:HG2 | 1.74 | 0.91 |
| 4:B:448:LYS:HD2 | 7:B:3017:HOH:O | 1.70 | 0.90 |
| 4:B:85:ILE:HG12 | 4:B:219:MET:SD | 2.11 | 0.90 |
| 4:A:103:PHE:O | 4:A:107:GLN:HG3 | 1.71 | 0.90 |
| 6:A:2000:APC:H4' | 7:A:3238:HOH:O | 1.70 | 0.90 |
| 4:A:423:ARG:NH2 | 4:A:784:HIS:ND1 | 2.18 | 0.90 |
| 4:C:751:PHE:HB3 | 4:C:752:LEU:HD12 | 1.51 | 0.90 |
| 4:A:294:LEU:HD13 | 4:A:429:VAL:HG21 | 1.52 | 0.90 |
| 4:A:829:ARG:HH11 | 4:A:829:ARG:CG | 1.84 | 0.90 |
| 4:C:460:LEU:HA | 4:C:534:LEU:HD21 | 1.54 | 0.90 |
| 4:B:137:VAL:HG12 | 4:B:217:ILE:HD11 | 1.54 | 0.90 |
| 4:A:464:GLY:HA3 | 4:A:514:PHE:CE2 | 2.07 | 0.90 |
| 4:C:536:PHE:HB3 | 4:C:882:PHE:CB | 2.01 | 0.90 |
| 4:D:273:VAL:HA | 4:D:415:TRP:CZ3 | 2.06 | 0.90 |
| 4:A:204:TRP:CH2 | 4:A:212:VAL:HG21 | 2.06 | 0.90 |
| 4:B:702:ALA:HB1 | 4:B:849:PHE:CE2 | 2.07 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:C:551:ARG:HH21 | 4:C:872:LEU:HD11 | 1.37 | 0.90 |
| 4:A:452:ILE:HG22 | 4:A:528:TYR:O | 1.72 | 0.89 |
| 4:B:163:LYS:NZ | 4:B:166:VAL:HB | 1.87 | 0.89 |
| 3:P:9:DC:H4' | 7:P:872:HOH:O | 1.72 | 0.89 |
| 4:B:793:LYS:HA | 7:B:3141:HOH:O | 1.71 | 0.89 |
| 4:D:473:VAL:HG22 | 4:D:477:GLU:HG3 | 1.54 | 0.89 |
| 4:B:296:LEU:HG | 4:B:296:LEU:O | 1.69 | 0.89 |
| 4:C:333:LYS:HB3 | 4:C:516:PHE:CD2 | 2.07 | 0.89 |
| 4:B:571:TYR:CE2 | 4:B:631:LYS:HG3 | 2.08 | 0.89 |
| 4:C:452:ILE:HD11 | 4:C:457:TYR:HA | 1.52 | 0.89 |
| 4:C:96:ARG:HB3 | 7:C:3133:HOH:O | 1.72 | 0.89 |
| 4:D:864:LEU:HA | 7:D:3079:HOH:O | 1.72 | 0.89 |
| 4:D:854:HIS:CD2 | 4:D:856:SER:H | 1.90 | 0.89 |
| 4:B:77:LEU:HD12 | 4:B:224:THR:HG21 | 1.55 | 0.88 |
| 4:B:236:VAL:HB | 4:B:239:GLN:HB2 | 1.54 | 0.88 |
| 4:B:430:SER:O | 4:B:431:MET:C | 2.09 | 0.88 |
| 4:C:109:ILE:HD11 | 4:C:149:ALA:HB2 | 1.54 | 0.88 |
| 4:A:154:ILE:HG23 | 4:A:190:MET:HE1 | 1.54 | 0.88 |
| 4:B:585:ASP:O | 4:B:614:LYS:HA | 1.73 | 0.88 |
| 4:B:452:ILE:HG23 | 4:B:453:GLY:H | 0.76 | 0.88 |
| 4:C:421:ASP:O | 4:C:423:ARG:N | 2.07 | 0.88 |
| 4:B:231:ARG:HG2 | 4:B:234:ALA:HB2 | 1.55 | 0.88 |
| 4:A:60:LYS:HZ1 | 4:A:61:ALA:HB2 | 1.39 | 0.88 |
| 4:A:546:PHE:HD2 | 4:A:692:ALA:HA | 1.39 | 0.88 |
| 1:H:12:DT:C4' | 4:B:423:ARG:HE | 1.86 | 0.88 |
| 4:A:105:PHE:HB3 | 4:A:204:TRP:CZ2 | 2.09 | 0.88 |
| 4:A:563:PRO:HB3 | 4:A:878:SER:HA | 1.55 | 0.88 |
| 4:B:110:LYS:HD3 | 4:B:111:PRO:HD2 | 1.55 | 0.88 |
| 4:B:695:ALA:O | 4:B:699:LEU:HD13 | 1.72 | 0.88 |
| 4:D:231:ARG:HG2 | 4:D:234:ALA:HB2 | 1.53 | 0.88 |
| 4:A:452:ILE:HD11 | 4:A:457:TYR:HB2 | 1.55 | 0.88 |
| 4:C:221:ILE:HG12 | 4:C:227:VAL:HG23 | 1.55 | 0.87 |
| 1:N:7:DC:H2'' | 1:N:8:DG:O5' | 1.73 | 0.87 |
| 4:B:264:ILE:HG23 | 4:B:292:ARG:HB2 | 1.56 | 0.87 |
| 1:N:2:DG:H2'' | 1:N:3:DG:H8 | 1.40 | 0.87 |
| 4:A:155:ARG:HB2 | 4:A:163:LYS:HE3 | 1.55 | 0.87 |
| 4:D:333:LYS:HB3 | 4:D:516:PHE:CE2 | 2.10 | 0.87 |
| 1:E:12:DT:C2' | 1:E:13:DC:H5' | 2.04 | 0.87 |
| 4:C:437:ASN:H | 4:C:437:ASN:ND2 | 1.70 | 0.87 |
| 4:A:308:TYR:O | 4:A:311:VAL:HG23 | 1.75 | 0.87 |
| 4:B:829:ARG:HG3 | 4:B:829:ARG:HH11 | 1.38 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:B:420:MET:HA | 4:B:425:ARG:O | 1.75 | 0.87 |
| 4:A:231:ARG:HG2 | 4:A:234:ALA:HB2 | 1.54 | 0.87 |
| 4:A:871:ASN:ND2 | 4:A:873:ARG:HB2 | 1.90 | 0.86 |
| 4:B:118:THR:HG23 | 4:B:141:ILE:HD13 | 1.55 | 0.86 |
| 4:B:408:PHE:HD1 | 4:B:414:ILE:HG21 | 1.40 | 0.86 |
| 4:D:536:PHE:HB3 | 4:D:882:PHE:HB3 | 1.57 | 0.86 |
| 1:H:2:DG:H2'' | 1:H:3:DG:C8 | 2.10 | 0.86 |
| 4:C:84:ARG:HD3 | 4:C:84:ARG:O | 1.75 | 0.86 |
| 4:D:437:ASN:ND2 | 4:D:440:THR:H | 1.73 | 0.86 |
| 4:D:89:PHE:O | 4:D:93:LYS:HG3 | 1.74 | 0.86 |
| 4:D:204:TRP:HE3 | 7:D:3053:HOH:O | 1.56 | 0.86 |
| 4:D:39:LEU:HD23 | 7:D:3105:HOH:O | 1.74 | 0.86 |
| 4:D:724:ALA:HB2 | 4:D:738:GLU:HG3 | 1.57 | 0.86 |
| 4:A:383:ALA:O | 4:A:385:TYR:N | 2.08 | 0.86 |
| 4:B:300:HIS:HE2 | 4:B:422:TRP:HZ3 | 1.21 | 0.86 |
| 4:C:828:VAL:HG23 | 4:C:829:ARG:H | 1.40 | 0.86 |
| 4:D:137:VAL:O | 4:D:141:ILE:HG13 | 1.75 | 0.86 |
| 4:A:791:LEU:HD11 | 4:A:809:LEU:HD22 | 1.55 | 0.86 |
| 4:C:317:TYR:O | 4:C:321:ASN:ND2 | 2.07 | 0.86 |
| 4:C:574:VAL:O | 4:C:578:VAL:HG23 | 1.75 | 0.86 |
| 4:B:706:LEU:HD21 | 4:B:849:PHE:CB | 2.05 | 0.86 |
| 4:C:570:ILE:HA | 4:C:573:ILE:CG2 | 2.05 | 0.86 |
| 4:D:308:TYR:HE2 | 4:D:734:PRO:HG2 | 1.39 | 0.86 |
| 4:A:109:ILE:HD11 | 4:A:145:ILE:O | 1.76 | 0.85 |
| 4:B:122:THR:HG21 | 4:B:226:MET:HE2 | 1.56 | 0.85 |
| 4:C:845:PHE:O | 4:C:848:GLN:HB2 | 1.75 | 0.85 |
| 4:C:84:ARG:NH1 | 4:C:87:ASP:HB2 | 1.91 | 0.85 |
| 4:B:463:HIS:CB | 4:B:534:LEU:HD22 | 2.06 | 0.85 |
| 4:C:690:VAL:O | 4:C:693:VAL:HB | 1.76 | 0.85 |
| 4:B:408:PHE:HD2 | 4:B:408:PHE:N | 1.72 | 0.85 |
| 4:D:804:ILE:HG23 | 4:D:816:THR:HG21 | 1.57 | 0.85 |
| 4:A:647:ARG:CD | 4:A:675:GLY:HA2 | 2.05 | 0.85 |
| 4:B:737:GLN:HE21 | 4:B:739:TYR:HE2 | 1.22 | 0.85 |
| 4:C:338:ALA:O | 4:C:340:VAL:N | 2.10 | 0.85 |
| 1:N:12:DT:H2'' | 1:N:13:DC:C5' | 2.06 | 0.85 |
| 4:C:227:VAL:HB | 4:C:244:ILE:HD12 | 1.58 | 0.85 |
| 4:C:276:LYS:HE2 | 7:C:3084:HOH:O | 1.76 | 0.85 |
| 3:P:1:DG:H1' | 3:P:2:DT:H71 | 1.56 | 0.85 |
| 4:A:59:LEU:HA | 4:A:64:VAL:CG2 | 2.06 | 0.85 |
| 4:B:37:LEU:H | 4:B:37:LEU:HD12 | 1.42 | 0.85 |
| 4:C:404:GLN:HE21 | 4:C:404:GLN:HA | 1.39 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:D:117:ILE:HG21 | 4:D:145:ILE:HD13 | 1.58 | 0.85 |
| 4:A:386:ARG:O | 4:A:389:LYS:N | 2.09 | 0.85 |
| 4:A:574:VAL:HG11 | 4:A:685:VAL:HG12 | 1.56 | 0.85 |
| 4:B:333:LYS:O | 4:B:337:VAL:HG23 | 1.77 | 0.85 |
| 4:B:111:PRO:HG2 | 4:B:112:GLU:OE1 | 1.77 | 0.84 |
| 4:D:705:LEU:HB3 | 4:D:857:GLN:NE2 | 1.92 | 0.84 |
| 4:B:473:VAL:HG13 | 4:B:474:PRO:CD | 2.07 | 0.84 |
| 4:A:256:THR:HG23 | 7:A:3067:HOH:O | 1.77 | 0.84 |
| 4:A:505:GLN:O | 4:A:507:SER:N | 2.10 | 0.84 |
| 4:C:232:GLN:HB2 | 4:C:241:SER:O | 1.77 | 0.84 |
| 4:B:423:ARG:HG3 | 4:B:781:ASN:HD22 | 1.40 | 0.84 |
| 4:C:452:ILE:HD11 | 4:C:457:TYR:CA | 2.07 | 0.84 |
| 4:A:881:ALA:O | 4:A:882:PHE:C | 2.14 | 0.84 |
| 4:C:158:GLU:CG | 4:C:195:LEU:HD22 | 2.01 | 0.84 |
| 4:C:278:TRP:CE3 | 4:C:284:GLY:HA3 | 2.13 | 0.84 |
| 4:C:92:VAL:CG1 | 4:C:99:ARG:HG3 | 2.06 | 0.84 |
| 1:H:9:DA:N6 | 3:J:1:DG:N2 | 2.26 | 0.84 |
| 4:A:727:TRP:CE2 | 4:A:735:VAL:HG11 | 2.12 | 0.84 |
| 4:C:559:VAL:HG23 | 4:C:561:LEU:HD13 | 1.58 | 0.84 |
| 4:A:452:ILE:HD11 | 4:A:457:TYR:CA | 2.07 | 0.84 |
| 4:B:168:GLU:O | 4:B:172:LYS:HG2 | 1.77 | 0.84 |
| 4:B:17:ALA:HA | 7:B:3012:HOH:O | 1.78 | 0.84 |
| 4:A:721:LYS:HD3 | 4:A:722:ARG:H | 1.41 | 0.84 |
| 4:B:632:ARG:HD2 | 6:B:2001:APC:HN61 | 1.43 | 0.84 |
| 4:B:728:VAL:HG22 | 4:B:734:PRO:HA | 1.60 | 0.84 |
| 4:B:816:THR:HG22 | 4:B:817:ILE:N | 1.91 | 0.84 |
| 4:B:201:TRP:HB3 | 7:B:3009:HOH:O | 1.78 | 0.83 |
| 4:C:423:ARG:NH1 | 4:C:423:ARG:HB2 | 1.93 | 0.83 |
| 4:A:816:THR:HG22 | 4:A:817:ILE:H | 1.43 | 0.83 |
| 4:C:636:THR:HG22 | 4:C:639:TYR:HD2 | 1.41 | 0.83 |
| 4:A:646:PHE:O | 4:A:650:VAL:HG23 | 1.78 | 0.83 |
| 4:A:731:ASP:OD1 | 4:A:792:ARG:NH2 | 2.11 | 0.83 |
| 4:A:720:ARG:HG2 | 4:A:720:ARG:HH11 | 1.42 | 0.83 |
| 4:B:574:VAL:HG21 | 4:B:685:VAL:HG12 | 1.57 | 0.83 |
| 4:B:339:ASN:O | 4:B:343:LYS:CD | 2.26 | 0.83 |
| 4:B:432:PHE:HE2 | 4:B:444:LEU:HD21 | 1.40 | 0.83 |
| 4:B:505:GLN:N | 4:B:505:GLN:HE21 | 1.75 | 0.83 |
| 4:C:275:PRO:HG2 | 4:C:324:GLN:HG2 | 1.61 | 0.83 |
| 4:A:386:ARG:HD2 | 7:A:3138:HOH:O | 1.76 | 0.83 |
| 4:A:574:VAL:O | 4:A:578:VAL:HG23 | 1.76 | 0.83 |
| 4:C:437:ASN:N | 4:C:437:ASN:HD22 | 1.72 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:744:GLN:HA | 4:D:756:ARG:CZ | 2.08 | 0.83 |
| 4:A:66:ASP:OD2 | 4:A:752:LEU:HD23 | 1.79 | 0.83 |
| 4:A:833:VAL:HG13 | 4:A:872:LEU:HB3 | 1.58 | 0.83 |
| 4:C:404:GLN:HG2 | 4:C:432:PHE:CB | 2.09 | 0.83 |
| 4:C:551:ARG:HE | 4:C:872:LEU:HD21 | 1.42 | 0.83 |
| 4:C:728:VAL:HG22 | 4:C:734:PRO:HA | 1.59 | 0.83 |
| 4:B:691:ALA:O | 4:B:694:GLU:HB2 | 1.79 | 0.83 |
| 4:A:280:GLY:HA2 | 4:A:317:TYR:CZ | 2.13 | 0.82 |
| 4:B:437:ASN:HD22 | 4:B:437:ASN:C | 1.81 | 0.82 |
| 4:B:172:LYS:HB3 | 4:B:172:LYS:NZ | 1.93 | 0.82 |
| 4:B:122:THR:HG21 | 4:B:226:MET:CE | 2.09 | 0.82 |
| 4:B:881:ALA:O | 4:B:882:PHE:C | 2.14 | 0.82 |
| 4:D:329:LYS:HG2 | 4:D:445:THR:O | 1.78 | 0.82 |
| 4:D:59:LEU:HD23 | 4:D:64:VAL:HG22 | 1.59 | 0.82 |
| 4:D:778:ILE:HG23 | 4:D:779:ALA:N | 1.93 | 0.82 |
| 4:B:846:TYR:HA | 4:B:849:PHE:HE1 | 1.42 | 0.82 |
| 4:C:582:LEU:HB3 | 4:C:621:LEU:HD21 | 1.62 | 0.82 |
| 4:C:663:LYS:HD3 | 4:C:664:GLY:H | 1.45 | 0.82 |
| 4:A:881:ALA:O | 4:A:882:PHE:O | 1.98 | 0.82 |
| 4:D:668:THR:HG22 | 4:D:669:GLN:HE21 | 1.45 | 0.82 |
| 4:A:278:TRP:CE3 | 4:A:284:GLY:HA3 | 2.15 | 0.82 |
| 4:B:345:LYS:NZ | 4:B:351:ASP:H | 1.77 | 0.82 |
| 4:B:574:VAL:CG1 | 4:B:574:VAL:O | 2.26 | 0.82 |
| 4:C:308:TYR:O | 4:C:311:VAL:HG23 | 1.79 | 0.82 |
| 4:D:828:VAL:HB | 4:D:883:ALA:HA | 1.61 | 0.82 |
| 1:E:14:DG:H2' | 1:E:15:DC:C6 | 2.15 | 0.82 |
| 4:B:298:ARG:HG3 | 4:B:420:MET:O | 1.78 | 0.82 |
| 4:B:574:VAL:HG12 | 4:B:574:VAL:O | 1.76 | 0.82 |
| 4:C:579:ASN:HA | 4:C:582:LEU:HD12 | 1.62 | 0.82 |
| 4:C:169:GLN:O | 4:C:173:ARG:HG2 | 1.80 | 0.82 |
| 4:D:275:PRO:HG2 | 4:D:324:GLN:HG2 | 1.61 | 0.82 |
| 4:D:470:VAL:HG12 | 4:D:473:VAL:HG11 | 1.61 | 0.82 |
| 4:A:486:HIS:HD2 | 4:A:518:TYR:CE1 | 1.98 | 0.82 |
| 4:A:512:LEU:HG | 4:A:516:PHE:HE1 | 1.43 | 0.82 |
| 4:B:231:ARG:HD2 | 4:B:240:ASP:OD2 | 1.80 | 0.82 |
| 4:B:408:PHE:CD2 | 4:B:408:PHE:N | 2.47 | 0.82 |
| 1:N:10:DT:H5' | 4:D:641:SER:CA | 2.09 | 0.82 |
| 4:A:19:ILE:HG13 | 7:A:3121:HOH:O | 1.78 | 0.81 |
| 4:C:236:VAL:CB | 4:C:239:GLN:HB2 | 2.10 | 0.81 |
| 4:D:486:HIS:HA | 4:D:489:ILE:HD12 | 1.59 | 0.81 |
| 4:B:229:LEU:HD11 | 4:B:242:GLU:HG2 | 1.61 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:D:342:THR:HG22 | 4:D:348:PRO:HG2 | 1.62 | 0.81 |
| 4:A:421:ASP:OD1 | 4:A:423:ARG:HD3 | 1.79 | 0.81 |
| 1:H:13:DC:O4' | 4:B:427:TYR:HE2 | 1.60 | 0.81 |
| 4:D:541:SER:HA | 4:D:544:GLN:NE2 | 1.95 | 0.81 |
| 4:D:870:LEU:HD22 | 4:D:872:LEU:HD23 | 1.62 | 0.81 |
| 4:C:231:ARG:HG2 | 4:C:234:ALA:HB2 | 1.63 | 0.81 |
| 4:C:271:CYS:SG | 4:C:417:PRO:HD3 | 2.20 | 0.81 |
| 2:I:4:G:H2' | 2:I:5:C:C6 | 2.16 | 0.81 |
| 4:B:51:PHE:O | 4:B:51:PHE:CD2 | 2.34 | 0.81 |
| 4:C:550:LEU:HD21 | 4:C:865:PRO:HG2 | 1.62 | 0.81 |
| 4:D:308:TYR:CE2 | 4:D:734:PRO:HG2 | 2.14 | 0.81 |
| 4:C:249:GLU:CD | 4:C:249:GLU:N | 2.31 | 0.81 |
| 4:A:401:MET:O | 4:A:403:GLU:N | 2.14 | 0.81 |
| 4:C:631:LYS:HZ3 | 6:C:2002:APC:H3A2 | 1.43 | 0.81 |
| 4:D:16:LEU:HD22 | 4:D:38:ALA:HA | 1.61 | 0.81 |
| 4:D:699:LEU:O | 4:D:778:ILE:HG21 | 1.80 | 0.81 |
| 4:B:632:ARG:O | 4:B:636:THR:HG23 | 1.79 | 0.81 |
| 4:B:742:PRO:HB3 | 4:B:744:GLN:OE1 | 1.81 | 0.81 |
| 4:A:583:GLN:HB2 | 7:A:3056:HOH:O | 1.79 | 0.81 |
| 4:D:80:LYS:HD3 | 4:D:224:THR:HB | 1.62 | 0.81 |
| 4:A:184:GLN:HG3 | 7:A:3137:HOH:O | 1.81 | 0.81 |
| 4:B:587:ILE:HG22 | 4:B:588:ASN:ND2 | 1.96 | 0.81 |
| 4:D:551:ARG:HB2 | 4:D:868:GLY:H | 1.45 | 0.81 |
| 4:A:303:LYS:HD2 | 7:D:3155:HOH:O | 1.81 | 0.80 |
| 4:B:470:VAL:HG12 | 4:B:470:VAL:O | 1.81 | 0.80 |
| 4:C:291:ARG:HG3 | 7:C:3104:HOH:O | 1.81 | 0.80 |
| 4:C:610:LYS:HE3 | 7:C:3172:HOH:O | 1.80 | 0.80 |
| 4:D:871:ASN:HD21 | 4:D:873:ARG:HB2 | 1.46 | 0.80 |
| 4:A:280:GLY:HA2 | 4:A:317:TYR:CE1 | 2.16 | 0.80 |
| 4:B:275:PRO:HD2 | 7:B:3116:HOH:O | 1.81 | 0.80 |
| 4:D:286:TYR:CE1 | 4:D:417:PRO:HG3 | 2.15 | 0.80 |
| 4:B:126:LEU:HD13 | 4:B:246:LEU:HB2 | 1.61 | 0.80 |
| 4:B:869:ASN:ND2 | 4:B:869:ASN:N | 2.28 | 0.80 |
| 4:A:15:GLU:HB3 | 4:A:19:ILE:HG12 | 1.63 | 0.80 |
| 4:D:840:ASP:O | 4:D:842:LEU:N | 2.14 | 0.80 |
| 4:A:669:GLN:HG2 | 4:A:672:GLN:HE21 | 1.47 | 0.80 |
| 4:A:801:LYS:HD3 | 4:A:801:LYS:C | 2.01 | 0.80 |
| 4:A:278:TRP:CZ3 | 4:A:284:GLY:HA3 | 2.17 | 0.80 |
| 4:A:624:GLY:HA3 | 7:A:3045:HOH:O | 1.79 | 0.80 |
| 4:D:582:LEU:HD11 | 4:D:625:VAL:HG21 | 1.62 | 0.80 |
| 4:A:502:TRP:CG | 4:A:512:LEU:HD13 | 2.16 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:B:158:GLU:HA | 4:B:195:LEU:HD13 | 1.63 | 0.80 |
| 4:C:631:LYS:CE | 6:C:2002:APC:H3A2 | 2.11 | 0.80 |
| 4:D:448:LYS:NZ | 4:D:806:SER:HB3 | 1.96 | 0.80 |
| 4:A:802:TYR:O | 4:A:804:ILE:N | 2.13 | 0.80 |
| 4:B:669:GLN:CG | 4:B:672:GLN:HG3 | 2.11 | 0.80 |
| 4:B:537:ASP:H | 4:B:882:PHE:HD2 | 1.28 | 0.80 |
| 4:C:211:HIS:O | 4:C:214:VAL:HG23 | 1.81 | 0.80 |
| 4:D:552:ASP:OD1 | 4:D:555:GLY:N | 2.11 | 0.80 |
| 1:H:6:DT:C6 | 1:H:6:DT:H5' | 2.16 | 0.80 |
| 7:I:777:HOH:O | 4:B:386:ARG:HD3 | 1.82 | 0.79 |
| 4:D:14:ILE:H | 4:D:14:ILE:HD12 | 1.45 | 0.79 |
| 4:D:281:ILE:HG22 | 4:D:282:THR:HG22 | 1.62 | 0.79 |
| 4:D:489:ILE:O | 4:D:492:CYS:SG | 2.40 | 0.79 |
| 1:N:2:DG:H2'' | 1:N:3:DG:C8 | 2.16 | 0.79 |
| 4:A:15:GLU:HG3 | 4:A:18:ALA:H | 1.45 | 0.79 |
| 4:A:610:LYS:HG2 | 4:A:610:LYS:O | 1.79 | 0.79 |
| 4:A:478:ARG:HH12 | 4:A:882:PHE:HZ | 1.29 | 0.79 |
| 4:C:214:VAL:HA | 4:C:217:ILE:HD12 | 1.65 | 0.79 |
| 4:D:125:CYS:O | 4:D:128:SER:HB3 | 1.81 | 0.79 |
| 4:D:490:MET:O | 4:D:493:ALA:HB3 | 1.81 | 0.79 |
| 4:A:462:ILE:HG12 | 4:A:479:ILE:HD11 | 1.64 | 0.79 |
| 4:B:881:ALA:O | 4:B:883:ALA:OXT | 1.99 | 0.79 |
| 4:A:157:LEU:HB3 | 7:A:3133:HOH:O | 1.80 | 0.79 |
| 4:A:452:ILE:HD11 | 4:A:457:TYR:CB | 2.13 | 0.79 |
| 4:A:526:LEU:N | 4:A:526:LEU:HD12 | 1.97 | 0.79 |
| 4:C:78:LEU:N | 4:C:79:PRO:HD2 | 1.97 | 0.79 |
| 4:D:804:ILE:HG12 | 4:D:820:ASP:HB3 | 1.63 | 0.79 |
| 4:A:119:ILE:O | 4:A:123:LEU:HD12 | 1.81 | 0.79 |
| 4:B:770:ASP:OD1 | 4:B:770:ASP:C | 2.21 | 0.79 |
| 1:H:14:DG:H2'' | 1:H:15:DC:C5' | 2.13 | 0.79 |
| 4:A:342:THR:HG21 | 4:A:398:LEU:HD21 | 1.61 | 0.79 |
| 4:D:860:LYS:O | 4:D:860:LYS:HD2 | 1.83 | 0.79 |
| 4:A:806:SER:O | 4:A:816:THR:HG23 | 1.82 | 0.79 |
| 4:B:748:ASN:ND2 | 4:B:751:PHE:HB2 | 1.98 | 0.79 |
| 4:C:158:GLU:HA | 4:C:195:LEU:HD13 | 1.63 | 0.79 |
| 4:C:19:ILE:HD13 | 7:C:3117:HOH:O | 1.83 | 0.79 |
| 4:C:59:LEU:HD22 | 4:C:64:VAL:HG13 | 1.65 | 0.79 |
| 4:D:139:SER:HB2 | 4:D:210:ILE:CD1 | 2.13 | 0.79 |
| 4:C:396:ILE:HG22 | 7:C:3188:HOH:O | 1.82 | 0.79 |
| 4:C:299:THR:HG22 | 4:C:300:HIS:N | 1.98 | 0.79 |
| 4:A:291:ARG:HB2 | 7:A:3193:HOH:O | 1.83 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:A:452:ILE:HD11 | 4:A:457:TYR:HA | 1.65 | 0.78 |
| 4:C:47:GLY:HA3 | 4:C:265:SER:O | 1.83 | 0.78 |
| 4:C:563:PRO:HB3 | 4:C:877:GLU:O | 1.82 | 0.78 |
| 4:A:16:LEU:HD13 | 4:A:38:ALA:CB | 2.13 | 0.78 |
| 4:B:24:LEU:HD13 | 4:B:37:LEU:HD11 | 1.62 | 0.78 |
| 4:B:712:ASP:HB3 | 7:B:3078:HOH:O | 1.84 | 0.78 |
| 4:B:814:PHE:HB3 | 4:B:824:LEU:HD21 | 1.65 | 0.78 |
| 4:D:475:PHE:HE2 | 4:D:879:ASP:HB3 | 1.48 | 0.78 |
| 4:A:871:ASN:HB3 | 4:A:874:ASP:OD2 | 1.83 | 0.78 |
| 4:B:816:THR:CG2 | 4:B:817:ILE:H | 1.89 | 0.78 |
| 4:A:133:THR:HA | 4:A:243:THR:HG22 | 1.65 | 0.78 |
| 4:B:449:GLY:HA3 | 4:B:529:ASN:ND2 | 1.99 | 0.78 |
| 4:C:404:GLN:HG2 | 4:C:432:PHE:HB2 | 1.65 | 0.78 |
| 4:C:778:ILE:CG2 | 4:C:779:ALA:N | 2.46 | 0.78 |
| 4:D:806:SER:O | 4:D:816:THR:HG23 | 1.81 | 0.78 |
| 4:A:748:ASN:ND2 | 4:A:751:PHE:H | 1.82 | 0.78 |
| 4:C:505:GLN:O | 4:C:508:PRO:HD3 | 1.82 | 0.78 |
| 4:A:546:PHE:CE1 | 4:A:783:VAL:CG2 | 2.63 | 0.78 |
| 4:A:791:LEU:CD1 | 4:A:809:LEU:HD22 | 2.14 | 0.78 |
| 4:B:446:LEU:HD12 | 4:B:817:ILE:HG23 | 1.64 | 0.78 |
| 4:C:84:ARG:HH11 | 4:C:84:ARG:HA | 1.47 | 0.78 |
| 1:K:11:DA:C8 | 4:C:639:TYR:HB3 | 2.18 | 0.78 |
| 4:A:44:TYR:OH | 4:A:292:ARG:HB3 | 1.83 | 0.78 |
| 4:A:475:PHE:O | 4:A:479:ILE:HG12 | 1.84 | 0.78 |
| 4:D:427:TYR:HA | 4:D:435:GLN:HE22 | 1.48 | 0.78 |
| 4:B:869:ASN:HD22 | 4:B:869:ASN:N | 1.81 | 0.78 |
| 4:C:448:LYS:HE3 | 4:C:806:SER:OG | 1.84 | 0.78 |
| 4:D:323:ALA:O | 4:D:325:ASN:N | 2.16 | 0.78 |
| 4:A:546:PHE:CZ | 4:A:783:VAL:HG22 | 2.19 | 0.78 |
| 4:A:562:LEU:HD21 | 4:A:870:LEU:HD12 | 1.65 | 0.78 |
| 4:A:860:LYS:HD2 | 4:A:860:LYS:O | 1.84 | 0.78 |
| 4:C:545:HIS:O | 4:C:549:MET:HG2 | 1.84 | 0.78 |
| 4:D:454:LYS:HG3 | 4:D:455:GLU:H | 1.48 | 0.78 |
| 4:D:475:PHE:CE2 | 4:D:879:ASP:HB3 | 2.19 | 0.77 |
| 1:N:15:DC:C2 | 1:N:16:DC:C5 | 2.72 | 0.77 |
| 4:B:423:ARG:HH12 | 4:B:784:HIS:HB3 | 1.48 | 0.77 |
| 4:B:398:LEU:HD21 | 4:B:439:MET:HE1 | 1.65 | 0.77 |
| 4:B:274:PRO:HD3 | 4:B:415:TRP:CZ3 | 2.19 | 0.77 |
| 4:C:706:LEU:HD22 | 4:C:725:VAL:HG22 | 1.67 | 0.77 |
| 4:A:727:TRP:HA | 4:A:848:GLN:HE21 | 1.46 | 0.77 |
| 4:B:80:LYS:O | 4:B:223:SER:HB2 | 1.83 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:D:159:ALA:O | 4:D:163:LYS:HB2 | 1.84 | 0.77 |
| 4:B:631:LYS:HE2 | 6:B:2001:APC:H3A2 | 1.67 | 0.77 |
| 4:C:155:ARG:HB2 | 4:C:163:LYS:NZ | 2.00 | 0.77 |
| 4:C:460:LEU:HG | 4:C:460:LEU:O | 1.84 | 0.77 |
| 1:H:2:DG:H2'' | 1:H:3:DG:H8 | 1.48 | 0.77 |
| 2:O:4:G:O2' | 2:O:5:C:H5' | 1.85 | 0.77 |
| 4:B:233:ASN:HD22 | 4:B:239:GLN:NE2 | 1.82 | 0.77 |
| 4:B:264:ILE:C | 4:B:266:PRO:HD3 | 2.05 | 0.77 |
| 4:B:273:VAL:O | 4:B:274:PRO:O | 2.02 | 0.77 |
| 4:C:181:ALA:O | 4:C:185:VAL:HG22 | 1.85 | 0.77 |
| 4:D:563:PRO:HB2 | 7:D:3032:HOH:O | 1.85 | 0.77 |
| 4:A:468:ALA:HB2 | 4:A:511:PHE:CE1 | 2.20 | 0.77 |
| 4:D:57:ARG:O | 4:D:60:LYS:HB3 | 1.85 | 0.77 |
| 4:A:141:ILE:HG22 | 4:A:145:ILE:HD11 | 1.66 | 0.77 |
| 4:A:664:GLY:HA2 | 4:A:667:PHE:HD2 | 1.50 | 0.77 |
| 4:B:407:LYS:HG2 | 4:B:408:PHE:CD2 | 2.19 | 0.77 |
| 4:B:489:ILE:HG22 | 4:B:515:CYS:HB3 | 1.67 | 0.77 |
| 4:B:663:LYS:HG2 | 4:B:664:GLY:H | 1.49 | 0.77 |
| 4:C:275:PRO:HB2 | 4:C:324:GLN:OE1 | 1.85 | 0.77 |
| 4:C:81:MET:O | 4:C:85:ILE:HG13 | 1.85 | 0.77 |
| 4:D:51:PHE:CE2 | 4:D:55:PHE:HB2 | 2.20 | 0.77 |
| 4:D:55:PHE:CZ | 4:D:59:LEU:HD21 | 2.20 | 0.77 |
| 4:D:720:ARG:HH11 | 4:D:720:ARG:CG | 1.86 | 0.77 |
| 4:B:5:ASN:HD22 | 4:B:8:LYS:HG3 | 1.49 | 0.77 |
| 4:C:337:VAL:HG21 | 4:C:512:LEU:HD21 | 1.66 | 0.77 |
| 4:C:433:ASN:CA | 7:C:3164:HOH:O | 2.33 | 0.77 |
| 1:H:14:DG:H2'' | 1:H:15:DC:H5' | 1.67 | 0.77 |
| 4:A:60:LYS:O | 4:A:60:LYS:NZ | 2.18 | 0.76 |
| 4:A:825:PHE:CZ | 4:A:829:ARG:NH2 | 2.52 | 0.76 |
| 4:D:744:GLN:HA | 4:D:756:ARG:NE | 2.00 | 0.76 |
| 1:K:11:DA:H2' | 1:K:12:DT:C7 | 2.14 | 0.76 |
| 4:C:401:MET:O | 4:C:404:GLN:HB3 | 1.85 | 0.76 |
| 4:C:516:PHE:O | 4:C:519:ALA:HB3 | 1.84 | 0.76 |
| 4:D:95:LYS:HD3 | 7:D:3062:HOH:O | 1.85 | 0.76 |
| 4:A:210:ILE:O | 4:A:214:VAL:HG23 | 1.85 | 0.76 |
| 4:A:390:ALA:O | 4:A:392:LYS:N | 2.18 | 0.76 |
| 4:A:495:SER:HA | 7:A:3203:HOH:O | 1.85 | 0.76 |
| 4:B:582:LEU:HB3 | 4:B:621:LEU:HD11 | 1.65 | 0.76 |
| 4:C:55:PHE:O | 4:C:58:GLN:HB2 | 1.85 | 0.76 |
| 4:D:473:VAL:N | 4:D:567:VAL:HG21 | 2.00 | 0.76 |
| 4:A:281:ILE:CG1 | 4:A:309:GLU:HA | 2.15 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:A:87:ASP:O | 4:A:91:GLU:HG3 | 1.85 | 0.76 |
| 4:B:423:ARG:CG | 4:B:781:ASN:HD22 | 1.98 | 0.76 |
| 4:D:651:LEU:O | 4:D:651:LEU:HD13 | 1.85 | 0.76 |
| 4:B:690:VAL:O | 4:B:693:VAL:HG23 | 1.84 | 0.76 |
| 4:A:512:LEU:HG | 4:A:516:PHE:CE1 | 2.21 | 0.76 |
| 4:B:784:HIS:O | 4:B:786:GLN:N | 2.18 | 0.76 |
| 4:B:790:HIS:HE1 | 4:B:831:THR:HG23 | 1.50 | 0.76 |
| 4:A:92:VAL:HG11 | 4:A:100:PRO:HD2 | 1.66 | 0.76 |
| 4:B:390:ALA:C | 4:B:392:LYS:H | 1.87 | 0.76 |
| 4:B:418:TYR:CD2 | 4:B:428:ALA:HA | 2.21 | 0.76 |
| 4:A:454:LYS:N | 4:A:526:LEU:HD23 | 2.00 | 0.76 |
| 4:C:15:GLU:HG3 | 4:C:18:ALA:H | 1.49 | 0.76 |
| 4:C:744:GLN:CB | 7:C:3076:HOH:O | 2.34 | 0.76 |
| 4:A:548:ALA:O | 4:A:550:LEU:N | 2.18 | 0.76 |
| 4:C:778:ILE:CG2 | 4:C:779:ALA:H | 1.99 | 0.76 |
| 4:D:790:HIS:CE1 | 4:D:831:THR:HG23 | 2.16 | 0.76 |
| 4:A:464:GLY:HA3 | 4:A:514:PHE:CZ | 2.21 | 0.75 |
| 4:C:308:TYR:OH | 4:C:734:PRO:O | 2.05 | 0.75 |
| 4:D:540:CYS:O | 4:D:542:GLY:N | 2.18 | 0.75 |
| 4:A:668:THR:HG22 | 4:A:669:GLN:OE1 | 1.86 | 0.75 |
| 4:A:825:PHE:CE1 | 4:A:829:ARG:CZ | 2.68 | 0.75 |
| 4:A:84:ARG:HD3 | 4:A:84:ARG:O | 1.87 | 0.75 |
| 4:A:290:GLY:O | 4:A:293:PRO:HD3 | 1.86 | 0.75 |
| 4:C:308:TYR:OH | 4:C:733:PHE:HE2 | 1.69 | 0.75 |
| 4:D:228:SER:HB3 | 7:D:3168:HOH:O | 1.86 | 0.75 |
| 4:A:457:TYR:HD1 | 4:A:521:VAL:HG21 | 1.52 | 0.75 |
| 4:A:816:THR:OG1 | 4:A:824:LEU:HD22 | 1.87 | 0.75 |
| 4:C:299:THR:HG22 | 4:C:300:HIS:H | 1.51 | 0.75 |
| 4:D:829:ARG:HG3 | 4:D:829:ARG:HH11 | 1.51 | 0.75 |
| 4:D:141:ILE:O | 4:D:145:ILE:HG12 | 1.87 | 0.75 |
| 4:B:719:LEU:HD23 | 4:B:854:HIS:NE2 | 2.01 | 0.75 |
| 4:C:5:ASN:HD21 | 4:C:7:ALA:HB3 | 1.50 | 0.75 |
| 4:D:465:ALA:CB | 4:D:478:ARG:HB3 | 2.16 | 0.75 |
| 4:D:871:ASN:ND2 | 4:D:873:ARG:HB2 | 2.00 | 0.75 |
| 4:A:280:GLY:CA | 4:A:317:TYR:OH | 2.35 | 0.75 |
| 4:B:391:ARG:HG3 | 7:B:3101:HOH:O | 1.86 | 0.75 |
| 4:B:463:HIS:HB2 | 4:B:534:LEU:HD22 | 1.68 | 0.75 |
| 4:C:539:SER:HA | 7:C:3124:HOH:O | 1.86 | 0.75 |
| 4:D:297:VAL:HG12 | 4:D:299:THR:HG22 | 1.68 | 0.75 |
| 4:A:273:VAL:O | 4:A:273:VAL:CG2 | 2.35 | 0.75 |
| 4:A:463:HIS:HA | 4:A:466:ASN:ND2 | 2.01 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:10:DT:H5' | 4:D:641:SER:N | 2.02 | 0.75 |
| 4:D:435:GLN:HB3 | 4:D:810:ILE:HG12 | 1.69 | 0.75 |
| 4:A:544:GLN:CG | 4:A:559:VAL:HG21 | 2.16 | 0.74 |
| 4:A:486:HIS:CD2 | 4:A:518:TYR:HE1 | 2.06 | 0.74 |
| 7:I:777:HOH:O | 4:B:386:ARG:CD | 2.33 | 0.74 |
| 4:B:55:PHE:O | 4:B:55:PHE:CD2 | 2.40 | 0.74 |
| 4:C:810:ILE:HG22 | 4:C:810:ILE:O | 1.86 | 0.74 |
| 1:H:15:DC:H2'' | 1:H:16:DC:C5' | 2.18 | 0.74 |
| 4:A:514:PHE:HD1 | 4:A:515:CYS:N | 1.85 | 0.74 |
| 4:A:793:LYS:O | 4:A:796:VAL:HG23 | 1.86 | 0.74 |
| 4:B:56:GLU:OE1 | 4:B:57:ARG:HA | 1.87 | 0.74 |
| 4:C:324:GLN:HE21 | 4:C:418:TYR:H | 1.36 | 0.74 |
| 4:C:4:ILE:HD12 | 4:C:256:THR:HG23 | 1.69 | 0.74 |
| 4:D:454:LYS:HG3 | 4:D:455:GLU:N | 2.03 | 0.74 |
| 4:A:825:PHE:CE1 | 4:A:829:ARG:NH2 | 2.55 | 0.74 |
| 4:B:871:ASN:HB3 | 4:B:874:ASP:OD2 | 1.88 | 0.74 |
| 4:B:92:VAL:HA | 7:B:3193:HOH:O | 1.88 | 0.74 |
| 4:D:351:ASP:HA | 7:D:3124:HOH:O | 1.86 | 0.74 |
| 4:B:143:ARG:O | 4:B:146:GLU:HB3 | 1.86 | 0.74 |
| 4:B:475:PHE:O | 4:B:476:PRO:C | 2.23 | 0.74 |
| 4:C:109:ILE:CD1 | 4:C:149:ALA:HB2 | 2.17 | 0.74 |
| 4:C:141:ILE:O | 4:C:145:ILE:HG12 | 1.86 | 0.74 |
| 4:A:77:LEU:HD23 | 4:A:119:ILE:HD12 | 1.70 | 0.74 |
| 4:A:418:TYR:HD2 | 4:A:426:VAL:CG1 | 2.01 | 0.74 |
| 4:A:60:LYS:O | 4:A:60:LYS:HG2 | 1.86 | 0.74 |
| 4:B:651:LEU:O | 4:B:651:LEU:HD22 | 1.86 | 0.74 |
| 4:C:749:LEU:HD12 | 4:C:750:MET:HG2 | 1.69 | 0.74 |
| 4:A:275:PRO:HD2 | 7:A:3206:HOH:O | 1.88 | 0.74 |
| 4:B:71:LYS:N | 4:B:72:PRO:HD2 | 2.03 | 0.74 |
| 4:B:846:TYR:HA | 4:B:849:PHE:CE1 | 2.23 | 0.74 |
| 4:B:855:GLU:O | 4:B:858:LEU:HD12 | 1.87 | 0.74 |
| 4:C:84:ARG:HH12 | 4:C:87:ASP:CB | 2.00 | 0.74 |
| 4:A:116:TYR:OH | 4:A:752:LEU:HD22 | 1.88 | 0.74 |
| 4:C:706:LEU:CD2 | 4:C:725:VAL:HG13 | 2.18 | 0.74 |
| 4:A:395:ARG:HG3 | 4:A:395:ARG:O | 1.88 | 0.74 |
| 4:B:537:ASP:O | 4:B:882:PHE:HB2 | 1.87 | 0.74 |
| 4:B:663:LYS:CG | 4:B:664:GLY:H | 2.00 | 0.74 |
| 4:C:738:GLU:HA | 4:C:774:GLN:HE22 | 1.53 | 0.74 |
| 4:C:744:GLN:HB3 | 4:C:756:ARG:HB3 | 1.70 | 0.74 |
| 4:D:250:TYR:O | 4:D:254:ILE:HG13 | 1.88 | 0.74 |
| 4:B:172:LYS:HZ2 | 4:B:172:LYS:HB3 | 1.52 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:B:636:THR:HG21 | 4:B:649:GLN:HE22 | 1.53 | 0.73 |
| 4:C:656:GLN:N | 4:C:657:PRO:HD2 | 2.02 | 0.73 |
| 4:D:663:LYS:HG2 | 4:D:664:GLY:H | 1.52 | 0.73 |
| 1:H:12:DT:H4' | 4:B:423:ARG:HE | 1.52 | 0.73 |
| 4:B:780:PRO:HA | 4:B:783:VAL:HG23 | 1.70 | 0.73 |
| 4:C:866:ALA:HB2 | 7:C:3189:HOH:O | 1.86 | 0.73 |
| 4:C:850:ALA:O | 4:C:853:LEU:HG | 1.89 | 0.73 |
| 4:B:226:MET:O | 4:B:247:ALA:HB2 | 1.88 | 0.73 |
| 4:B:278:TRP:CE3 | 4:B:284:GLY:HA3 | 2.23 | 0.73 |
| 4:B:557:ARG:O | 4:B:557:ARG:HG2 | 1.86 | 0.73 |
| 4:B:662:GLY:O | 4:B:663:LYS:O | 2.06 | 0.73 |
| 4:C:655:ILE:HD12 | 4:C:674:ALA:HB2 | 1.69 | 0.73 |
| 4:C:492:CYS:HA | 7:C:3071:HOH:O | 1.89 | 0.73 |
| 4:C:744:GLN:HB2 | 7:C:3076:HOH:O | 1.89 | 0.73 |
| 4:D:457:TYR:CE1 | 4:D:521:VAL:HG11 | 2.23 | 0.73 |
| 4:D:881:ALA:O | 4:D:882:PHE:C | 2.27 | 0.73 |
| 4:A:100:PRO:HG2 | 4:A:103:PHE:HB2 | 1.69 | 0.73 |
| 4:A:380:ALA:O | 4:A:384:VAL:HG23 | 1.87 | 0.73 |
| 4:C:210:ILE:O | 4:C:214:VAL:HG22 | 1.89 | 0.73 |
| 4:C:636:THR:HG22 | 4:C:639:TYR:CD2 | 2.22 | 0.73 |
| 4:C:778:ILE:HG23 | 4:C:779:ALA:H | 1.51 | 0.73 |
| 4:D:417:PRO:O | 4:D:429:VAL:HG23 | 1.87 | 0.73 |
| 4:D:457:TYR:CD1 | 4:D:521:VAL:HG11 | 2.24 | 0.73 |
| 1:K:13:DC:H2'' | 1:K:14:DG:C5' | 2.18 | 0.73 |
| 4:A:562:LEU:HD21 | 4:A:870:LEU:HD11 | 1.69 | 0.73 |
| 4:C:337:VAL:HG12 | 4:C:338:ALA:N | 2.03 | 0.73 |
| 4:A:54:MET:O | 4:A:58:GLN:HG2 | 1.89 | 0.73 |
| 4:C:281:ILE:HG12 | 4:C:309:GLU:HA | 1.70 | 0.73 |
| 4:C:70:ALA:C | 4:C:72:PRO:HD2 | 2.09 | 0.73 |
| 4:D:14:ILE:CG2 | 4:D:288:ALA:HB1 | 2.19 | 0.73 |
| 4:B:748:ASN:ND2 | 4:B:751:PHE:H | 1.86 | 0.73 |
| 4:D:330:ILE:HG13 | 4:D:408:PHE:O | 1.88 | 0.73 |
| 1:K:13:DC:H2'' | 1:K:14:DG:O5' | 1.89 | 0.73 |
| 4:A:138:ALA:O | 4:A:213:GLY:HA3 | 1.89 | 0.73 |
| 4:A:281:ILE:CG2 | 4:A:282:THR:HG23 | 2.11 | 0.73 |
| 4:B:291:ARG:HB2 | 7:B:3037:HOH:O | 1.89 | 0.73 |
| 4:C:739:TYR:HB2 | 4:C:774:GLN:OE1 | 1.89 | 0.73 |
| 4:D:623:TYR:HA | 4:D:666:MET:HE1 | 1.70 | 0.73 |
| 1:K:11:DA:H2' | 1:K:12:DT:H72 | 1.69 | 0.73 |
| 4:C:269:GLN:O | 4:C:430:SER:HB3 | 1.88 | 0.72 |
| 4:D:278:TRP:HB2 | 4:D:321:ASN:HD21 | 1.53 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:I:1:G:H5'' | 7:I:873:HOH:O | 1.89 | 0.72 |
| 4:A:514:PHE:CD1 | 4:A:515:CYS:N | 2.57 | 0.72 |
| 4:A:736:TRP:HB2 | 7:A:3116:HOH:O | 1.88 | 0.72 |
| 4:C:728:VAL:HG22 | 4:C:734:PRO:CA | 2.19 | 0.72 |
| 4:D:833:VAL:CG2 | 4:D:875:ILE:HB | 2.19 | 0.72 |
| 4:A:428:ALA:H | 4:A:435:GLN:HE22 | 1.34 | 0.72 |
| 4:A:829:ARG:NH1 | 4:A:829:ARG:HG3 | 1.98 | 0.72 |
| 4:B:345:LYS:HZ3 | 4:B:351:ASP:H | 1.37 | 0.72 |
| 4:B:418:TYR:HE2 | 4:B:428:ALA:CB | 2.01 | 0.72 |
| 4:A:59:LEU:HA | 4:A:64:VAL:HG22 | 1.70 | 0.72 |
| 4:B:119:ILE:O | 4:B:122:THR:HB | 1.88 | 0.72 |
| 4:B:395:ARG:O | 4:B:398:LEU:N | 2.22 | 0.72 |
| 4:B:454:LYS:HE2 | 7:B:3020:HOH:O | 1.88 | 0.72 |
| 4:C:423:ARG:NH2 | 4:C:784:HIS:ND1 | 2.37 | 0.72 |
| 4:D:39:LEU:HD22 | 4:D:272:VAL:CG2 | 2.19 | 0.72 |
| 2:F:1:G:H2' | 2:F:2:C:C6 | 2.24 | 0.72 |
| 4:D:272:VAL:O | 4:D:415:TRP:HZ3 | 1.72 | 0.72 |
| 4:D:505:GLN:N | 4:D:505:GLN:NE2 | 2.37 | 0.72 |
| 4:D:472:LYS:HA | 4:D:567:VAL:HG11 | 1.71 | 0.72 |
| 4:B:339:ASN:O | 4:B:343:LYS:HD2 | 1.88 | 0.72 |
| 4:A:113:ALA:O | 4:A:117:ILE:HG13 | 1.89 | 0.72 |
| 4:B:268:PHE:CB | 4:B:286:TYR:OH | 2.35 | 0.72 |
| 4:B:314:PRO:O | 4:B:316:VAL:N | 2.23 | 0.72 |
| 4:B:567:VAL:HG13 | 4:B:880:PHE:CG | 2.25 | 0.72 |
| 4:C:423:ARG:HD2 | 4:C:781:ASN:ND2 | 2.03 | 0.72 |
| 4:D:328:TRP:O | 4:D:414:ILE:N | 2.20 | 0.72 |
| 4:B:432:PHE:CE2 | 4:B:444:LEU:HD21 | 2.23 | 0.72 |
| 4:B:578:VAL:HG22 | 4:B:680:LEU:HB3 | 1.72 | 0.72 |
| 4:C:459:TRP:HB3 | 4:C:534:LEU:HD13 | 1.70 | 0.72 |
| 4:D:327:ALA:HB2 | 4:D:415:TRP:NE1 | 2.05 | 0.72 |
| 4:D:593:GLU:O | 4:D:610:LYS:N | 2.19 | 0.72 |
| 4:D:448:LYS:CE | 4:D:806:SER:HB3 | 2.19 | 0.72 |
| 1:H:3:DG:N3 | 7:H:1116:HOH:O | 2.22 | 0.72 |
| 4:A:182:PHE:O | 4:A:185:VAL:HG22 | 1.90 | 0.72 |
| 4:A:423:ARG:NH2 | 4:A:784:HIS:HB3 | 2.05 | 0.72 |
| 4:B:281:ILE:CD1 | 4:B:309:GLU:HA | 2.20 | 0.72 |
| 4:B:505:GLN:H | 4:B:505:GLN:HE21 | 1.36 | 0.72 |
| 4:B:741:LYS:HB2 | 4:B:770:ASP:HB2 | 1.70 | 0.72 |
| 4:C:420:MET:HA | 4:C:425:ARG:O | 1.89 | 0.72 |
| 4:D:766:ASP:HB3 | 7:D:3085:HOH:O | 1.88 | 0.72 |
| 4:A:502:TRP:CE2 | 4:A:512:LEU:HD13 | 2.25 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:A:84:ARG:HD3 | 4:A:84:ARG:C | 2.10 | 0.71 |
| 4:B:471:ASP:O | 4:B:472:LYS:HD2 | 1.90 | 0.71 |
| 4:C:335:LEU:HD21 | 4:C:339:ASN:HD22 | 1.55 | 0.71 |
| 4:A:421:ASP:O | 4:A:423:ARG:N | 2.22 | 0.71 |
| 4:B:300:HIS:NE2 | 4:B:422:TRP:CZ3 | 2.56 | 0.71 |
| 4:C:247:ALA:HB1 | 4:C:249:GLU:OE1 | 1.90 | 0.71 |
| 4:C:78:LEU:HG | 4:C:78:LEU:O | 1.88 | 0.71 |
| 4:D:352:ILE:N | 4:D:352:ILE:HD12 | 2.05 | 0.71 |
| 4:D:443:LEU:N | 4:D:443:LEU:HD23 | 2.04 | 0.71 |
| 4:B:281:ILE:HD13 | 4:B:309:GLU:HA | 1.72 | 0.71 |
| 4:C:291:ARG:HB2 | 7:C:3192:HOH:O | 1.89 | 0.71 |
| 4:C:433:ASN:OD1 | 4:C:435:GLN:N | 2.21 | 0.71 |
| 4:C:663:LYS:CD | 4:C:664:GLY:H | 2.03 | 0.71 |
| 4:C:797:TRP:CZ2 | 4:C:801:LYS:HG3 | 2.26 | 0.71 |
| 1:E:15:DC:H2'' | 1:E:16:DC:H5' | 1.71 | 0.71 |
| 4:B:609:VAL:O | 4:B:611:LEU:N | 2.23 | 0.71 |
| 4:B:423:ARG:CG | 4:B:781:ASN:ND2 | 2.53 | 0.71 |
| 4:C:551:ARG:HD2 | 7:C:3087:HOH:O | 1.91 | 0.71 |
| 4:A:666:MET:N | 4:A:666:MET:SD | 2.64 | 0.71 |
| 4:B:236:VAL:HG21 | 4:B:239:GLN:NE2 | 2.06 | 0.71 |
| 4:B:274:PRO:HD3 | 4:B:415:TRP:CH2 | 2.25 | 0.71 |
| 4:B:454:LYS:HB2 | 7:B:3020:HOH:O | 1.90 | 0.71 |
| 4:B:623:TYR:HA | 4:B:666:MET:HE1 | 1.71 | 0.71 |
| 4:C:557:ARG:HB2 | 4:C:562:LEU:HD12 | 1.70 | 0.71 |
| 4:A:457:TYR:CE1 | 4:A:521:VAL:HG11 | 2.25 | 0.71 |
| 4:A:5:ASN:ND2 | 4:A:7:ALA:HB3 | 2.06 | 0.71 |
| 4:B:308:TYR:CE2 | 4:B:734:PRO:HG2 | 2.25 | 0.71 |
| 4:B:617:ALA:HB2 | 4:B:676:TYR:OH | 1.91 | 0.71 |
| 4:D:541:SER:HA | 4:D:544:GLN:HE21 | 1.53 | 0.71 |
| 4:A:351:ASP:HA | 7:A:3222:HOH:O | 1.89 | 0.71 |
| 4:B:100:PRO:HG2 | 4:B:103:PHE:HB2 | 1.71 | 0.71 |
| 4:C:40:GLU:CD | 4:C:286:TYR:HB3 | 2.10 | 0.71 |
| 4:D:231:ARG:CG | 4:D:234:ALA:HB2 | 2.21 | 0.71 |
| 4:A:423:ARG:NH2 | 4:A:784:HIS:CG | 2.59 | 0.71 |
| 4:B:11:PHE:CZ | 4:B:44:TYR:HB3 | 2.24 | 0.71 |
| 4:B:564:SER:OG | 4:B:566:THR:N | 2.20 | 0.71 |
| 4:C:201:TRP:O | 4:C:204:TRP:HB2 | 1.90 | 0.71 |
| 4:C:828:VAL:O | 4:C:831:THR:HG22 | 1.89 | 0.71 |
| 4:D:257:ARG:O | 4:D:261:LEU:HB2 | 1.91 | 0.71 |
| 4:D:324:GLN:HG3 | 4:D:417:PRO:HA | 1.73 | 0.71 |
| 1:H:14:DG:H2'' | 1:H:15:DC:O5' | 1.90 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:A:720:ARG:NH1 | 4:A:720:ARG:HG2 | 2.03 | 0.71 |
| 4:B:816:THR:HG21 | 4:B:820:ASP:HB3 | 1.73 | 0.71 |
| 4:D:269:GLN:HE22 | 4:D:407:LYS:HE2 | 1.56 | 0.71 |
| 4:A:109:ILE:CD1 | 4:A:145:ILE:O | 2.39 | 0.71 |
| 4:A:643:GLU:HB2 | 7:A:3076:HOH:O | 1.90 | 0.71 |
| 4:A:786:GLN:NE2 | 4:A:786:GLN:HA | 2.03 | 0.71 |
| 4:A:828:VAL:HB | 4:A:883:ALA:HA | 1.73 | 0.71 |
| 4:B:390:ALA:O | 4:B:393:SER:N | 2.24 | 0.71 |
| 4:D:435:GLN:HA | 4:D:810:ILE:HD11 | 1.72 | 0.71 |
| 4:D:772:HIS:O | 4:D:773:LYS:C | 2.28 | 0.71 |
| 4:A:161:HIS:O | 4:A:164:LYS:HG2 | 1.90 | 0.70 |
| 4:A:786:GLN:OE1 | 4:A:841:VAL:HG11 | 1.91 | 0.70 |
| 4:B:213:GLY:O | 4:B:217:ILE:HG13 | 1.91 | 0.70 |
| 4:C:553:GLU:HA | 4:C:870:LEU:HD12 | 1.73 | 0.70 |
| 4:D:116:TYR:OH | 4:D:752:LEU:HD22 | 1.90 | 0.70 |
| 4:D:428:ALA:H | 4:D:435:GLN:NE2 | 1.89 | 0.70 |
| 4:A:633:SER:HB2 | 7:A:3199:HOH:O | 1.91 | 0.70 |
| 4:A:810:ILE:HB | 4:A:813:SER:HB3 | 1.72 | 0.70 |
| 4:B:849:PHE:O | 4:B:852:GLN:N | 2.22 | 0.70 |
| 4:C:120:LYS:HG3 | 4:C:752:LEU:HD11 | 1.74 | 0.70 |
| 4:A:827:ALA:O | 4:A:830:GLU:HB2 | 1.91 | 0.70 |
| 4:B:312:TYR:HA | 7:B:3069:HOH:O | 1.89 | 0.70 |
| 4:B:645:GLY:O | 4:B:647:ARG:N | 2.24 | 0.70 |
| 4:C:338:ALA:HB2 | 4:C:509:PHE:CE1 | 2.20 | 0.70 |
| 4:D:264:ILE:CG2 | 4:D:292:ARG:HB2 | 2.21 | 0.70 |
| 4:D:810:ILE:O | 4:D:810:ILE:HG22 | 1.89 | 0.70 |
| 4:A:89:PHE:HA | 4:A:103:PHE:CE1 | 2.26 | 0.70 |
| 4:A:158:GLU:HG2 | 4:A:195:LEU:HD23 | 1.74 | 0.70 |
| 4:A:281:ILE:HG12 | 4:A:309:GLU:HA | 1.73 | 0.70 |
| 4:A:720:ARG:O | 4:A:721:LYS:O | 2.09 | 0.70 |
| 4:B:475:PHE:O | 4:B:477:GLU:N | 2.25 | 0.70 |
| 4:B:777:GLY:O | 4:B:780:PRO:HD2 | 1.92 | 0.70 |
| 4:D:29:GLY:HA2 | 7:D:3080:HOH:O | 1.91 | 0.70 |
| 4:A:480:LYS:O | 4:A:484:GLU:HG3 | 1.91 | 0.70 |
| 4:C:40:GLU:OE2 | 4:C:286:TYR:HD1 | 1.74 | 0.70 |
| 4:C:572:GLY:O | 4:C:575:ALA:HB3 | 1.91 | 0.70 |
| 4:C:67:ASN:O | 4:C:69:ALA:N | 2.25 | 0.70 |
| 4:D:221:ILE:HG12 | 4:D:227:VAL:HG23 | 1.73 | 0.70 |
| 4:C:330:ILE:HG13 | 4:C:408:PHE:O | 1.91 | 0.70 |
| 4:D:306:MET:O | 4:D:308:TYR:N | 2.25 | 0.70 |
| 4:D:432:PHE:CE1 | 4:D:444:LEU:HD11 | 2.26 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:739:TYR:OH | 4:D:781:ASN:OD1 | 2.10 | 0.70 |
| 1:E:12:DT:H2'' | 1:E:13:DC:H5'' | 1.71 | 0.70 |
| 4:A:525:GLY:O | 4:A:527:SER:N | 2.24 | 0.70 |
| 4:A:78:LEU:N | 4:A:79:PRO:HD2 | 2.06 | 0.70 |
| 4:B:326:THR:HA | 7:B:3162:HOH:O | 1.90 | 0.70 |
| 4:C:333:LYS:HD3 | 4:C:516:PHE:CD2 | 2.22 | 0.70 |
| 4:C:703:ALA:HB2 | 4:C:778:ILE:HG12 | 1.73 | 0.70 |
| 4:D:36:GLN:CD | 4:D:273:VAL:HG22 | 2.12 | 0.70 |
| 4:D:268:PHE:CD2 | 4:D:429:VAL:HG12 | 2.26 | 0.70 |
| 4:A:16:LEU:HA | 4:A:37:LEU:HD22 | 1.73 | 0.70 |
| 4:A:4:ILE:HD12 | 7:A:3067:HOH:O | 1.92 | 0.70 |
| 4:B:632:ARG:HD3 | 6:B:2001:APC:N7 | 2.07 | 0.70 |
| 4:B:868:GLY:C | 4:B:869:ASN:HD22 | 1.95 | 0.70 |
| 4:C:105:PHE:HE1 | 4:C:208:ASP:HB3 | 1.56 | 0.70 |
| 4:D:14:ILE:HG23 | 4:D:288:ALA:HB1 | 1.74 | 0.70 |
| 4:A:611:LEU:HD12 | 4:A:669:GLN:HB2 | 1.74 | 0.70 |
| 4:A:647:ARG:HG3 | 4:A:674:ALA:O | 1.92 | 0.70 |
| 4:C:270:PRO:HG3 | 4:C:430:SER:OG | 1.92 | 0.70 |
| 4:D:402:LEU:HD23 | 4:D:443:LEU:CD1 | 2.22 | 0.70 |
| 4:B:416:PHE:CE1 | 4:B:433:ASN:HA | 2.26 | 0.70 |
| 4:B:544:GLN:HG3 | 4:B:561:LEU:HD11 | 1.74 | 0.70 |
| 4:B:557:ARG:HD3 | 7:B:3119:HOH:O | 1.91 | 0.70 |
| 4:B:734:PRO:HG2 | 4:B:734:PRO:O | 1.91 | 0.70 |
| 4:C:551:ARG:HH11 | 4:C:551:ARG:CG | 2.05 | 0.70 |
| 4:D:882:PHE:O | 4:D:883:ALA:HB3 | 1.92 | 0.70 |
| 2:I:1:G:H2' | 2:I:2:C:C6 | 2.27 | 0.70 |
| 4:A:746:ARG:HH12 | 4:A:754:GLN:H | 1.37 | 0.69 |
| 4:B:264:ILE:O | 4:B:266:PRO:HD3 | 1.92 | 0.69 |
| 4:B:298:ARG:HE | 4:B:419:ASN:HB3 | 1.57 | 0.69 |
| 4:B:647:ARG:O | 4:B:648:GLN:C | 2.31 | 0.69 |
| 4:B:788:GLY:O | 4:B:792:ARG:HG3 | 1.92 | 0.69 |
| 4:D:71:LYS:HD3 | 7:D:3030:HOH:O | 1.92 | 0.69 |
| 4:D:779:ALA:O | 4:D:783:VAL:HG22 | 1.90 | 0.69 |
| 1:K:11:DA:C2 | 1:K:12:DT:C4 | 2.80 | 0.69 |
| 4:A:273:VAL:O | 4:A:273:VAL:HG23 | 1.91 | 0.69 |
| 4:B:308:TYR:HA | 4:B:311:VAL:CG2 | 2.21 | 0.69 |
| 4:A:721:LYS:HD3 | 4:A:722:ARG:N | 2.07 | 0.69 |
| 4:B:278:TRP:HA | 7:B:3014:HOH:O | 1.92 | 0.69 |
| 4:C:322:ILE:HG13 | 7:C:3131:HOH:O | 1.91 | 0.69 |
| 4:C:570:ILE:O | 4:C:574:VAL:HG23 | 1.93 | 0.69 |
| 4:D:324:GLN:O | 4:D:324:GLN:HG2 | 1.91 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:471:ASP:O | 4:D:472:LYS:HD2 | 1.92 | 0.69 |
| 4:A:14:ILE:HD12 | 4:A:14:ILE:N | 2.07 | 0.69 |
| 4:A:19:ILE:HG23 | 4:A:20:PRO:HD2 | 1.73 | 0.69 |
| 4:A:275:PRO:HD3 | 4:A:415:TRP:HB3 | 1.74 | 0.69 |
| 4:B:307:ARG:HD3 | 4:B:736:TRP:CE3 | 2.28 | 0.69 |
| 4:B:390:ALA:C | 4:B:392:LYS:N | 2.46 | 0.69 |
| 4:B:824:LEU:O | 4:B:828:VAL:HG23 | 1.92 | 0.69 |
| 4:D:573:ILE:HA | 4:D:576:LYS:HD2 | 1.73 | 0.69 |
| 4:A:452:ILE:CD1 | 4:A:457:TYR:HB2 | 2.22 | 0.69 |
| 4:B:473:VAL:CG1 | 4:B:477:GLU:HB2 | 2.23 | 0.69 |
| 4:B:801:LYS:C | 4:B:801:LYS:HD3 | 2.13 | 0.69 |
| 4:C:29:GLY:HA3 | 7:C:3129:HOH:O | 1.93 | 0.69 |
| 4:B:512:LEU:O | 4:B:515:CYS:N | 2.25 | 0.69 |
| 4:B:829:ARG:NH2 | 4:B:882:PHE:CA | 2.54 | 0.69 |
| 4:D:158:GLU:HA | 4:D:195:LEU:HD22 | 1.75 | 0.69 |
| 4:A:236:VAL:HG11 | 4:A:239:GLN:CD | 2.13 | 0.69 |
| 4:A:6:ILE:O | 4:A:8:LYS:N | 2.22 | 0.69 |
| 1:H:12:DT:H4' | 4:B:423:ARG:NE | 2.08 | 0.69 |
| 4:B:418:TYR:CE2 | 4:B:428:ALA:HB2 | 2.18 | 0.69 |
| 4:D:274:PRO:HD3 | 4:D:415:TRP:CH2 | 2.27 | 0.69 |
| 4:A:474:PRO:HG2 | 4:A:477:GLU:HG3 | 1.75 | 0.69 |
| 4:B:549:MET:CE | 4:B:841:VAL:HG21 | 2.22 | 0.69 |
| 4:C:25:ALA:HA | 4:C:29:GLY:O | 1.92 | 0.69 |
| 4:C:308:TYR:HE2 | 4:C:734:PRO:HG2 | 1.57 | 0.69 |
| 4:D:120:LYS:HD2 | 4:D:752:LEU:HD11 | 1.73 | 0.69 |
| 4:D:206:LYS:H | 4:D:206:LYS:HD3 | 1.57 | 0.69 |
| 4:D:210:ILE:O | 4:D:214:VAL:HG23 | 1.93 | 0.69 |
| 4:D:657:PRO:O | 4:D:661:SER:HB2 | 1.92 | 0.69 |
| 1:K:7:DC:H2'' | 1:K:8:DG:O5' | 1.91 | 0.69 |
| 4:B:132:THR:HG21 | 7:B:3161:HOH:O | 1.92 | 0.69 |
| 4:B:390:ALA:O | 4:B:392:LYS:N | 2.25 | 0.69 |
| 4:B:423:ARG:HH12 | 4:B:784:HIS:CB | 2.06 | 0.69 |
| 4:D:337:VAL:HG21 | 4:D:512:LEU:HD21 | 1.74 | 0.69 |
| 4:A:311:VAL:HG12 | 4:A:312:TYR:N | 2.08 | 0.69 |
| 4:A:526:LEU:CD1 | 4:A:526:LEU:H | 2.06 | 0.69 |
| 4:A:665:LEU:HD12 | 4:A:665:LEU:H | 1.58 | 0.69 |
| 4:B:247:ALA:HB3 | 4:B:250:TYR:HB2 | 1.76 | 0.69 |
| 4:B:452:ILE:CG2 | 4:B:453:GLY:N | 2.33 | 0.69 |
| 4:D:333:LYS:NZ | 4:D:516:PHE:HB3 | 2.08 | 0.69 |
| 1:H:3:DG:N2 | 7:H:948:HOH:O | 2.25 | 0.69 |
| 4:A:308:TYR:CE2 | 4:A:734:PRO:HG2 | 2.21 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:B:109:ILE:N | 4:B:109:ILE:HD12 | 2.08 | 0.68 |
| 4:B:308:TYR:HA | 4:B:311:VAL:HG23 | 1.75 | 0.68 |
| 4:C:428:ALA:H | 4:C:435:GLN:NE2 | 1.90 | 0.68 |
| 4:D:390:ALA:HB1 | 4:D:394:ARG:HH21 | 1.58 | 0.68 |
| 4:D:470:VAL:HG12 | 4:D:473:VAL:CG1 | 2.23 | 0.68 |
| 4:A:275:PRO:HD3 | 4:A:415:TRP:CB | 2.22 | 0.68 |
| 4:A:236:VAL:HG11 | 4:A:239:GLN:CG | 2.24 | 0.68 |
| 4:A:4:ILE:HD11 | 4:A:256:THR:OG1 | 1.92 | 0.68 |
| 4:A:404:GLN:NE2 | 4:A:404:GLN:HA | 2.08 | 0.68 |
| 4:A:59:LEU:HD23 | 4:A:64:VAL:CG2 | 2.23 | 0.68 |
| 4:A:668:THR:HG22 | 4:A:669:GLN:CD | 2.14 | 0.68 |
| 4:C:840:ASP:O | 4:C:842:LEU:N | 2.27 | 0.68 |
| 4:D:433:ASN:HB2 | 4:D:434:PRO:CD | 2.23 | 0.68 |
| 4:B:571:TYR:HE1 | 7:B:3067:HOH:O | 1.75 | 0.68 |
| 4:B:261:LEU:O | 4:B:263:GLY:N | 2.27 | 0.68 |
| 4:B:301:SER:O | 4:B:304:ALA:N | 2.27 | 0.68 |
| 4:C:335:LEU:HD11 | 4:C:406:ASN:OD1 | 1.94 | 0.68 |
| 4:A:11:PHE:CE1 | 4:A:44:TYR:HB3 | 2.29 | 0.68 |
| 4:B:840:ASP:O | 4:B:842:LEU:N | 2.27 | 0.68 |
| 4:A:551:ARG:HB2 | 4:A:868:GLY:H | 1.58 | 0.68 |
| 4:B:31:ARG:HB3 | 4:B:31:ARG:HH11 | 1.59 | 0.68 |
| 4:B:720:ARG:NH1 | 4:B:720:ARG:HG2 | 1.92 | 0.68 |
| 4:B:730:PRO:CD | 4:B:786:GLN:HE21 | 2.06 | 0.68 |
| 4:B:801:LYS:HD3 | 4:B:801:LYS:O | 1.94 | 0.68 |
| 4:D:326:THR:O | 4:D:415:TRP:HD1 | 1.76 | 0.68 |
| 4:D:437:ASN:HD21 | 4:D:440:THR:H | 1.41 | 0.68 |
| 4:D:55:PHE:HA | 4:D:58:GLN:HG3 | 1.75 | 0.68 |
| 4:A:486:HIS:CD2 | 4:A:518:TYR:CE1 | 2.80 | 0.68 |
| 4:A:655:ILE:HD12 | 4:A:674:ALA:HB2 | 1.76 | 0.68 |
| 4:B:301:SER:O | 4:B:304:ALA:HB3 | 1.94 | 0.68 |
| 4:B:354:ALA:HA | 7:B:3118:HOH:O | 1.94 | 0.68 |
| 4:C:17:ALA:HB2 | 7:C:3201:HOH:O | 1.92 | 0.68 |
| 4:C:40:GLU:OE1 | 4:C:286:TYR:HB3 | 1.92 | 0.68 |
| 4:C:432:PHE:CZ | 4:C:444:LEU:HD21 | 2.28 | 0.68 |
| 4:C:465:ALA:O | 4:C:470:VAL:HG23 | 1.94 | 0.68 |
| 4:D:433:ASN:HB2 | 4:D:434:PRO:HD2 | 1.74 | 0.68 |
| 1:E:12:DT:H5" | 4:A:422:TRP:CH2 | 2.29 | 0.68 |
| 4:B:564:SER:OG | 4:B:565:GLU:N | 2.25 | 0.68 |
| 4:B:706:LEU:HD11 | 4:B:849:PHE:HD2 | 1.58 | 0.68 |
| 4:D:233:ASN:HD22 | 4:D:239:GLN:NE2 | 1.92 | 0.68 |
| 4:A:552:ASP:OD2 | 7:A:3223:HOH:O | 2.10 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:C:134:VAL:HG12 | 4:C:242:GLU:O | 1.94 | 0.68 |
| 4:C:159:ALA:O | 4:C:163:LYS:HB2 | 1.93 | 0.68 |
| 4:C:173:ARG:CZ | 4:C:182:PHE:HB2 | 2.23 | 0.68 |
| 4:A:404:GLN:HE21 | 4:A:404:GLN:CA | 2.02 | 0.67 |
| 4:B:299:THR:HG21 | 4:B:305:LEU:HA | 1.76 | 0.67 |
| 4:C:146:GLU:OE2 | 4:C:201:TRP:HB3 | 1.94 | 0.67 |
| 4:C:338:ALA:C | 4:C:340:VAL:N | 2.46 | 0.67 |
| 4:C:340:VAL:O | 4:C:342:THR:N | 2.27 | 0.67 |
| 4:C:514:PHE:CG | 4:C:514:PHE:O | 2.47 | 0.67 |
| 4:C:785:SER:HA | 7:C:3159:HOH:O | 1.93 | 0.67 |
| 4:C:475:PHE:CE2 | 4:C:879:ASP:HB3 | 2.29 | 0.67 |
| 4:D:100:PRO:HG2 | 4:D:103:PHE:CB | 2.23 | 0.67 |
| 4:D:161:HIS:O | 4:D:164:LYS:HG2 | 1.94 | 0.67 |
| 4:D:55:PHE:CE1 | 4:D:59:LEU:HD21 | 2.30 | 0.67 |
| 4:A:631:LYS:NZ | 6:A:2000:APC:C3A | 2.49 | 0.67 |
| 4:A:748:ASN:HD22 | 4:A:751:PHE:H | 1.40 | 0.67 |
| 4:B:418:TYR:HD2 | 4:B:428:ALA:HA | 1.59 | 0.67 |
| 4:B:571:TYR:OH | 4:B:635:MET:HE3 | 1.94 | 0.67 |
| 4:D:333:LYS:HB3 | 4:D:516:PHE:CD2 | 2.28 | 0.67 |
| 4:D:718:ILE:HD12 | 7:D:3025:HOH:O | 1.94 | 0.67 |
| 4:D:829:ARG:NH1 | 4:D:829:ARG:HG3 | 2.07 | 0.67 |
| 4:A:526:LEU:CD1 | 4:A:526:LEU:N | 2.57 | 0.67 |
| 4:A:744:GLN:HA | 4:A:756:ARG:NH2 | 2.09 | 0.67 |
| 4:B:552:ASP:C | 4:B:552:ASP:OD1 | 2.32 | 0.67 |
| 4:B:623:TYR:HA | 4:B:666:MET:CE | 2.23 | 0.67 |
| 4:C:50:ARG:HG2 | 4:C:50:ARG:NH1 | 2.07 | 0.67 |
| 4:C:866:ALA:HB1 | 7:C:3057:HOH:O | 1.94 | 0.67 |
| 4:A:464:GLY:CA | 4:A:514:PHE:CE2 | 2.78 | 0.67 |
| 4:A:551:ARG:NH2 | 4:A:872:LEU:HD11 | 2.10 | 0.67 |
| 4:A:423:ARG:NH2 | 4:A:784:HIS:CB | 2.58 | 0.67 |
| 4:A:78:LEU:HD21 | 4:A:116:TYR:HB2 | 1.74 | 0.67 |
| 4:B:269:GLN:NE2 | 4:B:407:LYS:NZ | 2.42 | 0.67 |
| 4:B:418:TYR:HD2 | 4:B:427:TYR:O | 1.78 | 0.67 |
| 4:C:32:LEU:HB2 | 7:C:3157:HOH:O | 1.94 | 0.67 |
| 4:C:475:PHE:HE2 | 4:C:879:ASP:HB3 | 1.58 | 0.67 |
| 4:D:330:ILE:HD11 | 4:D:405:ALA:HA | 1.75 | 0.67 |
| 4:D:855:GLU:O | 4:D:858:LEU:HD12 | 1.94 | 0.67 |
| 1:H:12:DT:O4' | 4:B:423:ARG:NH2 | 2.27 | 0.67 |
| 1:N:14:DG:N7 | 7:N:81:HOH:O | 2.27 | 0.67 |
| 4:A:495:SER:HB3 | 4:A:498:GLU:HG3 | 1.77 | 0.67 |
| 4:A:510:CYS:O | 4:A:513:ALA:N | 2.26 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:A:630:THR:O | 7:A:3199:HOH:O | 2.12 | 0.67 |
| 4:C:2:ASN:O | 7:C:3169:HOH:O | 2.11 | 0.67 |
| 4:C:59:LEU:CD2 | 4:C:64:VAL:HG13 | 2.24 | 0.67 |
| 4:A:109:ILE:HG13 | 4:A:149:ALA:HB2 | 1.75 | 0.67 |
| 4:A:428:ALA:HB3 | 4:A:433:ASN:HD22 | 1.57 | 0.67 |
| 4:B:449:GLY:HA3 | 4:B:529:ASN:HD21 | 1.58 | 0.67 |
| 4:B:829:ARG:HG3 | 4:B:829:ARG:NH1 | 2.05 | 0.67 |
| 4:C:24:LEU:HD21 | 4:C:287:TRP:CE2 | 2.29 | 0.67 |
| 4:C:330:ILE:CG1 | 4:C:408:PHE:O | 2.43 | 0.67 |
| 4:C:631:LYS:HZ1 | 6:C:2002:APC:C3A | 2.07 | 0.67 |
| 4:D:303:LYS:HG3 | 4:D:304:ALA:N | 2.10 | 0.67 |
| 4:A:716:GLY:HA3 | 7:A:3184:HOH:O | 1.93 | 0.67 |
| 4:A:802:TYR:N | 4:A:802:TYR:CD2 | 2.61 | 0.67 |
| 4:A:849:PHE:HD2 | 4:A:853:LEU:HD21 | 1.60 | 0.67 |
| 4:B:794:THR:OG1 | 4:B:831:THR:HG21 | 1.92 | 0.67 |
| 4:C:632:ARG:NH2 | 6:C:2002:APC:H5'1 | 2.08 | 0.67 |
| 4:D:778:ILE:CG2 | 4:D:779:ALA:N | 2.57 | 0.67 |
| 4:D:797:TRP:HE1 | 4:D:802:TYR:HE2 | 1.41 | 0.67 |
| 4:A:518:TYR:O | 4:A:518:TYR:CD1 | 2.48 | 0.67 |
| 4:C:279:THR:HG22 | 7:C:3038:HOH:O | 1.95 | 0.67 |
| 4:C:338:ALA:C | 4:C:340:VAL:H | 1.96 | 0.67 |
| 4:C:534:LEU:HD12 | 4:C:821:ALA:CB | 2.25 | 0.67 |
| 4:D:19:ILE:HD12 | 4:D:20:PRO:HD2 | 1.77 | 0.67 |
| 4:D:656:GLN:N | 4:D:657:PRO:HD2 | 2.10 | 0.67 |
| 4:D:769:ILE:H | 4:D:769:ILE:HD12 | 1.60 | 0.67 |
| 4:A:746:ARG:HG3 | 4:A:756:ARG:HB2 | 1.77 | 0.67 |
| 4:B:77:LEU:CD1 | 4:B:224:THR:HG21 | 2.25 | 0.67 |
| 4:B:423:ARG:HH11 | 4:B:423:ARG:CB | 2.08 | 0.67 |
| 4:B:449:GLY:CA | 4:B:529:ASN:HD21 | 2.08 | 0.67 |
| 4:B:64:VAL:HG21 | 4:B:127:THR:HG21 | 1.76 | 0.67 |
| 4:C:308:TYR:CZ | 4:C:733:PHE:HE2 | 2.12 | 0.67 |
| 4:C:349:VAL:HG11 | 4:C:508:PRO:HG3 | 1.77 | 0.67 |
| 4:C:9:ASN:HA | 4:C:12:SER:HB3 | 1.76 | 0.67 |
| 4:A:428:ALA:HB3 | 4:A:433:ASN:ND2 | 2.09 | 0.67 |
| 4:A:843:ALA:O | 4:A:846:TYR:N | 2.27 | 0.67 |
| 4:B:254:ILE:HG22 | 4:B:255:ALA:N | 2.10 | 0.67 |
| 4:B:720:ARG:HH11 | 4:B:720:ARG:CG | 2.03 | 0.67 |
| 4:B:549:MET:HE2 | 4:B:841:VAL:HG21 | 1.76 | 0.67 |
| 4:C:707:ALA:O | 4:C:722:ARG:HB3 | 1.95 | 0.67 |
| 4:C:77:LEU:C | 4:C:79:PRO:HD2 | 2.15 | 0.67 |
| 4:A:786:GLN:CA | 4:A:786:GLN:HE21 | 2.03 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:C:105:PHE:CE1 | 4:C:208:ASP:HB3 | 2.30 | 0.66 |
| 4:C:443:LEU:O | 4:C:444:LEU:HD23 | 1.95 | 0.66 |
| 4:C:460:LEU:HA | 4:C:534:LEU:CD2 | 2.24 | 0.66 |
| 4:D:635:MET:HE1 | 6:D:2003:APC:H3' | 1.77 | 0.66 |
| 4:D:39:LEU:HD22 | 4:D:272:VAL:HG23 | 1.76 | 0.66 |
| 4:D:272:VAL:O | 4:D:415:TRP:CZ3 | 2.47 | 0.66 |
| 4:A:46:MET:HG2 | 7:A:3162:HOH:O | 1.94 | 0.66 |
| 4:B:671:ASN:O | 4:B:674:ALA:HB3 | 1.96 | 0.66 |
| 4:B:850:ALA:O | 4:B:852:GLN:N | 2.28 | 0.66 |
| 4:C:706:LEU:HD22 | 4:C:725:VAL:CG1 | 2.24 | 0.66 |
| 4:A:548:ALA:C | 4:A:550:LEU:H | 1.97 | 0.66 |
| 4:A:669:GLN:O | 4:A:670:PRO:C | 2.33 | 0.66 |
| 4:B:35:GLU:O | 4:B:38:ALA:HB3 | 1.96 | 0.66 |
| 4:B:731:ASP:HB3 | 4:B:789:SER:OG | 1.96 | 0.66 |
| 4:D:89:PHE:HZ | 4:D:106:LEU:HB3 | 1.60 | 0.66 |
| 4:D:269:GLN:HG2 | 4:D:408:PHE:HZ | 1.59 | 0.66 |
| 4:A:881:ALA:O | 4:A:883:ALA:OXT | 2.14 | 0.66 |
| 4:C:551:ARG:CD | 4:C:872:LEU:HD21 | 2.24 | 0.66 |
| 4:D:109:ILE:HD13 | 4:D:114:VAL:HG22 | 1.76 | 0.66 |
| 4:D:744:GLN:HG2 | 4:D:756:ARG:HB3 | 1.75 | 0.66 |
| 4:D:829:ARG:HH22 | 4:D:882:PHE:HA | 1.61 | 0.66 |
| 4:A:308:TYR:OH | 4:A:734:PRO:O | 2.14 | 0.66 |
| 4:A:540:CYS:O | 4:A:541:SER:C | 2.33 | 0.66 |
| 4:A:828:VAL:HG23 | 4:A:829:ARG:N | 2.06 | 0.66 |
| 4:B:233:ASN:HD22 | 4:B:239:GLN:CD | 1.97 | 0.66 |
| 4:B:424:GLY:O | 4:B:792:ARG:NH1 | 2.29 | 0.66 |
| 4:C:105:PHE:O | 4:C:107:GLN:N | 2.29 | 0.66 |
| 4:C:50:ARG:HG2 | 4:C:50:ARG:HH11 | 1.60 | 0.66 |
| 4:C:50:ARG:CG | 4:C:50:ARG:HH11 | 2.08 | 0.66 |
| 4:D:275:PRO:HD2 | 7:D:3108:HOH:O | 1.94 | 0.66 |
| 4:D:560:ASN:OD1 | 4:D:568:GLN:HB2 | 1.95 | 0.66 |
| 4:D:84:ARG:HD3 | 4:D:84:ARG:O | 1.94 | 0.66 |
| 4:A:418:TYR:HD2 | 4:A:426:VAL:HG12 | 1.60 | 0.66 |
| 4:A:574:VAL:HG11 | 4:A:685:VAL:CG1 | 2.25 | 0.66 |
| 4:A:769:ILE:HD12 | 4:A:769:ILE:H | 1.60 | 0.66 |
| 4:B:437:ASN:HB2 | 7:B:3149:HOH:O | 1.95 | 0.66 |
| 4:A:157:LEU:HD23 | 7:A:3133:HOH:O | 1.95 | 0.66 |
| 4:A:44:TYR:CE2 | 4:A:266:PRO:HB3 | 2.31 | 0.66 |
| 4:A:30:GLU:HB3 | 4:A:34:ARG:NH2 | 2.10 | 0.66 |
| 4:B:525:GLY:O | 4:B:527:SER:N | 2.28 | 0.66 |
| 4:C:286:TYR:CZ | 4:C:417:PRO:HG3 | 2.31 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:C:36:GLN:HG3 | 4:C:273:VAL:HG22 | 1.78 | 0.66 |
| 4:C:553:GLU:HG2 | 4:C:554:VAL:H | 1.60 | 0.66 |
| 4:C:605:ILE:HG23 | 7:C:3098:HOH:O | 1.96 | 0.66 |
| 4:C:562:LEU:HD21 | 4:C:870:LEU:HG | 1.77 | 0.66 |
| 4:D:402:LEU:HD23 | 4:D:443:LEU:HD11 | 1.77 | 0.66 |
| 4:A:119:ILE:O | 4:A:122:THR:HB | 1.95 | 0.66 |
| 4:A:463:HIS:HD2 | 7:A:3167:HOH:O | 1.77 | 0.66 |
| 4:A:485:ASN:HB3 | 4:A:488:ASN:HD22 | 1.61 | 0.66 |
| 4:A:459:TRP:HE1 | 4:A:822:ALA:HA | 1.61 | 0.66 |
| 4:A:869:ASN:ND2 | 4:A:869:ASN:N | 2.44 | 0.66 |
| 4:B:336:ALA:O | 4:B:340:VAL:HG23 | 1.95 | 0.66 |
| 4:B:616:LEU:O | 4:B:619:GLN:N | 2.29 | 0.66 |
| 4:C:553:GLU:CD | 4:C:553:GLU:H | 1.99 | 0.66 |
| 4:D:23:THR:O | 4:D:27:HIS:HB2 | 1.96 | 0.66 |
| 4:D:337:VAL:O | 4:D:341:ILE:HG12 | 1.96 | 0.66 |
| 4:D:574:VAL:O | 4:D:578:VAL:HG23 | 1.95 | 0.66 |
| 4:A:281:ILE:HD11 | 4:A:309:GLU:N | 2.11 | 0.66 |
| 4:A:563:PRO:HB3 | 4:A:877:GLU:O | 1.96 | 0.66 |
| 4:B:825:PHE:O | 4:B:829:ARG:NH1 | 2.29 | 0.66 |
| 4:D:425:ARG:HB3 | 4:D:427:TYR:HE1 | 1.61 | 0.66 |
| 4:B:291:ARG:CG | 7:B:3037:HOH:O | 2.44 | 0.66 |
| 4:B:475:PHE:HA | 4:B:478:ARG:HD2 | 1.78 | 0.66 |
| 4:B:730:PRO:CD | 4:B:786:GLN:NE2 | 2.59 | 0.66 |
| 1:K:12:DT:C2 | 1:K:13:DC:C5 | 2.83 | 0.66 |
| 4:A:80:LYS:HD3 | 4:A:224:THR:HG22 | 1.76 | 0.65 |
| 4:B:173:ARG:HH11 | 4:B:182:PHE:HD1 | 1.44 | 0.65 |
| 4:B:273:VAL:O | 4:B:274:PRO:C | 2.32 | 0.65 |
| 4:B:536:PHE:HB3 | 4:B:882:PHE:HB3 | 1.76 | 0.65 |
| 4:A:475:PHE:HD2 | 7:A:3202:HOH:O | 1.79 | 0.65 |
| 4:A:737:GLN:O | 4:A:774:GLN:NE2 | 2.29 | 0.65 |
| 4:B:37:LEU:N | 4:B:37:LEU:HD12 | 2.09 | 0.65 |
| 4:B:639:TYR:HE1 | 7:B:3084:HOH:O | 1.79 | 0.65 |
| 4:B:726:HIS:CD2 | 4:B:735:VAL:O | 2.49 | 0.65 |
| 4:C:182:PHE:O | 4:C:186:VAL:HG23 | 1.97 | 0.65 |
| 4:C:340:VAL:O | 4:C:341:ILE:C | 2.33 | 0.65 |
| 4:C:551:ARG:HH11 | 4:C:551:ARG:HG3 | 1.61 | 0.65 |
| 4:D:718:ILE:CD1 | 7:D:3025:HOH:O | 2.43 | 0.65 |
| 4:A:433:ASN:C | 4:A:433:ASN:OD1 | 2.34 | 0.65 |
| 4:B:159:ALA:O | 4:B:160:LYS:C | 2.32 | 0.65 |
| 4:B:330:ILE:HD12 | 4:B:405:ALA:HB1 | 1.78 | 0.65 |
| 4:B:428:ALA:H | 4:B:435:GLN:HE22 | 1.43 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:C:551:ARG:NH2 | 4:C:872:LEU:HD11 | 2.11 | 0.65 |
| 4:D:106:LEU:HA | 4:D:109:ILE:HD11 | 1.78 | 0.65 |
| 4:D:252:GLU:O | 4:D:255:ALA:HB3 | 1.97 | 0.65 |
| 4:D:508:PRO:O | 4:D:511:PHE:N | 2.29 | 0.65 |
| 4:D:553:GLU:OE1 | 4:D:869:ASN:HB2 | 1.97 | 0.65 |
| 4:D:629:VAL:HG13 | 4:D:654:THR:HG21 | 1.77 | 0.65 |
| 4:A:24:LEU:HD21 | 4:A:287:TRP:CE2 | 2.31 | 0.65 |
| 4:A:668:THR:HG22 | 4:A:669:GLN:NE2 | 2.11 | 0.65 |
| 4:B:780:PRO:HD2 | 4:B:781:ASN:H | 1.61 | 0.65 |
| 4:C:64:VAL:HG21 | 4:C:127:THR:HG21 | 1.77 | 0.65 |
| 4:C:298:ARG:HB2 | 4:C:421:ASP:HA | 1.79 | 0.65 |
| 4:D:796:VAL:HA | 7:D:3013:HOH:O | 1.96 | 0.65 |
| 4:A:3:THR:HB | 4:A:52:ARG:NH1 | 2.12 | 0.65 |
| 4:B:236:VAL:HG21 | 4:B:239:GLN:HE21 | 1.60 | 0.65 |
| 4:B:266:PRO:HG2 | 4:B:268:PHE:CZ | 2.31 | 0.65 |
| 4:B:552:ASP:O | 4:B:552:ASP:OD1 | 2.14 | 0.65 |
| 4:B:663:LYS:HE2 | 4:B:666:MET:HE1 | 1.77 | 0.65 |
| 4:B:705:LEU:O | 4:B:707:ALA:N | 2.29 | 0.65 |
| 4:B:790:HIS:CE1 | 4:B:831:THR:HG23 | 2.30 | 0.65 |
| 4:D:236:VAL:HG21 | 4:D:239:GLN:NE2 | 2.11 | 0.65 |
| 1:E:5:DA:C2 | 3:G:7:DT:O2 | 2.50 | 0.65 |
| 4:A:141:ILE:O | 4:A:145:ILE:HG12 | 1.96 | 0.65 |
| 4:A:292:ARG:H | 4:A:293:PRO:HD3 | 1.62 | 0.65 |
| 4:A:632:ARG:O | 4:A:633:SER:C | 2.34 | 0.65 |
| 4:B:257:ARG:HG2 | 4:B:257:ARG:HH11 | 1.60 | 0.65 |
| 4:B:728:VAL:O | 7:B:3081:HOH:O | 2.15 | 0.65 |
| 4:C:631:LYS:HE2 | 4:C:635:MET:SD | 2.36 | 0.65 |
| 4:D:9:ASN:HA | 4:D:12:SER:HB2 | 1.79 | 0.65 |
| 1:N:16:DC:H2'' | 1:N:17:DG:O5' | 1.97 | 0.65 |
| 4:A:590:THR:HG1 | 4:A:613:THR:HG1 | 1.41 | 0.65 |
| 4:B:446:LEU:HD12 | 4:B:817:ILE:CG2 | 2.27 | 0.65 |
| 4:B:540:CYS:O | 4:B:541:SER:C | 2.35 | 0.65 |
| 4:C:551:ARG:NH2 | 4:C:836:TYR:O | 2.30 | 0.65 |
| 4:C:801:LYS:C | 4:C:801:LYS:HD3 | 2.17 | 0.65 |
| 4:D:109:ILE:HG12 | 4:D:145:ILE:HG22 | 1.79 | 0.65 |
| 4:D:475:PHE:N | 4:D:476:PRO:HD2 | 2.11 | 0.65 |
| 3:G:7:DT:H2'' | 3:G:8:DC:C6 | 2.31 | 0.65 |
| 1:K:13:DC:H2'' | 1:K:14:DG:H5' | 1.78 | 0.65 |
| 4:A:154:ILE:HG23 | 4:A:190:MET:HE2 | 1.76 | 0.65 |
| 4:B:119:ILE:N | 4:B:119:ILE:HD13 | 2.11 | 0.65 |
| 4:D:218:GLU:O | 4:D:222:GLU:HB2 | 1.95 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:D:428:ALA:H | 4:D:435:GLN:HE21 | 1.43 | 0.65 |
| 4:A:19:ILE:CG2 | 7:A:3120:HOH:O | 2.45 | 0.65 |
| 4:A:221:ILE:HG23 | 4:A:227:VAL:O | 1.97 | 0.65 |
| 4:A:744:GLN:HA | 4:A:756:ARG:CZ | 2.27 | 0.65 |
| 4:A:793:LYS:HA | 4:A:796:VAL:CG2 | 2.27 | 0.65 |
| 4:B:14:ILE:HD12 | 4:B:14:ILE:N | 2.08 | 0.65 |
| 4:B:631:LYS:CE | 6:B:2001:APC:H3A2 | 2.26 | 0.65 |
| 4:B:807:PHE:HA | 4:B:815:GLY:O | 1.96 | 0.65 |
| 4:C:474:PRO:HB2 | 4:C:476:PRO:HD2 | 1.78 | 0.65 |
| 4:D:340:VAL:O | 4:D:341:ILE:C | 2.35 | 0.65 |
| 4:A:16:LEU:HD22 | 4:A:38:ALA:HA | 1.77 | 0.65 |
| 4:B:296:LEU:CG | 4:B:296:LEU:O | 2.44 | 0.65 |
| 4:C:346:HIS:HA | 4:C:395:ARG:HH11 | 1.61 | 0.65 |
| 4:C:595:VAL:HG21 | 7:C:3085:HOH:O | 1.97 | 0.65 |
| 4:D:737:GLN:NE2 | 4:D:778:ILE:HA | 2.06 | 0.65 |
| 1:K:17:DG:H2" | 1:K:18:DC:C5 | 2.32 | 0.65 |
| 4:A:26:ASP:HB2 | 7:A:3183:HOH:O | 1.97 | 0.64 |
| 4:B:138:ALA:HB2 | 4:B:214:VAL:HG13 | 1.79 | 0.64 |
| 4:B:122:THR:CG2 | 4:B:226:MET:CE | 2.74 | 0.64 |
| 4:B:559:VAL:HG23 | 4:B:559:VAL:O | 1.98 | 0.64 |
| 4:B:435:GLN:CG | 4:B:810:ILE:HG23 | 2.20 | 0.64 |
| 4:C:727:TRP:CE3 | 4:C:735:VAL:HG13 | 2.32 | 0.64 |
| 4:D:564:SER:O | 7:D:3040:HOH:O | 2.14 | 0.64 |
| 4:A:40:GLU:HG2 | 4:A:286:TYR:HD1 | 1.62 | 0.64 |
| 4:A:421:ASP:O | 4:A:422:TRP:C | 2.31 | 0.64 |
| 4:B:281:ILE:CG2 | 4:B:282:THR:HG23 | 2.27 | 0.64 |
| 4:B:33:ALA:O | 4:B:37:LEU:HD13 | 1.97 | 0.64 |
| 4:B:828:VAL:CG1 | 4:B:883:ALA:HA | 2.28 | 0.64 |
| 4:D:134:VAL:H | 4:D:243:THR:HA | 1.62 | 0.64 |
| 4:D:426:VAL:HG21 | 4:D:791:LEU:HD21 | 1.78 | 0.64 |
| 4:A:50:ARG:NH1 | 4:A:50:ARG:HG2 | 2.11 | 0.64 |
| 4:A:78:LEU:N | 4:A:79:PRO:CD | 2.60 | 0.64 |
| 4:A:817:ILE:HB | 4:A:818:PRO:HD2 | 1.79 | 0.64 |
| 4:B:449:GLY:C | 4:B:529:ASN:HD21 | 2.01 | 0.64 |
| 4:C:746:ARG:HD3 | 4:C:755:PHE:O | 1.97 | 0.64 |
| 4:C:837:GLU:CG | 4:C:872:LEU:HD12 | 2.27 | 0.64 |
| 4:D:471:ASP:C | 4:D:472:LYS:HD2 | 2.17 | 0.64 |
| 4:B:275:PRO:O | 4:B:277:PRO:HD3 | 1.97 | 0.64 |
| 4:B:37:LEU:CD1 | 4:B:37:LEU:H | 2.10 | 0.64 |
| 4:B:58:GLN:HG3 | 4:B:67:ASN:HD22 | 1.63 | 0.64 |
| 4:B:702:ALA:O | 4:B:706:LEU:HD12 | 1.96 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:C:342:THR:HG22 | 4:C:348:PRO:CG | 2.24 | 0.64 |
| 4:C:400:PHE:CE1 | 4:C:431:MET:HE2 | 2.32 | 0.64 |
| 4:D:269:GLN:HG2 | 4:D:408:PHE:CZ | 2.33 | 0.64 |
| 4:D:326:THR:O | 4:D:415:TRP:CD1 | 2.50 | 0.64 |
| 4:D:402:LEU:CD2 | 4:D:443:LEU:HD11 | 2.28 | 0.64 |
| 4:D:438:ASP:OD2 | 4:D:508:PRO:HG2 | 1.97 | 0.64 |
| 4:D:471:ASP:OD1 | 4:D:472:LYS:HD3 | 1.97 | 0.64 |
| 1:E:14:DG:H2' | 1:E:15:DC:C5 | 2.31 | 0.64 |
| 4:A:274:PRO:HG3 | 4:A:415:TRP:CE2 | 2.32 | 0.64 |
| 4:A:476:PRO:O | 4:A:479:ILE:N | 2.28 | 0.64 |
| 4:B:473:VAL:CG1 | 4:B:474:PRO:N | 2.59 | 0.64 |
| 4:C:433:ASN:HA | 7:C:3164:HOH:O | 1.93 | 0.64 |
| 4:A:257:ARG:HG2 | 4:A:257:ARG:HH11 | 1.62 | 0.64 |
| 4:B:231:ARG:CG | 4:B:234:ALA:HB2 | 2.27 | 0.64 |
| 4:B:486:HIS:CE1 | 4:B:490:MET:HG3 | 2.32 | 0.64 |
| 4:B:401:MET:HE3 | 4:B:440:THR:HG21 | 1.80 | 0.64 |
| 4:B:423:ARG:NH1 | 4:B:784:HIS:HB3 | 2.13 | 0.64 |
| 4:B:46:MET:HE1 | 4:B:269:GLN:HE22 | 1.61 | 0.64 |
| 4:B:446:LEU:HB2 | 4:B:531:SER:O | 1.98 | 0.64 |
| 4:B:720:ARG:CG | 4:B:720:ARG:NH1 | 2.59 | 0.64 |
| 4:B:779:ALA:N | 4:B:780:PRO:CD | 2.60 | 0.64 |
| 4:C:475:PHE:N | 4:C:476:PRO:HD2 | 2.13 | 0.64 |
| 4:D:135:GLN:HG3 | 7:D:3160:HOH:O | 1.97 | 0.64 |
| 4:D:572:GLY:O | 4:D:575:ALA:N | 2.30 | 0.64 |
| 2:F:7:A:H2' | 2:F:8:U:H6 | 1.62 | 0.64 |
| 4:A:545:HIS:CE1 | 4:A:787:ASP:HA | 2.33 | 0.64 |
| 4:B:492:CYS:SG | 4:B:502:TRP:CD1 | 2.90 | 0.64 |
| 4:B:5:ASN:ND2 | 4:B:7:ALA:N | 2.46 | 0.64 |
| 4:D:281:ILE:HD12 | 4:D:317:TYR:OH | 1.96 | 0.64 |
| 4:A:10:ASP:O | 4:A:13:ASP:HB2 | 1.98 | 0.64 |
| 4:A:502:TRP:CD1 | 4:A:512:LEU:CD1 | 2.81 | 0.64 |
| 4:B:469:GLY:O | 4:B:471:ASP:N | 2.31 | 0.64 |
| 4:C:163:LYS:HB3 | 4:C:164:LYS:HZ3 | 1.63 | 0.64 |
| 4:D:161:HIS:HE1 | 7:D:3114:HOH:O | 1.80 | 0.64 |
| 4:D:421:ASP:O | 4:D:423:ARG:N | 2.31 | 0.64 |
| 4:C:744:GLN:HB3 | 7:C:3076:HOH:O | 1.96 | 0.64 |
| 4:C:423:ARG:HE | 4:C:781:ASN:HD22 | 1.45 | 0.64 |
| 4:D:311:VAL:HG12 | 4:D:312:TYR:N | 2.13 | 0.64 |
| 4:D:734:PRO:O | 4:D:734:PRO:HG2 | 1.97 | 0.64 |
| 4:A:582:LEU:HD11 | 4:A:625:VAL:HG21 | 1.78 | 0.63 |
| 4:B:433:ASN:CB | 4:B:434:PRO:CD | 2.63 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:B:5:ASN:HD21 | 4:B:7:ALA:N | 1.95 | 0.63 |
| 4:B:751:PHE:HB3 | 4:B:752:LEU:CD1 | 2.19 | 0.63 |
| 4:C:292:ARG:N | 4:C:293:PRO:HD3 | 2.13 | 0.63 |
| 4:C:423:ARG:HD2 | 4:C:781:ASN:CB | 2.27 | 0.63 |
| 1:K:17:DG:H2" | 1:K:18:DC:C6 | 2.33 | 0.63 |
| 4:B:217:ILE:O | 4:B:221:ILE:HG13 | 1.98 | 0.63 |
| 4:C:424:GLY:HA3 | 7:C:3159:HOH:O | 1.98 | 0.63 |
| 4:A:634:VAL:HG23 | 4:A:685:VAL:HG11 | 1.80 | 0.63 |
| 4:C:335:LEU:HD21 | 4:C:339:ASN:ND2 | 2.13 | 0.63 |
| 4:D:273:VAL:CA | 4:D:415:TRP:CZ3 | 2.82 | 0.63 |
| 4:D:804:ILE:CG2 | 4:D:816:THR:HG21 | 2.29 | 0.63 |
| 4:B:113:ALA:O | 4:B:117:ILE:HG13 | 1.98 | 0.63 |
| 4:B:463:HIS:HB3 | 4:B:534:LEU:HD22 | 1.79 | 0.63 |
| 4:B:537:ASP:N | 4:B:882:PHE:HD2 | 1.96 | 0.63 |
| 4:C:882:PHE:HD1 | 4:C:882:PHE:H | 1.44 | 0.63 |
| 4:C:881:ALA:O | 4:C:883:ALA:N | 2.31 | 0.63 |
| 4:D:10:ASP:O | 4:D:13:ASP:HB3 | 1.98 | 0.63 |
| 4:D:550:LEU:HD21 | 4:D:865:PRO:HG2 | 1.81 | 0.63 |
| 4:D:649:GLN:HA | 4:D:652:GLU:OE2 | 1.98 | 0.63 |
| 4:B:777:GLY:O | 4:B:781:ASN:HB2 | 1.98 | 0.63 |
| 4:C:423:ARG:NE | 4:C:781:ASN:HD22 | 1.96 | 0.63 |
| 4:A:92:VAL:HG12 | 4:A:99:ARG:HG3 | 1.80 | 0.63 |
| 4:B:51:PHE:CE2 | 4:B:55:PHE:HD1 | 2.16 | 0.63 |
| 4:B:860:LYS:O | 4:B:860:LYS:HD2 | 1.99 | 0.63 |
| 4:D:278:TRP:HB2 | 4:D:321:ASN:ND2 | 2.13 | 0.63 |
| 4:D:432:PHE:HE1 | 4:D:440:THR:HG23 | 1.64 | 0.63 |
| 4:D:552:ASP:CB | 4:D:691:ALA:HB2 | 2.28 | 0.63 |
| 4:A:65:ALA:HB3 | 4:A:120:LYS:HE3 | 1.79 | 0.63 |
| 4:A:871:ASN:ND2 | 4:A:871:ASN:O | 2.32 | 0.63 |
| 4:C:530:CYS:SG | 4:C:818:PRO:HG2 | 2.39 | 0.63 |
| 4:C:552:ASP:OD1 | 4:C:555:GLY:N | 2.27 | 0.63 |
| 4:C:881:ALA:O | 4:C:882:PHE:C | 2.37 | 0.63 |
| 4:D:141:ILE:HG22 | 4:D:145:ILE:HD11 | 1.80 | 0.63 |
| 4:D:274:PRO:HD3 | 4:D:415:TRP:CZ3 | 2.33 | 0.63 |
| 4:D:446:LEU:O | 4:D:531:SER:HB2 | 1.99 | 0.63 |
| 4:A:383:ALA:C | 4:A:385:TYR:N | 2.52 | 0.63 |
| 4:A:446:LEU:O | 4:A:531:SER:HB2 | 1.99 | 0.63 |
| 4:A:472:LYS:HA | 4:A:567:VAL:HG11 | 1.81 | 0.63 |
| 4:A:716:GLY:CA | 7:A:3184:HOH:O | 2.47 | 0.63 |
| 4:B:14:ILE:H | 4:B:14:ILE:CD1 | 2.03 | 0.63 |
| 4:B:281:ILE:HG22 | 4:B:282:THR:HG23 | 1.80 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:B:329:LYS:HD3 | 4:B:447:ALA:HA | 1.78 | 0.63 |
| 1:H:12:DT:C4' | 4:B:423:ARG:NE | 2.59 | 0.63 |
| 4:B:549:MET:HG2 | 4:B:836:TYR:HE1 | 1.63 | 0.63 |
| 4:B:830:GLU:HA | 4:B:876:LEU:HD21 | 1.80 | 0.63 |
| 4:C:296:LEU:HG | 4:C:296:LEU:O | 1.99 | 0.63 |
| 4:D:95:LYS:HB2 | 4:D:95:LYS:NZ | 2.13 | 0.63 |
| 4:A:304:ALA:O | 4:A:307:ARG:CG | 2.44 | 0.63 |
| 4:A:437:ASN:ND2 | 4:A:440:THR:OG1 | 2.32 | 0.63 |
| 4:A:478:ARG:O | 4:A:482:ILE:HG12 | 1.98 | 0.63 |
| 4:A:729:THR:N | 4:A:733:PHE:O | 2.31 | 0.63 |
| 4:B:278:TRP:CZ3 | 4:B:284:GLY:HA3 | 2.33 | 0.63 |
| 4:B:27:HIS:HA | 7:B:3169:HOH:O | 1.98 | 0.63 |
| 4:B:297:VAL:O | 4:B:297:VAL:HG12 | 1.95 | 0.63 |
| 4:B:626:THR:O | 4:B:628:SER:N | 2.31 | 0.63 |
| 4:B:730:PRO:HD2 | 4:B:786:GLN:NE2 | 2.13 | 0.63 |
| 4:C:110:LYS:HE2 | 4:C:112:GLU:OE1 | 1.98 | 0.63 |
| 4:D:221:ILE:HG12 | 4:D:227:VAL:O | 1.99 | 0.63 |
| 4:D:28:TYR:O | 4:D:32:LEU:HD13 | 1.99 | 0.63 |
| 4:D:452:ILE:HG23 | 4:D:453:GLY:H | 1.63 | 0.63 |
| 1:E:16:DC:H2'' | 1:E:17:DG:H5' | 1.81 | 0.63 |
| 4:A:280:GLY:O | 4:A:281:ILE:C | 2.35 | 0.62 |
| 4:A:270:PRO:HD2 | 4:A:408:PHE:CE2 | 2.34 | 0.62 |
| 4:A:459:TRP:O | 4:A:460:LEU:O | 2.16 | 0.62 |
| 4:A:570:ILE:O | 4:A:573:ILE:HG23 | 1.99 | 0.62 |
| 4:B:539:SER:OG | 4:B:560:ASN:ND2 | 2.32 | 0.62 |
| 4:C:163:LYS:HB3 | 4:C:164:LYS:NZ | 2.13 | 0.62 |
| 4:C:313:MET:HA | 7:C:3099:HOH:O | 1.99 | 0.62 |
| 4:C:317:TYR:C | 4:C:321:ASN:ND2 | 2.52 | 0.62 |
| 4:D:139:SER:HB2 | 4:D:210:ILE:HD13 | 1.81 | 0.62 |
| 4:A:118:THR:O | 4:A:122:THR:OG1 | 2.03 | 0.62 |
| 4:A:423:ARG:O | 4:A:785:SER:HA | 1.99 | 0.62 |
| 4:B:163:LYS:O | 4:B:166:VAL:HG23 | 1.98 | 0.62 |
| 4:C:824:LEU:O | 4:C:824:LEU:HD12 | 1.99 | 0.62 |
| 4:C:563:PRO:HD2 | 4:C:874:ASP:HB3 | 1.80 | 0.62 |
| 4:D:133:THR:HA | 4:D:243:THR:HG22 | 1.79 | 0.62 |
| 4:D:590:THR:O | 4:D:614:LYS:HB2 | 1.99 | 0.62 |
| 2:L:1:G:H2' | 2:L:2:C:C6 | 2.34 | 0.62 |
| 4:A:4:ILE:CD1 | 4:A:256:THR:HA | 2.29 | 0.62 |
| 4:A:630:THR:HA | 7:A:3199:HOH:O | 1.98 | 0.62 |
| 4:B:728:VAL:HG22 | 4:B:734:PRO:CA | 2.29 | 0.62 |
| 4:B:828:VAL:HG11 | 4:B:883:ALA:HA | 1.82 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:725:VAL:HB | 4:D:737:GLN:HB3 | 1.81 | 0.62 |
| 4:A:457:TYR:CE2 | 4:A:461:LYS:CD | 2.82 | 0.62 |
| 4:A:540:CYS:O | 4:A:542:GLY:N | 2.33 | 0.62 |
| 4:C:346:HIS:HA | 4:C:395:ARG:NH1 | 2.14 | 0.62 |
| 4:C:474:PRO:HB2 | 4:C:476:PRO:CG | 2.29 | 0.62 |
| 4:C:423:ARG:HD2 | 4:C:781:ASN:HB3 | 1.81 | 0.62 |
| 4:D:698:TRP:CE3 | 4:D:699:LEU:HD23 | 2.34 | 0.62 |
| 4:D:725:VAL:HG23 | 4:D:774:GLN:NE2 | 2.14 | 0.62 |
| 4:A:106:LEU:HD21 | 4:A:212:VAL:HG13 | 1.81 | 0.62 |
| 4:A:544:GLN:OE1 | 4:A:559:VAL:HG23 | 1.99 | 0.62 |
| 4:B:158:GLU:HG2 | 4:B:195:LEU:HD22 | 1.81 | 0.62 |
| 4:B:403:GLU:OE1 | 4:B:404:GLN:N | 2.32 | 0.62 |
| 4:B:571:TYR:CD2 | 4:B:631:LYS:HA | 2.35 | 0.62 |
| 4:B:668:THR:O | 4:B:670:PRO:HD3 | 1.99 | 0.62 |
| 1:H:10:DT:OP2 | 4:B:641:SER:CB | 2.48 | 0.62 |
| 4:A:632:ARG:HB3 | 4:A:649:GLN:HE21 | 1.63 | 0.62 |
| 4:B:508:PRO:O | 4:B:511:PHE:N | 2.32 | 0.62 |
| 4:B:553:GLU:HG3 | 7:B:3114:HOH:O | 2.00 | 0.62 |
| 4:B:610:LYS:O | 4:B:611:LEU:O | 2.17 | 0.62 |
| 4:B:569:ASP:CG | 4:B:627:ARG:HH21 | 2.02 | 0.62 |
| 4:C:137:VAL:O | 4:C:140:ALA:HB3 | 1.99 | 0.62 |
| 4:D:169:GLN:HB3 | 4:D:182:PHE:CE2 | 2.34 | 0.62 |
| 4:D:540:CYS:O | 4:D:541:SER:C | 2.37 | 0.62 |
| 4:A:11:PHE:HB3 | 4:A:41:HIS:CE1 | 2.34 | 0.62 |
| 4:A:823:ASN:O | 4:A:824:LEU:C | 2.36 | 0.62 |
| 4:B:578:VAL:HG13 | 4:B:680:LEU:HD23 | 1.80 | 0.62 |
| 4:D:327:ALA:HB2 | 4:D:415:TRP:HE1 | 1.61 | 0.62 |
| 4:D:582:LEU:CD1 | 4:D:625:VAL:HG21 | 2.28 | 0.62 |
| 4:A:392:LYS:O | 4:A:396:ILE:HG12 | 1.99 | 0.62 |
| 4:A:512:LEU:O | 4:A:516:PHE:CE1 | 2.53 | 0.62 |
| 4:A:540:CYS:HB3 | 4:A:543:ILE:HG13 | 1.82 | 0.62 |
| 4:A:793:LYS:HA | 4:A:796:VAL:HG23 | 1.82 | 0.62 |
| 4:A:425:ARG:HD3 | 4:A:811:HIS:CD2 | 2.35 | 0.62 |
| 4:B:122:THR:CG2 | 4:B:226:MET:HE1 | 2.28 | 0.62 |
| 4:C:303:LYS:CB | 4:C:303:LYS:NZ | 2.63 | 0.62 |
| 4:C:875:ILE:CG2 | 4:C:875:ILE:O | 2.48 | 0.62 |
| 2:L:6:G:OP1 | 4:C:394:ARG:NH1 | 2.32 | 0.62 |
| 4:A:132:THR:O | 4:A:132:THR:HG22 | 1.99 | 0.62 |
| 4:A:588:ASN:HB3 | 7:A:3224:HOH:O | 1.99 | 0.62 |
| 4:B:391:ARG:CG | 7:B:3101:HOH:O | 2.46 | 0.62 |
| 4:B:689:VAL:HG23 | 4:B:689:VAL:O | 1.99 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:B:748:ASN:HD22 | 4:B:751:PHE:H | 1.46 | 0.62 |
| 4:D:488:ASN:O | 4:D:491:ALA:HB3 | 2.00 | 0.62 |
| 4:A:632:ARG:HH21 | 6:A:2000:APC:C8 | 2.12 | 0.62 |
| 4:A:24:LEU:HD11 | 4:A:287:TRP:CG | 2.35 | 0.62 |
| 4:A:578:VAL:HG13 | 4:A:680:LEU:HB3 | 1.82 | 0.62 |
| 4:A:818:PRO:O | 4:A:821:ALA:HB3 | 1.98 | 0.62 |
| 4:B:26:ASP:HB3 | 7:B:3098:HOH:O | 2.00 | 0.62 |
| 4:B:475:PHE:O | 4:B:478:ARG:N | 2.32 | 0.62 |
| 4:B:792:ARG:O | 4:B:796:VAL:HG23 | 2.00 | 0.62 |
| 4:D:324:GLN:HA | 4:D:418:TYR:CD1 | 2.35 | 0.62 |
| 4:D:705:LEU:HD12 | 4:D:853:LEU:HD22 | 1.81 | 0.62 |
| 4:A:226:MET:HA | 4:A:250:TYR:CD1 | 2.35 | 0.61 |
| 4:B:24:LEU:HD22 | 4:B:33:ALA:HA | 1.80 | 0.61 |
| 4:B:464:GLY:HA3 | 4:B:514:PHE:CE2 | 2.35 | 0.61 |
| 4:C:557:ARG:HB3 | 4:C:557:ARG:HH11 | 1.64 | 0.61 |
| 4:A:704:LYS:HE3 | 4:A:860:LYS:NZ | 2.15 | 0.61 |
| 4:A:798:ALA:HB2 | 4:A:827:ALA:CB | 2.30 | 0.61 |
| 4:A:825:PHE:CD1 | 4:A:829:ARG:NH1 | 2.63 | 0.61 |
| 4:C:635:MET:CE | 6:C:2002:APC:H8 | 2.30 | 0.61 |
| 4:C:398:LEU:O | 4:C:398:LEU:HD23 | 1.99 | 0.61 |
| 4:C:549:MET:HE1 | 4:C:786:GLN:HG2 | 1.83 | 0.61 |
| 4:C:882:PHE:N | 4:C:882:PHE:CD1 | 2.68 | 0.61 |
| 1:H:6:DT:H6 | 1:H:6:DT:H5' | 1.65 | 0.61 |
| 4:A:112:GLU:O | 4:A:115:ALA:HB3 | 2.00 | 0.61 |
| 4:B:470:VAL:HG21 | 4:B:481:PHE:CD2 | 2.35 | 0.61 |
| 4:B:726:HIS:HD2 | 4:B:735:VAL:O | 1.82 | 0.61 |
| 4:C:730:PRO:HD3 | 4:C:786:GLN:HE22 | 1.66 | 0.61 |
| 4:D:304:ALA:HA | 4:D:307:ARG:HD2 | 1.81 | 0.61 |
| 4:A:231:ARG:CG | 4:A:234:ALA:HB2 | 2.30 | 0.61 |
| 4:A:347:CYS:O | 4:A:349:VAL:N | 2.33 | 0.61 |
| 4:A:786:GLN:OE1 | 4:A:841:VAL:HG21 | 2.00 | 0.61 |
| 4:B:88:TRP:CZ2 | 4:B:215:ARG:HD3 | 2.35 | 0.61 |
| 4:B:823:ASN:N | 4:B:823:ASN:HD22 | 1.98 | 0.61 |
| 4:C:19:ILE:HG12 | 4:C:20:PRO:CD | 2.20 | 0.61 |
| 4:C:14:ILE:CG2 | 4:C:288:ALA:HB1 | 2.31 | 0.61 |
| 4:C:728:VAL:HG22 | 4:C:734:PRO:CB | 2.30 | 0.61 |
| 4:D:273:VAL:HA | 4:D:415:TRP:HZ3 | 1.61 | 0.61 |
| 4:D:11:PHE:CE1 | 4:D:44:TYR:HB3 | 2.35 | 0.61 |
| 4:A:386:ARG:O | 4:A:388:ASP:N | 2.34 | 0.61 |
| 4:A:459:TRP:CZ3 | 4:A:475:PHE:HE1 | 2.18 | 0.61 |
| 4:A:563:PRO:HB3 | 4:A:878:SER:CA | 2.29 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:B:574:VAL:CG2 | 4:B:685:VAL:HG12 | 2.30 | 0.61 |
| 4:B:783:VAL:O | 4:B:786:GLN:N | 2.31 | 0.61 |
| 4:B:538:GLY:HA2 | 4:B:882:PHE:O | 2.00 | 0.61 |
| 4:D:139:SER:HB2 | 4:D:210:ILE:HD11 | 1.83 | 0.61 |
| 4:D:592:ASN:O | 4:D:593:GLU:HB2 | 2.00 | 0.61 |
| 4:B:292:ARG:O | 4:B:293:PRO:O | 2.19 | 0.61 |
| 4:B:485:ASN:O | 4:B:486:HIS:C | 2.39 | 0.61 |
| 4:C:291:ARG:HG2 | 7:C:3066:HOH:O | 2.00 | 0.61 |
| 4:C:455:GLU:O | 4:C:458:TYR:HB3 | 2.00 | 0.61 |
| 4:C:643:GLU:OE2 | 4:C:679:LYS:HD2 | 2.00 | 0.61 |
| 4:C:727:TRP:HB3 | 4:C:845:PHE:CD1 | 2.36 | 0.61 |
| 4:D:221:ILE:CG1 | 4:D:227:VAL:HG23 | 2.30 | 0.61 |
| 4:D:422:TRP:CD1 | 4:D:422:TRP:C | 2.74 | 0.61 |
| 4:A:459:TRP:O | 4:A:460:LEU:C | 2.36 | 0.61 |
| 4:A:778:ILE:HG23 | 4:A:779:ALA:N | 2.16 | 0.61 |
| 4:A:817:ILE:HB | 4:A:818:PRO:CD | 2.30 | 0.61 |
| 4:B:631:LYS:NZ | 6:B:2001:APC:H3A2 | 2.16 | 0.61 |
| 4:B:460:LEU:N | 4:B:534:LEU:HD11 | 2.15 | 0.61 |
| 4:B:676:TYR:CE1 | 4:B:680:LEU:HD11 | 2.36 | 0.61 |
| 4:C:495:SER:HB2 | 4:C:498:GLU:HB2 | 1.82 | 0.61 |
| 4:D:187:GLU:O | 4:D:191:LEU:HG | 2.00 | 0.61 |
| 4:D:329:LYS:HD2 | 4:D:447:ALA:HA | 1.82 | 0.61 |
| 4:B:571:TYR:CD2 | 4:B:631:LYS:HG3 | 2.34 | 0.61 |
| 4:B:682:TRP:O | 4:B:686:SER:OG | 2.16 | 0.61 |
| 4:B:706:LEU:O | 4:B:723:CYS:O | 2.19 | 0.61 |
| 4:C:405:ALA:HB2 | 4:C:443:LEU:HD13 | 1.81 | 0.61 |
| 4:D:448:LYS:HZ2 | 4:D:806:SER:HB3 | 1.64 | 0.61 |
| 4:D:573:ILE:O | 4:D:577:LYS:HG3 | 2.01 | 0.61 |
| 4:D:643:GLU:OE1 | 4:D:679:LYS:HD3 | 2.01 | 0.61 |
| 4:A:727:TRP:CD2 | 4:A:735:VAL:CG1 | 2.84 | 0.61 |
| 4:B:206:LYS:O | 4:B:210:ILE:HG12 | 2.01 | 0.61 |
| 4:B:55:PHE:CE2 | 4:B:59:LEU:HD11 | 2.36 | 0.61 |
| 4:C:292:ARG:HG3 | 4:C:292:ARG:O | 2.00 | 0.61 |
| 4:C:849:PHE:CD2 | 4:C:853:LEU:HD21 | 2.35 | 0.61 |
| 4:D:327:ALA:HA | 4:D:415:TRP:CD1 | 2.35 | 0.61 |
| 4:D:631:LYS:CE | 6:D:2003:APC:H3A2 | 2.31 | 0.61 |
| 4:A:390:ALA:O | 4:A:393:SER:N | 2.33 | 0.61 |
| 4:A:77:LEU:CD2 | 4:A:119:ILE:HD12 | 2.31 | 0.61 |
| 4:B:281:ILE:HG22 | 4:B:282:THR:N | 2.15 | 0.61 |
| 4:B:326:THR:O | 4:B:415:TRP:CD1 | 2.54 | 0.61 |
| 4:B:582:LEU:HD13 | 4:B:621:LEU:HD12 | 1.82 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:C:155:ARG:HB2 | 4:C:163:LYS:HZ2 | 1.65 | 0.61 |
| 4:C:303:LYS:HB2 | 4:C:303:LYS:HZ2 | 1.65 | 0.61 |
| 4:C:461:LYS:O | 4:C:464:GLY:N | 2.33 | 0.61 |
| 4:C:570:ILE:HA | 4:C:573:ILE:HG22 | 1.81 | 0.61 |
| 4:C:828:VAL:HG23 | 4:C:829:ARG:N | 2.12 | 0.61 |
| 4:D:330:ILE:HG21 | 4:D:409:ALA:HA | 1.81 | 0.61 |
| 4:D:432:PHE:CE1 | 4:D:440:THR:HG23 | 2.36 | 0.61 |
| 4:D:859:ASP:HA | 7:D:3136:HOH:O | 2.00 | 0.61 |
| 4:A:373:ALA:HB2 | 7:A:3006:HOH:O | 2.01 | 0.60 |
| 4:B:551:ARG:HG3 | 7:B:3047:HOH:O | 2.01 | 0.60 |
| 4:C:386:ARG:HB3 | 7:C:3082:HOH:O | 2.01 | 0.60 |
| 4:C:754:GLN:O | 4:C:755:PHE:O | 2.19 | 0.60 |
| 4:C:84:ARG:NH1 | 4:C:84:ARG:HA | 2.15 | 0.60 |
| 1:H:10:DT:H5' | 4:B:641:SER:N | 2.15 | 0.60 |
| 1:N:11:DA:C6 | 4:D:639:TYR:CE2 | 2.89 | 0.60 |
| 4:A:14:ILE:HA | 7:A:3082:HOH:O | 2.00 | 0.60 |
| 4:A:402:LEU:HG | 4:A:439:MET:CE | 2.31 | 0.60 |
| 4:A:457:TYR:OH | 4:A:461:LYS:HD3 | 2.00 | 0.60 |
| 4:A:516:PHE:N | 4:A:516:PHE:HD1 | 1.99 | 0.60 |
| 4:B:329:LYS:CG | 4:B:329:LYS:O | 2.49 | 0.60 |
| 4:A:316:VAL:HG13 | 4:A:792:ARG:HE | 1.66 | 0.60 |
| 4:A:488:ASN:O | 4:A:491:ALA:HB3 | 2.01 | 0.60 |
| 4:A:682:TRP:CG | 4:A:682:TRP:O | 2.54 | 0.60 |
| 4:B:345:LYS:NZ | 4:B:351:ASP:N | 2.48 | 0.60 |
| 4:B:269:GLN:HG2 | 4:B:404:GLN:OE1 | 2.00 | 0.60 |
| 4:B:423:ARG:CD | 4:B:781:ASN:ND2 | 2.64 | 0.60 |
| 4:B:427:TYR:CE1 | 4:B:811:HIS:NE2 | 2.69 | 0.60 |
| 4:B:439:MET:O | 4:B:442:GLY:N | 2.33 | 0.60 |
| 4:B:536:PHE:HE2 | 4:B:825:PHE:HB2 | 1.65 | 0.60 |
| 4:C:208:ASP:O | 4:C:212:VAL:HG23 | 2.01 | 0.60 |
| 4:C:236:VAL:O | 4:C:240:ASP:HB2 | 2.01 | 0.60 |
| 4:C:329:LYS:CD | 4:C:447:ALA:HA | 2.31 | 0.60 |
| 4:C:788:GLY:C | 4:C:792:ARG:NH1 | 2.54 | 0.60 |
| 4:C:823:ASN:O | 4:C:826:LYS:N | 2.32 | 0.60 |
| 4:A:25:ALA:O | 4:A:29:GLY:N | 2.32 | 0.60 |
| 4:A:496:PRO:HD2 | 7:A:3203:HOH:O | 2.00 | 0.60 |
| 4:A:802:TYR:OH | 4:A:830:GLU:OE2 | 2.20 | 0.60 |
| 4:B:677:MET:HG3 | 4:B:681:ILE:HD13 | 1.82 | 0.60 |
| 4:C:35:GLU:HG2 | 4:C:272:VAL:HG21 | 1.84 | 0.60 |
| 4:C:631:LYS:O | 4:C:632:ARG:C | 2.37 | 0.60 |
| 4:D:373:ALA:HB1 | 4:D:377:TRP:HE1 | 1.67 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:486:HIS:NE2 | 4:D:490:MET:HG3 | 2.16 | 0.60 |
| 7:N:1048:HOH:O | 4:D:772:HIS:HD2 | 1.83 | 0.60 |
| 1:N:15:DC:C2' | 1:N:16:DC:OP2 | 2.48 | 0.60 |
| 4:A:791:LEU:O | 4:A:795:VAL:HG23 | 2.02 | 0.60 |
| 4:B:347:CYS:HB3 | 4:B:350:GLU:CG | 2.32 | 0.60 |
| 4:B:433:ASN:CB | 4:B:434:PRO:HD3 | 2.11 | 0.60 |
| 4:B:875:ILE:HG22 | 4:B:876:LEU:N | 2.15 | 0.60 |
| 4:C:551:ARG:HE | 4:C:872:LEU:CD2 | 2.14 | 0.60 |
| 4:D:207:GLU:HB3 | 4:D:211:HIS:NE2 | 2.15 | 0.60 |
| 4:D:292:ARG:H | 4:D:293:PRO:HD3 | 1.65 | 0.60 |
| 1:H:3:DG:H2'' | 1:H:4:DA:C8 | 2.36 | 0.60 |
| 1:N:8:DG:H4' | 7:N:1048:HOH:O | 2.02 | 0.60 |
| 4:A:390:ALA:C | 4:A:392:LYS:N | 2.52 | 0.60 |
| 4:A:459:TRP:HZ3 | 4:A:475:PHE:HE1 | 1.50 | 0.60 |
| 4:A:882:PHE:H | 4:A:882:PHE:HD1 | 1.47 | 0.60 |
| 4:B:84:ARG:CD | 4:B:219:MET:HG2 | 2.25 | 0.60 |
| 4:B:320:ILE:O | 4:B:324:GLN:HB2 | 2.01 | 0.60 |
| 4:B:398:LEU:O | 4:B:398:LEU:HD23 | 2.01 | 0.60 |
| 4:C:266:PRO:HG2 | 4:C:268:PHE:CZ | 2.37 | 0.60 |
| 4:C:651:LEU:C | 4:C:651:LEU:HD13 | 2.22 | 0.60 |
| 4:A:159:ALA:O | 4:A:163:LYS:HB2 | 2.02 | 0.60 |
| 4:A:342:THR:HG22 | 4:A:348:PRO:HG3 | 1.83 | 0.60 |
| 4:A:47:GLY:O | 4:A:50:ARG:HB3 | 2.01 | 0.60 |
| 4:A:610:LYS:O | 4:A:611:LEU:C | 2.38 | 0.60 |
| 4:A:574:VAL:HG12 | 4:A:684:SER:HB3 | 1.82 | 0.60 |
| 4:A:546:PHE:CD2 | 4:A:692:ALA:HA | 2.30 | 0.60 |
| 4:B:454:LYS:HG3 | 4:B:455:GLU:N | 2.15 | 0.60 |
| 4:B:460:LEU:HA | 4:B:534:LEU:HD21 | 1.82 | 0.60 |
| 4:B:59:LEU:HA | 4:B:64:VAL:HG22 | 1.82 | 0.60 |
| 4:B:680:LEU:HD12 | 4:B:680:LEU:N | 2.15 | 0.60 |
| 4:B:120:LYS:NZ | 4:B:752:LEU:HD11 | 2.17 | 0.60 |
| 4:C:175:GLY:O | 4:C:176:HIS:C | 2.37 | 0.60 |
| 4:D:729:THR:HB | 4:D:789:SER:HB2 | 1.83 | 0.60 |
| 1:H:9:DA:N6 | 3:J:1:DG:H21 | 2.00 | 0.60 |
| 4:A:89:PHE:HA | 4:A:103:PHE:HE1 | 1.64 | 0.60 |
| 4:A:329:LYS:HG2 | 4:A:447:ALA:HA | 1.84 | 0.60 |
| 4:B:181:ALA:O | 4:B:185:VAL:HG13 | 2.00 | 0.60 |
| 4:B:291:ARG:HG3 | 7:B:3037:HOH:O | 2.00 | 0.60 |
| 4:B:437:ASN:C | 4:B:437:ASN:ND2 | 2.54 | 0.60 |
| 4:B:73:LEU:HD21 | 4:B:77:LEU:HD22 | 1.83 | 0.60 |
| 4:C:333:LYS:CB | 4:C:516:PHE:CD2 | 2.84 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:833:VAL:HG22 | 4:D:875:ILE:HB | 1.83 | 0.60 |
| 1:N:15:DC:H2'' | 1:N:16:DC:O5' | 2.01 | 0.60 |
| 4:A:633:SER:OG | 4:A:646:PHE:CG | 2.44 | 0.60 |
| 4:A:116:TYR:CE2 | 4:A:752:LEU:HD13 | 2.37 | 0.60 |
| 4:B:398:LEU:C | 4:B:398:LEU:HD23 | 2.21 | 0.60 |
| 4:C:492:CYS:SG | 4:C:501:TRP:HE3 | 2.25 | 0.60 |
| 4:D:113:ALA:O | 4:D:117:ILE:HG13 | 2.01 | 0.60 |
| 4:D:571:TYR:CD1 | 4:D:631:LYS:HA | 2.37 | 0.60 |
| 4:A:82:ILE:HG21 | 4:A:112:GLU:OE2 | 2.01 | 0.60 |
| 4:A:842:LEU:O | 4:A:845:PHE:HB3 | 2.02 | 0.60 |
| 4:A:536:PHE:HB3 | 4:A:882:PHE:HB3 | 1.84 | 0.60 |
| 4:B:292:ARG:N | 4:B:293:PRO:HD3 | 2.16 | 0.60 |
| 4:B:300:HIS:NE2 | 4:B:422:TRP:HZ3 | 1.97 | 0.60 |
| 4:C:14:ILE:HG21 | 4:C:288:ALA:HB1 | 1.83 | 0.60 |
| 4:D:213:GLY:O | 4:D:217:ILE:HG13 | 2.02 | 0.60 |
| 4:D:54:MET:O | 4:D:58:GLN:HG2 | 2.02 | 0.60 |
| 4:A:159:ALA:HB1 | 4:A:163:LYS:N | 2.17 | 0.59 |
| 4:A:342:THR:CG2 | 4:A:398:LEU:HD21 | 2.33 | 0.59 |
| 4:A:689:VAL:O | 4:A:690:VAL:C | 2.39 | 0.59 |
| 4:A:778:ILE:CG2 | 4:A:779:ALA:N | 2.65 | 0.59 |
| 4:B:571:TYR:CE1 | 7:B:3067:HOH:O | 2.51 | 0.59 |
| 4:B:780:PRO:O | 4:B:781:ASN:C | 2.35 | 0.59 |
| 4:C:324:GLN:HG3 | 4:C:417:PRO:HA | 1.84 | 0.59 |
| 4:D:646:PHE:O | 4:D:647:ARG:O | 2.19 | 0.59 |
| 4:A:380:ALA:O | 4:A:383:ALA:HB3 | 2.02 | 0.59 |
| 2:F:3:G:O2' | 4:A:389:LYS:NZ | 2.35 | 0.59 |
| 4:A:428:ALA:N | 4:A:435:GLN:HE22 | 2.00 | 0.59 |
| 4:A:669:GLN:CG | 4:A:672:GLN:HE21 | 2.15 | 0.59 |
| 4:A:712:ASP:HA | 7:A:3088:HOH:O | 2.00 | 0.59 |
| 4:B:66:ASP:OD1 | 4:B:120:LYS:HE3 | 2.01 | 0.59 |
| 4:B:698:TRP:O | 4:B:701:SER:N | 2.35 | 0.59 |
| 4:C:496:PRO:HA | 7:C:3071:HOH:O | 2.02 | 0.59 |
| 4:C:525:GLY:O | 4:C:527:SER:N | 2.35 | 0.59 |
| 4:D:846:TYR:HA | 4:D:849:PHE:CE1 | 2.36 | 0.59 |
| 4:D:95:LYS:HD2 | 7:D:3092:HOH:O | 2.02 | 0.59 |
| 4:A:741:LYS:HB2 | 4:A:770:ASP:HB2 | 1.84 | 0.59 |
| 4:B:163:LYS:HB3 | 4:B:164:LYS:NZ | 2.17 | 0.59 |
| 4:B:21:PHE:C | 4:B:23:THR:H | 2.05 | 0.59 |
| 4:B:418:TYR:CE2 | 4:B:428:ALA:CB | 2.82 | 0.59 |
| 4:B:473:VAL:CG1 | 4:B:474:PRO:CD | 2.79 | 0.59 |
| 4:C:299:THR:CG2 | 4:C:300:HIS:H | 2.13 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:C:333:LYS:NZ | 7:C:3010:HOH:O | 2.34 | 0.59 |
| 4:D:3:THR:HG23 | 7:D:3098:HOH:O | 2.00 | 0.59 |
| 2:O:4:G:H2' | 2:O:5:C:H6 | 1.67 | 0.59 |
| 4:A:585:ASP:O | 4:A:588:ASN:O | 2.19 | 0.59 |
| 4:B:398:LEU:HD21 | 4:B:439:MET:CE | 2.33 | 0.59 |
| 4:B:861:MET:O | 4:B:862:PRO:C | 2.40 | 0.59 |
| 4:B:561:LEU:HD23 | 4:B:875:ILE:HD11 | 1.84 | 0.59 |
| 4:C:78:LEU:HD11 | 4:C:115:ALA:HB3 | 1.84 | 0.59 |
| 4:C:330:ILE:HG12 | 7:C:3016:HOH:O | 2.02 | 0.59 |
| 4:C:695:ALA:O | 4:C:699:LEU:HD12 | 2.03 | 0.59 |
| 4:C:875:ILE:HG22 | 4:C:875:ILE:O | 2.01 | 0.59 |
| 4:D:322:ILE:HG22 | 4:D:323:ALA:N | 2.17 | 0.59 |
| 4:D:623:TYR:HA | 4:D:666:MET:CE | 2.32 | 0.59 |
| 4:A:205:HIS:HB3 | 4:A:207:GLU:HG2 | 1.84 | 0.59 |
| 4:A:849:PHE:CD2 | 4:A:853:LEU:HD21 | 2.37 | 0.59 |
| 4:C:14:ILE:HG21 | 4:C:288:ALA:CB | 2.33 | 0.59 |
| 4:C:318:LYS:HE2 | 4:C:796:VAL:HG13 | 1.84 | 0.59 |
| 4:D:19:ILE:HG23 | 4:D:20:PRO:HD2 | 1.84 | 0.59 |
| 4:D:229:LEU:HA | 4:D:244:ILE:HD13 | 1.84 | 0.59 |
| 4:D:53:LYS:O | 4:D:56:GLU:HB3 | 2.02 | 0.59 |
| 4:A:294:LEU:CD1 | 4:A:429:VAL:HG21 | 2.29 | 0.59 |
| 4:A:92:VAL:HG22 | 7:A:3011:HOH:O | 2.01 | 0.59 |
| 4:B:663:LYS:CG | 4:B:664:GLY:N | 2.66 | 0.59 |
| 4:B:751:PHE:C | 4:B:752:LEU:HD12 | 2.23 | 0.59 |
| 4:C:24:LEU:HD22 | 4:C:273:VAL:HG21 | 1.85 | 0.59 |
| 4:C:306:MET:O | 4:C:308:TYR:N | 2.35 | 0.59 |
| 4:C:706:LEU:O | 4:C:723:CYS:O | 2.20 | 0.59 |
| 4:C:726:HIS:HB2 | 4:C:736:TRP:CD1 | 2.37 | 0.59 |
| 4:C:78:LEU:N | 4:C:79:PRO:CD | 2.65 | 0.59 |
| 4:C:850:ALA:C | 4:C:852:GLN:H | 2.06 | 0.59 |
| 4:D:100:PRO:HG2 | 4:D:103:PHE:HB2 | 1.83 | 0.59 |
| 4:D:725:VAL:HG23 | 4:D:774:GLN:HE21 | 1.66 | 0.59 |
| 3:M:5:DA:H2'' | 3:M:6:DT:H72 | 1.84 | 0.59 |
| 4:A:143:ARG:HD3 | 7:A:3118:HOH:O | 2.01 | 0.59 |
| 4:A:15:GLU:HG2 | 4:A:18:ALA:O | 2.03 | 0.59 |
| 4:A:178:TYR:H | 4:A:178:TYR:HD1 | 1.47 | 0.59 |
| 4:A:96:ARG:NE | 7:A:3009:HOH:O | 2.33 | 0.59 |
| 4:C:837:GLU:HG3 | 4:C:872:LEU:HD12 | 1.85 | 0.59 |
| 4:D:710:VAL:CG1 | 4:D:720:ARG:HB3 | 2.33 | 0.59 |
| 4:A:629:VAL:HG12 | 4:A:629:VAL:O | 2.02 | 0.59 |
| 4:A:727:TRP:CH2 | 4:A:735:VAL:HG21 | 2.38 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:A:80:LYS:CD | 4:A:224:THR:HG22 | 2.32 | 0.59 |
| 4:B:36:GLN:HA | 4:B:36:GLN:OE1 | 2.03 | 0.59 |
| 4:B:770:ASP:OD1 | 4:B:772:HIS:N | 2.36 | 0.59 |
| 4:C:281:ILE:CG1 | 4:C:309:GLU:HA | 2.33 | 0.59 |
| 4:C:452:ILE:HD11 | 4:C:457:TYR:N | 2.18 | 0.59 |
| 4:D:273:VAL:C | 4:D:415:TRP:CE3 | 2.76 | 0.59 |
| 1:N:10:DT:H5' | 4:D:641:SER:HA | 1.83 | 0.59 |
| 2:I:5:C:N3 | 2:I:6:G:N7 | 2.50 | 0.59 |
| 4:A:660:ASP:HB3 | 7:A:3072:HOH:O | 2.02 | 0.59 |
| 4:A:727:TRP:CE3 | 4:A:735:VAL:HG13 | 2.37 | 0.59 |
| 4:A:802:TYR:HD2 | 4:A:802:TYR:N | 1.99 | 0.59 |
| 4:B:40:GLU:OE1 | 4:B:288:ALA:HB3 | 2.02 | 0.59 |
| 4:C:21:PHE:C | 4:C:23:THR:N | 2.54 | 0.59 |
| 4:C:308:TYR:HH | 4:C:733:PHE:HE2 | 1.49 | 0.59 |
| 4:A:720:ARG:HH21 | 4:A:857:GLN:HE22 | 1.51 | 0.59 |
| 4:B:473:VAL:HG12 | 4:B:474:PRO:N | 2.17 | 0.59 |
| 4:B:514:PHE:CG | 4:B:514:PHE:O | 2.56 | 0.59 |
| 4:B:576:LYS:O | 4:B:579:ASN:N | 2.36 | 0.59 |
| 4:C:724:ALA:HB2 | 4:C:738:GLU:HG3 | 1.85 | 0.59 |
| 4:D:479:ILE:HG22 | 4:D:483:GLU:CD | 2.23 | 0.59 |
| 4:D:726:HIS:CD2 | 4:D:736:TRP:CE2 | 2.90 | 0.59 |
| 3:J:1:DG:H1' | 3:J:2:DT:H71 | 1.83 | 0.59 |
| 4:A:425:ARG:NH2 | 4:A:784:HIS:CE1 | 2.71 | 0.58 |
| 4:C:268:PHE:HB3 | 4:C:430:SER:HA | 1.85 | 0.58 |
| 4:D:465:ALA:HB1 | 4:D:478:ARG:HB3 | 1.84 | 0.58 |
| 4:D:619:GLN:NE2 | 4:D:668:THR:H | 2.01 | 0.58 |
| 4:D:668:THR:HG22 | 4:D:669:GLN:NE2 | 2.17 | 0.58 |
| 4:D:616:LEU:HD13 | 4:D:676:TYR:HB2 | 1.85 | 0.58 |
| 1:H:13:DC:C4' | 4:B:427:TYR:HE2 | 2.15 | 0.58 |
| 1:K:9:DA:H5' | 7:K:731:HOH:O | 2.01 | 0.58 |
| 4:A:40:GLU:O | 4:A:43:SER:HB2 | 2.04 | 0.58 |
| 4:A:810:ILE:O | 4:A:812:ASP:N | 2.36 | 0.58 |
| 4:C:252:GLU:HG2 | 7:C:3072:HOH:O | 2.02 | 0.58 |
| 4:C:632:ARG:HA | 4:C:635:MET:HG2 | 1.85 | 0.58 |
| 4:C:728:VAL:HG13 | 4:C:733:PHE:C | 2.24 | 0.58 |
| 4:C:727:TRP:CZ2 | 4:C:735:VAL:HG11 | 2.38 | 0.58 |
| 4:D:472:LYS:HG3 | 4:D:567:VAL:HG11 | 1.84 | 0.58 |
| 4:A:108:GLU:HG3 | 7:A:3115:HOH:O | 2.02 | 0.58 |
| 4:A:404:GLN:HG2 | 4:A:432:PHE:CB | 2.33 | 0.58 |
| 4:A:549:MET:HB3 | 4:A:836:TYR:HE1 | 1.67 | 0.58 |
| 4:A:570:ILE:O | 4:A:574:VAL:HG23 | 2.02 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:A:619:GLN:O | 4:A:622:ALA:HB3 | 2.03 | 0.58 |
| 4:B:236:VAL:CB | 4:B:239:GLN:HB2 | 2.31 | 0.58 |
| 4:B:748:ASN:HD21 | 4:B:751:PHE:HB2 | 1.67 | 0.58 |
| 4:C:501:TRP:HB2 | 7:C:3116:HOH:O | 2.03 | 0.58 |
| 4:C:50:ARG:CZ | 4:C:267:MET:HE3 | 2.33 | 0.58 |
| 4:D:458:TYR:O | 4:D:462:ILE:HG12 | 2.03 | 0.58 |
| 4:D:473:VAL:CG2 | 4:D:477:GLU:HG3 | 2.32 | 0.58 |
| 4:D:560:ASN:O | 4:D:878:SER:OG | 2.18 | 0.58 |
| 4:A:48:GLU:O | 4:A:49:ALA:C | 2.42 | 0.58 |
| 4:B:585:ASP:OD2 | 4:B:613:THR:HB | 2.03 | 0.58 |
| 4:B:814:PHE:CE2 | 4:B:828:VAL:HG13 | 2.39 | 0.58 |
| 4:C:161:HIS:O | 4:C:163:LYS:N | 2.36 | 0.58 |
| 4:C:329:LYS:HG3 | 4:C:445:THR:CG2 | 2.32 | 0.58 |
| 4:C:588:ASN:N | 4:C:588:ASN:HD22 | 2.02 | 0.58 |
| 4:C:816:THR:HG22 | 4:C:817:ILE:HG13 | 1.86 | 0.58 |
| 4:C:92:VAL:HG12 | 4:C:99:ARG:CG | 2.27 | 0.58 |
| 4:D:475:PHE:O | 4:D:476:PRO:C | 2.37 | 0.58 |
| 4:D:496:PRO:HD2 | 7:D:3035:HOH:O | 2.02 | 0.58 |
| 3:G:4:DG:H1' | 3:G:5:DA:C8 | 2.38 | 0.58 |
| 4:A:516:PHE:CD1 | 4:A:516:PHE:N | 2.70 | 0.58 |
| 4:A:727:TRP:CD2 | 4:A:735:VAL:HG13 | 2.39 | 0.58 |
| 4:A:551:ARG:HH21 | 4:A:872:LEU:HD11 | 1.67 | 0.58 |
| 4:B:182:PHE:O | 4:B:185:VAL:HG22 | 2.02 | 0.58 |
| 4:B:46:MET:O | 4:B:49:ALA:HB3 | 2.03 | 0.58 |
| 4:B:55:PHE:O | 4:B:55:PHE:HD2 | 1.87 | 0.58 |
| 4:B:850:ALA:C | 4:B:852:GLN:H | 2.06 | 0.58 |
| 4:C:299:THR:HG21 | 4:C:304:ALA:HB3 | 1.85 | 0.58 |
| 4:C:319:ALA:CB | 4:C:792:ARG:HB3 | 2.34 | 0.58 |
| 4:C:322:ILE:HG21 | 4:C:795:VAL:HG12 | 1.85 | 0.58 |
| 4:C:477:GLU:HA | 4:C:480:LYS:HB3 | 1.86 | 0.58 |
| 4:C:882:PHE:O | 4:C:883:ALA:HB3 | 2.02 | 0.58 |
| 4:D:619:GLN:O | 4:D:622:ALA:HB3 | 2.03 | 0.58 |
| 4:A:502:TRP:CD1 | 4:A:512:LEU:HD13 | 2.39 | 0.58 |
| 4:B:206:LYS:HB2 | 7:B:3155:HOH:O | 2.02 | 0.58 |
| 4:B:389:LYS:O | 4:B:392:LYS:HB3 | 2.03 | 0.58 |
| 4:C:423:ARG:NH1 | 4:C:423:ARG:CB | 2.67 | 0.58 |
| 4:C:432:PHE:HZ | 4:C:444:LEU:HD21 | 1.67 | 0.58 |
| 4:C:579:ASN:HA | 4:C:582:LEU:HB2 | 1.86 | 0.58 |
| 4:D:40:GLU:OE1 | 4:D:288:ALA:N | 2.34 | 0.58 |
| 4:D:830:GLU:HG2 | 4:D:876:LEU:CD2 | 2.34 | 0.58 |
| 4:A:392:LYS:O | 4:A:392:LYS:HG2 | 2.03 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:A:461:LYS:O | 4:A:462:ILE:C | 2.40 | 0.58 |
| 4:A:582:LEU:HB2 | 4:A:621:LEU:HD21 | 1.86 | 0.58 |
| 4:A:792:ARG:HH11 | 4:A:792:ARG:HG3 | 1.68 | 0.58 |
| 4:B:162:PHE:CD1 | 4:B:190:MET:SD | 2.97 | 0.58 |
| 4:B:423:ARG:HD2 | 4:B:781:ASN:HD21 | 1.68 | 0.58 |
| 4:B:751:PHE:CB | 4:B:752:LEU:HD12 | 2.23 | 0.58 |
| 4:B:702:ALA:CB | 4:B:849:PHE:CE2 | 2.84 | 0.58 |
| 4:B:99:ARG:HG2 | 4:B:99:ARG:NH1 | 2.19 | 0.58 |
| 4:D:230:HIS:NE2 | 4:D:245:GLU:HB2 | 2.19 | 0.58 |
| 4:D:619:GLN:NE2 | 4:D:666:MET:O | 2.36 | 0.58 |
| 4:D:680:LEU:O | 4:D:683:GLU:N | 2.37 | 0.58 |
| 4:D:308:TYR:CE2 | 4:D:734:PRO:O | 2.56 | 0.58 |
| 4:D:77:LEU:HD11 | 4:D:224:THR:OG1 | 2.03 | 0.58 |
| 4:A:3:THR:HB | 4:A:52:ARG:HH12 | 1.69 | 0.58 |
| 4:B:54:MET:O | 4:B:58:GLN:HG2 | 2.03 | 0.58 |
| 4:B:423:ARG:HD2 | 4:B:781:ASN:ND2 | 2.18 | 0.58 |
| 4:B:5:ASN:HD21 | 4:B:7:ALA:CA | 2.17 | 0.58 |
| 4:C:19:ILE:CG1 | 4:C:20:PRO:HD2 | 2.20 | 0.58 |
| 4:C:452:ILE:HG22 | 4:C:528:TYR:O | 2.04 | 0.58 |
| 4:C:553:GLU:HG2 | 4:C:554:VAL:N | 2.19 | 0.58 |
| 4:C:849:PHE:HD2 | 4:C:853:LEU:HD21 | 1.68 | 0.58 |
| 4:A:270:PRO:HB3 | 4:A:416:PHE:CE1 | 2.39 | 0.58 |
| 4:A:400:PHE:O | 4:A:401:MET:C | 2.42 | 0.58 |
| 4:A:50:ARG:HH11 | 4:A:50:ARG:HG2 | 1.68 | 0.58 |
| 4:A:511:PHE:CD2 | 4:A:511:PHE:O | 2.57 | 0.58 |
| 4:B:753:GLY:O | 4:B:754:GLN:HG2 | 2.04 | 0.58 |
| 4:B:861:MET:O | 4:B:862:PRO:O | 2.21 | 0.58 |
| 4:B:843:ALA:HA | 4:B:864:LEU:HD21 | 1.85 | 0.58 |
| 4:C:433:ASN:HB2 | 4:C:434:PRO:HD2 | 1.85 | 0.58 |
| 4:C:701:SER:O | 4:C:704:LYS:HB3 | 2.04 | 0.58 |
| 4:C:727:TRP:NE1 | 4:C:782:PHE:CD1 | 2.72 | 0.58 |
| 4:D:292:ARG:N | 4:D:293:PRO:HD3 | 2.18 | 0.58 |
| 4:D:720:ARG:NH1 | 4:D:720:ARG:CG | 2.52 | 0.58 |
| 4:A:105:PHE:C | 4:A:107:GLN:H | 2.07 | 0.58 |
| 4:A:463:HIS:O | 4:A:466:ASN:N | 2.36 | 0.58 |
| 4:B:439:MET:HG3 | 4:B:509:PHE:CG | 2.38 | 0.58 |
| 4:C:401:MET:O | 4:C:404:GLN:CB | 2.52 | 0.58 |
| 4:C:476:PRO:HG2 | 4:C:477:GLU:H | 1.69 | 0.58 |
| 4:C:737:GLN:OE1 | 4:C:778:ILE:HD13 | 2.04 | 0.58 |
| 4:D:748:ASN:HB2 | 4:D:753:GLY:CA | 2.33 | 0.58 |
| 4:D:794:THR:OG1 | 4:D:831:THR:CG2 | 2.45 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:A:448:LYS:HG2 | 7:A:3094:HOH:O | 2.04 | 0.57 |
| 4:A:623:TYR:HD1 | 4:A:663:LYS:HE3 | 1.69 | 0.57 |
| 4:A:727:TRP:CZ2 | 4:A:735:VAL:HG11 | 2.39 | 0.57 |
| 4:A:788:GLY:C | 4:A:792:ARG:HH12 | 2.08 | 0.57 |
| 4:B:41:HIS:O | 4:B:42:GLU:C | 2.43 | 0.57 |
| 4:B:582:LEU:HD13 | 4:B:621:LEU:CD1 | 2.33 | 0.57 |
| 4:C:308:TYR:O | 4:C:310:ASP:N | 2.37 | 0.57 |
| 4:D:870:LEU:C | 4:D:870:LEU:HD23 | 2.25 | 0.57 |
| 4:A:135:GLN:HB2 | 7:A:3052:HOH:O | 2.02 | 0.57 |
| 4:A:416:PHE:CE2 | 4:A:434:PRO:HD3 | 2.40 | 0.57 |
| 4:A:471:ASP:OD1 | 4:A:472:LYS:CD | 2.38 | 0.57 |
| 4:A:669:GLN:HB3 | 4:A:672:GLN:HG3 | 1.86 | 0.57 |
| 4:B:123:LEU:O | 4:B:127:THR:HG23 | 2.04 | 0.57 |
| 4:B:436:GLY:HA3 | 7:B:3166:HOH:O | 2.03 | 0.57 |
| 4:B:450:LYS:HB3 | 4:B:819:ALA:HB3 | 1.86 | 0.57 |
| 4:B:823:ASN:O | 4:B:826:LYS:N | 2.36 | 0.57 |
| 4:B:99:ARG:HG2 | 4:B:99:ARG:HH11 | 1.68 | 0.57 |
| 4:C:67:ASN:C | 4:C:69:ALA:H | 2.06 | 0.57 |
| 4:D:84:ARG:HB2 | 4:D:223:SER:HB3 | 1.87 | 0.57 |
| 1:E:14:DG:C2' | 1:E:15:DC:C6 | 2.85 | 0.57 |
| 4:B:737:GLN:HG2 | 4:B:774:GLN:NE2 | 2.18 | 0.57 |
| 4:C:275:PRO:CG | 4:C:324:GLN:HG2 | 2.34 | 0.57 |
| 4:C:308:TYR:CE2 | 4:C:734:PRO:HG2 | 2.38 | 0.57 |
| 4:C:326:THR:O | 4:C:415:TRP:CD1 | 2.57 | 0.57 |
| 4:C:700:LYS:HA | 4:C:778:ILE:HG21 | 1.86 | 0.57 |
| 4:C:787:ASP:C | 4:C:787:ASP:OD1 | 2.42 | 0.57 |
| 4:D:100:PRO:O | 4:D:104:GLN:HG2 | 2.04 | 0.57 |
| 4:D:155:ARG:HA | 4:D:163:LYS:HE3 | 1.86 | 0.57 |
| 4:D:323:ALA:C | 4:D:325:ASN:H | 2.07 | 0.57 |
| 4:D:814:PHE:CE1 | 4:D:883:ALA:CB | 2.87 | 0.57 |
| 4:A:462:ILE:CD1 | 4:A:478:ARG:HD2 | 2.34 | 0.57 |
| 4:A:657:PRO:O | 4:A:661:SER:OG | 2.13 | 0.57 |
| 4:A:828:VAL:O | 4:A:831:THR:HG22 | 2.04 | 0.57 |
| 4:B:164:LYS:NZ | 4:B:164:LYS:N | 2.52 | 0.57 |
| 4:B:21:PHE:C | 4:B:23:THR:N | 2.58 | 0.57 |
| 4:B:492:CYS:SG | 4:B:502:TRP:HD1 | 2.25 | 0.57 |
| 4:B:642:LYS:HG2 | 4:B:682:TRP:CZ3 | 2.38 | 0.57 |
| 4:D:270:PRO:HD2 | 4:D:408:PHE:CE2 | 2.39 | 0.57 |
| 4:D:471:ASP:CG | 4:D:472:LYS:HD3 | 2.24 | 0.57 |
| 4:D:61:ALA:HB3 | 4:D:63:GLU:HG3 | 1.84 | 0.57 |
| 3:M:2:DT:H2'' | 3:M:3:DC:O5' | 2.02 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:A:651:LEU:HD11 | 4:A:656:GLN:HE22 | 1.70 | 0.57 |
| 4:A:712:ASP:O | 4:A:716:GLY:N | 2.36 | 0.57 |
| 4:B:261:LEU:C | 4:B:263:GLY:H | 2.07 | 0.57 |
| 4:B:281:ILE:HD11 | 4:B:308:TYR:C | 2.24 | 0.57 |
| 2:I:4:G:H5'' | 4:B:386:ARG:HD3 | 1.86 | 0.57 |
| 4:C:281:ILE:HG12 | 4:C:309:GLU:CA | 2.34 | 0.57 |
| 4:C:281:ILE:CD1 | 4:C:309:GLU:HA | 2.34 | 0.57 |
| 4:C:531:SER:OG | 7:C:3088:HOH:O | 2.17 | 0.57 |
| 4:C:583:GLN:O | 4:C:587:ILE:HG12 | 2.05 | 0.57 |
| 4:C:704:LYS:NZ | 4:C:775:GLU:OE2 | 2.32 | 0.57 |
| 4:D:486:HIS:NE2 | 4:D:490:MET:CG | 2.67 | 0.57 |
| 3:P:3:DC:H5' | 7:D:3034:HOH:O | 2.04 | 0.57 |
| 4:A:438:ASP:O | 4:A:439:MET:C | 2.42 | 0.57 |
| 4:A:849:PHE:O | 4:A:852:GLN:N | 2.38 | 0.57 |
| 4:A:882:PHE:N | 4:A:882:PHE:CD1 | 2.71 | 0.57 |
| 4:B:823:ASN:O | 4:B:824:LEU:C | 2.40 | 0.57 |
| 4:C:727:TRP:CE2 | 4:C:735:VAL:HG11 | 2.39 | 0.57 |
| 4:D:870:LEU:CD2 | 4:D:872:LEU:HD23 | 2.34 | 0.57 |
| 4:A:461:LYS:HE3 | 4:A:479:ILE:HG23 | 1.84 | 0.57 |
| 4:A:468:ALA:HB2 | 4:A:511:PHE:CD1 | 2.38 | 0.57 |
| 4:A:514:PHE:CD1 | 4:A:514:PHE:C | 2.76 | 0.57 |
| 4:B:298:ARG:HE | 4:B:419:ASN:CB | 2.18 | 0.57 |
| 4:B:828:VAL:O | 4:B:831:THR:HG22 | 2.05 | 0.57 |
| 4:C:10:ASP:OD1 | 7:C:3066:HOH:O | 2.18 | 0.57 |
| 4:D:632:ARG:HH22 | 6:D:2003:APC:C5' | 2.18 | 0.57 |
| 4:D:297:VAL:HG21 | 4:D:733:PHE:HZ | 1.69 | 0.57 |
| 4:D:543:ILE:HG22 | 4:D:543:ILE:O | 2.05 | 0.57 |
| 4:A:643:GLU:HG3 | 4:A:682:TRP:CG | 2.39 | 0.57 |
| 4:A:562:LEU:CD2 | 4:A:870:LEU:HD11 | 2.35 | 0.57 |
| 4:B:571:TYR:HD2 | 4:B:631:LYS:HA | 1.69 | 0.57 |
| 4:C:322:ILE:HG22 | 4:C:323:ALA:N | 2.19 | 0.57 |
| 4:D:19:ILE:CG2 | 7:D:3014:HOH:O | 2.51 | 0.57 |
| 4:D:720:ARG:NH1 | 4:D:721:LYS:O | 2.38 | 0.57 |
| 4:A:374:LEU:H | 4:A:374:LEU:HD12 | 1.68 | 0.57 |
| 4:A:404:GLN:HG2 | 4:A:432:PHE:HB2 | 1.86 | 0.57 |
| 4:B:557:ARG:HB2 | 4:B:562:LEU:HD12 | 1.86 | 0.57 |
| 4:B:677:MET:SD | 4:B:681:ILE:CD1 | 2.93 | 0.57 |
| 4:B:780:PRO:HA | 4:B:783:VAL:CG2 | 2.35 | 0.57 |
| 4:C:579:ASN:HA | 4:C:582:LEU:CD1 | 2.33 | 0.57 |
| 4:D:236:VAL:HB | 4:D:239:GLN:HB2 | 1.87 | 0.57 |
| 4:D:439:MET:HG3 | 4:D:509:PHE:CD2 | 2.40 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:88:TRP:O | 4:D:92:VAL:HG23 | 2.04 | 0.57 |
| 4:A:137:VAL:HG12 | 4:A:217:ILE:HD11 | 1.86 | 0.57 |
| 4:A:429:VAL:HG12 | 4:A:430:SER:N | 2.18 | 0.57 |
| 4:A:779:ALA:O | 4:A:783:VAL:HG23 | 2.05 | 0.57 |
| 4:B:162:PHE:HD1 | 4:B:190:MET:SD | 2.27 | 0.57 |
| 4:B:264:ILE:HG22 | 4:B:264:ILE:O | 2.05 | 0.57 |
| 4:B:702:ALA:HB1 | 4:B:849:PHE:HE2 | 1.67 | 0.57 |
| 4:C:711:LYS:HG2 | 4:C:718:ILE:HA | 1.87 | 0.57 |
| 4:D:338:ALA:HB2 | 4:D:509:PHE:CE1 | 2.40 | 0.57 |
| 4:D:42:GLU:O | 4:D:43:SER:C | 2.43 | 0.57 |
| 4:D:551:ARG:HB2 | 4:D:868:GLY:N | 2.16 | 0.57 |
| 4:A:109:ILE:CD1 | 4:A:149:ALA:HB2 | 2.35 | 0.56 |
| 4:A:312:TYR:CZ | 4:A:314:PRO:HG3 | 2.40 | 0.56 |
| 4:A:502:TRP:CG | 4:A:512:LEU:CD1 | 2.88 | 0.56 |
| 4:A:583:GLN:CB | 7:A:3056:HOH:O | 2.46 | 0.56 |
| 4:A:685:VAL:O | 4:A:687:VAL:N | 2.37 | 0.56 |
| 4:A:777:GLY:O | 4:A:781:ASN:OD1 | 2.23 | 0.56 |
| 4:A:828:VAL:CG2 | 4:A:829:ARG:H | 2.14 | 0.56 |
| 4:A:88:TRP:HE3 | 4:A:91:GLU:OE1 | 1.88 | 0.56 |
| 4:B:457:TYR:CE1 | 4:B:521:VAL:HG11 | 2.40 | 0.56 |
| 4:B:571:TYR:OH | 4:B:635:MET:CE | 2.52 | 0.56 |
| 4:B:734:PRO:O | 4:B:734:PRO:CG | 2.52 | 0.56 |
| 4:B:536:PHE:CE2 | 4:B:825:PHE:HD2 | 2.23 | 0.56 |
| 4:C:676:TYR:O | 4:C:677:MET:C | 2.43 | 0.56 |
| 4:C:721:LYS:HG2 | 4:C:722:ARG:N | 2.19 | 0.56 |
| 4:D:201:TRP:HA | 4:D:204:TRP:HD1 | 1.69 | 0.56 |
| 4:D:401:MET:HE3 | 4:D:440:THR:HG21 | 1.87 | 0.56 |
| 1:E:12:DT:C2' | 1:E:13:DC:C5' | 2.69 | 0.56 |
| 4:A:423:ARG:HG2 | 4:A:781:ASN:HD22 | 1.70 | 0.56 |
| 4:A:807:PHE:N | 4:A:807:PHE:CD1 | 2.73 | 0.56 |
| 4:B:163:LYS:NZ | 4:B:167:GLU:N | 2.54 | 0.56 |
| 4:B:42:GLU:O | 4:B:43:SER:C | 2.44 | 0.56 |
| 4:B:532:LEU:O | 4:B:818:PRO:HD3 | 2.04 | 0.56 |
| 4:C:5:ASN:ND2 | 4:C:7:ALA:HB3 | 2.19 | 0.56 |
| 4:C:632:ARG:HH22 | 6:C:2002:APC:C5' | 2.13 | 0.56 |
| 4:D:505:GLN:NE2 | 4:D:505:GLN:CA | 2.66 | 0.56 |
| 4:D:745:THR:HB | 4:D:756:ARG:NH1 | 2.21 | 0.56 |
| 4:A:383:ALA:O | 4:A:384:VAL:C | 2.41 | 0.56 |
| 4:A:579:ASN:HA | 4:A:582:LEU:CD1 | 2.35 | 0.56 |
| 4:A:308:TYR:CE2 | 4:A:736:TRP:HZ3 | 2.23 | 0.56 |
| 4:B:541:SER:O | 4:B:542:GLY:C | 2.43 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:B:841:VAL:HG12 | 7:B:3081:HOH:O | 2.05 | 0.56 |
| 4:C:831:THR:CG2 | 4:C:832:MET:N | 2.69 | 0.56 |
| 4:A:155:ARG:CB | 4:A:163:LYS:HE3 | 2.31 | 0.56 |
| 4:A:268:PHE:HB3 | 4:A:430:SER:HA | 1.86 | 0.56 |
| 4:A:379:ARG:HE | 4:A:656:GLN:HG2 | 1.70 | 0.56 |
| 4:A:820:ASP:O | 4:A:823:ASN:HB2 | 2.06 | 0.56 |
| 4:B:173:ARG:NH1 | 4:B:182:PHE:CD1 | 2.74 | 0.56 |
| 4:B:632:ARG:CD | 6:B:2001:APC:HN61 | 2.16 | 0.56 |
| 4:B:616:LEU:O | 4:B:618:GLY:N | 2.38 | 0.56 |
| 4:B:66:ASP:OD1 | 4:B:752:LEU:HD21 | 2.05 | 0.56 |
| 4:C:334:VAL:HG21 | 4:C:513:ALA:CB | 2.29 | 0.56 |
| 4:C:472:LYS:HE3 | 7:C:3049:HOH:O | 2.05 | 0.56 |
| 4:C:534:LEU:HD12 | 4:C:821:ALA:HB2 | 1.86 | 0.56 |
| 7:K:1088:HOH:O | 4:C:641:SER:HA | 2.06 | 0.56 |
| 4:D:420:MET:HA | 4:D:425:ARG:O | 2.04 | 0.56 |
| 4:D:512:LEU:O | 4:D:515:CYS:HB2 | 2.05 | 0.56 |
| 1:H:17:DG:H3' | 4:B:57:ARG:NH2 | 2.20 | 0.56 |
| 4:A:436:GLY:HA3 | 4:A:440:THR:HB | 1.87 | 0.56 |
| 4:A:508:PRO:HG2 | 4:A:509:PHE:H | 1.69 | 0.56 |
| 4:A:734:PRO:O | 4:A:734:PRO:HG2 | 2.05 | 0.56 |
| 4:A:816:THR:HG22 | 4:A:817:ILE:N | 2.18 | 0.56 |
| 4:B:233:ASN:CB | 4:B:239:GLN:HB3 | 2.35 | 0.56 |
| 4:B:335:LEU:HD21 | 4:B:406:ASN:OD1 | 2.06 | 0.56 |
| 4:B:465:ALA:O | 4:B:468:ALA:HB3 | 2.05 | 0.56 |
| 4:B:51:PHE:CD2 | 4:B:51:PHE:C | 2.78 | 0.56 |
| 4:B:541:SER:O | 4:B:544:GLN:HB3 | 2.04 | 0.56 |
| 4:B:56:GLU:OE1 | 4:B:57:ARG:CA | 2.53 | 0.56 |
| 4:B:634:VAL:O | 4:B:634:VAL:HG22 | 2.05 | 0.56 |
| 4:B:695:ALA:O | 4:B:699:LEU:CD1 | 2.50 | 0.56 |
| 4:B:846:TYR:CD2 | 4:B:864:LEU:HD11 | 2.40 | 0.56 |
| 4:C:152:GLY:O | 4:C:156:ASP:OD2 | 2.22 | 0.56 |
| 4:C:474:PRO:HB2 | 4:C:476:PRO:CD | 2.36 | 0.56 |
| 4:C:551:ARG:NH1 | 4:C:551:ARG:CG | 2.68 | 0.56 |
| 4:C:741:LYS:HB2 | 4:C:770:ASP:HB2 | 1.86 | 0.56 |
| 4:D:303:LYS:HG3 | 4:D:304:ALA:H | 1.68 | 0.56 |
| 4:D:390:ALA:HB1 | 4:D:394:ARG:NH2 | 2.19 | 0.56 |
| 4:A:109:ILE:HD13 | 4:A:145:ILE:CG2 | 2.20 | 0.56 |
| 4:A:14:ILE:HG13 | 7:A:3082:HOH:O | 2.05 | 0.56 |
| 4:A:792:ARG:O | 4:A:796:VAL:HG22 | 2.06 | 0.56 |
| 4:A:798:ALA:HB2 | 4:A:827:ALA:HB1 | 1.86 | 0.56 |
| 4:B:19:ILE:CD1 | 4:B:20:PRO:HD2 | 2.35 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:B:210:ILE:O | 4:B:214:VAL:HG22 | 2.06 | 0.56 |
| 4:B:446:LEU:HD13 | 4:B:806:SER:HB3 | 1.88 | 0.56 |
| 4:B:587:ILE:O | 4:B:614:LYS:HE3 | 2.05 | 0.56 |
| 4:B:620:TRP:CD2 | 4:B:677:MET:HE2 | 2.41 | 0.56 |
| 4:D:437:ASN:HD22 | 4:D:437:ASN:C | 2.07 | 0.56 |
| 4:A:143:ARG:HG2 | 7:A:3010:HOH:O | 2.05 | 0.56 |
| 4:A:314:PRO:HD2 | 4:A:315:GLU:H | 1.70 | 0.56 |
| 4:A:620:TRP:HA | 4:A:620:TRP:CE3 | 2.40 | 0.56 |
| 4:A:81:MET:SD | 4:A:85:ILE:HD11 | 2.45 | 0.56 |
| 4:B:89:PHE:HZ | 4:B:106:LEU:O | 1.89 | 0.56 |
| 4:B:5:ASN:HB3 | 4:B:8:LYS:HE3 | 1.88 | 0.56 |
| 4:B:783:VAL:O | 4:B:784:HIS:O | 2.24 | 0.56 |
| 4:B:827:ALA:O | 4:B:828:VAL:C | 2.44 | 0.56 |
| 4:C:335:LEU:HD21 | 4:C:406:ASN:OD1 | 2.06 | 0.56 |
| 4:D:669:GLN:HG3 | 4:D:672:GLN:NE2 | 2.21 | 0.56 |
| 4:D:712:ASP:HB2 | 4:D:719:LEU:HD11 | 1.88 | 0.56 |
| 4:D:828:VAL:HA | 4:D:831:THR:CG2 | 2.35 | 0.56 |
| 4:A:347:CYS:SG | 4:A:350:GLU:HG2 | 2.46 | 0.56 |
| 4:A:486:HIS:HE1 | 7:A:3212:HOH:O | 1.89 | 0.56 |
| 4:A:854:HIS:HD2 | 4:A:856:SER:OG | 1.89 | 0.56 |
| 4:B:109:ILE:HG13 | 4:B:149:ALA:HB2 | 1.88 | 0.56 |
| 4:B:199:GLU:HG2 | 4:B:201:TRP:HD1 | 1.70 | 0.56 |
| 4:B:550:LEU:HD11 | 4:B:695:ALA:HB2 | 1.88 | 0.56 |
| 4:B:795:VAL:O | 4:B:796:VAL:C | 2.39 | 0.56 |
| 4:B:804:ILE:HA | 7:B:3072:HOH:O | 2.04 | 0.56 |
| 4:C:275:PRO:HB2 | 4:C:324:GLN:CD | 2.25 | 0.56 |
| 4:C:421:ASP:O | 4:C:422:TRP:C | 2.44 | 0.56 |
| 4:C:42:GLU:O | 4:C:46:MET:HE2 | 2.06 | 0.56 |
| 4:C:452:ILE:HG13 | 4:C:456:GLY:HA3 | 1.86 | 0.56 |
| 4:C:485:ASN:O | 4:C:489:ILE:HG13 | 2.06 | 0.56 |
| 4:C:711:LYS:HG2 | 4:C:717:GLU:O | 2.06 | 0.56 |
| 4:D:199:GLU:OE2 | 4:D:202:SER:HB2 | 2.04 | 0.56 |
| 4:D:824:LEU:O | 4:D:828:VAL:HG22 | 2.06 | 0.56 |
| 4:A:316:VAL:HG13 | 4:A:792:ARG:NE | 2.20 | 0.56 |
| 4:A:390:ALA:C | 4:A:392:LYS:H | 2.10 | 0.56 |
| 4:A:534:LEU:HD23 | 4:A:534:LEU:N | 2.19 | 0.56 |
| 4:A:700:LYS:NZ | 7:A:3017:HOH:O | 2.25 | 0.56 |
| 4:B:173:ARG:NH1 | 4:B:182:PHE:HD1 | 2.03 | 0.56 |
| 4:B:478:ARG:O | 4:B:481:PHE:HB3 | 2.06 | 0.56 |
| 4:B:626:THR:O | 4:B:627:ARG:C | 2.43 | 0.56 |
| 4:B:86:ASN:HB3 | 7:B:3090:HOH:O | 2.04 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:C:278:TRP:CZ3 | 4:C:284:GLY:HA3 | 2.41 | 0.56 |
| 4:C:423:ARG:CD | 4:C:781:ASN:ND2 | 2.68 | 0.56 |
| 4:C:882:PHE:N | 4:C:882:PHE:HD1 | 2.02 | 0.56 |
| 4:D:421:ASP:OD1 | 4:D:421:ASP:O | 2.24 | 0.56 |
| 1:K:11:DA:H2' | 1:K:12:DT:H73 | 1.88 | 0.56 |
| 4:A:348:PRO:C | 4:A:349:VAL:CG2 | 2.74 | 0.56 |
| 4:A:656:GLN:N | 4:A:657:PRO:HD2 | 2.21 | 0.56 |
| 4:A:80:LYS:CE | 4:A:224:THR:HG22 | 2.36 | 0.56 |
| 4:B:620:TRP:O | 4:B:623:TYR:HB3 | 2.05 | 0.56 |
| 4:B:746:ARG:NH2 | 4:B:753:GLY:HA2 | 2.21 | 0.56 |
| 4:B:779:ALA:O | 4:B:783:VAL:HG22 | 2.06 | 0.56 |
| 4:B:730:PRO:HD2 | 4:B:786:GLN:HE21 | 1.69 | 0.56 |
| 4:B:846:TYR:CD1 | 4:B:850:ALA:HB2 | 2.41 | 0.56 |
| 4:B:89:PHE:CZ | 4:B:106:LEU:O | 2.58 | 0.56 |
| 4:C:273:VAL:O | 4:C:274:PRO:C | 2.42 | 0.56 |
| 4:C:281:ILE:HG22 | 4:C:282:THR:N | 2.21 | 0.56 |
| 4:C:322:ILE:HG21 | 4:C:795:VAL:CG1 | 2.36 | 0.56 |
| 4:D:313:MET:O | 4:D:317:TYR:HD2 | 1.89 | 0.56 |
| 4:D:432:PHE:CZ | 4:D:444:LEU:HD11 | 2.40 | 0.56 |
| 4:D:812:ASP:N | 4:D:812:ASP:OD1 | 2.38 | 0.56 |
| 4:A:281:ILE:HG13 | 4:A:309:GLU:HA | 1.88 | 0.56 |
| 4:A:333:LYS:CB | 4:A:516:PHE:CD2 | 2.89 | 0.56 |
| 4:B:329:LYS:HG2 | 4:B:445:THR:O | 2.05 | 0.56 |
| 4:B:639:TYR:HA | 7:B:3018:HOH:O | 2.04 | 0.56 |
| 4:B:737:GLN:HE22 | 4:B:777:GLY:C | 2.09 | 0.56 |
| 4:B:849:PHE:O | 4:B:852:GLN:HB2 | 2.06 | 0.56 |
| 4:C:341:ILE:CD1 | 4:C:348:PRO:HB3 | 2.29 | 0.56 |
| 4:C:416:PHE:HB2 | 4:C:418:TYR:HE1 | 1.70 | 0.56 |
| 4:C:512:LEU:O | 4:C:512:LEU:HD12 | 2.06 | 0.56 |
| 4:C:532:LEU:HD23 | 4:C:532:LEU:O | 2.06 | 0.56 |
| 4:D:30:GLU:HB3 | 4:D:34:ARG:HH21 | 1.70 | 0.56 |
| 1:E:9:DA:N6 | 3:G:1:DG:N2 | 2.54 | 0.56 |
| 4:A:433:ASN:HB2 | 4:A:434:PRO:HD2 | 1.88 | 0.55 |
| 4:A:545:HIS:HE1 | 4:A:787:ASP:HA | 1.71 | 0.55 |
| 4:C:116:TYR:OH | 4:C:752:LEU:HD22 | 2.06 | 0.55 |
| 4:C:205:HIS:O | 4:C:207:GLU:N | 2.39 | 0.55 |
| 4:C:543:ILE:HD13 | 4:C:689:VAL:HG11 | 1.88 | 0.55 |
| 4:C:571:TYR:CE2 | 4:C:631:LYS:HE3 | 2.42 | 0.55 |
| 4:C:814:PHE:N | 4:C:814:PHE:CD1 | 2.75 | 0.55 |
| 3:J:1:DG:H1' | 3:J:2:DT:C7 | 2.36 | 0.55 |
| 4:A:14:ILE:HD11 | 4:A:290:GLY:HA2 | 1.86 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:A:236:VAL:HB | 4:A:239:GLN:HB2 | 1.88 | 0.55 |
| 4:A:342:THR:HG22 | 4:A:348:PRO:CG | 2.35 | 0.55 |
| 4:A:715:THR:CG2 | 4:A:717:GLU:HB2 | 2.36 | 0.55 |
| 4:A:824:LEU:O | 4:A:827:ALA:N | 2.39 | 0.55 |
| 4:A:706:LEU:HD11 | 4:A:849:PHE:CD2 | 2.41 | 0.55 |
| 4:A:563:PRO:CB | 4:A:878:SER:HA | 2.33 | 0.55 |
| 4:B:407:LYS:CG | 4:B:408:PHE:CE2 | 2.85 | 0.55 |
| 4:B:576:LYS:NZ | 7:B:3102:HOH:O | 2.39 | 0.55 |
| 4:C:105:PHE:C | 4:C:107:GLN:H | 2.10 | 0.55 |
| 4:C:155:ARG:HG2 | 4:C:155:ARG:O | 2.06 | 0.55 |
| 4:C:16:LEU:HD21 | 4:C:41:HIS:ND1 | 2.20 | 0.55 |
| 4:C:423:ARG:HD2 | 4:C:781:ASN:CG | 2.26 | 0.55 |
| 4:C:421:ASP:C | 4:C:423:ARG:N | 2.57 | 0.55 |
| 4:C:50:ARG:CG | 4:C:50:ARG:NH1 | 2.69 | 0.55 |
| 4:D:744:GLN:HB3 | 4:D:756:ARG:HB2 | 1.88 | 0.55 |
| 1:N:12:DT:H5' | 4:D:781:ASN:HD21 | 1.71 | 0.55 |
| 4:A:292:ARG:N | 4:A:293:PRO:HD3 | 2.21 | 0.55 |
| 4:A:526:LEU:H | 4:A:526:LEU:HD12 | 1.66 | 0.55 |
| 4:B:182:PHE:O | 4:B:186:VAL:HG23 | 2.06 | 0.55 |
| 4:B:423:ARG:HH11 | 4:B:423:ARG:CG | 2.19 | 0.55 |
| 4:B:473:VAL:HG11 | 4:B:477:GLU:CB | 2.36 | 0.55 |
| 4:B:525:GLY:C | 4:B:527:SER:H | 2.10 | 0.55 |
| 4:B:698:TRP:CZ2 | 4:B:864:LEU:HG | 2.41 | 0.55 |
| 4:B:71:LYS:N | 4:B:72:PRO:CD | 2.69 | 0.55 |
| 4:C:711:LYS:CG | 4:C:718:ILE:HA | 2.36 | 0.55 |
| 4:D:505:GLN:N | 4:D:505:GLN:HE21 | 2.04 | 0.55 |
| 4:D:717:GLU:O | 4:D:719:LEU:HD12 | 2.07 | 0.55 |
| 4:D:772:HIS:O | 4:D:775:GLU:N | 2.38 | 0.55 |
| 4:A:59:LEU:HD23 | 4:A:64:VAL:HG22 | 1.88 | 0.55 |
| 4:A:650:VAL:O | 4:A:654:THR:HG22 | 2.07 | 0.55 |
| 4:A:578:VAL:CG1 | 4:A:680:LEU:HB3 | 2.36 | 0.55 |
| 4:B:291:ARG:CB | 7:B:3037:HOH:O | 2.51 | 0.55 |
| 4:B:411:HIS:O | 4:B:413:ALA:N | 2.40 | 0.55 |
| 4:B:489:ILE:CG2 | 4:B:515:CYS:HB3 | 2.37 | 0.55 |
| 4:B:492:CYS:O | 4:B:496:PRO:CD | 2.50 | 0.55 |
| 1:E:10:DT:OP2 | 4:A:645:GLY:HA3 | 2.05 | 0.55 |
| 1:N:9:DA:H2'' | 1:N:10:DT:OP1 | 2.05 | 0.55 |
| 4:A:778:ILE:CG2 | 4:A:779:ALA:H | 2.19 | 0.55 |
| 4:B:308:TYR:HE2 | 4:B:734:PRO:HG2 | 1.72 | 0.55 |
| 4:B:780:PRO:CD | 4:B:781:ASN:H | 2.19 | 0.55 |
| 4:D:817:ILE:HG12 | 4:D:820:ASP:OD2 | 2.05 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:9:DA:N6 | 3:M:1:DG:N2 | 2.54 | 0.55 |
| 4:A:474:PRO:HB2 | 4:A:476:PRO:HD2 | 1.88 | 0.55 |
| 4:A:632:ARG:HG2 | 7:A:3022:HOH:O | 2.06 | 0.55 |
| 4:B:588:ASN:O | 4:B:614:LYS:HD2 | 2.06 | 0.55 |
| 4:C:395:ARG:HE | 4:C:399:GLU:CG | 2.20 | 0.55 |
| 4:D:826:LYS:HD2 | 7:D:3041:HOH:O | 2.05 | 0.55 |
| 3:J:1:DG:H4' | 3:J:2:DT:H5' | 1.87 | 0.55 |
| 4:A:308:TYR:O | 4:A:311:VAL:N | 2.35 | 0.55 |
| 4:A:350:GLU:O | 7:A:3222:HOH:O | 2.18 | 0.55 |
| 4:A:401:MET:N | 4:A:401:MET:SD | 2.79 | 0.55 |
| 4:A:669:GLN:HG2 | 4:A:672:GLN:NE2 | 2.20 | 0.55 |
| 4:A:797:TRP:CZ2 | 4:A:801:LYS:HG3 | 2.40 | 0.55 |
| 4:B:137:VAL:HG12 | 4:B:217:ILE:CD1 | 2.34 | 0.55 |
| 4:B:275:PRO:CD | 7:B:3116:HOH:O | 2.48 | 0.55 |
| 4:B:285:GLY:HA2 | 4:B:324:GLN:HE22 | 1.71 | 0.55 |
| 4:B:854:HIS:HD1 | 4:B:855:GLU:H | 1.55 | 0.55 |
| 4:C:173:ARG:NH2 | 4:C:182:PHE:HB2 | 2.22 | 0.55 |
| 4:C:623:TYR:HA | 4:C:666:MET:HE1 | 1.89 | 0.55 |
| 4:C:582:LEU:HD11 | 4:C:625:VAL:HG21 | 1.88 | 0.55 |
| 4:C:807:PHE:N | 4:C:807:PHE:CD1 | 2.74 | 0.55 |
| 4:D:277:PRO:HA | 7:D:3029:HOH:O | 2.06 | 0.55 |
| 4:D:286:TYR:CZ | 4:D:417:PRO:HG3 | 2.41 | 0.55 |
| 4:A:707:ALA:O | 4:A:708:ALA:O | 2.25 | 0.55 |
| 4:B:345:LYS:HZ1 | 4:B:351:ASP:H | 1.55 | 0.55 |
| 4:B:569:ASP:OD1 | 4:B:569:ASP:O | 2.24 | 0.55 |
| 4:B:689:VAL:O | 4:B:690:VAL:C | 2.45 | 0.55 |
| 4:C:183:MET:HE3 | 4:C:186:VAL:HG21 | 1.89 | 0.55 |
| 4:C:744:GLN:HA | 4:C:756:ARG:HD3 | 1.89 | 0.55 |
| 4:D:743:ILE:O | 4:D:756:ARG:NH2 | 2.40 | 0.55 |
| 4:A:317:TYR:O | 4:A:321:ASN:ND2 | 2.33 | 0.55 |
| 4:A:619:GLN:O | 4:A:623:TYR:N | 2.37 | 0.55 |
| 4:A:630:THR:O | 4:A:631:LYS:O | 2.25 | 0.55 |
| 4:A:779:ALA:HB3 | 4:A:780:PRO:CD | 2.37 | 0.55 |
| 4:A:829:ARG:O | 4:A:833:VAL:HG23 | 2.06 | 0.55 |
| 4:B:345:LYS:O | 4:B:346:HIS:C | 2.45 | 0.55 |
| 4:B:76:THR:CG2 | 7:B:3212:HOH:O | 2.54 | 0.55 |
| 4:C:40:GLU:OE2 | 4:C:286:TYR:CD1 | 2.58 | 0.55 |
| 4:C:684:SER:O | 4:C:687:VAL:HG22 | 2.07 | 0.55 |
| 4:C:770:ASP:O | 4:C:770:ASP:OD1 | 2.25 | 0.55 |
| 4:D:652:GLU:O | 4:D:657:PRO:HD3 | 2.06 | 0.55 |
| 4:D:448:LYS:CD | 4:D:806:SER:HB3 | 2.36 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:A:14:ILE:CD1 | 4:A:14:ILE:N | 2.69 | 0.55 |
| 4:A:287:TRP:O | 4:A:288:ALA:O | 2.25 | 0.55 |
| 4:B:388:ASP:C | 4:B:388:ASP:OD1 | 2.45 | 0.55 |
| 4:B:803:GLY:O | 4:B:804:ILE:O | 2.25 | 0.55 |
| 4:B:813:SER:C | 4:B:814:PHE:CD1 | 2.81 | 0.55 |
| 4:C:106:LEU:HG | 4:C:212:VAL:HG13 | 1.89 | 0.55 |
| 4:C:579:ASN:OD1 | 4:C:582:LEU:HD12 | 2.07 | 0.55 |
| 4:C:710:VAL:HG13 | 4:C:710:VAL:O | 2.07 | 0.55 |
| 4:D:311:VAL:CG1 | 4:D:312:TYR:N | 2.70 | 0.55 |
| 4:D:816:THR:HG22 | 4:D:817:ILE:H | 1.71 | 0.55 |
| 4:A:177:VAL:HB | 7:A:3038:HOH:O | 2.06 | 0.54 |
| 4:B:419:ASN:O | 4:B:426:VAL:HA | 2.07 | 0.54 |
| 4:B:398:LEU:HG | 4:B:439:MET:HE2 | 1.89 | 0.54 |
| 4:B:587:ILE:HG22 | 4:B:588:ASN:HD22 | 1.71 | 0.54 |
| 4:C:21:PHE:C | 4:C:23:THR:H | 2.11 | 0.54 |
| 4:C:278:TRP:CD2 | 4:C:284:GLY:HA3 | 2.42 | 0.54 |
| 4:C:448:LYS:CE | 4:C:806:SER:OG | 2.54 | 0.54 |
| 4:D:241:SER:O | 4:D:243:THR:HG23 | 2.06 | 0.54 |
| 1:E:9:DA:C2 | 4:A:644:PHE:CD1 | 2.95 | 0.54 |
| 1:E:5:DA:H2 | 3:G:7:DT:O2 | 1.89 | 0.54 |
| 4:A:13:ASP:HB3 | 4:A:14:ILE:HD12 | 1.88 | 0.54 |
| 4:B:266:PRO:HG2 | 4:B:268:PHE:CE1 | 2.41 | 0.54 |
| 4:B:398:LEU:C | 4:B:398:LEU:CD2 | 2.75 | 0.54 |
| 4:B:532:LEU:HG | 4:B:533:PRO:HD2 | 1.90 | 0.54 |
| 4:B:545:HIS:O | 4:B:546:PHE:C | 2.42 | 0.54 |
| 4:B:662:GLY:C | 4:B:663:LYS:O | 2.45 | 0.54 |
| 4:B:849:PHE:O | 4:B:850:ALA:C | 2.46 | 0.54 |
| 4:C:340:VAL:C | 4:C:342:THR:N | 2.60 | 0.54 |
| 4:C:433:ASN:C | 4:C:433:ASN:OD1 | 2.46 | 0.54 |
| 4:C:45:GLU:O | 4:C:48:GLU:HB3 | 2.07 | 0.54 |
| 4:C:728:VAL:HG22 | 4:C:734:PRO:HB3 | 1.89 | 0.54 |
| 4:C:777:GLY:O | 4:C:781:ASN:OD1 | 2.25 | 0.54 |
| 4:C:814:PHE:CE1 | 4:C:883:ALA:CB | 2.91 | 0.54 |
| 4:D:155:ARG:CA | 4:D:163:LYS:HE3 | 2.37 | 0.54 |
| 4:D:558:ALA:HB1 | 4:D:570:ILE:HD13 | 1.88 | 0.54 |
| 4:A:641:SER:HB2 | 4:A:646:PHE:HE1 | 1.73 | 0.54 |
| 4:B:109:ILE:O | 4:B:110:LYS:C | 2.46 | 0.54 |
| 4:B:27:HIS:HD2 | 7:B:3169:HOH:O | 1.88 | 0.54 |
| 4:B:318:LYS:O | 4:B:319:ALA:C | 2.45 | 0.54 |
| 4:B:564:SER:HG | 4:B:566:THR:H | 1.53 | 0.54 |
| 4:C:278:TRP:CD1 | 4:C:320:ILE:HG22 | 2.43 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:C:334:VAL:CG2 | 4:C:513:ALA:HB2 | 2.29 | 0.54 |
| 4:C:84:ARG:HB2 | 4:C:223:SER:HB3 | 1.89 | 0.54 |
| 1:K:12:DT:H5'' | 4:C:422:TRP:CH2 | 2.42 | 0.54 |
| 4:A:35:GLU:O | 4:A:36:GLN:C | 2.46 | 0.54 |
| 4:A:640:GLY:O | 4:A:641:SER:C | 2.46 | 0.54 |
| 4:B:334:VAL:HG12 | 4:B:443:LEU:HD23 | 1.88 | 0.54 |
| 4:B:454:LYS:HG3 | 4:B:455:GLU:H | 1.72 | 0.54 |
| 4:B:639:TYR:CA | 7:B:3018:HOH:O | 2.55 | 0.54 |
| 4:B:423:ARG:NH2 | 4:B:784:HIS:ND1 | 2.53 | 0.54 |
| 4:B:784:HIS:O | 4:B:785:SER:C | 2.44 | 0.54 |
| 4:C:403:GLU:N | 7:C:3123:HOH:O | 2.39 | 0.54 |
| 4:C:508:PRO:HB2 | 4:C:509:PHE:HD2 | 1.71 | 0.54 |
| 4:C:509:PHE:H | 4:C:509:PHE:HD2 | 1.54 | 0.54 |
| 4:C:576:LYS:O | 4:C:580:GLU:HG3 | 2.07 | 0.54 |
| 4:D:577:LYS:O | 4:D:581:ILE:HG13 | 2.07 | 0.54 |
| 4:D:632:ARG:HH22 | 6:D:2003:APC:H5'2 | 1.72 | 0.54 |
| 1:H:12:DT:C2' | 1:H:13:DC:H6 | 2.19 | 0.54 |
| 3:P:9:DC:H2'' | 7:P:1110:HOH:O | 2.06 | 0.54 |
| 4:A:316:VAL:HG13 | 4:A:792:ARG:HD2 | 1.89 | 0.54 |
| 4:A:11:PHE:HB3 | 4:A:41:HIS:HE1 | 1.72 | 0.54 |
| 4:A:649:GLN:O | 4:A:650:VAL:C | 2.46 | 0.54 |
| 4:A:793:LYS:O | 4:A:794:THR:C | 2.45 | 0.54 |
| 4:B:181:ALA:HA | 4:B:184:GLN:NE2 | 2.22 | 0.54 |
| 4:B:573:ILE:HD13 | 7:B:3102:HOH:O | 2.07 | 0.54 |
| 4:B:677:MET:O | 4:B:678:ALA:C | 2.44 | 0.54 |
| 4:B:810:ILE:O | 4:B:813:SER:HB2 | 2.07 | 0.54 |
| 2:I:8:U:O3' | 4:B:812:ASP:OD2 | 2.24 | 0.54 |
| 4:C:833:VAL:HG22 | 4:C:872:LEU:O | 2.08 | 0.54 |
| 4:C:793:LYS:NZ | 4:C:835:THR:OG1 | 2.32 | 0.54 |
| 4:D:47:GLY:O | 4:D:50:ARG:HB3 | 2.08 | 0.54 |
| 4:D:446:LEU:HG | 4:D:533:PRO:HD3 | 1.90 | 0.54 |
| 4:A:13:ASP:CG | 4:A:291:ARG:HH21 | 2.10 | 0.54 |
| 4:A:204:TRP:HH2 | 4:A:212:VAL:HG21 | 1.67 | 0.54 |
| 4:A:555:GLY:O | 4:A:558:ALA:HB3 | 2.08 | 0.54 |
| 4:A:669:GLN:O | 4:A:672:GLN:N | 2.41 | 0.54 |
| 4:A:620:TRP:CE2 | 4:A:677:MET:HB2 | 2.43 | 0.54 |
| 4:A:76:THR:C | 4:A:79:PRO:HD2 | 2.27 | 0.54 |
| 4:A:720:ARG:HH21 | 4:A:857:GLN:NE2 | 2.06 | 0.54 |
| 4:B:473:VAL:HG11 | 4:B:477:GLU:HB2 | 1.88 | 0.54 |
| 4:B:742:PRO:HB3 | 4:B:744:GLN:CD | 2.27 | 0.54 |
| 4:B:803:GLY:O | 4:B:804:ILE:C | 2.46 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:C:656:GLN:HA | 4:C:656:GLN:HE21 | 1.72 | 0.54 |
| 4:D:258:ALA:O | 4:D:259:GLY:O | 2.26 | 0.54 |
| 4:D:50:ARG:NH1 | 4:D:267:MET:HG2 | 2.23 | 0.54 |
| 4:D:512:LEU:CA | 4:D:515:CYS:SG | 2.86 | 0.54 |
| 4:D:817:ILE:HB | 4:D:818:PRO:CD | 2.38 | 0.54 |
| 4:A:120:LYS:HG3 | 4:A:752:LEU:HD21 | 1.90 | 0.54 |
| 4:A:275:PRO:O | 4:A:277:PRO:HD3 | 2.07 | 0.54 |
| 4:A:471:ASP:O | 4:A:472:LYS:HG3 | 2.08 | 0.54 |
| 4:A:474:PRO:O | 4:A:477:GLU:HB2 | 2.07 | 0.54 |
| 4:A:88:TRP:CE3 | 4:A:91:GLU:OE1 | 2.61 | 0.54 |
| 4:B:211:HIS:O | 4:B:214:VAL:HG23 | 2.08 | 0.54 |
| 4:B:297:VAL:HG12 | 4:B:299:THR:HG22 | 1.88 | 0.54 |
| 4:B:790:HIS:HE1 | 4:B:831:THR:CG2 | 2.20 | 0.54 |
| 4:B:814:PHE:N | 4:B:814:PHE:CD1 | 2.76 | 0.54 |
| 4:C:273:VAL:HG23 | 4:C:274:PRO:O | 2.08 | 0.54 |
| 4:C:6:ILE:HD13 | 7:C:3031:HOH:O | 2.06 | 0.54 |
| 4:C:726:HIS:CD2 | 4:C:736:TRP:CE2 | 2.96 | 0.54 |
| 4:D:19:ILE:CD1 | 4:D:20:PRO:HD2 | 2.36 | 0.54 |
| 4:D:21:PHE:C | 4:D:23:THR:N | 2.61 | 0.54 |
| 4:D:744:GLN:HE21 | 4:D:756:ARG:H | 1.56 | 0.54 |
| 6:A:2000:APC:C4' | 7:A:3238:HOH:O | 2.41 | 0.54 |
| 4:A:636:THR:HG21 | 6:A:2000:APC:N6 | 2.23 | 0.54 |
| 4:A:216:CYS:O | 4:A:219:MET:N | 2.40 | 0.54 |
| 4:A:395:ARG:O | 4:A:399:GLU:HG3 | 2.08 | 0.54 |
| 4:A:428:ALA:H | 4:A:435:GLN:NE2 | 2.04 | 0.54 |
| 4:B:728:VAL:HG13 | 4:B:733:PHE:C | 2.28 | 0.54 |
| 4:B:823:ASN:O | 4:B:825:PHE:N | 2.40 | 0.54 |
| 4:B:882:PHE:HE2 | 7:B:3089:HOH:O | 1.90 | 0.54 |
| 4:C:161:HIS:C | 4:C:163:LYS:N | 2.62 | 0.54 |
| 4:C:474:PRO:CB | 4:C:476:PRO:HD2 | 2.37 | 0.54 |
| 4:D:882:PHE:O | 4:D:883:ALA:CB | 2.56 | 0.54 |
| 4:A:44:TYR:CD2 | 4:A:266:PRO:HB3 | 2.43 | 0.54 |
| 4:A:485:ASN:HD22 | 4:A:488:ASN:ND2 | 2.06 | 0.54 |
| 4:A:654:THR:O | 4:A:658:ALA:HB2 | 2.07 | 0.54 |
| 4:A:810:ILE:HG22 | 4:A:810:ILE:O | 2.07 | 0.54 |
| 4:B:201:TRP:CD2 | 7:B:3009:HOH:O | 2.61 | 0.54 |
| 4:B:754:GLN:O | 4:B:755:PHE:O | 2.25 | 0.54 |
| 4:C:120:LYS:HD2 | 4:C:751:PHE:HE2 | 1.72 | 0.54 |
| 4:C:199:GLU:HB2 | 7:C:3075:HOH:O | 2.08 | 0.54 |
| 4:C:312:TYR:CE1 | 4:C:314:PRO:HG3 | 2.42 | 0.54 |
| 4:C:457:TYR:CE1 | 4:C:521:VAL:CG1 | 2.87 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:201:TRP:O | 4:D:204:TRP:HB2 | 2.07 | 0.54 |
| 4:D:507:SER:O | 4:D:511:PHE:N | 2.41 | 0.54 |
| 1:H:15:DC:H2'' | 1:H:16:DC:H5' | 1.89 | 0.54 |
| 4:A:573:ILE:O | 4:A:576:LYS:HB2 | 2.07 | 0.54 |
| 4:A:656:GLN:O | 4:A:658:ALA:N | 2.41 | 0.54 |
| 4:B:144:ALA:O | 4:B:145:ILE:C | 2.46 | 0.54 |
| 4:B:163:LYS:C | 4:B:166:VAL:HG23 | 2.28 | 0.54 |
| 4:B:229:LEU:HD21 | 4:B:242:GLU:CD | 2.29 | 0.54 |
| 4:B:333:LYS:O | 4:B:337:VAL:CG2 | 2.54 | 0.54 |
| 4:B:42:GLU:HG2 | 4:B:46:MET:HE1 | 1.89 | 0.54 |
| 4:B:439:MET:O | 4:B:440:THR:C | 2.43 | 0.54 |
| 4:B:610:LYS:O | 4:B:611:LEU:C | 2.46 | 0.54 |
| 4:C:306:MET:C | 4:C:308:TYR:N | 2.61 | 0.54 |
| 4:C:830:GLU:O | 4:C:831:THR:C | 2.46 | 0.54 |
| 4:C:846:TYR:HA | 4:C:849:PHE:CE1 | 2.42 | 0.54 |
| 4:C:89:PHE:HZ | 4:C:106:LEU:O | 1.91 | 0.54 |
| 4:D:21:PHE:C | 4:D:23:THR:H | 2.10 | 0.54 |
| 4:D:551:ARG:HG3 | 4:D:551:ARG:HH11 | 1.73 | 0.54 |
| 4:D:594:VAL:HA | 4:D:609:VAL:HA | 1.90 | 0.54 |
| 4:D:530:CYS:HB3 | 4:D:818:PRO:HG2 | 1.90 | 0.54 |
| 4:D:829:ARG:O | 4:D:833:VAL:HG23 | 2.08 | 0.54 |
| 1:H:12:DT:H2'' | 1:H:13:DC:H5' | 1.89 | 0.54 |
| 3:M:8:DC:H2'' | 3:M:9:DC:OP2 | 2.07 | 0.54 |
| 4:A:134:VAL:O | 4:A:134:VAL:HG22 | 2.08 | 0.53 |
| 4:A:36:GLN:HG3 | 4:A:273:VAL:HG22 | 1.91 | 0.53 |
| 4:A:459:TRP:HZ3 | 4:A:475:PHE:CE1 | 2.25 | 0.53 |
| 4:A:544:GLN:OE1 | 4:A:559:VAL:CG2 | 2.56 | 0.53 |
| 4:A:648:GLN:O | 4:A:652:GLU:HG2 | 2.08 | 0.53 |
| 4:A:755:PHE:CD1 | 4:A:755:PHE:N | 2.77 | 0.53 |
| 4:A:882:PHE:N | 4:A:882:PHE:HD1 | 2.05 | 0.53 |
| 4:C:291:ARG:CG | 7:C:3066:HOH:O | 2.56 | 0.53 |
| 4:C:398:LEU:C | 4:C:398:LEU:HD23 | 2.29 | 0.53 |
| 4:C:539:SER:HB2 | 4:C:544:GLN:OE1 | 2.08 | 0.53 |
| 4:C:706:LEU:HD22 | 4:C:725:VAL:CG2 | 2.36 | 0.53 |
| 4:D:264:ILE:HG22 | 4:D:292:ARG:HG2 | 1.89 | 0.53 |
| 4:D:508:PRO:O | 4:D:510:CYS:N | 2.41 | 0.53 |
| 2:F:6:G:O2' | 2:F:7:A:H5' | 2.07 | 0.53 |
| 4:A:292:ARG:O | 4:A:292:ARG:HG3 | 2.09 | 0.53 |
| 4:A:594:VAL:HA | 4:A:609:VAL:HA | 1.89 | 0.53 |
| 4:A:316:VAL:HG13 | 4:A:792:ARG:CD | 2.38 | 0.53 |
| 4:A:825:PHE:C | 4:A:825:PHE:CD1 | 2.81 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:A:78:LEU:O | 4:A:82:ILE:HG13 | 2.08 | 0.53 |
| 4:A:563:PRO:HB3 | 4:A:877:GLU:C | 2.28 | 0.53 |
| 4:B:645:GLY:C | 4:B:647:ARG:N | 2.60 | 0.53 |
| 4:B:76:THR:HG22 | 7:B:3212:HOH:O | 2.07 | 0.53 |
| 4:B:730:PRO:HD3 | 4:B:786:GLN:NE2 | 2.24 | 0.53 |
| 4:B:816:THR:HG21 | 4:B:820:ASP:CB | 2.38 | 0.53 |
| 4:B:843:ALA:HA | 4:B:864:LEU:CD2 | 2.38 | 0.53 |
| 4:C:514:PHE:CD1 | 4:C:514:PHE:C | 2.81 | 0.53 |
| 4:C:705:LEU:HD21 | 4:C:860:LYS:HE3 | 1.90 | 0.53 |
| 4:D:19:ILE:HG21 | 7:D:3014:HOH:O | 2.08 | 0.53 |
| 4:D:274:PRO:HB3 | 4:D:325:ASN:OD1 | 2.07 | 0.53 |
| 4:D:523:HIS:O | 4:D:524:HIS:ND1 | 2.41 | 0.53 |
| 1:N:11:DA:C5 | 4:D:639:TYR:CE2 | 2.96 | 0.53 |
| 4:A:105:PHE:O | 4:A:107:GLN:N | 2.41 | 0.53 |
| 4:A:19:ILE:HG22 | 7:A:3120:HOH:O | 2.04 | 0.53 |
| 4:A:236:VAL:HG11 | 4:A:239:GLN:HG3 | 1.89 | 0.53 |
| 4:B:201:TRP:CG | 7:B:3009:HOH:O | 2.60 | 0.53 |
| 4:B:710:VAL:O | 4:B:710:VAL:HG13 | 2.08 | 0.53 |
| 4:B:840:ASP:O | 4:B:841:VAL:C | 2.46 | 0.53 |
| 4:C:421:ASP:C | 4:C:423:ARG:H | 2.10 | 0.53 |
| 4:C:739:TYR:HD2 | 4:C:774:GLN:HA | 1.73 | 0.53 |
| 4:C:791:LEU:C | 4:C:791:LEU:HD23 | 2.29 | 0.53 |
| 4:D:14:ILE:HG21 | 4:D:288:ALA:HB1 | 1.89 | 0.53 |
| 4:D:302:LYS:HE3 | 4:D:306:MET:CE | 2.38 | 0.53 |
| 4:A:328:TRP:HA | 4:A:446:LEU:HA | 1.91 | 0.53 |
| 4:A:333:LYS:HB2 | 4:A:516:PHE:CD2 | 2.43 | 0.53 |
| 4:A:651:LEU:CD1 | 4:A:656:GLN:NE2 | 2.72 | 0.53 |
| 4:A:546:PHE:CZ | 4:A:783:VAL:CG2 | 2.88 | 0.53 |
| 4:B:112:GLU:H | 4:B:112:GLU:CD | 2.11 | 0.53 |
| 4:B:465:ALA:HB1 | 4:B:470:VAL:HB | 1.89 | 0.53 |
| 4:B:633:SER:HB3 | 4:B:646:PHE:CD1 | 2.43 | 0.53 |
| 4:B:69:ALA:O | 4:B:72:PRO:HD2 | 2.08 | 0.53 |
| 4:C:826:LYS:O | 4:C:830:GLU:HG3 | 2.08 | 0.53 |
| 4:C:840:ASP:O | 4:C:843:ALA:N | 2.41 | 0.53 |
| 4:D:419:ASN:HD22 | 4:D:419:ASN:N | 2.06 | 0.53 |
| 4:A:229:LEU:HD13 | 4:A:244:ILE:HD13 | 1.90 | 0.53 |
| 4:A:374:LEU:C | 4:A:376:ALA:H | 2.12 | 0.53 |
| 4:A:423:ARG:HH21 | 4:A:784:HIS:CB | 2.22 | 0.53 |
| 4:A:11:PHE:CZ | 4:A:44:TYR:HB3 | 2.43 | 0.53 |
| 4:A:643:GLU:HG3 | 4:A:682:TRP:CB | 2.39 | 0.53 |
| 4:A:809:LEU:C | 4:A:810:ILE:HG13 | 2.28 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:B:427:TYR:HE1 | 4:B:811:HIS:NE2 | 2.06 | 0.53 |
| 4:C:452:ILE:HG23 | 4:C:453:GLY:H | 1.74 | 0.53 |
| 4:C:719:LEU:N | 4:C:719:LEU:HD12 | 2.24 | 0.53 |
| 4:C:830:GLU:HG2 | 4:C:876:LEU:CD2 | 2.38 | 0.53 |
| 4:C:88:TRP:O | 4:C:92:VAL:HG23 | 2.07 | 0.53 |
| 4:D:677:MET:O | 4:D:680:LEU:HB2 | 2.08 | 0.53 |
| 4:D:810:ILE:HB | 4:D:813:SER:CB | 2.39 | 0.53 |
| 2:I:5:C:C2 | 2:I:6:G:C8 | 2.96 | 0.53 |
| 4:A:796:VAL:O | 4:A:797:TRP:C | 2.45 | 0.53 |
| 4:A:881:ALA:C | 4:A:882:PHE:O | 2.45 | 0.53 |
| 7:I:777:HOH:O | 4:B:386:ARG:HD2 | 2.02 | 0.53 |
| 4:B:430:SER:O | 4:B:430:SER:OG | 2.21 | 0.53 |
| 4:B:50:ARG:HH11 | 4:B:50:ARG:CG | 2.22 | 0.53 |
| 4:B:696:MET:O | 4:B:700:LYS:HB2 | 2.08 | 0.53 |
| 4:B:795:VAL:O | 4:B:796:VAL:O | 2.27 | 0.53 |
| 4:B:99:ARG:NH2 | 7:B:3046:HOH:O | 2.40 | 0.53 |
| 4:D:537:ASP:O | 4:D:882:PHE:HB2 | 2.08 | 0.53 |
| 4:D:619:GLN:HG2 | 4:D:666:MET:O | 2.09 | 0.53 |
| 4:A:165:ASN:N | 4:A:165:ASN:OD1 | 2.35 | 0.53 |
| 4:A:457:TYR:HE1 | 4:A:521:VAL:HG11 | 1.70 | 0.53 |
| 4:A:729:THR:OG1 | 4:A:733:PHE:HB3 | 2.08 | 0.53 |
| 4:B:278:TRP:N | 4:B:321:ASN:OD1 | 2.27 | 0.53 |
| 4:B:631:LYS:O | 4:B:632:ARG:C | 2.47 | 0.53 |
| 4:C:118:THR:HG23 | 4:C:141:ILE:HD13 | 1.90 | 0.53 |
| 4:C:14:ILE:HA | 7:C:3014:HOH:O | 2.09 | 0.53 |
| 4:C:553:GLU:O | 4:C:554:VAL:C | 2.47 | 0.53 |
| 4:D:754:GLN:O | 4:D:755:PHE:O | 2.27 | 0.53 |
| 4:A:136:ALA:O | 4:A:139:SER:HB3 | 2.08 | 0.53 |
| 4:A:30:GLU:HB2 | 7:A:3035:HOH:O | 2.09 | 0.53 |
| 4:A:828:VAL:C | 4:A:830:GLU:N | 2.61 | 0.53 |
| 4:B:21:PHE:HD1 | 4:B:21:PHE:O | 1.91 | 0.53 |
| 1:H:10:DT:H4' | 4:B:639:TYR:O | 2.08 | 0.53 |
| 4:B:68:ALA:HB3 | 4:B:261:LEU:HD21 | 1.91 | 0.53 |
| 4:C:80:LYS:HD2 | 4:C:224:THR:CG2 | 2.39 | 0.53 |
| 4:C:472:LYS:HA | 4:C:567:VAL:HG11 | 1.89 | 0.53 |
| 4:C:592:ASN:O | 4:C:593:GLU:HB2 | 2.09 | 0.53 |
| 4:C:849:PHE:O | 4:C:852:GLN:N | 2.42 | 0.53 |
| 4:C:90:GLU:OE2 | 4:C:93:LYS:HD2 | 2.08 | 0.53 |
| 4:D:230:HIS:O | 4:D:230:HIS:ND1 | 2.41 | 0.53 |
| 4:D:281:ILE:HD12 | 4:D:317:TYR:HH | 1.73 | 0.53 |
| 2:L:4:G:H1' | 4:C:389:LYS:NZ | 2.23 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:N:10:DT:H3 | 6:D:2003:APC:HN62 | 1.56 | 0.53 |
| 4:A:446:LEU:HB2 | 4:A:531:SER:O | 2.09 | 0.53 |
| 4:B:407:LYS:HE2 | 4:B:408:PHE:CE2 | 2.44 | 0.53 |
| 1:H:13:DC:H4' | 4:B:427:TYR:CE2 | 2.44 | 0.53 |
| 4:B:737:GLN:NE2 | 4:B:739:TYR:HE2 | 1.99 | 0.53 |
| 4:C:737:GLN:OE1 | 4:C:778:ILE:HA | 2.08 | 0.53 |
| 4:C:96:ARG:HG2 | 4:C:96:ARG:HH11 | 1.74 | 0.53 |
| 4:D:402:LEU:O | 4:D:403:GLU:C | 2.47 | 0.53 |
| 4:D:428:ALA:N | 4:D:435:GLN:NE2 | 2.55 | 0.53 |
| 4:D:854:HIS:CG | 4:D:855:GLU:N | 2.76 | 0.53 |
| 4:A:502:TRP:O | 4:A:505:GLN:HB2 | 2.09 | 0.53 |
| 4:B:416:PHE:HE1 | 4:B:432:PHE:O | 1.92 | 0.53 |
| 4:B:423:ARG:NH1 | 4:B:784:HIS:CB | 2.71 | 0.53 |
| 4:B:793:LYS:HG3 | 7:B:3181:HOH:O | 2.08 | 0.53 |
| 4:C:509:PHE:N | 4:C:509:PHE:CD2 | 2.76 | 0.53 |
| 4:C:512:LEU:O | 4:C:516:PHE:HD1 | 1.92 | 0.53 |
| 4:C:698:TRP:CZ2 | 4:C:864:LEU:HG | 2.44 | 0.53 |
| 4:C:82:ILE:CD1 | 4:C:112:GLU:HA | 2.39 | 0.53 |
| 4:D:100:PRO:HG2 | 4:D:103:PHE:HB3 | 1.90 | 0.53 |
| 4:D:32:LEU:CD1 | 4:D:32:LEU:H | 2.08 | 0.53 |
| 4:D:349:VAL:HG12 | 4:D:349:VAL:O | 2.09 | 0.53 |
| 4:D:570:ILE:HA | 4:D:573:ILE:HG22 | 1.91 | 0.53 |
| 4:D:571:TYR:HD1 | 4:D:631:LYS:HA | 1.72 | 0.53 |
| 4:D:711:LYS:C | 4:D:719:LEU:HD13 | 2.29 | 0.53 |
| 4:D:817:ILE:HB | 4:D:818:PRO:HD2 | 1.90 | 0.53 |
| 4:D:849:PHE:O | 4:D:852:GLN:N | 2.34 | 0.53 |
| 3:M:5:DA:H2'' | 3:M:6:DT:C7 | 2.39 | 0.53 |
| 4:A:109:ILE:CG1 | 4:A:149:ALA:HB2 | 2.39 | 0.52 |
| 4:B:11:PHE:CE1 | 4:B:44:TYR:HB3 | 2.43 | 0.52 |
| 4:B:663:LYS:HG2 | 4:B:664:GLY:N | 2.21 | 0.52 |
| 4:B:669:GLN:CB | 4:B:672:GLN:HE21 | 2.22 | 0.52 |
| 4:C:158:GLU:OE1 | 4:C:195:LEU:HB3 | 2.08 | 0.52 |
| 4:C:871:ASN:ND2 | 4:C:873:ARG:HB2 | 2.24 | 0.52 |
| 4:D:233:ASN:HD22 | 4:D:239:GLN:HE21 | 1.56 | 0.52 |
| 4:D:543:ILE:HG21 | 4:D:689:VAL:HG11 | 1.91 | 0.52 |
| 4:D:744:GLN:CA | 4:D:756:ARG:CZ | 2.85 | 0.52 |
| 3:J:4:DG:H1' | 3:J:5:DA:C8 | 2.44 | 0.52 |
| 4:A:569:ASP:O | 4:A:573:ILE:HG22 | 2.08 | 0.52 |
| 4:A:664:GLY:HA2 | 4:A:667:PHE:CD2 | 2.39 | 0.52 |
| 4:A:727:TRP:CE2 | 4:A:735:VAL:CG1 | 2.88 | 0.52 |
| 4:B:307:ARG:HB3 | 4:B:736:TRP:CZ3 | 2.44 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:B:486:HIS:HE1 | 4:B:490:MET:HG3 | 1.73 | 0.52 |
| 4:C:19:ILE:HG23 | 4:C:20:PRO:N | 2.23 | 0.52 |
| 4:C:36:GLN:HG3 | 4:C:273:VAL:CG2 | 2.38 | 0.52 |
| 4:C:320:ILE:O | 4:C:324:GLN:HB2 | 2.09 | 0.52 |
| 4:C:845:PHE:O | 4:C:848:GLN:N | 2.41 | 0.52 |
| 4:D:114:VAL:HA | 4:D:117:ILE:HD12 | 1.91 | 0.52 |
| 4:D:545:HIS:O | 4:D:546:PHE:C | 2.47 | 0.52 |
| 4:D:557:ARG:NH2 | 7:D:3021:HOH:O | 2.43 | 0.52 |
| 4:D:739:TYR:HD2 | 4:D:774:GLN:HA | 1.74 | 0.52 |
| 2:O:2:C:H5 | 7:O:443:HOH:O | 1.92 | 0.52 |
| 4:A:626:THR:O | 4:A:627:ARG:C | 2.48 | 0.52 |
| 4:A:646:PHE:O | 4:A:647:ARG:C | 2.48 | 0.52 |
| 4:A:755:PHE:N | 4:A:755:PHE:HD1 | 2.07 | 0.52 |
| 4:B:122:THR:HG22 | 4:B:123:LEU:N | 2.24 | 0.52 |
| 4:B:146:GLU:O | 4:B:147:ASP:C | 2.46 | 0.52 |
| 4:B:21:PHE:C | 4:B:21:PHE:CD1 | 2.82 | 0.52 |
| 4:B:272:VAL:HG11 | 4:B:411:HIS:HD2 | 1.73 | 0.52 |
| 4:C:205:HIS:C | 4:C:207:GLU:H | 2.12 | 0.52 |
| 4:C:322:ILE:CG2 | 4:C:795:VAL:CG1 | 2.88 | 0.52 |
| 4:C:474:PRO:O | 4:C:478:ARG:HG3 | 2.09 | 0.52 |
| 4:C:788:GLY:O | 4:C:792:ARG:NH1 | 2.42 | 0.52 |
| 4:C:830:GLU:HG2 | 4:C:876:LEU:HD21 | 1.91 | 0.52 |
| 4:C:551:ARG:HD3 | 4:C:872:LEU:HD21 | 1.91 | 0.52 |
| 4:D:154:ILE:O | 4:D:159:ALA:HB3 | 2.09 | 0.52 |
| 4:D:751:PHE:HB3 | 4:D:752:LEU:HD12 | 1.90 | 0.52 |
| 4:D:731:ASP:OD1 | 4:D:792:ARG:NH2 | 2.42 | 0.52 |
| 1:E:11:DA:H2' | 1:E:12:DT:C7 | 2.39 | 0.52 |
| 3:J:5:DA:H2'' | 3:J:6:DT:H72 | 1.91 | 0.52 |
| 1:N:6:DT:C6 | 1:N:6:DT:H5' | 2.44 | 0.52 |
| 4:A:383:ALA:C | 4:A:385:TYR:H | 2.11 | 0.52 |
| 4:A:269:GLN:O | 4:A:430:SER:HB2 | 2.10 | 0.52 |
| 4:A:544:GLN:HG2 | 4:A:559:VAL:CG2 | 2.30 | 0.52 |
| 4:A:551:ARG:O | 4:A:868:GLY:HA3 | 2.08 | 0.52 |
| 4:B:19:ILE:HG23 | 4:B:20:PRO:CD | 2.39 | 0.52 |
| 1:H:12:DT:C5' | 4:B:423:ARG:HE | 2.22 | 0.52 |
| 4:C:278:TRP:CD1 | 4:C:320:ILE:CG2 | 2.92 | 0.52 |
| 4:C:770:ASP:O | 4:C:772:HIS:N | 2.42 | 0.52 |
| 4:C:315:GLU:OE1 | 4:C:796:VAL:HG11 | 2.08 | 0.52 |
| 4:C:794:THR:OG1 | 4:C:831:THR:HG21 | 2.09 | 0.52 |
| 4:C:843:ALA:HA | 4:C:864:LEU:HD21 | 1.92 | 0.52 |
| 4:D:207:GLU:O | 4:D:211:HIS:CE1 | 2.63 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:323:ALA:C | 4:D:325:ASN:N | 2.61 | 0.52 |
| 4:D:384:VAL:HA | 7:D:3158:HOH:O | 2.10 | 0.52 |
| 4:D:458:TYR:CD2 | 4:D:458:TYR:C | 2.82 | 0.52 |
| 4:D:833:VAL:O | 4:D:837:GLU:HG3 | 2.09 | 0.52 |
| 4:A:476:PRO:HG2 | 4:A:477:GLU:H | 1.74 | 0.52 |
| 4:A:546:PHE:HE2 | 4:A:696:MET:CG | 2.22 | 0.52 |
| 4:A:694:GLU:OE1 | 4:A:865:PRO:HB3 | 2.10 | 0.52 |
| 4:B:231:ARG:HG2 | 4:B:234:ALA:CB | 2.35 | 0.52 |
| 4:B:407:LYS:HG2 | 4:B:408:PHE:HE2 | 1.66 | 0.52 |
| 4:B:430:SER:O | 4:B:432:PHE:N | 2.43 | 0.52 |
| 4:B:327:ALA:HB1 | 4:B:447:ALA:HB3 | 1.91 | 0.52 |
| 4:B:569:ASP:O | 4:B:572:GLY:N | 2.41 | 0.52 |
| 4:B:810:ILE:N | 4:B:813:SER:HB3 | 2.25 | 0.52 |
| 4:C:116:TYR:O | 4:C:119:ILE:HG12 | 2.10 | 0.52 |
| 4:C:325:ASN:O | 4:C:415:TRP:CD1 | 2.62 | 0.52 |
| 4:C:433:ASN:N | 7:C:3164:HOH:O | 2.41 | 0.52 |
| 4:D:116:TYR:CE2 | 4:D:752:LEU:HD22 | 2.44 | 0.52 |
| 1:H:18:DC:H2'' | 4:B:63:GLU:OE1 | 2.10 | 0.52 |
| 2:O:6:G:O2' | 2:O:7:A:H5' | 2.09 | 0.52 |
| 4:A:34:ARG:NH2 | 7:A:3166:HOH:O | 2.43 | 0.52 |
| 4:A:422:TRP:CD1 | 4:A:423:ARG:HG3 | 2.45 | 0.52 |
| 4:A:42:GLU:O | 4:A:45:GLU:N | 2.42 | 0.52 |
| 4:A:433:ASN:OD1 | 4:A:435:GLN:N | 2.41 | 0.52 |
| 4:B:278:TRP:CD2 | 4:B:284:GLY:HA3 | 2.44 | 0.52 |
| 4:B:422:TRP:CD1 | 4:B:422:TRP:C | 2.83 | 0.52 |
| 4:B:473:VAL:HG12 | 4:B:477:GLU:HB2 | 1.91 | 0.52 |
| 4:B:58:GLN:NE2 | 7:B:3136:HOH:O | 2.41 | 0.52 |
| 4:B:720:ARG:NH1 | 4:B:721:LYS:O | 2.43 | 0.52 |
| 4:C:591:ASP:OD1 | 7:C:3122:HOH:O | 2.19 | 0.52 |
| 4:D:232:GLN:HB2 | 4:D:241:SER:O | 2.09 | 0.52 |
| 4:D:322:ILE:HG21 | 4:D:795:VAL:HG12 | 1.92 | 0.52 |
| 4:D:506:ASP:O | 4:D:508:PRO:HD2 | 2.09 | 0.52 |
| 4:D:777:GLY:O | 4:D:778:ILE:C | 2.46 | 0.52 |
| 3:G:5:DA:N6 | 7:G:73:HOH:O | 2.43 | 0.52 |
| 1:K:14:DG:H3' | 7:K:520:HOH:O | 2.08 | 0.52 |
| 4:A:134:VAL:HA | 4:A:137:VAL:HB | 1.92 | 0.52 |
| 4:A:16:LEU:HB3 | 4:A:37:LEU:HB3 | 1.92 | 0.52 |
| 4:A:299:THR:HG22 | 4:A:300:HIS:H | 1.75 | 0.52 |
| 4:B:330:ILE:HD11 | 4:B:405:ALA:HA | 1.90 | 0.52 |
| 4:B:267:MET:HE3 | 4:B:431:MET:SD | 2.50 | 0.52 |
| 4:B:699:LEU:HD11 | 4:B:842:LEU:HD11 | 1.90 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:B:872:LEU:O | 4:B:874:ASP:N | 2.43 | 0.52 |
| 4:B:882:PHE:O | 4:B:883:ALA:HB3 | 2.09 | 0.52 |
| 4:D:95:LYS:HB2 | 4:D:95:LYS:HZ2 | 1.75 | 0.52 |
| 4:A:141:ILE:CG2 | 4:A:145:ILE:HD11 | 2.39 | 0.52 |
| 4:A:627:ARG:NH2 | 6:A:2000:APC:O2G | 2.43 | 0.52 |
| 4:A:596:THR:HG23 | 4:A:606:SER:O | 2.09 | 0.52 |
| 4:A:830:GLU:O | 4:A:831:THR:C | 2.47 | 0.52 |
| 4:B:276:LYS:HB2 | 4:B:287:TRP:CD2 | 2.45 | 0.52 |
| 4:B:403:GLU:O | 4:B:404:GLN:C | 2.48 | 0.52 |
| 4:B:422:TRP:NE1 | 4:B:781:ASN:ND2 | 2.57 | 0.52 |
| 4:C:685:VAL:C | 4:C:687:VAL:H | 2.13 | 0.52 |
| 4:C:846:TYR:HD2 | 4:C:864:LEU:HD11 | 1.74 | 0.52 |
| 4:D:337:VAL:HG12 | 4:D:341:ILE:HD11 | 1.92 | 0.52 |
| 4:D:809:LEU:O | 4:D:810:ILE:HG13 | 2.10 | 0.52 |
| 4:D:848:GLN:OE1 | 4:D:848:GLN:HA | 2.09 | 0.52 |
| 3:G:4:DG:H2'' | 3:G:5:DA:C8 | 2.45 | 0.52 |
| 1:N:11:DA:H2'' | 1:N:12:DT:O5' | 2.10 | 0.52 |
| 4:A:166:VAL:O | 4:A:167:GLU:C | 2.47 | 0.52 |
| 4:A:206:LYS:O | 4:A:210:ILE:HG12 | 2.10 | 0.52 |
| 4:A:437:ASN:O | 4:A:438:ASP:C | 2.46 | 0.52 |
| 4:A:620:TRP:CZ2 | 4:A:677:MET:HB2 | 2.45 | 0.52 |
| 4:A:871:ASN:O | 4:A:874:ASP:OD2 | 2.28 | 0.52 |
| 4:B:157:LEU:O | 4:B:160:LYS:N | 2.32 | 0.52 |
| 4:B:48:GLU:HG3 | 4:B:262:ALA:HB1 | 1.92 | 0.52 |
| 4:B:780:PRO:HB3 | 7:B:3018:HOH:O | 2.10 | 0.52 |
| 4:B:779:ALA:N | 4:B:780:PRO:HD3 | 2.25 | 0.52 |
| 4:B:849:PHE:H | 4:B:849:PHE:HD1 | 1.56 | 0.52 |
| 4:C:455:GLU:OE1 | 4:C:455:GLU:HA | 2.09 | 0.52 |
| 4:C:4:ILE:CD1 | 4:C:256:THR:HG23 | 2.37 | 0.52 |
| 4:C:333:LYS:CD | 4:C:516:PHE:HD2 | 2.15 | 0.52 |
| 4:D:404:GLN:HG2 | 4:D:432:PHE:CB | 2.40 | 0.52 |
| 4:A:281:ILE:HG13 | 4:A:309:GLU:CG | 2.40 | 0.52 |
| 4:A:281:ILE:HG22 | 4:A:282:THR:N | 2.23 | 0.52 |
| 4:A:459:TRP:CH2 | 4:A:825:PHE:CE2 | 2.98 | 0.52 |
| 4:B:450:LYS:N | 4:B:529:ASN:HD21 | 2.07 | 0.52 |
| 4:B:471:ASP:C | 4:B:472:LYS:HD2 | 2.31 | 0.52 |
| 4:B:722:ARG:NH1 | 4:B:768:GLU:OE2 | 2.42 | 0.52 |
| 4:D:236:VAL:O | 4:D:240:ASP:HB2 | 2.09 | 0.52 |
| 4:D:501:TRP:HA | 4:D:504:GLU:CD | 2.30 | 0.52 |
| 4:D:613:THR:HG22 | 4:D:676:TYR:HE1 | 1.75 | 0.52 |
| 4:D:582:LEU:HD22 | 4:D:620:TRP:HB2 | 1.92 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:66:ASP:OD2 | 4:D:752:LEU:HD23 | 2.10 | 0.52 |
| 2:I:5:C:N3 | 2:I:6:G:C8 | 2.78 | 0.52 |
| 4:A:270:PRO:HB3 | 4:A:416:PHE:CD1 | 2.45 | 0.51 |
| 4:A:457:TYR:CD1 | 4:A:521:VAL:HG21 | 2.40 | 0.51 |
| 4:A:521:VAL:HG12 | 4:A:522:GLN:N | 2.24 | 0.51 |
| 4:A:810:ILE:CD1 | 7:A:3145:HOH:O | 2.58 | 0.51 |
| 4:B:105:PHE:C | 4:B:107:GLN:H | 2.13 | 0.51 |
| 4:B:194:GLY:O | 4:B:196:LEU:HD23 | 2.11 | 0.51 |
| 4:C:404:GLN:NE2 | 4:C:404:GLN:HA | 2.19 | 0.51 |
| 4:C:42:GLU:OE1 | 4:C:46:MET:HE1 | 2.09 | 0.51 |
| 4:C:569:ASP:O | 4:C:572:GLY:N | 2.43 | 0.51 |
| 4:C:649:GLN:O | 4:C:650:VAL:C | 2.48 | 0.51 |
| 4:C:93:LYS:HA | 4:C:99:ARG:NH2 | 2.25 | 0.51 |
| 4:D:466:ASN:OD1 | 4:D:478:ARG:NH1 | 2.44 | 0.51 |
| 1:H:9:DA:N6 | 3:J:1:DG:H22 | 2.05 | 0.51 |
| 4:A:459:TRP:CZ3 | 4:A:475:PHE:CE1 | 2.99 | 0.51 |
| 4:B:516:PHE:O | 4:B:519:ALA:HB3 | 2.10 | 0.51 |
| 4:C:155:ARG:HB2 | 4:C:163:LYS:HZ3 | 1.74 | 0.51 |
| 4:C:215:ARG:O | 4:C:218:GLU:HB2 | 2.10 | 0.51 |
| 4:C:405:ALA:CB | 4:C:443:LEU:HD13 | 2.41 | 0.51 |
| 4:C:579:ASN:O | 4:C:582:LEU:HB2 | 2.09 | 0.51 |
| 4:C:729:THR:OG1 | 4:C:733:PHE:N | 2.40 | 0.51 |
| 4:D:745:THR:CG2 | 7:D:3056:HOH:O | 2.59 | 0.51 |
| 4:A:379:ARG:HE | 4:A:656:GLN:CG | 2.23 | 0.51 |
| 4:A:50:ARG:CG | 4:A:50:ARG:HH11 | 2.23 | 0.51 |
| 4:A:812:ASP:OD1 | 4:A:812:ASP:N | 2.38 | 0.51 |
| 4:B:194:GLY:O | 4:B:196:LEU:CD2 | 2.59 | 0.51 |
| 4:B:704:LYS:HG3 | 4:B:775:GLU:OE1 | 2.10 | 0.51 |
| 4:B:875:ILE:O | 4:B:877:GLU:N | 2.43 | 0.51 |
| 4:C:15:GLU:CG | 4:C:18:ALA:H | 2.22 | 0.51 |
| 4:C:668:THR:HB | 4:C:669:GLN:NE2 | 2.25 | 0.51 |
| 4:D:84:ARG:CB | 4:D:223:SER:HB3 | 2.41 | 0.51 |
| 4:D:814:PHE:CE1 | 4:D:883:ALA:HB1 | 2.45 | 0.51 |
| 1:E:3:DG:H2" | 1:E:4:DA:C8 | 2.45 | 0.51 |
| 4:A:551:ARG:HB2 | 4:A:868:GLY:N | 2.24 | 0.51 |
| 4:A:729:THR:HB | 4:A:789:SER:HB2 | 1.92 | 0.51 |
| 4:B:339:ASN:O | 4:B:343:LYS:CG | 2.59 | 0.51 |
| 4:B:381:ALA:C | 4:B:383:ALA:H | 2.14 | 0.51 |
| 4:B:639:TYR:C | 7:B:3018:HOH:O | 2.48 | 0.51 |
| 4:C:51:PHE:CZ | 4:C:261:LEU:HD23 | 2.45 | 0.51 |
| 4:C:32:LEU:N | 7:C:3157:HOH:O | 2.29 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:C:36:GLN:HA | 4:C:36:GLN:OE1 | 2.10 | 0.51 |
| 4:C:400:PHE:CZ | 4:C:431:MET:HE2 | 2.44 | 0.51 |
| 4:D:338:ALA:O | 4:D:342:THR:HG23 | 2.10 | 0.51 |
| 4:D:472:LYS:CA | 4:D:567:VAL:HG11 | 2.38 | 0.51 |
| 1:H:17:DG:H2'' | 1:H:18:DC:C5 | 2.46 | 0.51 |
| 4:A:292:ARG:N | 4:A:293:PRO:CD | 2.73 | 0.51 |
| 4:A:513:ALA:O | 7:A:3098:HOH:O | 2.19 | 0.51 |
| 4:A:689:VAL:O | 4:A:691:ALA:N | 2.44 | 0.51 |
| 4:A:754:GLN:O | 4:A:755:PHE:O | 2.28 | 0.51 |
| 4:B:112:GLU:CD | 4:B:112:GLU:N | 2.63 | 0.51 |
| 4:B:136:ALA:O | 4:B:139:SER:HB3 | 2.10 | 0.51 |
| 4:B:322:ILE:HG22 | 4:B:323:ALA:N | 2.24 | 0.51 |
| 4:B:432:PHE:CE2 | 4:B:444:LEU:HD11 | 2.44 | 0.51 |
| 4:B:580:GLU:O | 4:B:581:ILE:C | 2.47 | 0.51 |
| 4:C:239:GLN:O | 4:C:241:SER:N | 2.43 | 0.51 |
| 4:C:643:GLU:OE2 | 4:C:679:LYS:HA | 2.11 | 0.51 |
| 4:D:475:PHE:HE2 | 4:D:879:ASP:CB | 2.21 | 0.51 |
| 4:D:486:HIS:O | 4:D:487:GLU:C | 2.47 | 0.51 |
| 4:D:578:VAL:HG13 | 4:D:680:LEU:HB3 | 1.93 | 0.51 |
| 4:D:724:ALA:HB1 | 4:D:737:GLN:O | 2.10 | 0.51 |
| 4:D:849:PHE:O | 4:D:850:ALA:C | 2.48 | 0.51 |
| 4:D:6:ILE:C | 4:D:8:LYS:H | 2.13 | 0.51 |
| 1:H:12:DT:H2'' | 1:H:13:DC:H6 | 1.76 | 0.51 |
| 1:H:15:DC:C2 | 1:H:16:DC:C5 | 2.99 | 0.51 |
| 1:K:11:DA:C8 | 4:C:639:TYR:CG | 2.98 | 0.51 |
| 1:N:12:DT:H4' | 4:D:423:ARG:HD2 | 1.93 | 0.51 |
| 4:A:213:GLY:O | 4:A:217:ILE:HG13 | 2.11 | 0.51 |
| 4:A:430:SER:OG | 4:A:431:MET:N | 2.41 | 0.51 |
| 4:A:439:MET:HG3 | 4:A:509:PHE:CD2 | 2.45 | 0.51 |
| 4:B:417:PRO:O | 4:B:429:VAL:HG23 | 2.10 | 0.51 |
| 4:B:55:PHE:CD2 | 4:B:59:LEU:HD11 | 2.45 | 0.51 |
| 4:B:854:HIS:ND1 | 4:B:855:GLU:N | 2.58 | 0.51 |
| 4:C:109:ILE:H | 4:C:109:ILE:HD12 | 1.74 | 0.51 |
| 4:C:294:LEU:HD23 | 4:C:294:LEU:N | 2.25 | 0.51 |
| 4:C:462:ILE:O | 4:C:465:ALA:HB3 | 2.11 | 0.51 |
| 4:D:15:GLU:OE2 | 4:D:18:ALA:HB3 | 2.11 | 0.51 |
| 4:D:308:TYR:HE2 | 4:D:734:PRO:O | 1.94 | 0.51 |
| 4:D:538:GLY:O | 4:D:539:SER:C | 2.49 | 0.51 |
| 4:D:726:HIS:CD2 | 4:D:736:TRP:NE1 | 2.78 | 0.51 |
| 4:D:859:ASP:C | 4:D:861:MET:H | 2.14 | 0.51 |
| 2:L:4:G:O2' | 2:L:5:C:H5' | 2.10 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:A:40:GLU:OE1 | 4:A:286:TYR:HB3 | 2.10 | 0.51 |
| 4:B:157:LEU:O | 4:B:158:GLU:C | 2.48 | 0.51 |
| 4:B:172:LYS:HB3 | 4:B:172:LYS:HZ3 | 1.76 | 0.51 |
| 4:B:19:ILE:HG23 | 4:B:20:PRO:HD2 | 1.92 | 0.51 |
| 4:B:576:LYS:O | 4:B:577:LYS:C | 2.49 | 0.51 |
| 4:C:59:LEU:HD22 | 4:C:64:VAL:CG1 | 2.39 | 0.51 |
| 4:D:259:GLY:O | 4:D:262:ALA:N | 2.43 | 0.51 |
| 4:D:277:PRO:CA | 7:D:3029:HOH:O | 2.59 | 0.51 |
| 4:D:306:MET:O | 4:D:309:GLU:N | 2.42 | 0.51 |
| 4:D:324:GLN:HA | 4:D:418:TYR:CE1 | 2.45 | 0.51 |
| 4:D:835:THR:HG22 | 4:D:836:TYR:CD2 | 2.46 | 0.51 |
| 4:A:268:PHE:CB | 4:A:430:SER:HA | 2.40 | 0.51 |
| 4:A:303:LYS:NZ | 7:A:3108:HOH:O | 2.42 | 0.51 |
| 4:A:726:HIS:HB2 | 4:A:736:TRP:CD1 | 2.45 | 0.51 |
| 4:A:746:ARG:HH12 | 4:A:754:GLN:N | 2.06 | 0.51 |
| 4:A:843:ALA:O | 4:A:844:ASP:C | 2.48 | 0.51 |
| 4:B:308:TYR:HA | 4:B:311:VAL:HG21 | 1.91 | 0.51 |
| 4:B:505:GLN:N | 4:B:505:GLN:CD | 2.58 | 0.51 |
| 4:B:585:ASP:OD2 | 4:B:613:THR:CB | 2.58 | 0.51 |
| 4:B:744:GLN:HB3 | 4:B:756:ARG:HB3 | 1.92 | 0.51 |
| 4:B:82:ILE:CD1 | 4:B:112:GLU:HG3 | 2.41 | 0.51 |
| 4:C:308:TYR:CZ | 4:C:733:PHE:CE2 | 2.97 | 0.51 |
| 4:C:437:ASN:ND2 | 4:C:440:THR:OG1 | 2.44 | 0.51 |
| 4:C:840:ASP:O | 4:C:841:VAL:C | 2.50 | 0.51 |
| 4:D:207:GLU:O | 4:D:211:HIS:CG | 2.64 | 0.51 |
| 4:D:221:ILE:HA | 4:D:224:THR:O | 2.11 | 0.51 |
| 1:N:11:DA:C4' | 4:D:780:PRO:HG3 | 2.40 | 0.51 |
| 4:D:797:TRP:NE1 | 4:D:802:TYR:HE2 | 2.08 | 0.51 |
| 6:A:2000:APC:H5'2 | 7:A:3048:HOH:O | 2.11 | 0.51 |
| 4:A:418:TYR:HD2 | 4:A:426:VAL:HG11 | 1.75 | 0.51 |
| 4:A:548:ALA:C | 4:A:550:LEU:N | 2.63 | 0.51 |
| 4:B:158:GLU:HG2 | 4:B:195:LEU:CB | 2.41 | 0.51 |
| 4:B:571:TYR:HE2 | 4:B:631:LYS:HG3 | 1.68 | 0.51 |
| 4:B:61:ALA:C | 4:B:63:GLU:H | 2.14 | 0.51 |
| 4:B:729:THR:HG23 | 4:B:733:PHE:O | 2.10 | 0.51 |
| 4:B:783:VAL:O | 4:B:784:HIS:C | 2.48 | 0.51 |
| 4:C:345:LYS:NZ | 4:C:352:ILE:HG12 | 2.24 | 0.51 |
| 4:C:824:LEU:O | 4:C:828:VAL:HG22 | 2.10 | 0.51 |
| 4:D:327:ALA:CB | 4:D:415:TRP:NE1 | 2.73 | 0.51 |
| 4:D:455:GLU:O | 4:D:458:TYR:HB3 | 2.11 | 0.51 |
| 4:D:843:ALA:O | 4:D:846:TYR:N | 2.42 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:A:115:ALA:O | 4:A:119:ILE:HG12 | 2.11 | 0.51 |
| 4:A:480:LYS:HE3 | 4:A:484:GLU:CD | 2.31 | 0.51 |
| 4:A:514:PHE:O | 4:A:515:CYS:C | 2.45 | 0.51 |
| 4:A:721:LYS:CD | 4:A:722:ARG:H | 2.17 | 0.51 |
| 4:B:4:ILE:HD12 | 4:B:256:THR:HG23 | 1.92 | 0.51 |
| 4:B:535:ALA:HA | 4:B:815:GLY:HA2 | 1.94 | 0.51 |
| 4:B:871:ASN:O | 4:B:872:LEU:C | 2.49 | 0.51 |
| 4:C:313:MET:O | 4:C:317:TYR:HD2 | 1.94 | 0.51 |
| 4:D:7:ALA:HA | 4:D:11:PHE:HD2 | 1.76 | 0.51 |
| 1:N:15:DC:H2'' | 1:N:16:DC:OP2 | 2.09 | 0.51 |
| 4:B:40:GLU:O | 4:B:41:HIS:C | 2.48 | 0.50 |
| 4:B:42:GLU:HG2 | 4:B:46:MET:CE | 2.41 | 0.50 |
| 4:C:307:ARG:HD3 | 4:C:736:TRP:CD2 | 2.45 | 0.50 |
| 4:C:333:LYS:CD | 4:C:516:PHE:CD2 | 2.93 | 0.50 |
| 4:C:442:GLY:O | 4:C:444:LEU:N | 2.44 | 0.50 |
| 4:C:329:LYS:HG3 | 4:C:445:THR:HG23 | 1.93 | 0.50 |
| 4:C:852:GLN:NE2 | 7:C:3094:HOH:O | 2.21 | 0.50 |
| 4:D:377:TRP:HA | 7:D:3074:HOH:O | 2.10 | 0.50 |
| 4:D:452:ILE:HD11 | 4:D:457:TYR:HA | 1.94 | 0.50 |
| 4:D:71:LYS:N | 4:D:72:PRO:HD2 | 2.25 | 0.50 |
| 1:H:14:DG:C4 | 1:H:15:DC:C5 | 2.99 | 0.50 |
| 1:K:15:DC:H5' | 1:K:15:DC:H6 | 1.75 | 0.50 |
| 4:A:308:TYR:HE2 | 4:A:734:PRO:CG | 2.12 | 0.50 |
| 4:A:651:LEU:HD11 | 4:A:656:GLN:NE2 | 2.25 | 0.50 |
| 4:A:685:VAL:C | 4:A:687:VAL:H | 2.13 | 0.50 |
| 4:B:478:ARG:O | 4:B:479:ILE:C | 2.48 | 0.50 |
| 4:B:780:PRO:CD | 4:B:781:ASN:N | 2.73 | 0.50 |
| 4:B:777:GLY:C | 4:B:780:PRO:HD2 | 2.31 | 0.50 |
| 4:C:205:HIS:C | 4:C:207:GLU:N | 2.64 | 0.50 |
| 4:C:291:ARG:CB | 7:C:3192:HOH:O | 2.54 | 0.50 |
| 4:C:60:LYS:O | 4:C:60:LYS:HG2 | 2.12 | 0.50 |
| 1:K:10:DT:H4' | 4:C:639:TYR:O | 2.12 | 0.50 |
| 4:C:737:GLN:HE22 | 4:C:777:GLY:C | 2.14 | 0.50 |
| 4:C:120:LYS:HD2 | 4:C:751:PHE:CE2 | 2.46 | 0.50 |
| 4:C:779:ALA:N | 4:C:780:PRO:HD2 | 2.26 | 0.50 |
| 4:C:837:GLU:HG2 | 4:C:872:LEU:HD12 | 1.93 | 0.50 |
| 4:D:676:TYR:CZ | 4:D:680:LEU:HD11 | 2.46 | 0.50 |
| 1:H:9:DA:C2 | 4:B:644:PHE:CD1 | 2.98 | 0.50 |
| 1:H:9:DA:C5' | 7:H:484:HOH:O | 2.32 | 0.50 |
| 4:A:223:SER:OG | 4:A:224:THR:HG23 | 2.11 | 0.50 |
| 4:A:421:ASP:OD2 | 4:A:427:TYR:HE1 | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:A:611:LEU:HD11 | 4:A:669:GLN:NE2 | 2.27 | 0.50 |
| 4:B:422:TRP:CE2 | 4:B:781:ASN:ND2 | 2.79 | 0.50 |
| 4:B:426:VAL:C | 4:B:427:TYR:HD1 | 2.14 | 0.50 |
| 4:B:505:GLN:H | 4:B:505:GLN:NE2 | 1.94 | 0.50 |
| 4:B:70:ALA:C | 4:B:72:PRO:HD2 | 2.31 | 0.50 |
| 4:B:791:LEU:O | 4:B:794:THR:N | 2.42 | 0.50 |
| 4:B:821:ALA:O | 4:B:822:ALA:C | 2.49 | 0.50 |
| 4:B:824:LEU:O | 4:B:824:LEU:HG | 2.11 | 0.50 |
| 4:C:569:ASP:O | 4:C:573:ILE:HG22 | 2.11 | 0.50 |
| 4:D:158:GLU:HA | 4:D:195:LEU:HD13 | 1.94 | 0.50 |
| 4:D:215:ARG:HA | 4:D:218:GLU:OE1 | 2.10 | 0.50 |
| 4:D:275:PRO:HG2 | 4:D:324:GLN:CG | 2.38 | 0.50 |
| 4:D:448:LYS:NZ | 4:D:806:SER:CB | 2.73 | 0.50 |
| 4:D:789:SER:HA | 4:D:792:ARG:CZ | 2.41 | 0.50 |
| 4:A:82:ILE:CG2 | 4:A:112:GLU:OE2 | 2.59 | 0.50 |
| 4:A:281:ILE:HD11 | 4:A:309:GLU:H | 1.75 | 0.50 |
| 4:B:632:ARG:HH11 | 6:B:2001:APC:C8 | 2.24 | 0.50 |
| 4:B:508:PRO:O | 4:B:509:PHE:C | 2.49 | 0.50 |
| 4:B:120:LYS:HG3 | 4:B:752:LEU:HD11 | 1.94 | 0.50 |
| 4:C:291:ARG:C | 4:C:293:PRO:HD3 | 2.31 | 0.50 |
| 4:D:205:HIS:C | 4:D:207:GLU:H | 2.14 | 0.50 |
| 4:D:236:VAL:HG11 | 4:D:239:GLN:CD | 2.31 | 0.50 |
| 4:A:463:HIS:O | 4:A:464:GLY:C | 2.48 | 0.50 |
| 4:A:610:LYS:CG | 4:A:610:LYS:O | 2.51 | 0.50 |
| 4:B:159:ALA:HA | 4:B:162:PHE:HB3 | 1.94 | 0.50 |
| 4:B:272:VAL:CG1 | 4:B:411:HIS:HD2 | 2.25 | 0.50 |
| 4:B:422:TRP:CD1 | 4:B:423:ARG:N | 2.80 | 0.50 |
| 4:B:470:VAL:HG11 | 4:B:478:ARG:HA | 1.93 | 0.50 |
| 4:B:770:ASP:OD1 | 4:B:770:ASP:O | 2.29 | 0.50 |
| 4:C:43:SER:OG | 4:C:269:GLN:HG3 | 2.12 | 0.50 |
| 4:C:672:GLN:HG3 | 7:C:3033:HOH:O | 2.10 | 0.50 |
| 4:D:19:ILE:HG23 | 4:D:20:PRO:CD | 2.41 | 0.50 |
| 1:N:12:DT:O4' | 4:D:423:ARG:CZ | 2.58 | 0.50 |
| 4:D:665:LEU:HB2 | 7:D:3125:HOH:O | 2.12 | 0.50 |
| 4:D:70:ALA:C | 4:D:72:PRO:HD2 | 2.32 | 0.50 |
| 4:D:828:VAL:HA | 4:D:831:THR:HG22 | 1.93 | 0.50 |
| 4:D:706:LEU:HD11 | 4:D:849:PHE:CG | 2.46 | 0.50 |
| 4:D:702:ALA:HB2 | 4:D:861:MET:CE | 2.41 | 0.50 |
| 1:K:11:DA:C8 | 4:C:639:TYR:CB | 2.93 | 0.50 |
| 1:K:11:DA:C2' | 1:K:12:DT:C7 | 2.89 | 0.50 |
| 4:A:386:ARG:CD | 7:A:3138:HOH:O | 2.45 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:A:572:GLY:O | 4:A:576:LYS:HG3 | 2.12 | 0.50 |
| 4:B:631:LYS:HZ1 | 6:B:2001:APC:H3A2 | 1.76 | 0.50 |
| 4:B:14:ILE:HG23 | 4:B:288:ALA:HB1 | 1.93 | 0.50 |
| 4:B:51:PHE:O | 4:B:55:PHE:HB2 | 2.11 | 0.50 |
| 4:B:638:ALA:O | 4:B:780:PRO:HB3 | 2.11 | 0.50 |
| 4:B:84:ARG:C | 4:B:84:ARG:HD3 | 2.31 | 0.50 |
| 4:C:474:PRO:C | 4:C:476:PRO:HD2 | 2.32 | 0.50 |
| 4:C:9:ASN:CA | 4:C:12:SER:HB3 | 2.41 | 0.50 |
| 4:D:150:ARG:HG3 | 4:D:201:TRP:CD1 | 2.46 | 0.50 |
| 4:D:209:SER:HB2 | 7:D:3053:HOH:O | 2.11 | 0.50 |
| 4:D:335:LEU:O | 4:D:339:ASN:HB2 | 2.12 | 0.50 |
| 4:D:685:VAL:C | 4:D:687:VAL:H | 2.15 | 0.50 |
| 4:D:706:LEU:HD23 | 4:D:853:LEU:HD23 | 1.94 | 0.50 |
| 4:A:42:GLU:O | 4:A:43:SER:C | 2.50 | 0.50 |
| 4:A:333:LYS:CB | 4:A:516:PHE:HD2 | 2.23 | 0.50 |
| 4:A:579:ASN:HA | 4:A:582:LEU:HG | 1.93 | 0.50 |
| 4:B:405:ALA:O | 4:B:409:ALA:N | 2.45 | 0.50 |
| 4:B:412:LYS:O | 4:B:413:ALA:HB2 | 2.12 | 0.50 |
| 4:B:475:PHE:HB2 | 4:B:476:PRO:CD | 2.42 | 0.50 |
| 4:B:479:ILE:O | 4:B:480:LYS:C | 2.49 | 0.50 |
| 4:C:446:LEU:H | 4:C:533:PRO:HD3 | 1.76 | 0.50 |
| 4:C:446:LEU:HD12 | 4:C:817:ILE:HG23 | 1.93 | 0.50 |
| 4:D:304:ALA:HB1 | 7:D:3038:HOH:O | 2.10 | 0.50 |
| 4:D:485:ASN:O | 4:D:489:ILE:HG13 | 2.12 | 0.50 |
| 4:D:585:ASP:O | 4:D:614:LYS:HA | 2.12 | 0.50 |
| 4:D:706:LEU:HD21 | 4:D:849:PHE:HD2 | 1.76 | 0.50 |
| 4:D:92:VAL:CG1 | 4:D:99:ARG:HG3 | 2.41 | 0.50 |
| 4:A:19:ILE:HG23 | 4:A:20:PRO:CD | 2.39 | 0.50 |
| 4:A:21:PHE:C | 4:A:23:THR:N | 2.64 | 0.50 |
| 4:B:159:ALA:HB1 | 4:B:163:LYS:N | 2.27 | 0.50 |
| 4:B:162:PHE:HE1 | 4:B:190:MET:HG2 | 1.76 | 0.50 |
| 4:B:450:LYS:N | 4:B:529:ASN:ND2 | 2.60 | 0.50 |
| 4:B:500:THR:O | 4:B:503:ALA:HB3 | 2.11 | 0.50 |
| 4:C:248:PRO:HB2 | 4:C:249:GLU:OE2 | 2.12 | 0.50 |
| 4:C:22:ASN:O | 4:C:26:ASP:HB3 | 2.11 | 0.50 |
| 4:C:306:MET:O | 4:C:307:ARG:C | 2.51 | 0.50 |
| 4:C:490:MET:HE3 | 4:C:490:MET:HA | 1.94 | 0.50 |
| 1:K:11:DA:H8 | 4:C:639:TYR:HB3 | 1.74 | 0.50 |
| 4:C:656:GLN:N | 4:C:657:PRO:CD | 2.75 | 0.50 |
| 4:D:402:LEU:CD2 | 4:D:443:LEU:CD1 | 2.88 | 0.50 |
| 4:D:794:THR:O | 4:D:795:VAL:C | 2.49 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:857:GLN:C | 4:D:859:ASP:H | 2.15 | 0.50 |
| 3:J:5:DA:C2 | 3:J:6:DT:C2 | 2.99 | 0.50 |
| 1:K:16:DC:H2'' | 1:K:17:DG:H5' | 1.93 | 0.50 |
| 4:A:422:TRP:HD1 | 7:A:3029:HOH:O | 1.95 | 0.50 |
| 4:A:42:GLU:HG2 | 4:A:46:MET:CE | 2.42 | 0.50 |
| 4:A:846:TYR:CD1 | 4:A:850:ALA:HB2 | 2.47 | 0.50 |
| 4:A:719:LEU:HD22 | 4:A:854:HIS:CE1 | 2.47 | 0.50 |
| 4:A:829:ARG:NE | 4:A:878:SER:O | 2.42 | 0.50 |
| 4:B:268:PHE:HD2 | 4:B:429:VAL:HG12 | 1.77 | 0.50 |
| 1:K:10:DT:H5' | 4:C:641:SER:CA | 2.42 | 0.50 |
| 4:D:115:ALA:O | 4:D:119:ILE:HG12 | 2.11 | 0.50 |
| 4:D:433:ASN:CB | 4:D:434:PRO:CD | 2.88 | 0.50 |
| 4:D:508:PRO:O | 4:D:509:PHE:C | 2.48 | 0.50 |
| 1:H:10:DT:OP2 | 4:B:641:SER:HB3 | 2.12 | 0.50 |
| 3:P:4:DG:H2'' | 3:P:5:DA:C8 | 2.47 | 0.50 |
| 4:A:273:VAL:O | 4:A:274:PRO:C | 2.50 | 0.49 |
| 4:A:338:ALA:C | 4:A:340:VAL:N | 2.66 | 0.49 |
| 4:A:786:GLN:C | 4:A:788:GLY:N | 2.63 | 0.49 |
| 4:B:92:VAL:HG11 | 4:B:100:PRO:HD2 | 1.94 | 0.49 |
| 4:C:632:ARG:CZ | 6:C:2002:APC:C8 | 2.90 | 0.49 |
| 4:C:221:ILE:HG23 | 4:C:227:VAL:O | 2.12 | 0.49 |
| 4:C:232:GLN:NE2 | 7:C:3040:HOH:O | 2.45 | 0.49 |
| 4:C:272:VAL:HG13 | 4:C:411:HIS:HD2 | 1.76 | 0.49 |
| 4:C:14:ILE:HG12 | 4:C:288:ALA:HB1 | 1.94 | 0.49 |
| 4:C:417:PRO:O | 4:C:429:VAL:HG23 | 2.12 | 0.49 |
| 4:C:668:THR:HB | 4:C:669:GLN:HE22 | 1.75 | 0.49 |
| 4:D:72:PRO:HG3 | 4:D:257:ARG:HG3 | 1.94 | 0.49 |
| 4:D:404:GLN:HG2 | 4:D:432:PHE:HB2 | 1.94 | 0.49 |
| 4:D:489:ILE:HA | 4:D:492:CYS:SG | 2.52 | 0.49 |
| 1:N:10:DT:C5' | 4:D:641:SER:N | 2.75 | 0.49 |
| 4:D:797:TRP:CH2 | 4:D:801:LYS:HG3 | 2.47 | 0.49 |
| 4:D:560:ASN:C | 4:D:881:ALA:HB2 | 2.30 | 0.49 |
| 1:H:15:DC:OP2 | 7:H:411:HOH:O | 2.19 | 0.49 |
| 1:K:16:DC:H2'' | 1:K:17:DG:C5' | 2.42 | 0.49 |
| 4:A:401:MET:C | 4:A:403:GLU:H | 2.14 | 0.49 |
| 4:A:704:LYS:O | 4:A:707:ALA:HB3 | 2.12 | 0.49 |
| 4:A:71:LYS:N | 4:A:72:PRO:HD2 | 2.27 | 0.49 |
| 4:B:261:LEU:C | 4:B:263:GLY:N | 2.63 | 0.49 |
| 4:B:51:PHE:HE2 | 4:B:55:PHE:HD1 | 1.57 | 0.49 |
| 4:B:578:VAL:HG13 | 4:B:680:LEU:CD2 | 2.40 | 0.49 |
| 1:H:18:DC:C2' | 4:B:63:GLU:OE1 | 2.60 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:B:860:LYS:O | 4:B:862:PRO:HD2 | 2.12 | 0.49 |
| 4:D:544:GLN:HG2 | 4:D:561:LEU:HD11 | 1.93 | 0.49 |
| 4:D:745:THR:H | 4:D:756:ARG:HD3 | 1.76 | 0.49 |
| 1:H:13:DC:C4' | 4:B:427:TYR:CE2 | 2.95 | 0.49 |
| 1:H:14:DG:H2'' | 1:H:15:DC:H6 | 1.77 | 0.49 |
| 3:J:6:DT:H2'' | 3:J:7:DT:H71 | 1.94 | 0.49 |
| 1:K:5:DA:N6 | 3:M:5:DA:N6 | 2.60 | 0.49 |
| 4:A:182:PHE:O | 4:A:185:VAL:CG2 | 2.59 | 0.49 |
| 4:A:344:TRP:O | 4:A:345:LYS:HG3 | 2.12 | 0.49 |
| 4:A:473:VAL:CG1 | 4:A:473:VAL:O | 2.60 | 0.49 |
| 4:A:543:ILE:O | 4:A:544:GLN:C | 2.50 | 0.49 |
| 4:A:715:THR:HB | 4:A:717:GLU:HB2 | 1.94 | 0.49 |
| 4:A:84:ARG:HG3 | 4:A:222:GLU:HG2 | 1.93 | 0.49 |
| 4:B:155:ARG:HH21 | 4:B:749:LEU:HB2 | 1.77 | 0.49 |
| 4:B:55:PHE:CD2 | 4:B:55:PHE:C | 2.84 | 0.49 |
| 4:B:647:ARG:HD3 | 7:B:3138:HOH:O | 2.11 | 0.49 |
| 4:B:829:ARG:CG | 4:B:829:ARG:NH1 | 2.68 | 0.49 |
| 4:C:316:VAL:O | 4:C:317:TYR:C | 2.50 | 0.49 |
| 4:C:474:PRO:HB2 | 4:C:476:PRO:HG2 | 1.94 | 0.49 |
| 4:C:458:TYR:CE1 | 4:C:479:ILE:HD11 | 2.47 | 0.49 |
| 4:C:711:LYS:HE2 | 4:C:716:GLY:O | 2.12 | 0.49 |
| 4:C:870:LEU:HA | 7:C:3053:HOH:O | 2.11 | 0.49 |
| 3:G:6:DT:H2'' | 3:G:7:DT:OP2 | 2.12 | 0.49 |
| 1:N:15:DC:N3 | 1:N:16:DC:C4 | 2.80 | 0.49 |
| 4:A:136:ALA:HA | 7:A:3053:HOH:O | 2.11 | 0.49 |
| 4:A:425:ARG:HD3 | 4:A:811:HIS:HD2 | 1.76 | 0.49 |
| 4:A:488:ASN:O | 4:A:491:ALA:N | 2.45 | 0.49 |
| 4:A:720:ARG:HE | 4:A:854:HIS:H | 1.60 | 0.49 |
| 4:B:193:LYS:HG3 | 4:B:194:GLY:H | 1.77 | 0.49 |
| 4:B:203:SER:O | 4:B:205:HIS:N | 2.38 | 0.49 |
| 4:B:232:GLN:HG3 | 4:B:243:THR:CG2 | 2.43 | 0.49 |
| 4:B:826:LYS:HG2 | 4:B:830:GLU:HG3 | 1.94 | 0.49 |
| 4:C:250:TYR:O | 4:C:254:ILE:HG13 | 2.12 | 0.49 |
| 4:C:461:LYS:O | 4:C:462:ILE:C | 2.49 | 0.49 |
| 4:C:669:GLN:N | 4:C:669:GLN:NE2 | 2.60 | 0.49 |
| 4:C:854:HIS:O | 4:C:857:GLN:HG2 | 2.13 | 0.49 |
| 4:D:379:ARG:HD2 | 7:D:3122:HOH:O | 2.12 | 0.49 |
| 4:D:551:ARG:O | 4:D:868:GLY:HA3 | 2.12 | 0.49 |
| 4:A:402:LEU:HG | 4:A:439:MET:HE1 | 1.94 | 0.49 |
| 4:A:460:LEU:O | 4:A:461:LYS:C | 2.50 | 0.49 |
| 4:A:60:LYS:O | 4:A:60:LYS:CG | 2.56 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:A:772:HIS:O | 4:A:773:LYS:C | 2.50 | 0.49 |
| 4:B:272:VAL:HG11 | 4:B:411:HIS:CD2 | 2.48 | 0.49 |
| 4:B:421:ASP:O | 4:B:424:GLY:N | 2.45 | 0.49 |
| 4:B:485:ASN:ND2 | 4:B:501:TRP:CZ2 | 2.80 | 0.49 |
| 4:B:459:TRP:CZ3 | 4:B:536:PHE:CZ | 3.01 | 0.49 |
| 4:C:324:GLN:CG | 4:C:417:PRO:HA | 2.42 | 0.49 |
| 4:C:345:LYS:HZ3 | 4:C:352:ILE:HG12 | 1.77 | 0.49 |
| 4:D:10:ASP:O | 4:D:13:ASP:CB | 2.61 | 0.49 |
| 4:D:139:SER:CA | 4:D:210:ILE:HD13 | 2.42 | 0.49 |
| 4:D:830:GLU:HG2 | 4:D:876:LEU:HD21 | 1.94 | 0.49 |
| 3:M:5:DA:C2' | 3:M:6:DT:H72 | 2.42 | 0.49 |
| 4:A:264:ILE:HG22 | 4:A:292:ARG:HD3 | 1.95 | 0.49 |
| 4:A:465:ALA:CB | 4:A:478:ARG:HB3 | 2.43 | 0.49 |
| 4:A:480:LYS:HG2 | 7:A:3046:HOH:O | 2.13 | 0.49 |
| 4:A:524:HIS:O | 4:A:525:GLY:O | 2.30 | 0.49 |
| 4:A:629:VAL:HG11 | 4:A:677:MET:CE | 2.43 | 0.49 |
| 4:A:643:GLU:OE2 | 4:A:679:LYS:HA | 2.13 | 0.49 |
| 4:B:334:VAL:HG12 | 4:B:443:LEU:CD2 | 2.42 | 0.49 |
| 4:B:512:LEU:C | 4:B:514:PHE:N | 2.64 | 0.49 |
| 4:B:454:LYS:N | 4:B:526:LEU:HD22 | 2.27 | 0.49 |
| 4:B:544:GLN:HA | 4:B:559:VAL:HG21 | 1.94 | 0.49 |
| 4:B:560:ASN:OD1 | 4:B:568:GLN:HB2 | 2.12 | 0.49 |
| 4:B:60:LYS:HE2 | 4:B:61:ALA:HB2 | 1.95 | 0.49 |
| 4:C:423:ARG:CD | 4:C:781:ASN:HD22 | 2.25 | 0.49 |
| 4:C:84:ARG:CA | 4:C:84:ARG:HH11 | 2.22 | 0.49 |
| 4:D:330:ILE:CG1 | 4:D:408:PHE:O | 2.60 | 0.49 |
| 4:D:646:PHE:O | 4:D:647:ARG:C | 2.51 | 0.49 |
| 4:D:810:ILE:CB | 4:D:813:SER:OG | 2.53 | 0.49 |
| 4:D:814:PHE:CE1 | 4:D:883:ALA:HB2 | 2.47 | 0.49 |
| 1:E:15:DC:H2'' | 1:E:16:DC:C5' | 2.41 | 0.49 |
| 2:F:1:G:C2 | 2:F:2:C:C2 | 3.01 | 0.49 |
| 4:A:169:GLN:O | 4:A:173:ARG:CG | 2.50 | 0.49 |
| 4:A:401:MET:C | 4:A:403:GLU:N | 2.63 | 0.49 |
| 4:A:462:ILE:O | 4:A:465:ALA:N | 2.45 | 0.49 |
| 4:A:485:ASN:HA | 7:A:3028:HOH:O | 2.12 | 0.49 |
| 4:B:292:ARG:CG | 4:B:292:ARG:O | 2.61 | 0.49 |
| 4:B:726:HIS:CD2 | 4:B:736:TRP:CE2 | 3.01 | 0.49 |
| 4:B:546:PHE:CE1 | 4:B:783:VAL:HG13 | 2.47 | 0.49 |
| 4:C:24:LEU:CD2 | 4:C:273:VAL:HG21 | 2.42 | 0.49 |
| 4:D:259:GLY:O | 4:D:260:ALA:C | 2.50 | 0.49 |
| 4:D:518:TYR:O | 4:D:522:GLN:HG2 | 2.13 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:810:ILE:N | 4:D:813:SER:OG | 2.46 | 0.49 |
| 4:B:111:PRO:HG2 | 4:B:112:GLU:CD | 2.33 | 0.49 |
| 4:B:281:ILE:HD11 | 4:B:309:GLU:N | 2.28 | 0.49 |
| 4:B:388:ASP:O | 4:B:389:LYS:C | 2.51 | 0.49 |
| 4:B:404:GLN:HB3 | 4:B:432:PHE:CD1 | 2.48 | 0.49 |
| 4:B:703:ALA:O | 4:B:704:LYS:C | 2.50 | 0.49 |
| 4:B:804:ILE:CG2 | 4:B:807:PHE:CE2 | 2.96 | 0.49 |
| 4:B:826:LYS:O | 4:B:830:GLU:HG3 | 2.13 | 0.49 |
| 4:C:340:VAL:HA | 4:C:343:LYS:HD3 | 1.95 | 0.49 |
| 4:C:734:PRO:HG2 | 4:C:734:PRO:O | 2.13 | 0.49 |
| 4:C:786:GLN:O | 4:C:789:SER:HB3 | 2.12 | 0.49 |
| 4:C:549:MET:HB3 | 4:C:836:TYR:CE1 | 2.48 | 0.49 |
| 4:D:381:ALA:O | 4:D:384:VAL:HB | 2.12 | 0.49 |
| 4:D:78:LEU:N | 4:D:79:PRO:HD2 | 2.27 | 0.49 |
| 4:D:840:ASP:C | 4:D:842:LEU:N | 2.65 | 0.49 |
| 1:K:7:DC:C6 | 1:K:8:DG:N7 | 2.80 | 0.49 |
| 4:A:617:ALA:O | 4:A:620:TRP:N | 2.46 | 0.49 |
| 4:B:105:PHE:HB3 | 4:B:204:TRP:CZ2 | 2.48 | 0.49 |
| 4:B:810:ILE:O | 4:B:811:HIS:HB2 | 2.11 | 0.49 |
| 4:B:846:TYR:O | 4:B:847:ASP:C | 2.50 | 0.49 |
| 4:C:151:PHE:O | 4:C:154:ILE:HG13 | 2.13 | 0.49 |
| 4:C:552:ASP:HB2 | 4:C:691:ALA:HB2 | 1.94 | 0.49 |
| 4:C:846:TYR:CD1 | 4:C:850:ALA:HB2 | 2.48 | 0.49 |
| 4:D:452:ILE:HG23 | 4:D:526:LEU:O | 2.13 | 0.49 |
| 1:H:15:DC:N3 | 1:H:16:DC:C4 | 2.80 | 0.49 |
| 1:H:3:DG:H1' | 7:H:1116:HOH:O | 2.12 | 0.49 |
| 4:A:159:ALA:HA | 4:A:162:PHE:HB3 | 1.94 | 0.49 |
| 4:A:178:TYR:CD1 | 4:A:178:TYR:N | 2.77 | 0.49 |
| 4:A:51:PHE:CZ | 4:A:261:LEU:HB3 | 2.47 | 0.49 |
| 4:A:631:LYS:HG2 | 4:A:632:ARG:N | 2.28 | 0.49 |
| 4:A:721:LYS:HE2 | 7:A:3021:HOH:O | 2.12 | 0.49 |
| 4:B:263:GLY:C | 7:B:3137:HOH:O | 2.51 | 0.49 |
| 4:B:292:ARG:HG3 | 4:B:292:ARG:O | 2.13 | 0.49 |
| 4:B:463:HIS:O | 4:B:467:CYS:SG | 2.71 | 0.49 |
| 4:C:36:GLN:CG | 4:C:273:VAL:HG22 | 2.41 | 0.49 |
| 4:C:475:PHE:O | 4:C:479:ILE:HG12 | 2.13 | 0.49 |
| 4:C:553:GLU:CG | 4:C:554:VAL:H | 2.25 | 0.49 |
| 4:C:730:PRO:HD3 | 4:C:786:GLN:NE2 | 2.27 | 0.49 |
| 4:D:84:ARG:CG | 4:D:223:SER:HB3 | 2.43 | 0.49 |
| 4:D:275:PRO:HB2 | 4:D:324:GLN:CD | 2.33 | 0.49 |
| 4:D:116:TYR:HE2 | 4:D:752:LEU:HD13 | 1.77 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:17:DG:H2'' | 1:H:18:DC:C6 | 2.47 | 0.49 |
| 4:A:89:PHE:HA | 4:A:103:PHE:CZ | 2.47 | 0.48 |
| 4:A:532:LEU:HA | 4:A:533:PRO:HD2 | 1.64 | 0.48 |
| 4:A:619:GLN:NE2 | 4:A:666:MET:O | 2.46 | 0.48 |
| 4:B:13:ASP:O | 4:B:15:GLU:N | 2.43 | 0.48 |
| 4:B:301:SER:O | 4:B:304:ALA:CB | 2.59 | 0.48 |
| 1:H:9:DA:C5 | 4:B:644:PHE:CZ | 3.01 | 0.48 |
| 4:B:698:TRP:O | 4:B:701:SER:HB2 | 2.12 | 0.48 |
| 4:C:82:ILE:HD13 | 4:C:112:GLU:HA | 1.95 | 0.48 |
| 4:C:786:GLN:NE2 | 4:C:841:VAL:HG11 | 2.28 | 0.48 |
| 4:C:871:ASN:HD21 | 4:C:873:ARG:HB2 | 1.78 | 0.48 |
| 4:D:347:CYS:O | 4:D:349:VAL:N | 2.46 | 0.48 |
| 4:D:646:PHE:O | 4:D:650:VAL:HG23 | 2.13 | 0.48 |
| 1:E:16:DC:H2'' | 1:E:17:DG:C5' | 2.42 | 0.48 |
| 1:K:9:DA:N6 | 3:M:1:DG:H22 | 2.11 | 0.48 |
| 4:A:340:VAL:O | 4:A:341:ILE:C | 2.49 | 0.48 |
| 4:A:559:VAL:HG23 | 4:A:559:VAL:O | 2.12 | 0.48 |
| 4:A:634:VAL:O | 4:A:637:LEU:HB3 | 2.13 | 0.48 |
| 4:A:720:ARG:HG2 | 4:A:720:ARG:O | 2.13 | 0.48 |
| 4:A:797:TRP:CZ2 | 4:A:830:GLU:OE1 | 2.67 | 0.48 |
| 4:B:32:LEU:HA | 4:B:32:LEU:HD12 | 1.67 | 0.48 |
| 4:B:418:TYR:HB3 | 4:B:426:VAL:CG1 | 2.44 | 0.48 |
| 4:B:549:MET:HG2 | 4:B:836:TYR:CE1 | 2.46 | 0.48 |
| 4:B:680:LEU:H | 4:B:680:LEU:HD12 | 1.75 | 0.48 |
| 4:C:330:ILE:HG12 | 4:C:408:PHE:O | 2.13 | 0.48 |
| 4:D:92:VAL:HG11 | 4:D:103:PHE:CG | 2.48 | 0.48 |
| 4:D:158:GLU:CA | 4:D:195:LEU:HD22 | 2.43 | 0.48 |
| 4:D:231:ARG:HG2 | 4:D:234:ALA:CB | 2.36 | 0.48 |
| 4:D:338:ALA:C | 4:D:340:VAL:H | 2.16 | 0.48 |
| 1:H:16:DC:H2'' | 1:H:17:DG:OP2 | 2.13 | 0.48 |
| 1:K:13:DC:C2 | 1:K:14:DG:C8 | 3.00 | 0.48 |
| 1:N:14:DG:C4 | 1:N:15:DC:C5 | 3.02 | 0.48 |
| 4:A:6:ILE:HD11 | 4:A:259:GLY:C | 2.33 | 0.48 |
| 4:A:333:LYS:HB3 | 4:A:516:PHE:CD2 | 2.48 | 0.48 |
| 4:A:39:LEU:O | 4:A:42:GLU:N | 2.46 | 0.48 |
| 4:A:463:HIS:O | 4:A:465:ALA:N | 2.46 | 0.48 |
| 4:A:512:LEU:O | 4:A:516:PHE:CD1 | 2.66 | 0.48 |
| 4:A:633:SER:HB3 | 4:A:646:PHE:CE2 | 2.48 | 0.48 |
| 4:A:637:LEU:O | 4:A:637:LEU:HG | 2.11 | 0.48 |
| 4:A:668:THR:HG22 | 4:A:669:GLN:HE22 | 1.79 | 0.48 |
| 4:A:670:PRO:O | 4:A:671:ASN:C | 2.52 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:A:744:GLN:H | 4:A:744:GLN:HG3 | 1.36 | 0.48 |
| 4:A:745:THR:HG22 | 4:A:746:ARG:N | 2.28 | 0.48 |
| 4:A:777:GLY:O | 4:A:781:ASN:HB2 | 2.12 | 0.48 |
| 4:A:85:ILE:O | 4:A:85:ILE:HG22 | 2.13 | 0.48 |
| 4:A:89:PHE:CZ | 4:A:106:LEU:O | 2.65 | 0.48 |
| 4:B:109:ILE:HG22 | 4:B:110:LYS:O | 2.13 | 0.48 |
| 4:B:109:ILE:CD1 | 4:B:109:ILE:N | 2.75 | 0.48 |
| 4:B:347:CYS:HA | 4:B:348:PRO:HD3 | 1.68 | 0.48 |
| 4:B:428:ALA:N | 4:B:435:GLN:HE22 | 2.08 | 0.48 |
| 4:B:546:PHE:CE2 | 4:B:696:MET:HG3 | 2.48 | 0.48 |
| 4:B:556:GLY:C | 4:B:558:ALA:H | 2.17 | 0.48 |
| 4:B:670:PRO:O | 4:B:671:ASN:C | 2.48 | 0.48 |
| 4:B:794:THR:CG2 | 4:B:828:VAL:HA | 2.43 | 0.48 |
| 4:B:860:LYS:O | 4:B:862:PRO:CD | 2.61 | 0.48 |
| 4:C:252:GLU:HA | 7:C:3072:HOH:O | 2.13 | 0.48 |
| 4:C:297:VAL:HG21 | 4:C:733:PHE:HZ | 1.78 | 0.48 |
| 4:C:846:TYR:CD2 | 4:C:864:LEU:HD11 | 2.48 | 0.48 |
| 4:D:230:HIS:HB3 | 7:D:3168:HOH:O | 2.13 | 0.48 |
| 4:D:269:GLN:NE2 | 4:D:407:LYS:HE2 | 2.25 | 0.48 |
| 4:D:485:ASN:OD1 | 4:D:485:ASN:N | 2.46 | 0.48 |
| 4:D:62:GLY:C | 4:D:64:VAL:H | 2.17 | 0.48 |
| 4:D:745:THR:HG21 | 7:D:3056:HOH:O | 2.13 | 0.48 |
| 1:K:11:DA:H2'' | 1:K:12:DT:O5' | 2.12 | 0.48 |
| 4:A:401:MET:HG3 | 4:A:440:THR:HG23 | 1.96 | 0.48 |
| 4:A:477:GLU:O | 4:A:480:LYS:N | 2.46 | 0.48 |
| 4:A:619:GLN:O | 4:A:622:ALA:N | 2.47 | 0.48 |
| 4:B:264:ILE:O | 4:B:292:ARG:NH1 | 2.45 | 0.48 |
| 4:B:84:ARG:HD3 | 4:B:84:ARG:O | 2.13 | 0.48 |
| 4:B:850:ALA:C | 4:B:852:GLN:N | 2.64 | 0.48 |
| 4:C:303:LYS:HB2 | 4:C:303:LYS:NZ | 2.28 | 0.48 |
| 4:C:490:MET:O | 4:C:493:ALA:HB3 | 2.14 | 0.48 |
| 4:C:502:TRP:CZ3 | 4:C:503:ALA:HB2 | 2.48 | 0.48 |
| 4:C:512:LEU:HG | 4:C:516:PHE:HE1 | 1.77 | 0.48 |
| 4:C:706:LEU:CD2 | 4:C:725:VAL:HG22 | 2.42 | 0.48 |
| 4:C:78:LEU:HD21 | 4:C:82:ILE:HD11 | 1.96 | 0.48 |
| 4:C:850:ALA:O | 4:C:852:GLN:N | 2.42 | 0.48 |
| 4:D:84:ARG:HG3 | 4:D:223:SER:HB3 | 1.95 | 0.48 |
| 4:D:273:VAL:CA | 4:D:415:TRP:CE3 | 2.96 | 0.48 |
| 4:D:468:ALA:HA | 4:D:505:GLN:HB3 | 1.96 | 0.48 |
| 4:D:779:ALA:O | 4:D:783:VAL:CG2 | 2.61 | 0.48 |
| 4:A:193:LYS:HA | 7:A:3220:HOH:O | 2.12 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:A:304:ALA:HA | 4:A:307:ARG:HD2 | 1.96 | 0.48 |
| 4:A:274:PRO:HD3 | 4:A:415:TRP:CZ3 | 2.48 | 0.48 |
| 4:A:639:TYR:HA | 4:A:780:PRO:HB3 | 1.95 | 0.48 |
| 4:A:770:ASP:O | 4:A:772:HIS:N | 2.47 | 0.48 |
| 4:A:817:ILE:CB | 4:A:818:PRO:CD | 2.89 | 0.48 |
| 4:B:116:TYR:CE2 | 4:B:120:LYS:HB2 | 2.48 | 0.48 |
| 4:B:126:LEU:CD1 | 4:B:246:LEU:HB2 | 2.39 | 0.48 |
| 4:B:450:LYS:HG2 | 4:B:451:PRO:HD2 | 1.94 | 0.48 |
| 4:B:787:ASP:OD1 | 4:B:788:GLY:N | 2.46 | 0.48 |
| 4:C:489:ILE:O | 4:C:492:CYS:HB2 | 2.13 | 0.48 |
| 4:C:464:GLY:HA3 | 4:C:514:PHE:CE2 | 2.48 | 0.48 |
| 4:C:755:PHE:N | 4:C:755:PHE:CD1 | 2.80 | 0.48 |
| 4:D:161:HIS:C | 4:D:163:LYS:H | 2.17 | 0.48 |
| 4:D:490:MET:C | 4:D:493:ALA:HB3 | 2.33 | 0.48 |
| 4:D:544:GLN:HG2 | 4:D:561:LEU:CD1 | 2.43 | 0.48 |
| 3:J:2:DT:H2'' | 3:J:3:DC:O5' | 2.14 | 0.48 |
| 2:L:8:U:O4 | 6:C:2002:APC:H1' | 2.14 | 0.48 |
| 4:A:65:ALA:HB3 | 4:A:120:LYS:CE | 2.42 | 0.48 |
| 4:A:105:PHE:CB | 4:A:204:TRP:CZ2 | 2.89 | 0.48 |
| 4:A:278:TRP:CZ3 | 4:A:284:GLY:CA | 2.93 | 0.48 |
| 4:A:546:PHE:HE2 | 4:A:696:MET:HG3 | 1.78 | 0.48 |
| 4:B:34:ARG:O | 4:B:38:ALA:HB2 | 2.14 | 0.48 |
| 4:B:705:LEU:C | 4:B:707:ALA:H | 2.17 | 0.48 |
| 4:C:173:ARG:NH1 | 4:C:182:PHE:HB2 | 2.28 | 0.48 |
| 4:C:36:GLN:HE21 | 4:C:273:VAL:HG22 | 1.78 | 0.48 |
| 4:C:299:THR:HG21 | 4:C:304:ALA:CB | 2.44 | 0.48 |
| 4:D:452:ILE:HG23 | 4:D:453:GLY:N | 2.28 | 0.48 |
| 4:D:502:TRP:CD1 | 4:D:512:LEU:HD13 | 2.49 | 0.48 |
| 4:D:631:LYS:O | 4:D:632:ARG:C | 2.51 | 0.48 |
| 4:D:88:TRP:CZ2 | 4:D:215:ARG:NH2 | 2.81 | 0.48 |
| 2:F:4:G:H2' | 2:F:5:C:O4' | 2.13 | 0.48 |
| 4:A:617:ALA:O | 4:A:618:GLY:C | 2.52 | 0.48 |
| 4:A:649:GLN:O | 4:A:653:ASP:HB2 | 2.14 | 0.48 |
| 4:A:680:LEU:O | 4:A:681:ILE:C | 2.50 | 0.48 |
| 4:A:709:GLU:HB2 | 4:A:722:ARG:HE | 1.79 | 0.48 |
| 4:A:794:THR:O | 4:A:795:VAL:C | 2.51 | 0.48 |
| 4:A:81:MET:O | 4:A:85:ILE:HG13 | 2.14 | 0.48 |
| 4:B:304:ALA:O | 4:B:307:ARG:HB2 | 2.13 | 0.48 |
| 4:B:422:TRP:CZ2 | 4:B:781:ASN:ND2 | 2.82 | 0.48 |
| 4:B:616:LEU:C | 4:B:618:GLY:N | 2.66 | 0.48 |
| 4:B:787:ASP:O | 4:B:790:HIS:HB3 | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:C:183:MET:HA | 4:C:186:VAL:HB | 1.96 | 0.48 |
| 4:C:400:PHE:CZ | 4:C:431:MET:CE | 2.96 | 0.48 |
| 4:C:404:GLN:CG | 4:C:432:PHE:HB2 | 2.41 | 0.48 |
| 4:C:473:VAL:O | 4:C:474:PRO:O | 2.32 | 0.48 |
| 4:C:689:VAL:O | 4:C:690:VAL:C | 2.52 | 0.48 |
| 4:C:711:LYS:HG2 | 4:C:717:GLU:C | 2.34 | 0.48 |
| 4:D:121:THR:O | 4:D:124:ALA:HB3 | 2.14 | 0.48 |
| 4:D:261:LEU:C | 4:D:263:GLY:N | 2.66 | 0.48 |
| 4:D:387:LYS:HD3 | 7:D:3157:HOH:O | 2.12 | 0.48 |
| 4:D:752:LEU:HD12 | 4:D:752:LEU:N | 2.29 | 0.48 |
| 4:D:828:VAL:CA | 4:D:831:THR:HG22 | 2.43 | 0.48 |
| 2:F:5:C:O2 | 2:F:5:C:H2' | 2.14 | 0.48 |
| 1:K:11:DA:C4 | 1:K:12:DT:H72 | 2.48 | 0.48 |
| 1:K:5:DA:H2'' | 1:K:6:DT:OP2 | 2.13 | 0.48 |
| 4:A:418:TYR:CD2 | 4:A:426:VAL:HG12 | 2.47 | 0.48 |
| 4:A:540:CYS:HB3 | 4:A:543:ILE:CG1 | 2.44 | 0.48 |
| 4:A:864:LEU:HD12 | 4:A:864:LEU:N | 2.29 | 0.48 |
| 4:B:467:CYS:O | 4:B:506:ASP:HB2 | 2.14 | 0.48 |
| 4:B:457:TYR:CD1 | 4:B:521:VAL:HG11 | 2.49 | 0.48 |
| 4:B:535:ALA:O | 4:B:536:PHE:HD1 | 1.96 | 0.48 |
| 4:B:823:ASN:ND2 | 4:B:823:ASN:N | 2.60 | 0.48 |
| 2:L:8:U:O4 | 6:C:2002:APC:N3 | 2.47 | 0.48 |
| 4:C:298:ARG:HA | 7:C:3165:HOH:O | 2.14 | 0.48 |
| 4:C:324:GLN:HE21 | 4:C:418:TYR:N | 2.09 | 0.48 |
| 4:C:307:ARG:HD3 | 4:C:736:TRP:CE3 | 2.49 | 0.48 |
| 4:C:744:GLN:HB2 | 4:C:744:GLN:HE21 | 1.46 | 0.48 |
| 4:C:97:GLY:O | 4:C:98:LYS:C | 2.52 | 0.48 |
| 4:D:442:GLY:C | 4:D:444:LEU:H | 2.17 | 0.48 |
| 4:D:477:GLU:HG2 | 4:D:477:GLU:H | 1.37 | 0.48 |
| 4:D:783:VAL:O | 4:D:786:GLN:HB2 | 2.14 | 0.48 |
| 4:A:82:ILE:HG12 | 4:A:115:ALA:CB | 2.44 | 0.48 |
| 4:A:138:ALA:HB1 | 4:A:214:VAL:HG23 | 1.96 | 0.48 |
| 4:A:786:GLN:CA | 4:A:786:GLN:NE2 | 2.70 | 0.48 |
| 6:B:2001:APC:O2B | 6:B:2001:APC:O1A | 2.32 | 0.48 |
| 4:B:552:ASP:OD1 | 4:B:554:VAL:N | 2.46 | 0.48 |
| 4:C:199:GLU:HG2 | 4:C:201:TRP:HD1 | 1.78 | 0.48 |
| 4:C:392:LYS:O | 4:C:396:ILE:HG12 | 2.14 | 0.48 |
| 4:C:629:VAL:O | 4:C:629:VAL:HG12 | 2.14 | 0.48 |
| 4:C:646:PHE:O | 4:C:649:GLN:HB2 | 2.14 | 0.48 |
| 4:D:343:LYS:HA | 7:D:3020:HOH:O | 2.13 | 0.48 |
| 4:D:646:PHE:HE2 | 4:D:682:TRP:HE3 | 1.60 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:A:19:ILE:HG21 | 7:A:3120:HOH:O | 2.08 | 0.48 |
| 4:A:393:SER:O | 4:A:396:ILE:N | 2.45 | 0.48 |
| 4:A:647:ARG:O | 4:A:648:GLN:C | 2.53 | 0.48 |
| 4:B:525:GLY:C | 4:B:527:SER:N | 2.66 | 0.48 |
| 4:B:642:LYS:HG2 | 4:B:682:TRP:HZ3 | 1.77 | 0.48 |
| 4:B:790:HIS:ND1 | 4:B:790:HIS:C | 2.67 | 0.48 |
| 4:B:810:ILE:H | 4:B:813:SER:HB3 | 1.79 | 0.48 |
| 4:C:101:THR:HA | 4:C:104:GLN:NE2 | 2.28 | 0.48 |
| 4:C:349:VAL:HG12 | 4:C:349:VAL:O | 2.13 | 0.48 |
| 4:C:435:GLN:HA | 4:C:810:ILE:HD11 | 1.96 | 0.48 |
| 4:C:515:CYS:O | 4:C:516:PHE:C | 2.51 | 0.48 |
| 4:C:54:MET:SD | 4:C:54:MET:C | 2.93 | 0.48 |
| 4:D:134:VAL:HG12 | 4:D:242:GLU:O | 2.13 | 0.48 |
| 4:D:322:ILE:HG13 | 7:D:3013:HOH:O | 2.13 | 0.48 |
| 4:D:579:ASN:HD21 | 4:D:625:VAL:HG12 | 1.79 | 0.48 |
| 4:D:752:LEU:HB2 | 4:D:753:GLY:H | 1.54 | 0.48 |
| 1:H:12:DT:H2' | 1:H:13:DC:C6 | 2.49 | 0.48 |
| 4:A:379:ARG:HD3 | 4:A:660:ASP:CG | 2.34 | 0.47 |
| 4:A:286:TYR:CE2 | 4:A:417:PRO:HG3 | 2.49 | 0.47 |
| 4:A:502:TRP:CG | 4:A:503:ALA:N | 2.81 | 0.47 |
| 4:A:438:ASP:OD1 | 4:A:507:SER:HB3 | 2.14 | 0.47 |
| 4:A:530:CYS:HB3 | 4:A:818:PRO:HG2 | 1.96 | 0.47 |
| 4:A:580:GLU:HG3 | 7:A:3111:HOH:O | 2.13 | 0.47 |
| 4:A:77:LEU:HD11 | 4:A:226:MET:SD | 2.54 | 0.47 |
| 4:B:21:PHE:O | 4:B:21:PHE:CD1 | 2.67 | 0.47 |
| 4:B:687:VAL:HG23 | 4:B:687:VAL:O | 2.14 | 0.47 |
| 4:B:5:ASN:HD21 | 4:B:7:ALA:C | 2.17 | 0.47 |
| 4:B:840:ASP:O | 4:B:843:ALA:N | 2.47 | 0.47 |
| 4:C:292:ARG:O | 4:C:292:ARG:CG | 2.62 | 0.47 |
| 4:C:36:GLN:HG2 | 4:C:273:VAL:HG13 | 1.96 | 0.47 |
| 4:C:391:ARG:O | 4:C:391:ARG:HG2 | 2.14 | 0.47 |
| 4:C:397:SER:OG | 4:C:398:LEU:N | 2.42 | 0.47 |
| 4:C:421:ASP:OD2 | 4:C:423:ARG:NH1 | 2.44 | 0.47 |
| 4:C:657:PRO:HG2 | 4:C:658:ALA:H | 1.79 | 0.47 |
| 4:C:816:THR:HG22 | 4:C:817:ILE:N | 2.29 | 0.47 |
| 4:D:564:SER:C | 7:D:3040:HOH:O | 2.51 | 0.47 |
| 4:D:647:ARG:O | 4:D:649:GLN:N | 2.47 | 0.47 |
| 4:D:833:VAL:HG22 | 4:D:875:ILE:HD12 | 1.95 | 0.47 |
| 4:A:216:CYS:HA | 4:A:219:MET:CE | 2.44 | 0.47 |
| 4:A:277:PRO:HA | 4:A:321:ASN:OD1 | 2.14 | 0.47 |
| 4:A:518:TYR:C | 4:A:518:TYR:CD1 | 2.87 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:A:632:ARG:HA | 4:A:635:MET:HG2 | 1.96 | 0.47 |
| 4:B:199:GLU:O | 4:B:201:TRP:N | 2.41 | 0.47 |
| 4:B:201:TRP:CB | 7:B:3009:HOH:O | 2.50 | 0.47 |
| 4:B:423:ARG:HG3 | 4:B:781:ASN:ND2 | 2.14 | 0.47 |
| 4:B:439:MET:HG3 | 4:B:509:PHE:CD2 | 2.49 | 0.47 |
| 4:B:470:VAL:CG1 | 4:B:470:VAL:O | 2.52 | 0.47 |
| 4:B:501:TRP:O | 4:B:505:GLN:NE2 | 2.47 | 0.47 |
| 4:B:592:ASN:N | 4:B:592:ASN:OD1 | 2.47 | 0.47 |
| 4:B:67:ASN:O | 4:B:69:ALA:N | 2.47 | 0.47 |
| 4:C:416:PHE:CZ | 4:C:434:PRO:HD3 | 2.49 | 0.47 |
| 4:C:831:THR:HG22 | 4:C:832:MET:N | 2.29 | 0.47 |
| 4:D:120:LYS:HG3 | 4:D:752:LEU:CD2 | 2.27 | 0.47 |
| 4:D:445:THR:OG1 | 4:D:533:PRO:HD2 | 2.15 | 0.47 |
| 4:D:569:ASP:OD2 | 4:D:572:GLY:N | 2.45 | 0.47 |
| 4:A:30:GLU:OE1 | 4:A:30:GLU:HA | 2.13 | 0.47 |
| 4:A:403:GLU:O | 4:A:404:GLN:C | 2.52 | 0.47 |
| 4:A:274:PRO:HD3 | 4:A:415:TRP:CH2 | 2.48 | 0.47 |
| 4:A:416:PHE:CE2 | 4:A:434:PRO:CD | 2.98 | 0.47 |
| 4:A:751:PHE:HB3 | 4:A:752:LEU:HD12 | 1.96 | 0.47 |
| 4:A:318:LYS:HE3 | 4:A:800:GLU:OE2 | 2.14 | 0.47 |
| 4:A:829:ARG:NH2 | 4:A:878:SER:O | 2.47 | 0.47 |
| 4:B:106:LEU:HD11 | 4:B:212:VAL:HG13 | 1.95 | 0.47 |
| 4:B:461:LYS:HG2 | 4:B:482:ILE:HG21 | 1.96 | 0.47 |
| 4:B:504:GLU:HB3 | 7:B:3140:HOH:O | 2.13 | 0.47 |
| 4:B:155:ARG:NE | 4:B:749:LEU:HD23 | 2.28 | 0.47 |
| 4:C:557:ARG:HD3 | 7:C:3150:HOH:O | 2.15 | 0.47 |
| 4:C:575:ALA:O | 4:C:578:VAL:HB | 2.13 | 0.47 |
| 4:C:811:HIS:N | 4:C:811:HIS:CD2 | 2.82 | 0.47 |
| 4:D:345:LYS:NZ | 4:D:351:ASP:O | 2.43 | 0.47 |
| 4:D:592:ASN:OD1 | 4:D:611:LEU:HA | 2.15 | 0.47 |
| 1:K:8:DG:H2" | 1:K:9:DA:C8 | 2.49 | 0.47 |
| 4:A:418:TYR:CD2 | 4:A:426:VAL:CG1 | 2.90 | 0.47 |
| 4:A:545:HIS:O | 4:A:546:PHE:C | 2.52 | 0.47 |
| 4:A:60:LYS:HG3 | 7:A:3125:HOH:O | 2.14 | 0.47 |
| 4:A:629:VAL:HG11 | 4:A:677:MET:HE2 | 1.96 | 0.47 |
| 4:B:272:VAL:CG1 | 4:B:411:HIS:CD2 | 2.98 | 0.47 |
| 4:B:329:LYS:O | 4:B:330:ILE:C | 2.52 | 0.47 |
| 4:C:686:SER:HA | 4:C:693:VAL:HG21 | 1.96 | 0.47 |
| 4:C:777:GLY:C | 4:C:780:PRO:HD2 | 2.35 | 0.47 |
| 4:C:794:THR:O | 4:C:795:VAL:C | 2.50 | 0.47 |
| 4:D:830:GLU:HA | 4:D:876:LEU:HD21 | 1.95 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:A:105:PHE:C | 4:A:107:GLN:N | 2.67 | 0.47 |
| 4:A:152:GLY:O | 4:A:156:ASP:OD2 | 2.32 | 0.47 |
| 4:A:559:VAL:O | 4:A:560:ASN:HB2 | 2.14 | 0.47 |
| 4:A:59:LEU:CA | 4:A:64:VAL:HG22 | 2.41 | 0.47 |
| 4:A:739:TYR:HB2 | 4:A:774:GLN:OE1 | 2.14 | 0.47 |
| 4:B:512:LEU:O | 4:B:513:ALA:C | 2.49 | 0.47 |
| 4:B:51:PHE:HE2 | 4:B:55:PHE:CD1 | 2.33 | 0.47 |
| 4:B:669:GLN:HB3 | 4:B:672:GLN:HB2 | 1.97 | 0.47 |
| 4:B:696:MET:HG2 | 4:B:779:ALA:HB1 | 1.95 | 0.47 |
| 4:C:161:HIS:O | 4:C:164:LYS:HG2 | 2.14 | 0.47 |
| 4:C:727:TRP:NE1 | 4:C:782:PHE:HD1 | 2.11 | 0.47 |
| 4:D:168:GLU:O | 4:D:172:LYS:HG2 | 2.15 | 0.47 |
| 4:D:720:ARG:HD2 | 4:D:852:GLN:O | 2.14 | 0.47 |
| 4:A:85:ILE:HG23 | 4:A:219:MET:SD | 2.54 | 0.47 |
| 4:A:313:MET:HG3 | 4:A:313:MET:O | 2.15 | 0.47 |
| 4:A:473:VAL:HG13 | 4:A:477:GLU:HB2 | 1.96 | 0.47 |
| 4:A:477:GLU:O | 4:A:480:LYS:HB3 | 2.13 | 0.47 |
| 4:B:308:TYR:CA | 4:B:311:VAL:HG23 | 2.44 | 0.47 |
| 4:B:634:VAL:O | 4:B:637:LEU:HB2 | 2.14 | 0.47 |
| 4:B:726:HIS:CD2 | 4:B:736:TRP:CD2 | 3.03 | 0.47 |
| 4:B:794:THR:HG21 | 4:B:828:VAL:HA | 1.97 | 0.47 |
| 4:C:180:LYS:O | 4:C:183:MET:N | 2.41 | 0.47 |
| 4:C:183:MET:O | 4:C:186:VAL:HB | 2.15 | 0.47 |
| 4:C:39:LEU:HD22 | 4:C:272:VAL:HG23 | 1.95 | 0.47 |
| 4:C:559:VAL:CG2 | 4:C:561:LEU:HD13 | 2.37 | 0.47 |
| 4:D:387:LYS:HE2 | 7:D:3158:HOH:O | 2.14 | 0.47 |
| 4:D:333:LYS:HZ2 | 4:D:516:PHE:HB3 | 1.78 | 0.47 |
| 4:D:631:LYS:HE2 | 4:D:635:MET:SD | 2.55 | 0.47 |
| 1:K:11:DA:C2 | 1:K:12:DT:N3 | 2.83 | 0.47 |
| 1:K:2:DG:H1' | 7:K:268:HOH:O | 2.14 | 0.47 |
| 2:L:6:G:C2 | 2:L:7:A:C8 | 3.03 | 0.47 |
| 3:M:4:DG:H4' | 3:M:5:DA:OP1 | 2.15 | 0.47 |
| 1:N:4:DA:C6 | 1:N:5:DA:C6 | 3.02 | 0.47 |
| 4:A:141:ILE:HB | 4:A:213:GLY:HA2 | 1.97 | 0.47 |
| 4:A:80:LYS:HE2 | 4:A:224:THR:HG22 | 1.96 | 0.47 |
| 4:A:42:GLU:O | 4:A:46:MET:N | 2.44 | 0.47 |
| 4:A:632:ARG:HH22 | 6:A:2000:APC:H5'2 | 1.79 | 0.47 |
| 4:A:791:LEU:HA | 4:A:814:PHE:HE2 | 1.80 | 0.47 |
| 4:A:869:ASN:HD22 | 4:A:869:ASN:N | 2.13 | 0.47 |
| 4:A:99:ARG:N | 4:A:99:ARG:HD2 | 2.29 | 0.47 |
| 4:B:652:GLU:O | 4:B:657:PRO:HD3 | 2.13 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:C:109:ILE:HD12 | 4:C:109:ILE:N | 2.29 | 0.47 |
| 4:C:616:LEU:HD13 | 4:C:676:TYR:HB2 | 1.95 | 0.47 |
| 4:D:236:VAL:CG2 | 4:D:239:GLN:HB2 | 2.45 | 0.47 |
| 4:D:316:VAL:O | 4:D:317:TYR:C | 2.52 | 0.47 |
| 4:D:435:GLN:HA | 4:D:810:ILE:CD1 | 2.43 | 0.47 |
| 4:D:797:TRP:CZ2 | 4:D:801:LYS:HG3 | 2.50 | 0.47 |
| 1:N:2:DG:C2' | 1:N:3:DG:C8 | 2.95 | 0.47 |
| 4:A:103:PHE:O | 4:A:107:GLN:NE2 | 2.44 | 0.47 |
| 4:A:190:MET:HB3 | 7:A:3103:HOH:O | 2.14 | 0.47 |
| 4:A:676:TYR:O | 4:A:677:MET:C | 2.51 | 0.47 |
| 4:A:828:VAL:CB | 4:A:883:ALA:HA | 2.44 | 0.47 |
| 4:B:159:ALA:O | 4:B:161:HIS:N | 2.47 | 0.47 |
| 4:B:279:THR:HG22 | 7:B:3148:HOH:O | 2.14 | 0.47 |
| 4:B:44:TYR:HD1 | 4:B:44:TYR:H | 1.63 | 0.47 |
| 4:B:469:GLY:C | 4:B:471:ASP:H | 2.15 | 0.47 |
| 4:C:101:THR:HA | 4:C:104:GLN:CD | 2.35 | 0.47 |
| 4:C:71:LYS:N | 4:C:72:PRO:HD2 | 2.30 | 0.47 |
| 4:D:143:ARG:O | 4:D:147:ASP:OD2 | 2.32 | 0.47 |
| 4:D:14:ILE:N | 4:D:14:ILE:HD12 | 2.23 | 0.47 |
| 4:D:515:CYS:O | 4:D:516:PHE:C | 2.51 | 0.47 |
| 4:D:521:VAL:O | 4:D:525:GLY:N | 2.46 | 0.47 |
| 4:D:558:ALA:CB | 4:D:570:ILE:HD13 | 2.45 | 0.47 |
| 4:D:629:VAL:HG22 | 4:D:654:THR:HG21 | 1.95 | 0.47 |
| 4:D:836:TYR:CD2 | 4:D:836:TYR:N | 2.81 | 0.47 |
| 2:I:2:C:H2' | 2:I:3:G:H8 | 1.80 | 0.47 |
| 3:J:7:DT:H2'' | 3:J:8:DC:C6 | 2.49 | 0.47 |
| 2:L:2:C:O5' | 2:L:2:C:H6 | 1.98 | 0.47 |
| 4:A:280:GLY:HA2 | 4:A:317:TYR:HE1 | 1.74 | 0.47 |
| 4:A:801:LYS:C | 4:A:801:LYS:CD | 2.80 | 0.47 |
| 4:A:86:ASN:O | 4:A:90:GLU:HG2 | 2.15 | 0.47 |
| 4:B:24:LEU:O | 4:B:25:ALA:C | 2.52 | 0.47 |
| 4:B:314:PRO:C | 4:B:316:VAL:N | 2.65 | 0.47 |
| 4:B:428:ALA:H | 4:B:435:GLN:NE2 | 2.11 | 0.47 |
| 4:B:647:ARG:O | 4:B:650:VAL:N | 2.48 | 0.47 |
| 4:B:656:GLN:N | 4:B:657:PRO:HD2 | 2.29 | 0.47 |
| 4:B:806:SER:O | 4:B:816:THR:HG23 | 2.14 | 0.47 |
| 4:C:117:ILE:HG21 | 4:C:145:ILE:HD13 | 1.97 | 0.47 |
| 4:C:337:VAL:HG12 | 4:C:338:ALA:H | 1.79 | 0.47 |
| 4:C:417:PRO:O | 4:C:418:TYR:HD1 | 1.98 | 0.47 |
| 4:C:579:ASN:HA | 4:C:582:LEU:CG | 2.45 | 0.47 |
| 4:C:651:LEU:HB2 | 4:C:674:ALA:CB | 2.45 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:C:830:GLU:HA | 4:C:876:LEU:HD21 | 1.96 | 0.47 |
| 4:D:159:ALA:HB3 | 4:D:163:LYS:HD3 | 1.96 | 0.47 |
| 4:D:472:LYS:C | 4:D:567:VAL:HG21 | 2.35 | 0.47 |
| 4:D:631:LYS:HD3 | 4:D:635:MET:SD | 2.54 | 0.47 |
| 4:D:308:TYR:OH | 4:D:734:PRO:O | 2.26 | 0.47 |
| 3:P:5:DA:H2" | 3:P:6:DT:H72 | 1.97 | 0.47 |
| 4:A:77:LEU:CD1 | 4:A:226:MET:SD | 3.03 | 0.47 |
| 4:A:311:VAL:HG12 | 4:A:312:TYR:H | 1.77 | 0.47 |
| 4:A:631:LYS:O | 4:A:632:ARG:C | 2.53 | 0.47 |
| 4:A:635:MET:HE1 | 6:A:2000:APC:H3' | 1.97 | 0.47 |
| 4:A:797:TRP:CH2 | 4:A:801:LYS:HG3 | 2.50 | 0.47 |
| 4:A:706:LEU:HD11 | 4:A:849:PHE:CG | 2.50 | 0.47 |
| 4:B:166:VAL:O | 4:B:167:GLU:C | 2.53 | 0.47 |
| 4:B:485:ASN:N | 4:B:485:ASN:OD1 | 2.44 | 0.47 |
| 4:B:49:ALA:O | 4:B:50:ARG:C | 2.52 | 0.47 |
| 4:B:56:GLU:CD | 4:B:57:ARG:N | 2.68 | 0.47 |
| 4:B:778:ILE:HG13 | 4:B:778:ILE:O | 2.14 | 0.47 |
| 4:C:452:ILE:HG23 | 4:C:453:GLY:N | 2.29 | 0.47 |
| 4:C:517:GLU:OE1 | 4:C:517:GLU:HA | 2.14 | 0.47 |
| 4:D:166:VAL:O | 4:D:167:GLU:C | 2.53 | 0.47 |
| 4:D:31:ARG:O | 4:D:32:LEU:C | 2.53 | 0.47 |
| 4:D:374:LEU:O | 4:D:378:LYS:HB2 | 2.14 | 0.47 |
| 4:D:416:PHE:O | 4:D:418:TYR:CE1 | 2.68 | 0.47 |
| 4:D:647:ARG:O | 4:D:648:GLN:C | 2.53 | 0.47 |
| 4:A:679:LYS:O | 4:A:680:LEU:C | 2.51 | 0.47 |
| 4:A:794:THR:HG1 | 4:A:831:THR:HG21 | 1.76 | 0.47 |
| 4:B:411:HIS:C | 4:B:413:ALA:N | 2.67 | 0.47 |
| 4:B:492:CYS:SG | 4:B:502:TRP:HB3 | 2.55 | 0.47 |
| 4:B:567:VAL:HG13 | 4:B:880:PHE:CD2 | 2.50 | 0.47 |
| 4:B:648:GLN:O | 4:B:649:GLN:C | 2.53 | 0.47 |
| 4:C:274:PRO:HA | 4:C:275:PRO:HD3 | 1.77 | 0.47 |
| 4:C:314:PRO:HD3 | 7:C:3099:HOH:O | 2.13 | 0.47 |
| 4:C:727:TRP:HB3 | 4:C:845:PHE:CE1 | 2.50 | 0.47 |
| 4:C:746:ARG:NH1 | 4:C:754:GLN:O | 2.47 | 0.47 |
| 4:C:870:LEU:HD23 | 4:C:871:ASN:C | 2.35 | 0.47 |
| 4:D:419:ASN:ND2 | 4:D:429:VAL:HG22 | 2.30 | 0.47 |
| 4:D:448:LYS:HZ1 | 4:D:806:SER:HA | 1.79 | 0.47 |
| 4:A:390:ALA:O | 4:A:391:ARG:C | 2.52 | 0.46 |
| 4:A:420:MET:HA | 4:A:425:ARG:O | 2.15 | 0.46 |
| 4:A:439:MET:HG3 | 4:A:509:PHE:CE2 | 2.49 | 0.46 |
| 4:A:647:ARG:CG | 4:A:675:GLY:HA2 | 2.45 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-------------------|--------------------------|-------------------|
| 4:A:711:LYS:CB | 4:A:711:LYS:NZ | 2.78 | 0.46 |
| 4:B:254:ILE:O | 4:B:255:ALA:C | 2.52 | 0.46 |
| 4:B:36:GLN:OE1 | 4:B:36:GLN:CA | 2.63 | 0.46 |
| 4:B:403:GLU:O | 4:B:405:ALA:N | 2.48 | 0.46 |
| 4:B:570:ILE:O | 4:B:570:ILE:HG13 | 2.14 | 0.46 |
| 4:B:675:GLY:O | 4:B:678:ALA:HB3 | 2.15 | 0.46 |
| 4:B:729:THR:HB | 4:B:789:SER:HB2 | 1.96 | 0.46 |
| 4:C:404:GLN:CA | 4:C:404:GLN:HE21 | 2.15 | 0.46 |
| 4:C:4:ILE:CD1 | 7:C:3146:HOH:O | 2.62 | 0.46 |
| 4:C:616:LEU:O | 4:C:617:ALA:C | 2.53 | 0.46 |
| 4:D:631:LYS:HE2 | 6:D:2003:APC:H3A2 | 1.97 | 0.46 |
| 4:D:706:LEU:CD2 | 4:D:853:LEU:HD23 | 2.44 | 0.46 |
| 4:D:782:PHE:CE2 | 4:D:786:GLN:OE1 | 2.68 | 0.46 |
| 4:D:823:ASN:O | 4:D:826:LYS:N | 2.48 | 0.46 |
| 1:E:14:DG:C2' | 1:E:15:DC:H6 | 2.28 | 0.46 |
| 3:G:4:DG:C1' | 3:G:5:DA:C8 | 2.98 | 0.46 |
| 4:A:303:LYS:HE2 | 4:A:740:LYS:HZ1 | 1.81 | 0.46 |
| 4:A:308:TYR:CE2 | 4:A:736:TRP:CZ3 | 3.03 | 0.46 |
| 4:A:311:VAL:CG1 | 4:A:312:TYR:N | 2.77 | 0.46 |
| 4:A:410:ASN:N | 4:A:410:ASN:HD22 | 2.12 | 0.46 |
| 4:B:116:TYR:CD2 | 4:B:116:TYR:C | 2.89 | 0.46 |
| 4:B:247:ALA:CB | 4:B:250:TYR:CD1 | 2.99 | 0.46 |
| 4:B:268:PHE:CD2 | 4:B:429:VAL:HG12 | 2.51 | 0.46 |
| 4:B:787:ASP:O | 4:B:790:HIS:N | 2.48 | 0.46 |
| 4:C:140:ALA:O | 4:C:143:ARG:N | 2.48 | 0.46 |
| 4:C:84:ARG:HD2 | 4:C:222:GLU:OE1 | 2.14 | 0.46 |
| 4:C:246:LEU:HG | 4:C:247:ALA:N | 2.29 | 0.46 |
| 4:C:540:CYS:O | 4:C:541:SER:C | 2.54 | 0.46 |
| 4:C:598:THR:OG1 | 4:C:605:ILE:HD13 | 2.16 | 0.46 |
| 4:C:623:TYR:HD1 | 4:C:663:LYS:HE2 | 1.80 | 0.46 |
| 4:D:828:VAL:O | 4:D:831:THR:HG22 | 2.16 | 0.46 |
| 1:H:12:DT:C2' | 1:H:13:DC:C6 | 2.98 | 0.46 |
| 4:A:347:CYS:HB3 | 4:A:350:GLU:CG | 2.45 | 0.46 |
| 4:A:347:CYS:HB3 | 4:A:350:GLU:HB2 | 1.97 | 0.46 |
| 4:A:386:ARG:C | 4:A:388:ASP:N | 2.68 | 0.46 |
| 4:A:403:GLU:O | 4:A:406:ASN:N | 2.48 | 0.46 |
| 4:A:473:VAL:HA | 4:A:474:PRO:HD2 | 1.62 | 0.46 |
| 4:A:711:LYS:HB2 | 4:A:711:LYS:NZ | 2.30 | 0.46 |
| 4:A:871:ASN:O | 4:A:872:LEU:C | 2.54 | 0.46 |
| 4:B:643:GLU:C | 4:B:645:GLY:N | 2.66 | 0.46 |
| 4:C:416:PHE:HB2 | 4:C:418:TYR:CE1 | 2.51 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:C:450:LYS:HD2 | 4:C:817:ILE:CD1 | 2.46 | 0.46 |
| 4:C:659:ILE:HG22 | 4:C:660:ASP:N | 2.29 | 0.46 |
| 4:D:21:PHE:CD1 | 4:D:21:PHE:O | 2.68 | 0.46 |
| 4:D:373:ALA:O | 4:D:377:TRP:CD1 | 2.68 | 0.46 |
| 4:D:739:TYR:CD2 | 4:D:774:GLN:HA | 2.50 | 0.46 |
| 4:D:784:HIS:O | 4:D:787:ASP:N | 2.49 | 0.46 |
| 2:F:7:A:H2' | 2:F:8:U:C6 | 2.46 | 0.46 |
| 4:A:261:LEU:C | 4:A:263:GLY:H | 2.19 | 0.46 |
| 4:A:281:ILE:HG22 | 4:A:282:THR:HG22 | 1.86 | 0.46 |
| 4:A:59:LEU:HD23 | 4:A:64:VAL:CG1 | 2.46 | 0.46 |
| 4:A:796:VAL:O | 4:A:799:HIS:N | 2.40 | 0.46 |
| 4:B:324:GLN:HG3 | 4:B:418:TYR:H | 1.80 | 0.46 |
| 4:B:450:LYS:HB3 | 4:B:819:ALA:CB | 2.45 | 0.46 |
| 4:B:520:GLY:HA3 | 4:B:528:TYR:CE1 | 2.50 | 0.46 |
| 4:B:549:MET:HE1 | 4:B:782:PHE:HE2 | 1.81 | 0.46 |
| 4:C:729:THR:O | 4:C:732:GLY:N | 2.29 | 0.46 |
| 4:C:92:VAL:HG12 | 4:C:92:VAL:O | 2.15 | 0.46 |
| 4:D:390:ALA:CB | 4:D:394:ARG:HH21 | 2.28 | 0.46 |
| 4:D:684:SER:O | 4:D:687:VAL:HG22 | 2.16 | 0.46 |
| 4:A:274:PRO:HA | 4:A:415:TRP:CG | 2.50 | 0.46 |
| 4:A:646:PHE:O | 4:A:647:ARG:O | 2.33 | 0.46 |
| 4:A:726:HIS:CD2 | 4:A:736:TRP:CE2 | 3.03 | 0.46 |
| 4:A:89:PHE:HZ | 4:A:106:LEU:O | 1.99 | 0.46 |
| 4:B:158:GLU:HA | 4:B:195:LEU:CD1 | 2.42 | 0.46 |
| 4:B:469:GLY:C | 4:B:471:ASP:N | 2.68 | 0.46 |
| 4:B:644:PHE:CD2 | 4:B:644:PHE:C | 2.89 | 0.46 |
| 4:C:165:ASN:ND2 | 7:C:3138:HOH:O | 2.48 | 0.46 |
| 4:C:475:PHE:N | 4:C:476:PRO:CD | 2.78 | 0.46 |
| 4:C:698:TRP:O | 4:C:701:SER:HB2 | 2.16 | 0.46 |
| 4:C:777:GLY:O | 4:C:781:ASN:CG | 2.54 | 0.46 |
| 4:C:727:TRP:CD1 | 4:C:782:PHE:HE1 | 2.33 | 0.46 |
| 4:C:549:MET:CE | 4:C:786:GLN:HG2 | 2.46 | 0.46 |
| 4:D:21:PHE:CD1 | 4:D:21:PHE:C | 2.89 | 0.46 |
| 4:D:328:TRP:CG | 4:D:416:PHE:HE2 | 2.33 | 0.46 |
| 4:D:541:SER:O | 4:D:542:GLY:C | 2.53 | 0.46 |
| 4:D:593:GLU:O | 4:D:610:LYS:HB3 | 2.16 | 0.46 |
| 4:D:588:ASN:O | 4:D:614:LYS:HG3 | 2.15 | 0.46 |
| 4:D:632:ARG:HG2 | 4:D:653:ASP:OD2 | 2.15 | 0.46 |
| 4:D:76:THR:C | 4:D:79:PRO:HD2 | 2.36 | 0.46 |
| 4:D:797:TRP:HD1 | 4:D:827:ALA:HB1 | 1.81 | 0.46 |
| 3:M:9:DC:H2'' | 7:M:350:HOH:O | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:12:DT:C2' | 1:N:13:DC:H5' | 2.22 | 0.46 |
| 4:A:109:ILE:HG12 | 4:A:148:GLU:HB3 | 1.97 | 0.46 |
| 4:A:520:GLY:HA3 | 4:A:528:TYR:CE2 | 2.50 | 0.46 |
| 4:A:727:TRP:CH2 | 4:A:735:VAL:CG2 | 2.99 | 0.46 |
| 4:B:432:PHE:C | 4:B:432:PHE:CD2 | 2.89 | 0.46 |
| 4:B:60:LYS:O | 4:B:60:LYS:HG2 | 2.15 | 0.46 |
| 4:B:459:TRP:CH2 | 4:B:825:PHE:CD2 | 3.04 | 0.46 |
| 4:C:329:LYS:HD3 | 4:C:447:ALA:HA | 1.98 | 0.46 |
| 4:C:338:ALA:O | 4:C:339:ASN:C | 2.43 | 0.46 |
| 4:C:268:PHE:O | 4:C:430:SER:HB2 | 2.15 | 0.46 |
| 4:C:655:ILE:O | 4:C:655:ILE:HG22 | 2.15 | 0.46 |
| 4:C:754:GLN:HB3 | 4:C:755:PHE:HD1 | 1.80 | 0.46 |
| 4:C:82:ILE:HA | 4:C:85:ILE:HD12 | 1.96 | 0.46 |
| 4:C:829:ARG:NH2 | 4:C:878:SER:O | 2.47 | 0.46 |
| 4:D:89:PHE:CZ | 4:D:106:LEU:HB3 | 2.46 | 0.46 |
| 4:D:476:PRO:HG2 | 4:D:477:GLU:OE2 | 2.15 | 0.46 |
| 4:D:613:THR:HG22 | 4:D:676:TYR:CE1 | 2.51 | 0.46 |
| 4:D:81:MET:O | 4:D:85:ILE:HG13 | 2.15 | 0.46 |
| 3:G:1:DG:H1' | 3:G:2:DT:H72 | 1.98 | 0.46 |
| 1:H:3:DG:N2 | 3:J:9:DC:O2 | 2.48 | 0.46 |
| 4:A:139:SER:HB2 | 4:A:210:ILE:CD1 | 2.46 | 0.46 |
| 4:A:446:LEU:HD12 | 4:A:531:SER:O | 2.15 | 0.46 |
| 4:A:541:SER:O | 4:A:542:GLY:C | 2.52 | 0.46 |
| 4:A:577:LYS:HB3 | 4:A:684:SER:OG | 2.15 | 0.46 |
| 4:A:829:ARG:NH1 | 4:A:829:ARG:CG | 2.57 | 0.46 |
| 4:B:172:LYS:NZ | 4:B:172:LYS:CB | 2.70 | 0.46 |
| 4:B:482:ILE:O | 4:B:485:ASN:N | 2.48 | 0.46 |
| 4:B:680:LEU:H | 4:B:680:LEU:CD1 | 2.29 | 0.46 |
| 4:B:748:ASN:ND2 | 4:B:751:PHE:N | 2.60 | 0.46 |
| 4:C:349:VAL:HG13 | 4:C:503:ALA:O | 2.16 | 0.46 |
| 4:C:551:ARG:HH12 | 4:C:867:LYS:HZ3 | 1.63 | 0.46 |
| 4:C:577:LYS:O | 4:C:581:ILE:HG13 | 2.15 | 0.46 |
| 4:C:840:ASP:OD2 | 4:C:867:LYS:NZ | 2.49 | 0.46 |
| 4:C:849:PHE:O | 4:C:850:ALA:C | 2.54 | 0.46 |
| 4:D:122:THR:O | 4:D:125:CYS:N | 2.48 | 0.46 |
| 4:D:205:HIS:C | 4:D:207:GLU:N | 2.69 | 0.46 |
| 4:D:422:TRP:CD1 | 4:D:422:TRP:O | 2.69 | 0.46 |
| 4:A:230:HIS:CE1 | 4:A:232:GLN:HE21 | 2.34 | 0.46 |
| 4:A:404:GLN:NE2 | 4:A:404:GLN:CA | 2.73 | 0.46 |
| 4:A:429:VAL:O | 4:A:430:SER:O | 2.33 | 0.46 |
| 4:A:517:GLU:OE1 | 4:A:517:GLU:HA | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:A:644:PHE:C | 4:A:644:PHE:CD2 | 2.88 | 0.46 |
| 4:B:105:PHE:O | 4:B:107:GLN:N | 2.49 | 0.46 |
| 4:B:229:LEU:CD1 | 4:B:242:GLU:HG2 | 2.41 | 0.46 |
| 4:B:460:LEU:HD12 | 4:B:460:LEU:O | 2.15 | 0.46 |
| 4:B:475:PHE:HB2 | 4:B:476:PRO:HD2 | 1.98 | 0.46 |
| 4:B:556:GLY:HA2 | 4:B:561:LEU:HD13 | 1.98 | 0.46 |
| 4:B:55:PHE:HE2 | 4:B:59:LEU:HD11 | 1.79 | 0.46 |
| 4:B:727:TRP:CZ2 | 4:B:782:PHE:HA | 2.51 | 0.46 |
| 4:C:42:GLU:HG2 | 4:C:46:MET:HE2 | 1.96 | 0.46 |
| 4:C:550:LEU:C | 4:C:867:LYS:HG3 | 2.36 | 0.46 |
| 4:D:221:ILE:HG23 | 4:D:227:VAL:O | 2.16 | 0.46 |
| 4:D:502:TRP:CG | 4:D:512:LEU:HD13 | 2.50 | 0.46 |
| 4:D:55:PHE:CZ | 4:D:59:LEU:HD11 | 2.51 | 0.46 |
| 4:D:825:PHE:O | 4:D:828:VAL:HG23 | 2.16 | 0.46 |
| 4:A:475:PHE:O | 4:A:476:PRO:C | 2.50 | 0.46 |
| 4:B:164:LYS:HZ2 | 4:B:164:LYS:N | 2.13 | 0.46 |
| 4:B:30:GLU:O | 4:B:31:ARG:C | 2.53 | 0.46 |
| 4:B:408:PHE:CD1 | 4:B:414:ILE:HG21 | 2.31 | 0.46 |
| 4:B:67:ASN:O | 4:B:68:ALA:C | 2.54 | 0.46 |
| 4:C:257:ARG:HH11 | 4:C:257:ARG:HG2 | 1.81 | 0.46 |
| 4:C:418:TYR:HD2 | 4:C:426:VAL:HG11 | 1.80 | 0.46 |
| 4:C:435:GLN:HG2 | 4:C:810:ILE:HG12 | 1.97 | 0.46 |
| 4:C:506:ASP:O | 4:C:508:PRO:HD2 | 2.15 | 0.46 |
| 4:C:534:LEU:CD1 | 4:C:818:PRO:HA | 2.46 | 0.46 |
| 4:C:786:GLN:O | 4:C:788:GLY:N | 2.49 | 0.46 |
| 4:C:319:ALA:HB2 | 4:C:792:ARG:HB3 | 1.97 | 0.46 |
| 4:C:848:GLN:OE1 | 4:C:848:GLN:HA | 2.15 | 0.46 |
| 4:D:281:ILE:HG12 | 4:D:309:GLU:HA | 1.97 | 0.46 |
| 4:D:470:VAL:CG1 | 4:D:473:VAL:HG11 | 2.40 | 0.46 |
| 4:D:543:ILE:HG21 | 4:D:689:VAL:CG1 | 2.45 | 0.46 |
| 4:D:744:GLN:HB3 | 4:D:756:ARG:CB | 2.45 | 0.46 |
| 4:A:147:ASP:HB3 | 4:A:750:MET:CE | 2.46 | 0.46 |
| 4:A:404:GLN:O | 4:A:407:LYS:HB3 | 2.16 | 0.46 |
| 4:A:656:GLN:C | 4:A:658:ALA:N | 2.68 | 0.46 |
| 4:A:746:ARG:CZ | 4:A:746:ARG:HB3 | 2.45 | 0.46 |
| 4:A:831:THR:CG2 | 4:A:832:MET:N | 2.78 | 0.46 |
| 4:B:163:LYS:HA | 4:B:163:LYS:HD2 | 1.71 | 0.46 |
| 4:B:72:PRO:HG3 | 4:B:257:ARG:HG3 | 1.97 | 0.46 |
| 4:B:322:ILE:O | 4:B:323:ALA:C | 2.52 | 0.46 |
| 4:B:433:ASN:HB2 | 4:B:434:PRO:HD2 | 1.88 | 0.46 |
| 4:C:14:ILE:CG2 | 4:C:288:ALA:CB | 2.91 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:C:180:LYS:O | 4:C:181:ALA:C | 2.54 | 0.46 |
| 4:C:462:ILE:CD1 | 4:C:479:ILE:HD11 | 2.45 | 0.46 |
| 4:C:646:PHE:HD1 | 4:C:649:GLN:OE1 | 1.99 | 0.46 |
| 4:C:700:LYS:O | 4:C:701:SER:C | 2.54 | 0.46 |
| 4:C:809:LEU:HA | 4:C:813:SER:O | 2.17 | 0.46 |
| 4:D:135:GLN:HB3 | 7:D:3160:HOH:O | 2.15 | 0.46 |
| 4:D:139:SER:CB | 4:D:210:ILE:HD13 | 2.45 | 0.46 |
| 4:D:182:PHE:O | 4:D:186:VAL:HG23 | 2.16 | 0.46 |
| 4:D:468:ALA:HB2 | 4:D:511:PHE:CE1 | 2.51 | 0.46 |
| 4:D:699:LEU:HD11 | 4:D:782:PHE:CD2 | 2.50 | 0.46 |
| 4:A:158:GLU:CD | 4:A:195:LEU:HB3 | 2.37 | 0.45 |
| 4:A:480:LYS:HG3 | 4:A:484:GLU:OE1 | 2.16 | 0.45 |
| 4:B:164:LYS:HA | 4:B:164:LYS:HD3 | 1.78 | 0.45 |
| 4:B:163:LYS:HB3 | 4:B:164:LYS:HZ2 | 1.79 | 0.45 |
| 4:B:199:GLU:C | 4:B:201:TRP:H | 2.20 | 0.45 |
| 4:B:620:TRP:CD2 | 4:B:677:MET:CE | 2.99 | 0.45 |
| 4:B:676:TYR:O | 4:B:677:MET:C | 2.53 | 0.45 |
| 4:B:797:TRP:CZ2 | 4:B:801:LYS:HG3 | 2.51 | 0.45 |
| 4:C:148:GLU:OE1 | 4:C:749:LEU:HB2 | 2.15 | 0.45 |
| 4:C:164:LYS:N | 4:C:164:LYS:HZ3 | 2.14 | 0.45 |
| 4:C:551:ARG:HE | 4:C:872:LEU:HD11 | 1.80 | 0.45 |
| 4:C:89:PHE:CZ | 4:C:106:LEU:O | 2.68 | 0.45 |
| 4:D:236:VAL:O | 4:D:240:ASP:CB | 2.64 | 0.45 |
| 4:D:460:LEU:HD13 | 4:D:532:LEU:HD23 | 1.97 | 0.45 |
| 4:D:116:TYR:HH | 4:D:752:LEU:HD22 | 1.82 | 0.45 |
| 1:K:15:DC:C5' | 1:K:15:DC:H6 | 2.28 | 0.45 |
| 4:A:704:LYS:HE3 | 4:A:860:LYS:CE | 2.46 | 0.45 |
| 4:A:801:LYS:HD3 | 4:A:801:LYS:O | 2.13 | 0.45 |
| 4:A:798:ALA:HB1 | 4:A:804:ILE:HD12 | 1.98 | 0.45 |
| 4:A:828:VAL:C | 4:A:830:GLU:H | 2.19 | 0.45 |
| 4:A:92:VAL:CG1 | 4:A:99:ARG:HG3 | 2.45 | 0.45 |
| 4:B:257:ARG:HG2 | 4:B:257:ARG:NH1 | 2.30 | 0.45 |
| 4:B:279:THR:O | 4:B:279:THR:HG23 | 2.15 | 0.45 |
| 4:B:373:ALA:O | 4:B:377:TRP:CD1 | 2.70 | 0.45 |
| 4:B:384:VAL:O | 4:B:384:VAL:HG12 | 2.16 | 0.45 |
| 4:C:110:LYS:O | 4:C:114:VAL:HG23 | 2.16 | 0.45 |
| 4:C:334:VAL:O | 4:C:337:VAL:HB | 2.16 | 0.45 |
| 4:C:432:PHE:HE1 | 4:C:440:THR:HG23 | 1.81 | 0.45 |
| 4:C:437:ASN:ND2 | 4:C:440:THR:H | 2.13 | 0.45 |
| 4:C:548:ALA:C | 4:C:550:LEU:H | 2.19 | 0.45 |
| 4:C:882:PHE:O | 4:C:883:ALA:CB | 2.64 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:501:TRP:HA | 4:D:504:GLU:OE2 | 2.16 | 0.45 |
| 4:D:705:LEU:HB3 | 4:D:857:GLN:HE22 | 1.78 | 0.45 |
| 1:E:4:DA:H2'' | 1:E:5:DA:OP2 | 2.15 | 0.45 |
| 1:H:9:DA:H62 | 3:J:1:DG:H22 | 1.64 | 0.45 |
| 1:K:2:DG:H2'' | 1:K:3:DG:C8 | 2.52 | 0.45 |
| 2:L:1:G:C2 | 2:L:2:C:C2 | 3.04 | 0.45 |
| 4:A:113:ALA:O | 4:A:114:VAL:C | 2.54 | 0.45 |
| 4:A:153:ARG:HD2 | 7:A:3089:HOH:O | 2.17 | 0.45 |
| 4:A:261:LEU:O | 4:A:263:GLY:N | 2.50 | 0.45 |
| 4:A:416:PHE:HA | 4:A:417:PRO:HD2 | 1.75 | 0.45 |
| 4:B:552:ASP:HB3 | 4:B:691:ALA:HB2 | 1.99 | 0.45 |
| 4:C:556:GLY:HA3 | 4:C:561:LEU:HD22 | 1.91 | 0.45 |
| 4:C:567:VAL:HG12 | 4:C:567:VAL:O | 2.15 | 0.45 |
| 4:C:656:GLN:H | 4:C:657:PRO:HD2 | 1.78 | 0.45 |
| 4:D:126:LEU:HD11 | 4:D:227:VAL:HG12 | 1.97 | 0.45 |
| 4:D:47:GLY:HA3 | 4:D:265:SER:O | 2.16 | 0.45 |
| 4:D:342:THR:CG2 | 4:D:348:PRO:HG2 | 2.41 | 0.45 |
| 4:D:440:THR:O | 4:D:444:LEU:HD12 | 2.16 | 0.45 |
| 4:D:656:GLN:N | 4:D:657:PRO:CD | 2.77 | 0.45 |
| 4:D:696:MET:O | 4:D:700:LYS:HB2 | 2.16 | 0.45 |
| 4:D:704:LYS:HE3 | 4:D:860:LYS:NZ | 2.32 | 0.45 |
| 4:D:709:GLU:O | 4:D:711:LYS:HG3 | 2.16 | 0.45 |
| 1:H:14:DG:H8 | 1:H:14:DG:H5' | 1.82 | 0.45 |
| 4:A:145:ILE:H | 4:A:145:ILE:HG12 | 1.55 | 0.45 |
| 4:A:281:ILE:HG13 | 4:A:309:GLU:HG2 | 1.98 | 0.45 |
| 4:B:232:GLN:HG3 | 4:B:243:THR:HG23 | 1.98 | 0.45 |
| 4:B:314:PRO:C | 4:B:316:VAL:H | 2.20 | 0.45 |
| 4:B:577:LYS:O | 4:B:580:GLU:HB2 | 2.16 | 0.45 |
| 4:B:690:VAL:C | 4:B:693:VAL:HG23 | 2.36 | 0.45 |
| 4:B:698:TRP:O | 4:B:699:LEU:C | 2.54 | 0.45 |
| 4:B:770:ASP:OD2 | 4:B:773:LYS:HD2 | 2.17 | 0.45 |
| 4:C:425:ARG:NH2 | 4:C:787:ASP:OD2 | 2.49 | 0.45 |
| 4:C:433:ASN:C | 7:C:3164:HOH:O | 2.52 | 0.45 |
| 4:D:669:GLN:HG3 | 4:D:672:GLN:HE21 | 1.80 | 0.45 |
| 1:E:2:DG:C2 | 7:E:42:HOH:O | 2.56 | 0.45 |
| 4:A:112:GLU:H | 4:A:112:GLU:CD | 2.19 | 0.45 |
| 4:A:278:TRP:CD2 | 4:A:284:GLY:HA3 | 2.49 | 0.45 |
| 4:A:462:ILE:HG22 | 4:A:463:HIS:N | 2.31 | 0.45 |
| 4:A:664:GLY:O | 4:A:667:PHE:HB2 | 2.17 | 0.45 |
| 4:B:167:GLU:O | 4:B:168:GLU:C | 2.54 | 0.45 |
| 4:B:225:GLY:HA2 | 7:B:3035:HOH:O | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:B:685:VAL:O | 4:B:687:VAL:N | 2.49 | 0.45 |
| 4:C:164:LYS:N | 4:C:164:LYS:NZ | 2.64 | 0.45 |
| 2:L:4:G:H1' | 4:C:389:LYS:HZ1 | 1.80 | 0.45 |
| 4:C:814:PHE:CE1 | 4:C:883:ALA:HB1 | 2.52 | 0.45 |
| 4:D:322:ILE:HG21 | 7:D:3013:HOH:O | 2.16 | 0.45 |
| 4:D:42:GLU:O | 4:D:45:GLU:N | 2.50 | 0.45 |
| 3:J:5:DA:C2' | 3:J:6:DT:H72 | 2.47 | 0.45 |
| 4:A:109:ILE:HG13 | 4:A:149:ALA:CB | 2.46 | 0.45 |
| 4:A:208:ASP:OD2 | 4:A:208:ASP:N | 2.50 | 0.45 |
| 4:A:330:ILE:HA | 4:A:330:ILE:HD13 | 1.39 | 0.45 |
| 4:A:416:PHE:CZ | 4:A:434:PRO:HD3 | 2.51 | 0.45 |
| 4:A:518:TYR:HD1 | 4:A:518:TYR:O | 1.98 | 0.45 |
| 4:A:148:GLU:OE2 | 4:A:749:LEU:HB2 | 2.15 | 0.45 |
| 4:A:746:ARG:NH1 | 4:A:754:GLN:H | 2.11 | 0.45 |
| 4:A:423:ARG:O | 4:A:785:SER:HB2 | 2.16 | 0.45 |
| 4:B:404:GLN:HE21 | 4:B:404:GLN:HB2 | 1.35 | 0.45 |
| 4:B:436:GLY:O | 4:B:441:LYS:HE2 | 2.15 | 0.45 |
| 4:B:552:ASP:CB | 4:B:691:ALA:HB2 | 2.46 | 0.45 |
| 4:B:6:ILE:C | 4:B:8:LYS:H | 2.19 | 0.45 |
| 4:C:140:ALA:O | 4:C:141:ILE:C | 2.55 | 0.45 |
| 7:M:542:HOH:O | 4:C:164:LYS:HB3 | 2.16 | 0.45 |
| 4:D:316:VAL:HG22 | 4:D:731:ASP:OD2 | 2.15 | 0.45 |
| 4:D:322:ILE:HD13 | 4:D:322:ILE:HA | 1.79 | 0.45 |
| 4:D:448:LYS:HZ2 | 4:D:806:SER:CB | 2.29 | 0.45 |
| 4:D:6:ILE:O | 4:D:8:LYS:N | 2.39 | 0.45 |
| 1:K:12:DT:N3 | 1:K:13:DC:C5 | 2.85 | 0.45 |
| 1:K:16:DC:H2'' | 1:K:17:DG:O5' | 2.15 | 0.45 |
| 4:A:385:TYR:CD2 | 4:A:385:TYR:C | 2.90 | 0.45 |
| 4:A:778:ILE:O | 4:A:779:ALA:C | 2.54 | 0.45 |
| 4:A:849:PHE:O | 4:A:850:ALA:C | 2.55 | 0.45 |
| 4:B:334:VAL:CG1 | 4:B:443:LEU:HD23 | 2.46 | 0.45 |
| 4:B:36:GLN:HB3 | 4:B:37:LEU:HD12 | 1.97 | 0.45 |
| 4:B:402:LEU:HA | 4:B:402:LEU:HD23 | 1.45 | 0.45 |
| 4:B:418:TYR:HE1 | 7:B:3028:HOH:O | 1.99 | 0.45 |
| 4:B:455:GLU:O | 4:B:458:TYR:HB3 | 2.16 | 0.45 |
| 1:H:9:DA:C6 | 4:B:644:PHE:CE1 | 3.04 | 0.45 |
| 4:B:726:HIS:HB2 | 4:B:736:TRP:CD1 | 2.52 | 0.45 |
| 4:B:804:ILE:HG22 | 4:B:807:PHE:CE2 | 2.52 | 0.45 |
| 4:B:459:TRP:HH2 | 4:B:825:PHE:CE2 | 2.34 | 0.45 |
| 4:C:279:THR:CG2 | 7:C:3038:HOH:O | 2.59 | 0.45 |
| 4:D:220:LEU:HD21 | 4:D:226:MET:HE2 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:633:SER:HA | 4:D:649:GLN:HE22 | 1.82 | 0.45 |
| 4:D:84:ARG:HH11 | 4:D:84:ARG:HA | 1.80 | 0.45 |
| 4:D:859:ASP:OD2 | 4:D:860:LYS:N | 2.50 | 0.45 |
| 4:A:318:LYS:O | 4:A:319:ALA:C | 2.55 | 0.45 |
| 4:A:421:ASP:C | 4:A:423:ARG:N | 2.70 | 0.45 |
| 4:A:473:VAL:HG13 | 4:A:473:VAL:O | 2.17 | 0.45 |
| 4:B:19:ILE:O | 4:B:21:PHE:N | 2.42 | 0.45 |
| 4:B:486:HIS:ND1 | 4:B:486:HIS:C | 2.71 | 0.45 |
| 4:B:620:TRP:CH2 | 4:B:677:MET:HE3 | 2.52 | 0.45 |
| 4:C:161:HIS:C | 4:C:163:LYS:H | 2.20 | 0.45 |
| 4:C:269:GLN:HB3 | 4:C:269:GLN:HE21 | 1.56 | 0.45 |
| 4:D:246:LEU:HD23 | 4:D:247:ALA:O | 2.17 | 0.45 |
| 4:D:462:ILE:HD12 | 4:D:475:PHE:HD1 | 1.82 | 0.45 |
| 4:D:702:ALA:O | 4:D:703:ALA:C | 2.55 | 0.45 |
| 1:H:15:DC:H3' | 7:H:334:HOH:O | 2.16 | 0.45 |
| 4:A:786:GLN:O | 4:A:787:ASP:C | 2.54 | 0.45 |
| 4:B:205:HIS:O | 4:B:207:GLU:N | 2.50 | 0.45 |
| 4:B:400:PHE:O | 4:B:401:MET:C | 2.50 | 0.45 |
| 4:B:419:ASN:O | 4:B:420:MET:CG | 2.65 | 0.45 |
| 1:H:10:DT:H5' | 4:B:641:SER:H | 1.79 | 0.45 |
| 4:C:287:TRP:O | 4:C:288:ALA:O | 2.35 | 0.45 |
| 4:C:507:SER:HA | 4:C:508:PRO:HD2 | 1.62 | 0.45 |
| 4:C:849:PHE:O | 4:C:852:GLN:HB2 | 2.17 | 0.45 |
| 4:D:5:ASN:HA | 4:D:52:ARG:NH1 | 2.32 | 0.45 |
| 4:D:829:ARG:HH12 | 4:D:883:ALA:H | 1.64 | 0.45 |
| 3:G:4:DG:H2'' | 3:G:5:DA:H8 | 1.81 | 0.45 |
| 1:N:10:DT:H5' | 4:D:641:SER:CB | 2.46 | 0.45 |
| 4:A:8:LYS:O | 4:A:12:SER:HB2 | 2.16 | 0.45 |
| 4:A:60:LYS:HG3 | 7:A:3023:HOH:O | 2.16 | 0.45 |
| 4:A:688:THR:CG2 | 4:A:689:VAL:HG13 | 2.30 | 0.45 |
| 4:A:802:TYR:C | 4:A:804:ILE:H | 2.17 | 0.45 |
| 4:B:267:MET:HB3 | 4:B:267:MET:HE3 | 1.83 | 0.45 |
| 4:B:345:LYS:HZ1 | 4:B:351:ASP:N | 2.13 | 0.45 |
| 4:B:50:ARG:HH11 | 4:B:50:ARG:HG2 | 1.82 | 0.45 |
| 4:B:549:MET:HE1 | 4:B:841:VAL:HG21 | 1.96 | 0.45 |
| 4:C:323:ALA:O | 4:C:324:GLN:C | 2.55 | 0.45 |
| 4:C:329:LYS:HG3 | 4:C:445:THR:HG22 | 1.99 | 0.45 |
| 4:C:3:THR:HB | 4:C:52:ARG:CZ | 2.46 | 0.45 |
| 4:C:432:PHE:CE1 | 4:C:440:THR:HG23 | 2.51 | 0.45 |
| 4:C:553:GLU:CG | 4:C:554:VAL:N | 2.80 | 0.45 |
| 4:D:331:ASN:ND2 | 4:D:334:VAL:HG23 | 2.32 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:402:LEU:HD21 | 4:D:439:MET:HE3 | 1.99 | 0.45 |
| 4:D:439:MET:CE | 4:D:443:LEU:HD11 | 2.47 | 0.45 |
| 4:D:502:TRP:CE3 | 4:D:503:ALA:N | 2.85 | 0.45 |
| 4:D:816:THR:HG22 | 4:D:817:ILE:N | 2.32 | 0.45 |
| 1:E:6:DT:H2' | 1:E:6:DT:H6 | 1.55 | 0.45 |
| 1:H:15:DC:N3 | 1:H:16:DC:C5 | 2.85 | 0.45 |
| 4:A:47:GLY:HA3 | 4:A:265:SER:O | 2.18 | 0.44 |
| 4:A:474:PRO:C | 4:A:476:PRO:HD2 | 2.37 | 0.44 |
| 4:A:554:VAL:O | 4:A:557:ARG:HB3 | 2.17 | 0.44 |
| 4:B:138:ALA:O | 4:B:213:GLY:HA3 | 2.17 | 0.44 |
| 4:B:164:LYS:N | 4:B:164:LYS:HZ3 | 2.15 | 0.44 |
| 4:B:347:CYS:HB3 | 4:B:350:GLU:HG3 | 1.99 | 0.44 |
| 4:B:532:LEU:HG | 4:B:533:PRO:CD | 2.47 | 0.44 |
| 4:B:571:TYR:H | 4:B:571:TYR:HD1 | 1.65 | 0.44 |
| 4:B:579:ASN:HA | 4:B:582:LEU:HB2 | 1.98 | 0.44 |
| 4:B:643:GLU:HG3 | 4:B:682:TRP:HB3 | 1.99 | 0.44 |
| 4:C:488:ASN:O | 4:C:491:ALA:HB3 | 2.16 | 0.44 |
| 4:C:651:LEU:C | 4:C:651:LEU:CD1 | 2.86 | 0.44 |
| 4:C:845:PHE:O | 4:C:848:GLN:CB | 2.57 | 0.44 |
| 4:D:729:THR:HG23 | 4:D:733:PHE:O | 2.17 | 0.44 |
| 4:A:19:ILE:HA | 4:A:19:ILE:HD13 | 1.89 | 0.44 |
| 4:A:205:HIS:C | 4:A:207:GLU:N | 2.70 | 0.44 |
| 4:A:572:GLY:O | 4:A:575:ALA:HB3 | 2.18 | 0.44 |
| 4:B:194:GLY:O | 4:B:195:LEU:C | 2.56 | 0.44 |
| 4:B:404:GLN:HG3 | 4:B:404:GLN:O | 2.17 | 0.44 |
| 4:B:416:PHE:HD1 | 4:B:430:SER:OG | 2.01 | 0.44 |
| 4:B:570:ILE:HA | 4:B:573:ILE:HG22 | 1.98 | 0.44 |
| 4:B:640:GLY:O | 4:B:641:SER:O | 2.36 | 0.44 |
| 4:B:643:GLU:HG3 | 4:B:682:TRP:CB | 2.47 | 0.44 |
| 4:B:784:HIS:C | 4:B:786:GLN:N | 2.69 | 0.44 |
| 4:C:210:ILE:O | 4:C:214:VAL:CG2 | 2.63 | 0.44 |
| 4:C:313:MET:O | 4:C:317:TYR:CD2 | 2.70 | 0.44 |
| 4:C:323:ALA:O | 4:C:325:ASN:N | 2.49 | 0.44 |
| 4:C:460:LEU:O | 4:C:514:PHE:CE2 | 2.70 | 0.44 |
| 4:C:71:LYS:N | 4:C:72:PRO:CD | 2.81 | 0.44 |
| 4:D:133:THR:C | 4:D:135:GLN:N | 2.71 | 0.44 |
| 4:D:340:VAL:O | 4:D:343:LYS:HG2 | 2.17 | 0.44 |
| 4:D:345:LYS:O | 4:D:346:HIS:C | 2.51 | 0.44 |
| 4:D:511:PHE:O | 4:D:514:PHE:HB3 | 2.16 | 0.44 |
| 4:D:631:LYS:HD2 | 4:D:632:ARG:NH1 | 2.32 | 0.44 |
| 4:A:417:PRO:C | 4:A:418:TYR:HD1 | 2.21 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:A:505:GLN:O | 4:A:506:ASP:C | 2.51 | 0.44 |
| 4:A:333:LYS:HB3 | 4:A:516:PHE:CE2 | 2.52 | 0.44 |
| 4:A:56:GLU:HB2 | 7:A:3057:HOH:O | 2.17 | 0.44 |
| 4:A:746:ARG:NH1 | 4:A:746:ARG:HB3 | 2.32 | 0.44 |
| 4:A:739:TYR:CD2 | 4:A:773:LYS:HB3 | 2.52 | 0.44 |
| 4:B:473:VAL:HG12 | 4:B:474:PRO:O | 2.18 | 0.44 |
| 4:B:685:VAL:C | 4:B:687:VAL:N | 2.70 | 0.44 |
| 4:B:701:SER:O | 4:B:702:ALA:C | 2.55 | 0.44 |
| 4:C:14:ILE:HG22 | 4:C:14:ILE:O | 2.18 | 0.44 |
| 4:C:155:ARG:CG | 4:C:155:ARG:O | 2.65 | 0.44 |
| 4:C:617:ALA:O | 4:C:621:LEU:HG | 2.18 | 0.44 |
| 4:C:620:TRP:CZ3 | 4:C:667:PHE:HZ | 2.35 | 0.44 |
| 4:D:306:MET:C | 4:D:308:TYR:N | 2.70 | 0.44 |
| 4:D:327:ALA:CA | 4:D:415:TRP:NE1 | 2.81 | 0.44 |
| 4:D:443:LEU:H | 4:D:443:LEU:HD23 | 1.81 | 0.44 |
| 4:D:706:LEU:HD21 | 4:D:849:PHE:CD2 | 2.53 | 0.44 |
| 4:A:42:GLU:C | 4:A:46:MET:HE2 | 2.38 | 0.44 |
| 4:A:308:TYR:OH | 4:A:733:PHE:CE2 | 2.70 | 0.44 |
| 4:A:788:GLY:O | 4:A:789:SER:C | 2.56 | 0.44 |
| 4:A:846:TYR:HD1 | 4:A:850:ALA:HB2 | 1.82 | 0.44 |
| 4:B:169:GLN:HB3 | 4:B:169:GLN:HE21 | 1.51 | 0.44 |
| 4:B:19:ILE:HD13 | 4:B:20:PRO:HD2 | 1.98 | 0.44 |
| 4:B:430:SER:OG | 4:B:432:PHE:O | 2.34 | 0.44 |
| 4:B:460:LEU:CA | 4:B:534:LEU:HD11 | 2.48 | 0.44 |
| 4:B:570:ILE:O | 4:B:570:ILE:CG1 | 2.59 | 0.44 |
| 4:B:609:VAL:O | 4:B:609:VAL:HG22 | 2.17 | 0.44 |
| 4:B:626:THR:C | 4:B:628:SER:N | 2.70 | 0.44 |
| 4:C:536:PHE:HB3 | 4:C:882:PHE:HB2 | 1.94 | 0.44 |
| 4:C:728:VAL:CG2 | 4:C:734:PRO:HB3 | 2.47 | 0.44 |
| 4:D:300:HIS:HA | 7:D:3088:HOH:O | 2.17 | 0.44 |
| 4:D:326:THR:C | 4:D:415:TRP:CD1 | 2.91 | 0.44 |
| 4:D:49:ALA:O | 4:D:52:ARG:HB2 | 2.17 | 0.44 |
| 4:D:502:TRP:CZ3 | 4:D:503:ALA:HB2 | 2.52 | 0.44 |
| 4:D:795:VAL:HG12 | 7:D:3013:HOH:O | 2.18 | 0.44 |
| 4:D:857:GLN:C | 4:D:859:ASP:N | 2.70 | 0.44 |
| 2:F:4:G:H4' | 4:A:389:LYS:HD3 | 1.99 | 0.44 |
| 1:K:15:DC:H2'' | 1:K:16:DC:C5' | 2.46 | 0.44 |
| 1:K:6:DT:H5' | 1:K:6:DT:C6 | 2.52 | 0.44 |
| 4:A:631:LYS:NZ | 6:A:2000:APC:O2A | 2.39 | 0.44 |
| 4:A:286:TYR:CD2 | 4:A:286:TYR:N | 2.86 | 0.44 |
| 4:A:400:PHE:O | 4:A:401:MET:O | 2.36 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:A:60:LYS:NZ | 4:A:61:ALA:HB2 | 2.22 | 0.44 |
| 4:A:697:ASN:O | 4:A:698:TRP:C | 2.55 | 0.44 |
| 4:A:86:ASN:HD22 | 4:A:86:ASN:N | 2.15 | 0.44 |
| 4:B:273:VAL:C | 4:B:274:PRO:O | 2.56 | 0.44 |
| 4:B:340:VAL:O | 4:B:343:LYS:HG3 | 2.17 | 0.44 |
| 4:B:421:ASP:OD2 | 4:B:425:ARG:HB2 | 2.17 | 0.44 |
| 4:B:665:LEU:HD23 | 4:B:665:LEU:HA | 1.82 | 0.44 |
| 4:B:823:ASN:C | 4:B:825:PHE:N | 2.70 | 0.44 |
| 4:C:305:LEU:C | 4:C:305:LEU:CD2 | 2.86 | 0.44 |
| 4:D:482:ILE:HD12 | 4:D:514:PHE:HZ | 1.83 | 0.44 |
| 4:D:646:PHE:HA | 4:D:649:GLN:OE1 | 2.17 | 0.44 |
| 1:H:15:DC:OP1 | 7:H:313:HOH:O | 2.21 | 0.44 |
| 4:A:16:LEU:HA | 4:A:37:LEU:CD2 | 2.46 | 0.44 |
| 4:A:264:ILE:O | 4:A:264:ILE:HG22 | 2.18 | 0.44 |
| 4:A:699:LEU:O | 4:A:702:ALA:HB3 | 2.18 | 0.44 |
| 4:A:710:VAL:HG13 | 4:A:710:VAL:O | 2.18 | 0.44 |
| 4:A:794:THR:OG1 | 4:A:831:THR:CG2 | 2.48 | 0.44 |
| 4:A:797:TRP:CZ3 | 4:A:801:LYS:HB2 | 2.52 | 0.44 |
| 4:B:278:TRP:CZ3 | 4:B:284:GLY:CA | 2.99 | 0.44 |
| 4:B:329:LYS:O | 4:B:445:THR:HG23 | 2.17 | 0.44 |
| 4:B:460:LEU:HA | 4:B:534:LEU:HD11 | 1.99 | 0.44 |
| 4:B:512:LEU:O | 4:B:514:PHE:N | 2.51 | 0.44 |
| 4:B:556:GLY:O | 4:B:558:ALA:N | 2.51 | 0.44 |
| 4:B:737:GLN:C | 4:B:774:GLN:HE22 | 2.21 | 0.44 |
| 4:B:780:PRO:HD2 | 4:B:781:ASN:N | 2.31 | 0.44 |
| 4:B:796:VAL:HG21 | 7:B:3141:HOH:O | 2.18 | 0.44 |
| 4:C:270:PRO:HD2 | 4:C:408:PHE:CE2 | 2.53 | 0.44 |
| 4:C:291:ARG:HD2 | 7:C:3077:HOH:O | 2.17 | 0.44 |
| 4:C:307:ARG:HG3 | 4:C:307:ARG:HH11 | 1.82 | 0.44 |
| 4:C:571:TYR:HD1 | 4:C:634:VAL:HG11 | 1.83 | 0.44 |
| 4:C:69:ALA:HA | 4:C:257:ARG:HD2 | 1.99 | 0.44 |
| 4:C:308:TYR:CE2 | 4:C:734:PRO:O | 2.71 | 0.44 |
| 4:C:824:LEU:C | 4:C:824:LEU:HD12 | 2.37 | 0.44 |
| 4:D:14:ILE:HG21 | 4:D:288:ALA:CB | 2.48 | 0.44 |
| 4:D:338:ALA:C | 4:D:340:VAL:N | 2.70 | 0.44 |
| 4:D:486:HIS:NE2 | 4:D:490:MET:HG2 | 2.33 | 0.44 |
| 4:D:333:LYS:HZ1 | 4:D:516:PHE:HB3 | 1.83 | 0.44 |
| 4:D:611:LEU:HB2 | 4:D:616:LEU:HD21 | 2.00 | 0.44 |
| 4:D:870:LEU:HD23 | 4:D:871:ASN:N | 2.33 | 0.44 |
| 1:K:13:DC:C2' | 1:K:14:DG:H5' | 2.45 | 0.44 |
| 4:A:133:THR:O | 4:A:137:VAL:HG23 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:A:320:ILE:HG23 | 4:A:418:TYR:O | 2.18 | 0.44 |
| 4:B:170:LEU:C | 4:B:170:LEU:HD13 | 2.38 | 0.44 |
| 4:B:199:GLU:HG2 | 4:B:201:TRP:CD1 | 2.51 | 0.44 |
| 4:B:220:LEU:O | 4:B:223:SER:N | 2.46 | 0.44 |
| 4:B:269:GLN:NE2 | 4:B:407:LYS:HZ3 | 2.15 | 0.44 |
| 4:B:40:GLU:O | 4:B:43:SER:HB2 | 2.17 | 0.44 |
| 4:B:296:LEU:O | 4:B:420:MET:HE2 | 2.18 | 0.44 |
| 4:B:50:ARG:NH1 | 4:B:50:ARG:HG2 | 2.33 | 0.44 |
| 4:B:651:LEU:HA | 4:B:655:ILE:HD12 | 1.99 | 0.44 |
| 4:B:699:LEU:HD12 | 4:B:699:LEU:H | 1.82 | 0.44 |
| 4:C:685:VAL:O | 4:C:687:VAL:N | 2.51 | 0.44 |
| 4:D:14:ILE:CG2 | 4:D:288:ALA:CB | 2.91 | 0.44 |
| 4:D:743:ILE:HD12 | 4:D:766:ASP:HB3 | 2.00 | 0.44 |
| 4:D:804:ILE:H | 4:D:804:ILE:HG13 | 1.47 | 0.44 |
| 4:D:840:ASP:O | 4:D:841:VAL:C | 2.54 | 0.44 |
| 4:A:347:CYS:C | 4:A:349:VAL:N | 2.68 | 0.44 |
| 4:A:436:GLY:HA3 | 4:A:440:THR:CB | 2.48 | 0.44 |
| 4:A:462:ILE:O | 4:A:463:HIS:C | 2.55 | 0.44 |
| 4:A:578:VAL:O | 4:A:581:ILE:N | 2.50 | 0.44 |
| 4:A:802:TYR:H | 4:A:802:TYR:HD2 | 1.63 | 0.44 |
| 4:A:446:LEU:HD13 | 4:A:817:ILE:HG23 | 1.99 | 0.44 |
| 4:B:164:LYS:HZ3 | 4:B:164:LYS:H | 1.65 | 0.44 |
| 4:B:505:GLN:HG3 | 4:B:511:PHE:CD2 | 2.53 | 0.44 |
| 4:C:236:VAL:CG1 | 4:C:239:GLN:HB2 | 2.48 | 0.44 |
| 4:C:450:LYS:O | 4:C:529:ASN:HA | 2.18 | 0.44 |
| 4:C:550:LEU:O | 4:C:867:LYS:HG3 | 2.18 | 0.44 |
| 4:D:161:HIS:C | 4:D:163:LYS:N | 2.71 | 0.44 |
| 4:D:233:ASN:O | 4:D:236:VAL:HG23 | 2.17 | 0.44 |
| 4:D:523:HIS:C | 4:D:524:HIS:HD1 | 2.21 | 0.44 |
| 4:A:282:THR:OG1 | 4:A:283:GLY:N | 2.45 | 0.44 |
| 4:A:676:TYR:O | 4:A:678:ALA:N | 2.50 | 0.44 |
| 4:A:73:LEU:C | 4:A:75:THR:H | 2.20 | 0.44 |
| 4:B:227:VAL:HB | 4:B:245:GLU:O | 2.17 | 0.44 |
| 4:B:322:ILE:HD13 | 4:B:322:ILE:HA | 1.73 | 0.44 |
| 4:B:495:SER:N | 4:B:496:PRO:CD | 2.80 | 0.44 |
| 4:B:570:ILE:HG23 | 4:B:571:TYR:N | 2.32 | 0.44 |
| 4:B:752:LEU:HB2 | 4:B:753:GLY:H | 1.69 | 0.44 |
| 4:C:296:LEU:HD12 | 4:C:296:LEU:HA | 1.85 | 0.44 |
| 4:C:269:GLN:C | 4:C:430:SER:HB3 | 2.38 | 0.44 |
| 1:K:10:DT:H5' | 4:C:641:SER:HA | 1.99 | 0.44 |
| 4:C:832:MET:O | 4:C:833:VAL:C | 2.56 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:459:TRP:O | 4:D:462:ILE:N | 2.51 | 0.44 |
| 1:N:10:DT:H4' | 4:D:639:TYR:O | 2.17 | 0.44 |
| 4:D:778:ILE:O | 4:D:782:PHE:HB2 | 2.18 | 0.44 |
| 1:E:12:DT:C2 | 1:E:13:DC:C6 | 3.06 | 0.44 |
| 1:K:3:DG:H5' | 7:K:268:HOH:O | 2.17 | 0.44 |
| 4:A:78:LEU:CD1 | 4:A:119:ILE:HG13 | 2.48 | 0.43 |
| 4:A:215:ARG:NH1 | 4:A:218:GLU:OE2 | 2.47 | 0.43 |
| 4:A:226:MET:O | 4:A:247:ALA:CB | 2.66 | 0.43 |
| 4:A:286:TYR:HD2 | 4:A:286:TYR:H | 1.66 | 0.43 |
| 4:A:620:TRP:NE1 | 4:A:677:MET:HB2 | 2.33 | 0.43 |
| 4:A:713:LYS:O | 4:A:714:LYS:HD3 | 2.18 | 0.43 |
| 4:B:421:ASP:O | 4:B:422:TRP:C | 2.55 | 0.43 |
| 4:B:398:LEU:CD2 | 4:B:439:MET:CE | 2.96 | 0.43 |
| 4:B:556:GLY:O | 4:B:559:VAL:N | 2.51 | 0.43 |
| 4:B:616:LEU:O | 4:B:617:ALA:C | 2.56 | 0.43 |
| 4:B:84:ARG:NH1 | 4:B:84:ARG:O | 2.51 | 0.43 |
| 4:C:402:LEU:HD23 | 4:C:402:LEU:HA | 1.79 | 0.43 |
| 4:D:268:PHE:CD2 | 4:D:429:VAL:CG1 | 3.00 | 0.43 |
| 1:E:13:DC:H6 | 1:E:13:DC:H5' | 1.82 | 0.43 |
| 1:E:15:DC:H2' | 1:E:16:DC:C6 | 2.53 | 0.43 |
| 4:A:110:LYS:O | 4:A:113:ALA:HB3 | 2.18 | 0.43 |
| 4:A:276:LYS:O | 4:A:277:PRO:C | 2.57 | 0.43 |
| 4:A:388:ASP:O | 4:A:388:ASP:CG | 2.56 | 0.43 |
| 4:A:320:ILE:CG2 | 4:A:418:TYR:O | 2.67 | 0.43 |
| 4:A:804:ILE:HG23 | 4:A:816:THR:HG21 | 2.00 | 0.43 |
| 4:A:826:LYS:O | 4:A:827:ALA:C | 2.56 | 0.43 |
| 4:B:233:ASN:HB3 | 4:B:239:GLN:HB3 | 2.00 | 0.43 |
| 4:C:136:ALA:HA | 7:C:3021:HOH:O | 2.17 | 0.43 |
| 4:C:220:LEU:HD21 | 4:C:226:MET:CE | 2.49 | 0.43 |
| 4:C:317:TYR:C | 4:C:321:ASN:HD21 | 2.21 | 0.43 |
| 4:C:462:ILE:CD1 | 4:C:479:ILE:CD1 | 2.96 | 0.43 |
| 4:C:462:ILE:HG23 | 4:C:478:ARG:HD2 | 2.00 | 0.43 |
| 4:C:66:ASP:OD2 | 4:C:66:ASP:N | 2.51 | 0.43 |
| 4:C:721:LYS:HG2 | 4:C:722:ARG:H | 1.81 | 0.43 |
| 4:C:818:PRO:O | 4:C:821:ALA:HB3 | 2.18 | 0.43 |
| 4:C:706:LEU:HD11 | 4:C:849:PHE:CG | 2.54 | 0.43 |
| 4:C:698:TRP:NE1 | 4:C:864:LEU:HA | 2.33 | 0.43 |
| 4:D:422:TRP:O | 4:D:422:TRP:HD1 | 2.00 | 0.43 |
| 4:D:532:LEU:HA | 4:D:533:PRO:HD2 | 1.58 | 0.43 |
| 1:K:2:DG:N2 | 7:K:239:HOH:O | 2.50 | 0.43 |
| 1:K:7:DC:H6 | 1:K:7:DC:H2' | 1.47 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:A:125:CYS:O | 4:A:128:SER:HB3 | 2.18 | 0.43 |
| 4:A:320:ILE:HD12 | 4:A:320:ILE:HG23 | 1.74 | 0.43 |
| 4:A:521:VAL:O | 4:A:525:GLY:N | 2.51 | 0.43 |
| 4:A:647:ARG:HD2 | 4:A:675:GLY:CA | 2.25 | 0.43 |
| 4:A:780:PRO:O | 4:A:784:HIS:HB2 | 2.18 | 0.43 |
| 4:B:46:MET:CE | 4:B:269:GLN:HE22 | 2.30 | 0.43 |
| 4:B:459:TRP:O | 4:B:460:LEU:C | 2.56 | 0.43 |
| 4:B:556:GLY:C | 4:B:558:ALA:N | 2.72 | 0.43 |
| 4:B:582:LEU:HD23 | 4:B:582:LEU:HA | 1.86 | 0.43 |
| 4:C:231:ARG:CG | 4:C:234:ALA:HB2 | 2.42 | 0.43 |
| 4:C:532:LEU:HA | 4:C:533:PRO:HD2 | 1.77 | 0.43 |
| 4:C:541:SER:O | 4:C:542:GLY:C | 2.56 | 0.43 |
| 4:C:570:ILE:O | 4:C:573:ILE:HG23 | 2.18 | 0.43 |
| 4:C:592:ASN:ND2 | 4:C:611:LEU:CD2 | 2.81 | 0.43 |
| 4:C:727:TRP:CD2 | 4:C:735:VAL:CG1 | 3.01 | 0.43 |
| 4:C:737:GLN:O | 4:C:774:GLN:NE2 | 2.51 | 0.43 |
| 4:C:808:ALA:HB3 | 4:C:815:GLY:HA3 | 2.00 | 0.43 |
| 4:D:122:THR:HG21 | 4:D:226:MET:CE | 2.48 | 0.43 |
| 4:D:232:GLN:O | 4:D:233:ASN:C | 2.56 | 0.43 |
| 4:D:402:LEU:CD2 | 4:D:439:MET:HE3 | 2.48 | 0.43 |
| 4:D:379:ARG:HD3 | 4:D:660:ASP:OD2 | 2.18 | 0.43 |
| 4:D:794:THR:HA | 4:D:797:TRP:HB3 | 1.99 | 0.43 |
| 4:A:65:ALA:CB | 4:A:120:LYS:HG2 | 2.48 | 0.43 |
| 4:A:234:ALA:HA | 4:A:240:ASP:OD2 | 2.18 | 0.43 |
| 4:A:276:LYS:O | 4:A:277:PRO:O | 2.36 | 0.43 |
| 4:A:422:TRP:C | 4:A:422:TRP:CD1 | 2.91 | 0.43 |
| 4:A:651:LEU:HA | 4:A:655:ILE:HB | 1.99 | 0.43 |
| 4:A:820:ASP:OD1 | 4:A:820:ASP:N | 2.51 | 0.43 |
| 4:B:577:LYS:CB | 4:B:684:SER:HB3 | 2.47 | 0.43 |
| 4:B:86:ASN:ND2 | 7:B:3033:HOH:O | 2.37 | 0.43 |
| 4:C:298:ARG:HG3 | 4:C:420:MET:O | 2.17 | 0.43 |
| 4:C:308:TYR:HA | 4:C:311:VAL:CG2 | 2.48 | 0.43 |
| 4:C:306:MET:C | 4:C:308:TYR:H | 2.20 | 0.43 |
| 4:C:646:PHE:O | 4:C:647:ARG:C | 2.56 | 0.43 |
| 4:C:68:ALA:O | 4:C:257:ARG:HD2 | 2.17 | 0.43 |
| 4:D:169:GLN:HB3 | 4:D:182:PHE:CZ | 2.53 | 0.43 |
| 4:D:545:HIS:O | 4:D:549:MET:HG2 | 2.18 | 0.43 |
| 4:D:744:GLN:HA | 4:D:756:ARG:NH2 | 2.33 | 0.43 |
| 4:D:825:PHE:O | 4:D:828:VAL:CG2 | 2.67 | 0.43 |
| 4:D:829:ARG:HB3 | 4:D:876:LEU:HD23 | 2.00 | 0.43 |
| 1:K:11:DA:N1 | 1:K:12:DT:C4 | 2.86 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:A:204:TRP:CZ3 | 4:A:212:VAL:HG21 | 2.50 | 0.43 |
| 4:A:51:PHE:HZ | 4:A:261:LEU:HD23 | 1.83 | 0.43 |
| 4:A:643:GLU:OE2 | 4:A:679:LYS:CA | 2.67 | 0.43 |
| 4:B:324:GLN:HE21 | 4:B:417:PRO:HA | 1.84 | 0.43 |
| 4:B:394:ARG:HB2 | 4:B:394:ARG:HE | 1.49 | 0.43 |
| 4:B:307:ARG:HD3 | 4:B:736:TRP:CD2 | 2.52 | 0.43 |
| 4:C:47:GLY:CA | 4:C:265:SER:O | 2.59 | 0.43 |
| 4:C:374:LEU:C | 4:C:376:ALA:H | 2.22 | 0.43 |
| 4:C:269:GLN:C | 4:C:430:SER:CB | 2.87 | 0.43 |
| 4:C:452:ILE:CG1 | 4:C:457:TYR:N | 2.81 | 0.43 |
| 4:C:696:MET:O | 4:C:700:LYS:HB2 | 2.18 | 0.43 |
| 4:C:755:PHE:N | 4:C:755:PHE:HD1 | 2.16 | 0.43 |
| 4:C:778:ILE:HD12 | 4:C:778:ILE:HA | 1.65 | 0.43 |
| 4:D:401:MET:HG3 | 4:D:440:THR:OG1 | 2.19 | 0.43 |
| 4:D:461:LYS:HE3 | 4:D:479:ILE:HG23 | 2.00 | 0.43 |
| 4:D:554:VAL:O | 4:D:557:ARG:HB3 | 2.19 | 0.43 |
| 4:D:743:ILE:HG22 | 4:D:743:ILE:O | 2.19 | 0.43 |
| 4:D:830:GLU:HG2 | 4:D:876:LEU:HD22 | 2.00 | 0.43 |
| 4:A:147:ASP:HB3 | 4:A:750:MET:HE1 | 2.01 | 0.43 |
| 4:A:73:LEU:HD11 | 4:A:254:ILE:HG13 | 2.00 | 0.43 |
| 4:A:77:LEU:C | 4:A:79:PRO:HD2 | 2.39 | 0.43 |
| 4:B:306:MET:O | 4:B:308:TYR:N | 2.52 | 0.43 |
| 4:B:341:ILE:O | 4:B:343:LYS:N | 2.51 | 0.43 |
| 4:B:831:THR:HG23 | 4:B:832:MET:N | 2.33 | 0.43 |
| 4:C:248:PRO:HD2 | 4:C:249:GLU:OE2 | 2.19 | 0.43 |
| 4:C:50:ARG:NH1 | 4:C:267:MET:HE3 | 2.33 | 0.43 |
| 4:C:397:SER:O | 4:C:398:LEU:C | 2.56 | 0.43 |
| 4:C:485:ASN:OD1 | 4:C:485:ASN:N | 2.51 | 0.43 |
| 4:C:563:PRO:HD3 | 4:C:874:ASP:O | 2.19 | 0.43 |
| 4:D:276:LYS:O | 4:D:277:PRO:C | 2.56 | 0.43 |
| 4:D:489:ILE:HG13 | 4:D:489:ILE:H | 1.40 | 0.43 |
| 4:D:472:LYS:CG | 4:D:567:VAL:HG11 | 2.49 | 0.43 |
| 4:D:837:GLU:HG2 | 4:D:872:LEU:HD12 | 2.01 | 0.43 |
| 1:H:9:DA:H2" | 1:H:10:DT:OP1 | 2.18 | 0.43 |
| 4:A:109:ILE:O | 4:A:110:LYS:C | 2.55 | 0.43 |
| 4:A:122:THR:O | 4:A:126:LEU:HG | 2.19 | 0.43 |
| 4:A:178:TYR:O | 4:A:181:ALA:HB3 | 2.18 | 0.43 |
| 4:A:274:PRO:HA | 4:A:275:PRO:HD3 | 1.89 | 0.43 |
| 4:A:308:TYR:HA | 4:A:311:VAL:HG23 | 1.99 | 0.43 |
| 4:A:344:TRP:O | 4:A:345:LYS:CB | 2.66 | 0.43 |
| 4:A:461:LYS:HE3 | 4:A:479:ILE:CG2 | 2.48 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:A:465:ALA:HB2 | 4:A:482:ILE:HD11 | 2.00 | 0.43 |
| 4:A:502:TRP:CE2 | 4:A:512:LEU:CD1 | 2.97 | 0.43 |
| 4:A:545:HIS:H | 4:A:545:HIS:CD2 | 2.36 | 0.43 |
| 4:A:549:MET:HB3 | 4:A:836:TYR:CE1 | 2.51 | 0.43 |
| 4:A:635:MET:HE1 | 6:A:2000:APC:C3' | 2.49 | 0.43 |
| 4:A:459:TRP:NE1 | 4:A:822:ALA:HA | 2.29 | 0.43 |
| 4:A:8:LYS:HB3 | 4:A:9:ASN:H | 1.49 | 0.43 |
| 4:B:400:PHE:C | 4:B:400:PHE:CD1 | 2.91 | 0.43 |
| 4:B:407:LYS:CG | 4:B:408:PHE:HE2 | 2.27 | 0.43 |
| 4:B:416:PHE:CD1 | 4:B:430:SER:OG | 2.71 | 0.43 |
| 4:B:504:GLU:C | 4:B:505:GLN:O | 2.56 | 0.43 |
| 4:B:78:LEU:N | 4:B:79:PRO:HD2 | 2.34 | 0.43 |
| 4:B:435:GLN:HG2 | 4:B:810:ILE:HG12 | 2.00 | 0.43 |
| 4:C:502:TRP:O | 4:C:504:GLU:N | 2.51 | 0.43 |
| 4:C:555:GLY:O | 4:C:556:GLY:C | 2.57 | 0.43 |
| 4:D:21:PHE:CE1 | 4:D:25:ALA:HB2 | 2.54 | 0.43 |
| 4:D:485:ASN:O | 4:D:486:HIS:C | 2.57 | 0.43 |
| 4:D:452:ILE:HG22 | 4:D:528:TYR:O | 2.18 | 0.43 |
| 4:D:583:GLN:HB3 | 7:D:3135:HOH:O | 2.19 | 0.43 |
| 4:D:78:LEU:O | 4:D:82:ILE:HG13 | 2.18 | 0.43 |
| 4:D:95:LYS:HE3 | 7:D:3065:HOH:O | 2.17 | 0.43 |
| 3:J:5:DA:H2'' | 3:J:6:DT:C7 | 2.48 | 0.43 |
| 2:L:5:C:H5'' | 4:C:390:ALA:HB1 | 2.01 | 0.43 |
| 4:A:396:ILE:HG23 | 4:A:396:ILE:HD12 | 1.65 | 0.43 |
| 4:A:402:LEU:HG | 4:A:439:MET:HE3 | 2.01 | 0.43 |
| 4:A:793:LYS:CA | 4:A:796:VAL:HG23 | 2.48 | 0.43 |
| 4:B:13:ASP:OD1 | 4:B:14:ILE:N | 2.51 | 0.43 |
| 4:B:163:LYS:HA | 4:B:166:VAL:HG23 | 2.00 | 0.43 |
| 4:B:220:LEU:C | 4:B:222:GLU:N | 2.70 | 0.43 |
| 4:B:233:ASN:ND2 | 4:B:239:GLN:CD | 2.70 | 0.43 |
| 4:B:865:PRO:HA | 7:B:3135:HOH:O | 2.19 | 0.43 |
| 4:C:105:PHE:C | 4:C:107:GLN:N | 2.70 | 0.43 |
| 4:C:246:LEU:HD12 | 4:C:247:ALA:H | 1.83 | 0.43 |
| 4:C:412:LYS:O | 4:C:413:ALA:HB2 | 2.19 | 0.43 |
| 4:C:70:ALA:O | 4:C:73:LEU:HB2 | 2.18 | 0.43 |
| 4:C:846:TYR:O | 4:C:847:ASP:C | 2.57 | 0.43 |
| 4:C:881:ALA:O | 4:C:883:ALA:OXT | 2.37 | 0.43 |
| 4:D:159:ALA:CB | 4:D:163:LYS:HD3 | 2.49 | 0.43 |
| 4:D:419:ASN:HB3 | 4:D:420:MET:H | 1.53 | 0.43 |
| 4:D:741:LYS:HA | 4:D:742:PRO:HD3 | 1.79 | 0.43 |
| 4:D:744:GLN:NE2 | 4:D:756:ARG:H | 2.16 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:A:78:LEU:HD13 | 4:A:119:ILE:HG13 | 2.00 | 0.43 |
| 4:A:201:TRP:O | 4:A:204:TRP:HB2 | 2.19 | 0.43 |
| 4:A:219:MET:O | 4:A:222:GLU:HB3 | 2.19 | 0.43 |
| 4:A:525:GLY:O | 4:A:526:LEU:C | 2.57 | 0.43 |
| 4:A:57:ARG:HA | 4:A:60:LYS:HB3 | 2.01 | 0.43 |
| 4:A:615:ALA:O | 4:A:618:GLY:N | 2.51 | 0.43 |
| 4:A:630:THR:O | 4:A:631:LYS:C | 2.55 | 0.43 |
| 4:B:109:ILE:H | 4:B:109:ILE:HD12 | 1.78 | 0.43 |
| 4:B:122:THR:HG22 | 4:B:226:MET:HE1 | 2.01 | 0.43 |
| 4:B:261:LEU:HD12 | 4:B:261:LEU:HA | 1.81 | 0.43 |
| 4:B:421:ASP:OD1 | 4:B:424:GLY:N | 2.50 | 0.43 |
| 4:B:437:ASN:O | 4:B:441:LYS:HG2 | 2.19 | 0.43 |
| 4:B:61:ALA:C | 4:B:63:GLU:N | 2.71 | 0.43 |
| 4:B:724:ALA:HB2 | 4:B:738:GLU:HG3 | 2.00 | 0.43 |
| 4:B:455:GLU:HG2 | 4:B:822:ALA:HB2 | 2.00 | 0.43 |
| 4:C:120:LYS:HG3 | 4:C:752:LEU:CD1 | 2.46 | 0.43 |
| 4:C:289:ASN:HB2 | 7:C:3014:HOH:O | 2.17 | 0.43 |
| 4:C:308:TYR:O | 4:C:309:GLU:C | 2.56 | 0.43 |
| 4:C:373:ALA:O | 4:C:377:TRP:CD1 | 2.71 | 0.43 |
| 4:C:531:SER:O | 4:C:817:ILE:HG22 | 2.18 | 0.43 |
| 4:C:548:ALA:O | 4:C:550:LEU:N | 2.52 | 0.43 |
| 4:C:67:ASN:C | 4:C:69:ALA:N | 2.69 | 0.43 |
| 4:D:126:LEU:HD13 | 4:D:246:LEU:HB2 | 2.00 | 0.43 |
| 3:G:8:DC:H2" | 3:G:9:DC:OP2 | 2.19 | 0.43 |
| 4:A:14:ILE:CD1 | 4:A:14:ILE:H | 2.32 | 0.43 |
| 4:A:159:ALA:HB3 | 4:A:163:LYS:HD3 | 2.01 | 0.43 |
| 4:A:223:SER:HA | 7:A:3147:HOH:O | 2.19 | 0.43 |
| 4:A:517:GLU:O | 4:A:520:GLY:N | 2.42 | 0.43 |
| 4:A:546:PHE:HA | 4:A:549:MET:HG2 | 2.01 | 0.43 |
| 4:A:619:GLN:HA | 4:A:622:ALA:HB3 | 2.01 | 0.43 |
| 4:B:141:ILE:O | 4:B:145:ILE:HG12 | 2.19 | 0.43 |
| 4:B:14:ILE:HG22 | 4:B:14:ILE:O | 2.19 | 0.43 |
| 4:B:158:GLU:HG2 | 4:B:195:LEU:CD2 | 2.47 | 0.43 |
| 4:B:520:GLY:HA3 | 4:B:528:TYR:CZ | 2.54 | 0.43 |
| 4:B:56:GLU:OE1 | 4:B:57:ARG:N | 2.52 | 0.43 |
| 4:B:596:THR:CG2 | 4:B:605:ILE:HG23 | 2.49 | 0.43 |
| 4:B:643:GLU:HB2 | 7:B:3053:HOH:O | 2.19 | 0.43 |
| 4:B:726:HIS:CD2 | 4:B:736:TRP:CD1 | 3.06 | 0.43 |
| 4:C:164:LYS:C | 4:C:166:VAL:H | 2.22 | 0.43 |
| 4:C:727:TRP:CD1 | 4:C:782:PHE:CE1 | 3.06 | 0.43 |
| 4:C:710:VAL:HG21 | 4:C:856:SER:OG | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:C:9:ASN:HA | 4:C:12:SER:CB | 2.47 | 0.43 |
| 4:D:164:LYS:NZ | 7:D:3179:HOH:O | 2.50 | 0.43 |
| 4:D:306:MET:O | 4:D:309:GLU:HB2 | 2.19 | 0.43 |
| 4:D:303:LYS:HE2 | 4:D:307:ARG:HH12 | 1.84 | 0.43 |
| 4:A:617:ALA:C | 4:A:621:LEU:HD12 | 2.40 | 0.42 |
| 4:A:631:LYS:HZ2 | 6:A:2000:APC:PA | 2.41 | 0.42 |
| 4:A:742:PRO:HB3 | 4:A:744:GLN:OE1 | 2.19 | 0.42 |
| 4:A:840:ASP:O | 4:A:841:VAL:C | 2.56 | 0.42 |
| 4:B:6:ILE:HG23 | 4:B:10:ASP:CG | 2.39 | 0.42 |
| 4:B:110:LYS:CD | 4:B:111:PRO:HD2 | 2.39 | 0.42 |
| 4:B:17:ALA:O | 4:B:21:PHE:HE2 | 2.02 | 0.42 |
| 4:B:620:TRP:CE2 | 4:B:677:MET:HE2 | 2.54 | 0.42 |
| 4:B:623:TYR:HA | 4:B:666:MET:HE2 | 2.00 | 0.42 |
| 4:B:744:GLN:HA | 4:B:756:ARG:HD3 | 2.01 | 0.42 |
| 4:B:80:LYS:HD3 | 4:B:224:THR:HG23 | 1.99 | 0.42 |
| 4:C:786:GLN:O | 4:C:789:SER:N | 2.51 | 0.42 |
| 4:C:8:LYS:HB2 | 7:C:3187:HOH:O | 2.18 | 0.42 |
| 4:D:134:VAL:HB | 4:D:244:ILE:HG12 | 2.01 | 0.42 |
| 4:D:352:ILE:HA | 4:D:353:PRO:HD2 | 1.54 | 0.42 |
| 4:D:478:ARG:O | 4:D:481:PHE:HB3 | 2.19 | 0.42 |
| 4:D:340:VAL:HG11 | 4:D:497:LEU:HD11 | 2.01 | 0.42 |
| 4:D:520:GLY:O | 4:D:524:HIS:HB2 | 2.18 | 0.42 |
| 4:D:535:ALA:HA | 4:D:814:PHE:O | 2.19 | 0.42 |
| 4:A:246:LEU:HD23 | 4:A:251:ALA:HB2 | 2.01 | 0.42 |
| 4:A:24:LEU:O | 4:A:25:ALA:C | 2.56 | 0.42 |
| 4:A:266:PRO:HD2 | 4:A:292:ARG:NH1 | 2.34 | 0.42 |
| 4:A:610:LYS:O | 4:A:611:LEU:O | 2.37 | 0.42 |
| 4:A:640:GLY:O | 4:A:641:SER:O | 2.37 | 0.42 |
| 4:A:89:PHE:O | 4:A:93:LYS:HG3 | 2.19 | 0.42 |
| 4:B:142:GLY:O | 4:B:143:ARG:C | 2.57 | 0.42 |
| 4:B:259:GLY:O | 4:B:262:ALA:N | 2.52 | 0.42 |
| 4:B:31:ARG:HB3 | 4:B:31:ARG:NH1 | 2.32 | 0.42 |
| 4:B:504:GLU:O | 4:B:505:GLN:O | 2.37 | 0.42 |
| 4:B:714:LYS:HD3 | 4:B:714:LYS:HA | 1.77 | 0.42 |
| 4:B:798:ALA:O | 4:B:802:TYR:O | 2.38 | 0.42 |
| 4:B:864:LEU:O | 4:B:865:PRO:O | 2.36 | 0.42 |
| 4:C:632:ARG:NH1 | 6:C:2002:APC:C8 | 2.83 | 0.42 |
| 4:D:106:LEU:HD11 | 4:D:215:ARG:HG2 | 2.01 | 0.42 |
| 4:D:231:ARG:NH1 | 4:D:242:GLU:HB2 | 2.34 | 0.42 |
| 4:D:337:VAL:HG12 | 4:D:341:ILE:CD1 | 2.48 | 0.42 |
| 4:D:442:GLY:O | 4:D:444:LEU:N | 2.52 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:677:MET:O | 4:D:678:ALA:C | 2.55 | 0.42 |
| 4:D:861:MET:HA | 4:D:862:PRO:HD2 | 1.84 | 0.42 |
| 4:A:205:HIS:O | 4:A:208:ASP:N | 2.52 | 0.42 |
| 4:A:331:ASN:O | 4:A:333:LYS:N | 2.53 | 0.42 |
| 4:A:347:CYS:C | 4:A:349:VAL:H | 2.22 | 0.42 |
| 4:A:703:ALA:O | 4:A:704:LYS:C | 2.57 | 0.42 |
| 4:A:720:ARG:O | 4:A:721:LYS:C | 2.57 | 0.42 |
| 4:A:810:ILE:N | 4:A:813:SER:O | 2.46 | 0.42 |
| 4:A:84:ARG:NH1 | 4:A:91:GLU:OE2 | 2.52 | 0.42 |
| 4:B:150:ARG:C | 4:B:152:GLY:N | 2.70 | 0.42 |
| 4:B:152:GLY:C | 4:B:154:ILE:N | 2.72 | 0.42 |
| 4:B:301:SER:O | 4:B:302:LYS:C | 2.56 | 0.42 |
| 4:B:305:LEU:O | 4:B:307:ARG:N | 2.53 | 0.42 |
| 4:B:613:THR:HG21 | 7:B:3104:HOH:O | 2.19 | 0.42 |
| 4:B:682:TRP:C | 4:B:682:TRP:CD1 | 2.90 | 0.42 |
| 4:B:533:PRO:HA | 4:B:816:THR:O | 2.18 | 0.42 |
| 4:C:305:LEU:HD23 | 4:C:305:LEU:O | 2.19 | 0.42 |
| 4:C:326:THR:O | 4:C:415:TRP:HD1 | 1.99 | 0.42 |
| 4:C:428:ALA:H | 4:C:435:GLN:HE22 | 1.66 | 0.42 |
| 4:C:699:LEU:O | 4:C:778:ILE:HG12 | 2.19 | 0.42 |
| 4:C:318:LYS:HE2 | 4:C:796:VAL:CG1 | 2.48 | 0.42 |
| 4:D:125:CYS:O | 4:D:128:SER:CB | 2.62 | 0.42 |
| 4:D:334:VAL:HG12 | 4:D:443:LEU:HD22 | 2.01 | 0.42 |
| 4:D:474:PRO:HA | 4:D:880:PHE:CE1 | 2.54 | 0.42 |
| 4:D:68:ALA:HB3 | 4:D:261:LEU:HD21 | 2.01 | 0.42 |
| 3:M:4:DG:C2 | 3:M:5:DA:C2 | 3.07 | 0.42 |
| 4:A:308:TYR:OH | 4:A:733:PHE:HE2 | 2.02 | 0.42 |
| 4:A:675:GLY:O | 4:A:678:ALA:HB3 | 2.18 | 0.42 |
| 4:A:801:LYS:HD3 | 4:A:802:TYR:CD2 | 2.54 | 0.42 |
| 4:A:793:LYS:HB3 | 4:A:831:THR:OG1 | 2.19 | 0.42 |
| 4:B:144:ALA:O | 4:B:147:ASP:N | 2.53 | 0.42 |
| 4:B:19:ILE:HG23 | 4:B:20:PRO:N | 2.34 | 0.42 |
| 4:B:36:GLN:O | 4:B:39:LEU:N | 2.45 | 0.42 |
| 4:B:511:PHE:O | 4:B:514:PHE:HB3 | 2.19 | 0.42 |
| 4:B:51:PHE:CE2 | 4:B:55:PHE:CD1 | 3.03 | 0.42 |
| 4:B:749:LEU:HD12 | 4:B:750:MET:HG3 | 2.01 | 0.42 |
| 4:C:162:PHE:CE2 | 4:C:165:ASN:HB2 | 2.54 | 0.42 |
| 4:C:36:GLN:NE2 | 4:C:273:VAL:HG22 | 2.34 | 0.42 |
| 4:C:462:ILE:HG12 | 4:C:479:ILE:HD11 | 2.02 | 0.42 |
| 4:C:512:LEU:O | 4:C:516:PHE:CD1 | 2.71 | 0.42 |
| 4:C:693:VAL:HG12 | 4:C:694:GLU:N | 2.34 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:207:GLU:O | 4:D:211:HIS:CD2 | 2.73 | 0.42 |
| 4:D:247:ALA:HA | 4:D:248:PRO:HD3 | 1.80 | 0.42 |
| 4:D:486:HIS:HA | 4:D:489:ILE:CD1 | 2.40 | 0.42 |
| 4:D:579:ASN:ND2 | 4:D:625:VAL:HG12 | 2.35 | 0.42 |
| 4:D:147:ASP:HB3 | 4:D:750:MET:HE2 | 2.01 | 0.42 |
| 4:D:89:PHE:CD2 | 4:D:107:GLN:OE1 | 2.73 | 0.42 |
| 4:A:226:MET:HG3 | 4:A:250:TYR:HD1 | 1.83 | 0.42 |
| 4:A:236:VAL:HG11 | 4:A:239:GLN:OE1 | 2.19 | 0.42 |
| 4:A:276:LYS:HB2 | 4:A:287:TRP:CD2 | 2.54 | 0.42 |
| 4:A:395:ARG:O | 4:A:399:GLU:CG | 2.68 | 0.42 |
| 4:A:704:LYS:O | 4:A:707:ALA:N | 2.47 | 0.42 |
| 4:A:830:GLU:O | 4:A:832:MET:N | 2.51 | 0.42 |
| 4:C:205:HIS:HB3 | 4:C:208:ASP:OD2 | 2.18 | 0.42 |
| 4:C:41:HIS:CD2 | 4:C:41:HIS:C | 2.92 | 0.42 |
| 4:C:650:VAL:HG11 | 4:C:674:ALA:HA | 2.00 | 0.42 |
| 4:C:698:TRP:O | 4:C:701:SER:N | 2.53 | 0.42 |
| 4:C:714:LYS:HA | 4:C:714:LYS:HD3 | 1.74 | 0.42 |
| 4:C:799:HIS:HA | 4:C:804:ILE:O | 2.20 | 0.42 |
| 4:D:122:THR:O | 4:D:125:CYS:HB2 | 2.19 | 0.42 |
| 4:D:64:VAL:HG21 | 4:D:127:THR:HG21 | 2.01 | 0.42 |
| 4:D:303:LYS:HE2 | 4:D:307:ARG:NH1 | 2.34 | 0.42 |
| 4:D:326:THR:C | 4:D:415:TRP:HD1 | 2.22 | 0.42 |
| 4:D:727:TRP:CE2 | 4:D:735:VAL:CG1 | 3.03 | 0.42 |
| 4:D:116:TYR:CZ | 4:D:752:LEU:HD22 | 2.54 | 0.42 |
| 3:G:3:DC:C4 | 3:G:4:DG:N7 | 2.88 | 0.42 |
| 1:H:14:DG:H2' | 1:H:15:DC:C5 | 2.55 | 0.42 |
| 4:A:163:LYS:HA | 4:A:163:LYS:HD2 | 1.93 | 0.42 |
| 4:A:166:VAL:HG12 | 4:A:170:LEU:HD12 | 2.01 | 0.42 |
| 4:A:333:LYS:HE3 | 4:A:516:PHE:HB3 | 2.01 | 0.42 |
| 4:A:333:LYS:CB | 4:A:516:PHE:CE2 | 3.03 | 0.42 |
| 4:A:556:GLY:CA | 4:A:561:LEU:HB2 | 2.49 | 0.42 |
| 4:A:722:ARG:CB | 4:A:769:ILE:HD13 | 2.19 | 0.42 |
| 4:A:832:MET:O | 4:A:834:ASP:N | 2.53 | 0.42 |
| 4:A:88:TRP:HA | 4:A:91:GLU:CD | 2.40 | 0.42 |
| 4:B:264:ILE:CG2 | 4:B:292:ARG:HB2 | 2.39 | 0.42 |
| 4:B:305:LEU:O | 4:B:306:MET:C | 2.57 | 0.42 |
| 4:B:381:ALA:C | 4:B:383:ALA:N | 2.71 | 0.42 |
| 4:B:39:LEU:O | 4:B:40:GLU:C | 2.57 | 0.42 |
| 4:B:518:TYR:CE1 | 4:B:522:GLN:NE2 | 2.88 | 0.42 |
| 4:B:690:VAL:O | 4:B:691:ALA:C | 2.58 | 0.42 |
| 4:C:322:ILE:HA | 4:C:322:ILE:HD13 | 1.74 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:C:286:TYR:CE2 | 4:C:417:PRO:HG3 | 2.54 | 0.42 |
| 4:C:329:LYS:HD2 | 4:C:447:ALA:HA | 2.02 | 0.42 |
| 4:C:556:GLY:C | 4:C:561:LEU:HB2 | 2.40 | 0.42 |
| 4:C:834:ASP:O | 4:C:837:GLU:N | 2.44 | 0.42 |
| 4:C:833:VAL:HG11 | 4:C:873:ARG:HD3 | 2.01 | 0.42 |
| 4:D:113:ALA:O | 4:D:114:VAL:C | 2.57 | 0.42 |
| 4:D:257:ARG:NH1 | 4:D:261:LEU:HD13 | 2.34 | 0.42 |
| 4:D:384:VAL:O | 4:D:384:VAL:HG12 | 2.19 | 0.42 |
| 4:D:425:ARG:HB3 | 4:D:427:TYR:CE1 | 2.49 | 0.42 |
| 4:D:579:ASN:OD1 | 4:D:625:VAL:HB | 2.18 | 0.42 |
| 4:D:631:LYS:CD | 4:D:635:MET:SD | 3.08 | 0.42 |
| 4:D:794:THR:CB | 4:D:831:THR:HG21 | 2.47 | 0.42 |
| 4:D:836:TYR:HD2 | 4:D:836:TYR:N | 2.16 | 0.42 |
| 4:A:121:THR:OG1 | 4:A:751:PHE:HE1 | 2.02 | 0.42 |
| 4:A:215:ARG:O | 4:A:219:MET:HG3 | 2.20 | 0.42 |
| 4:A:348:PRO:C | 4:A:349:VAL:HG23 | 2.37 | 0.42 |
| 4:A:407:LYS:HB2 | 4:A:407:LYS:HE3 | 1.85 | 0.42 |
| 4:A:457:TYR:C | 4:A:457:TYR:CD2 | 2.93 | 0.42 |
| 4:A:471:ASP:OD1 | 4:A:471:ASP:C | 2.55 | 0.42 |
| 4:A:488:ASN:O | 4:A:491:ALA:CB | 2.67 | 0.42 |
| 4:A:510:CYS:O | 4:A:512:LEU:N | 2.53 | 0.42 |
| 4:A:543:ILE:O | 4:A:544:GLN:O | 2.37 | 0.42 |
| 4:A:656:GLN:C | 4:A:658:ALA:H | 2.22 | 0.42 |
| 4:A:779:ALA:HB3 | 4:A:780:PRO:HD3 | 2.02 | 0.42 |
| 4:B:208:ASP:OD2 | 4:B:208:ASP:N | 2.53 | 0.42 |
| 4:B:432:PHE:HD2 | 4:B:432:PHE:O | 2.01 | 0.42 |
| 4:B:545:HIS:HE1 | 4:B:787:ASP:HA | 1.84 | 0.42 |
| 4:B:581:ILE:O | 4:B:584:ALA:HB3 | 2.20 | 0.42 |
| 4:B:643:GLU:O | 4:B:644:PHE:C | 2.56 | 0.42 |
| 4:B:793:LYS:CG | 7:B:3181:HOH:O | 2.66 | 0.42 |
| 4:B:804:ILE:HG21 | 4:B:807:PHE:CE2 | 2.54 | 0.42 |
| 4:B:840:ASP:HB3 | 4:B:843:ALA:HB3 | 2.02 | 0.42 |
| 4:B:567:VAL:CG1 | 4:B:880:PHE:CG | 3.01 | 0.42 |
| 4:C:132:THR:HG21 | 4:C:244:ILE:O | 2.20 | 0.42 |
| 4:C:161:HIS:O | 4:C:162:PHE:C | 2.58 | 0.42 |
| 4:C:247:ALA:HA | 4:C:248:PRO:HD3 | 1.89 | 0.42 |
| 4:C:257:ARG:HG2 | 4:C:257:ARG:NH1 | 2.34 | 0.42 |
| 4:C:631:LYS:NZ | 6:C:2002:APC:C3A | 2.47 | 0.42 |
| 4:C:756:ARG:HG3 | 7:C:3143:HOH:O | 2.20 | 0.42 |
| 4:D:166:VAL:HG11 | 4:D:183:MET:CE | 2.50 | 0.42 |
| 4:D:239:GLN:O | 4:D:241:SER:N | 2.52 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:D:396:ILE:HA | 4:D:396:ILE:HD13 | 1.84 | 0.42 |
| 4:D:473:VAL:N | 4:D:567:VAL:CG2 | 2.79 | 0.42 |
| 4:D:631:LYS:HE2 | 4:D:635:MET:CE | 2.50 | 0.42 |
| 4:D:643:GLU:HB2 | 4:D:682:TRP:CD1 | 2.54 | 0.42 |
| 4:D:712:ASP:O | 4:D:716:GLY:N | 2.46 | 0.42 |
| 4:D:728:VAL:HG22 | 4:D:734:PRO:HA | 2.01 | 0.42 |
| 4:D:745:THR:O | 4:D:746:ARG:HG3 | 2.20 | 0.42 |
| 4:A:13:ASP:OD2 | 4:A:291:ARG:NH2 | 2.50 | 0.42 |
| 4:A:19:ILE:O | 4:A:21:PHE:N | 2.49 | 0.42 |
| 4:A:281:ILE:HG23 | 4:A:305:LEU:HD11 | 2.01 | 0.42 |
| 4:A:308:TYR:C | 4:A:311:VAL:HG23 | 2.37 | 0.42 |
| 4:A:65:ALA:HB3 | 4:A:120:LYS:CD | 2.49 | 0.42 |
| 4:A:668:THR:CG2 | 4:A:669:GLN:HE22 | 2.32 | 0.42 |
| 4:A:686:SER:HA | 4:A:693:VAL:HG21 | 2.01 | 0.42 |
| 4:B:205:HIS:C | 4:B:207:GLU:N | 2.72 | 0.42 |
| 4:B:19:ILE:CG2 | 4:B:20:PRO:N | 2.83 | 0.42 |
| 4:B:661:SER:CB | 7:B:3192:HOH:O | 2.68 | 0.42 |
| 4:B:709:GLU:HG2 | 4:B:709:GLU:O | 2.20 | 0.42 |
| 4:B:726:HIS:CD2 | 4:B:736:TRP:CG | 3.08 | 0.42 |
| 4:B:530:CYS:SG | 4:B:818:PRO:HG2 | 2.60 | 0.42 |
| 4:C:109:ILE:HD13 | 4:C:145:ILE:HG22 | 2.01 | 0.42 |
| 4:C:191:LEU:O | 4:C:196:LEU:HD22 | 2.20 | 0.42 |
| 4:C:322:ILE:CG1 | 7:C:3131:HOH:O | 2.59 | 0.42 |
| 4:C:330:ILE:HA | 4:C:330:ILE:HD13 | 1.74 | 0.42 |
| 4:C:42:GLU:HG2 | 4:C:46:MET:CE | 2.49 | 0.42 |
| 4:D:133:THR:HA | 4:D:243:THR:CG2 | 2.48 | 0.42 |
| 4:D:161:HIS:CE1 | 7:D:3114:HOH:O | 2.64 | 0.42 |
| 4:D:339:ASN:O | 4:D:343:LYS:HD3 | 2.20 | 0.42 |
| 4:D:36:GLN:HE21 | 4:D:36:GLN:CA | 2.28 | 0.42 |
| 4:D:632:ARG:HH22 | 6:D:2003:APC:H5'1 | 1.85 | 0.42 |
| 2:L:3:G:H5'' | 4:C:172:LYS:CD | 2.50 | 0.42 |
| 1:N:12:DT:H5' | 4:D:781:ASN:ND2 | 2.34 | 0.42 |
| 4:A:254:ILE:HG22 | 4:A:255:ALA:N | 2.34 | 0.42 |
| 4:A:333:LYS:O | 4:A:334:VAL:C | 2.58 | 0.42 |
| 4:A:505:GLN:O | 4:A:508:PRO:HD3 | 2.19 | 0.42 |
| 4:B:11:PHE:C | 4:B:13:ASP:N | 2.73 | 0.42 |
| 4:B:19:ILE:HG22 | 4:B:21:PHE:HB3 | 2.01 | 0.42 |
| 4:B:19:ILE:HD12 | 4:B:20:PRO:HD2 | 2.00 | 0.42 |
| 4:B:280:GLY:HA2 | 4:B:317:TYR:OH | 2.20 | 0.42 |
| 4:B:347:CYS:HB3 | 4:B:350:GLU:HG2 | 2.00 | 0.42 |
| 4:B:308:TYR:CE2 | 4:B:734:PRO:O | 2.73 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:11:DA:N3 | 4:B:784:HIS:HE1 | 2.17 | 0.42 |
| 4:C:101:THR:HG23 | 4:C:104:GLN:HE22 | 1.84 | 0.42 |
| 4:C:216:CYS:O | 4:C:217:ILE:C | 2.57 | 0.42 |
| 4:C:303:LYS:HB3 | 4:C:303:LYS:NZ | 2.35 | 0.42 |
| 4:C:571:TYR:HD1 | 4:C:634:VAL:CG1 | 2.33 | 0.42 |
| 4:C:63:GLU:O | 4:C:66:ASP:HB2 | 2.20 | 0.42 |
| 4:C:713:LYS:HD2 | 4:C:713:LYS:HA | 1.83 | 0.42 |
| 4:C:789:SER:O | 4:C:793:LYS:HG3 | 2.19 | 0.42 |
| 4:C:845:PHE:O | 4:C:846:TYR:C | 2.58 | 0.42 |
| 4:D:423:ARG:NH2 | 4:D:784:HIS:ND1 | 2.67 | 0.42 |
| 4:D:809:LEU:HA | 4:D:813:SER:O | 2.19 | 0.42 |
| 4:D:854:HIS:HD2 | 4:D:856:SER:H | 1.55 | 0.42 |
| 4:A:100:PRO:HG2 | 4:A:103:PHE:CB | 2.46 | 0.42 |
| 4:A:254:ILE:O | 4:A:255:ALA:C | 2.58 | 0.42 |
| 4:A:292:ARG:O | 4:A:292:ARG:CG | 2.63 | 0.42 |
| 4:A:481:PHE:O | 4:A:482:ILE:C | 2.54 | 0.42 |
| 4:A:489:ILE:O | 4:A:490:MET:C | 2.56 | 0.42 |
| 4:A:553:GLU:OE1 | 4:A:553:GLU:N | 2.53 | 0.42 |
| 4:A:71:LYS:N | 4:A:72:PRO:CD | 2.82 | 0.42 |
| 4:A:801:LYS:CD | 4:A:802:TYR:CD2 | 3.02 | 0.42 |
| 4:B:170:LEU:HD22 | 4:B:179:LYS:HG2 | 2.01 | 0.42 |
| 4:B:158:GLU:HA | 4:B:195:LEU:HD22 | 2.01 | 0.42 |
| 4:B:247:ALA:HB3 | 4:B:250:TYR:CD1 | 2.55 | 0.42 |
| 4:B:339:ASN:O | 4:B:343:LYS:HD3 | 2.15 | 0.42 |
| 4:B:352:ILE:HA | 4:B:353:PRO:HD2 | 1.69 | 0.42 |
| 4:B:561:LEU:HD12 | 4:B:561:LEU:N | 2.35 | 0.42 |
| 4:B:6:ILE:O | 4:B:8:LYS:N | 2.44 | 0.42 |
| 4:C:260:ALA:O | 4:C:261:LEU:C | 2.59 | 0.42 |
| 4:C:329:LYS:HD3 | 4:C:446:LEU:O | 2.20 | 0.42 |
| 4:C:553:GLU:CD | 4:C:553:GLU:N | 2.71 | 0.42 |
| 4:D:281:ILE:HG22 | 4:D:282:THR:CG2 | 2.42 | 0.42 |
| 4:A:108:GLU:CG | 7:A:3115:HOH:O | 2.63 | 0.41 |
| 4:A:21:PHE:C | 4:A:23:THR:H | 2.23 | 0.41 |
| 4:A:291:ARG:CB | 7:A:3193:HOH:O | 2.56 | 0.41 |
| 4:A:291:ARG:CG | 7:A:3193:HOH:O | 2.67 | 0.41 |
| 4:A:330:ILE:HG21 | 4:A:409:ALA:HA | 2.02 | 0.41 |
| 4:A:659:ILE:HG22 | 4:A:660:ASP:N | 2.35 | 0.41 |
| 4:A:864:LEU:H | 4:A:864:LEU:HD12 | 1.84 | 0.41 |
| 4:B:179:LYS:O | 4:B:750:MET:SD | 2.78 | 0.41 |
| 4:B:247:ALA:CB | 4:B:250:TYR:HD1 | 2.33 | 0.41 |
| 4:B:416:PHE:N | 4:B:416:PHE:CD2 | 2.88 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:B:578:VAL:HG21 | 4:B:681:ILE:HD12 | 2.01 | 0.41 |
| 4:C:9:ASN:C | 4:C:12:SER:HB3 | 2.40 | 0.41 |
| 4:C:292:ARG:N | 4:C:293:PRO:CD | 2.82 | 0.41 |
| 4:C:385:TYR:O | 4:C:386:ARG:C | 2.56 | 0.41 |
| 4:C:402:LEU:HG | 4:C:439:MET:CE | 2.50 | 0.41 |
| 4:C:473:VAL:HA | 4:C:474:PRO:HD2 | 1.90 | 0.41 |
| 4:C:610:LYS:HD2 | 7:C:3085:HOH:O | 2.19 | 0.41 |
| 4:C:619:GLN:O | 4:C:666:MET:HG3 | 2.20 | 0.41 |
| 4:C:870:LEU:HD23 | 4:C:871:ASN:N | 2.35 | 0.41 |
| 4:D:161:HIS:O | 4:D:163:LYS:N | 2.53 | 0.41 |
| 4:D:264:ILE:O | 4:D:264:ILE:HG22 | 2.19 | 0.41 |
| 4:D:32:LEU:HD12 | 4:D:32:LEU:N | 2.12 | 0.41 |
| 4:D:459:TRP:O | 4:D:460:LEU:C | 2.56 | 0.41 |
| 1:N:11:DA:H4' | 4:D:780:PRO:HG3 | 2.00 | 0.41 |
| 3:P:7:DT:H2'' | 3:P:8:DC:OP2 | 2.21 | 0.41 |
| 4:A:244:ILE:HG22 | 4:A:245:GLU:N | 2.34 | 0.41 |
| 4:A:348:PRO:HB2 | 4:A:349:VAL:HG23 | 2.03 | 0.41 |
| 4:A:401:MET:O | 4:A:404:GLN:N | 2.53 | 0.41 |
| 4:A:421:ASP:OD2 | 4:A:427:TYR:CE1 | 2.71 | 0.41 |
| 4:A:693:VAL:HG12 | 4:A:694:GLU:N | 2.35 | 0.41 |
| 4:B:6:ILE:O | 4:B:10:ASP:HB3 | 2.19 | 0.41 |
| 4:B:472:LYS:C | 4:B:567:VAL:HG21 | 2.40 | 0.41 |
| 4:B:541:SER:O | 4:B:542:GLY:O | 2.38 | 0.41 |
| 4:B:650:VAL:O | 4:B:654:THR:HG23 | 2.20 | 0.41 |
| 4:B:155:ARG:NH2 | 4:B:749:LEU:HB2 | 2.34 | 0.41 |
| 4:B:773:LYS:HE3 | 7:B:3124:HOH:O | 2.19 | 0.41 |
| 4:B:864:LEU:HA | 4:B:865:PRO:HD2 | 1.72 | 0.41 |
| 4:B:537:ASP:N | 4:B:882:PHE:CD2 | 2.73 | 0.41 |
| 4:C:635:MET:HG3 | 6:C:2002:APC:N7 | 2.36 | 0.41 |
| 4:C:261:LEU:O | 4:C:263:GLY:N | 2.52 | 0.41 |
| 4:C:437:ASN:ND2 | 4:C:440:THR:CB | 2.83 | 0.41 |
| 4:C:420:MET:SD | 4:C:733:PHE:CE1 | 3.13 | 0.41 |
| 4:C:850:ALA:C | 4:C:852:GLN:N | 2.72 | 0.41 |
| 4:D:291:ARG:O | 4:D:292:ARG:HB2 | 2.20 | 0.41 |
| 1:K:14:DG:C4 | 1:K:15:DC:C5 | 3.08 | 0.41 |
| 4:A:40:GLU:HG2 | 4:A:286:TYR:CD1 | 2.49 | 0.41 |
| 4:A:482:ILE:O | 4:A:482:ILE:HG22 | 2.20 | 0.41 |
| 4:A:454:LYS:H | 4:A:526:LEU:HD23 | 1.81 | 0.41 |
| 4:A:706:LEU:HD11 | 4:A:849:PHE:HB2 | 2.02 | 0.41 |
| 4:B:115:ALA:O | 4:B:119:ILE:HG12 | 2.21 | 0.41 |
| 4:B:345:LYS:HB3 | 4:B:345:LYS:HE2 | 1.68 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:B:381:ALA:O | 4:B:383:ALA:N | 2.53 | 0.41 |
| 4:B:587:ILE:HD13 | 4:B:587:ILE:HA | 1.83 | 0.41 |
| 4:B:655:ILE:HG12 | 4:B:667:PHE:CE1 | 2.55 | 0.41 |
| 4:B:738:GLU:HG2 | 4:B:738:GLU:O | 2.20 | 0.41 |
| 4:B:537:ASP:O | 4:B:882:PHE:CD2 | 2.72 | 0.41 |
| 4:C:423:ARG:HD2 | 4:C:781:ASN:HD22 | 1.81 | 0.41 |
| 4:C:461:LYS:O | 4:C:463:HIS:N | 2.53 | 0.41 |
| 4:C:55:PHE:CE2 | 4:C:59:LEU:HD21 | 2.55 | 0.41 |
| 4:C:58:GLN:NE2 | 4:C:58:GLN:HA | 2.35 | 0.41 |
| 4:C:727:TRP:CD2 | 4:C:735:VAL:HG13 | 2.55 | 0.41 |
| 4:C:738:GLU:CA | 4:C:774:GLN:HE22 | 2.28 | 0.41 |
| 4:C:448:LYS:CG | 4:C:806:SER:OG | 2.69 | 0.41 |
| 4:D:570:ILE:HG23 | 4:D:571:TYR:N | 2.35 | 0.41 |
| 4:D:733:PHE:HA | 4:D:734:PRO:HD2 | 1.93 | 0.41 |
| 4:D:116:TYR:HE2 | 4:D:752:LEU:HD22 | 1.86 | 0.41 |
| 1:H:13:DC:O4' | 4:B:427:TYR:CE2 | 2.53 | 0.41 |
| 1:K:3:DG:C2 | 1:K:4:DA:C2 | 3.08 | 0.41 |
| 4:A:261:LEU:C | 4:A:263:GLY:N | 2.72 | 0.41 |
| 4:A:314:PRO:CD | 4:A:315:GLU:H | 2.33 | 0.41 |
| 4:A:462:ILE:CD1 | 4:A:475:PHE:CD1 | 3.03 | 0.41 |
| 4:A:475:PHE:HD2 | 4:A:475:PHE:H | 1.68 | 0.41 |
| 4:A:668:THR:O | 4:A:670:PRO:HD3 | 2.20 | 0.41 |
| 4:B:250:TYR:O | 4:B:251:ALA:C | 2.59 | 0.41 |
| 4:B:464:GLY:HA3 | 4:B:514:PHE:CZ | 2.55 | 0.41 |
| 4:B:592:ASN:O | 4:B:593:GLU:HB2 | 2.20 | 0.41 |
| 4:B:617:ALA:O | 4:B:621:LEU:HD12 | 2.19 | 0.41 |
| 4:B:745:THR:O | 4:B:746:ARG:HB2 | 2.20 | 0.41 |
| 4:B:793:LYS:HE2 | 4:B:835:THR:OG1 | 2.20 | 0.41 |
| 4:B:881:ALA:O | 4:B:883:ALA:N | 2.52 | 0.41 |
| 4:C:278:TRP:HB2 | 4:C:321:ASN:OD1 | 2.20 | 0.41 |
| 4:C:330:ILE:HG13 | 4:C:409:ALA:HA | 2.00 | 0.41 |
| 4:C:788:GLY:C | 4:C:792:ARG:HH12 | 2.24 | 0.41 |
| 4:D:191:LEU:HD23 | 4:D:195:LEU:O | 2.21 | 0.41 |
| 4:D:19:ILE:HD13 | 4:D:19:ILE:HA | 1.95 | 0.41 |
| 4:D:146:GLU:HG3 | 4:D:204:TRP:CE2 | 2.55 | 0.41 |
| 4:D:19:ILE:CG2 | 4:D:20:PRO:N | 2.84 | 0.41 |
| 4:D:261:LEU:C | 4:D:263:GLY:H | 2.23 | 0.41 |
| 4:D:717:GLU:HA | 7:D:3025:HOH:O | 2.20 | 0.41 |
| 4:D:734:PRO:O | 4:D:734:PRO:CG | 2.65 | 0.41 |
| 4:D:735:VAL:HG23 | 4:D:736:TRP:N | 2.35 | 0.41 |
| 1:K:14:DG:H2'' | 1:K:15:DC:C6 | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:L:7:A:H2' | 2:L:8:U:H6 | 1.85 | 0.41 |
| 4:A:31:ARG:NH2 | 4:A:32:LEU:HD11 | 2.34 | 0.41 |
| 4:A:59:LEU:HD23 | 4:A:64:VAL:HG21 | 1.99 | 0.41 |
| 4:A:689:VAL:C | 4:A:691:ALA:N | 2.72 | 0.41 |
| 4:A:743:ILE:HA | 7:A:3130:HOH:O | 2.19 | 0.41 |
| 4:A:873:ARG:O | 4:A:876:LEU:HD12 | 2.20 | 0.41 |
| 4:B:111:PRO:HG2 | 4:B:112:GLU:H | 1.86 | 0.41 |
| 4:B:451:PRO:O | 4:B:452:ILE:C | 2.58 | 0.41 |
| 4:B:569:ASP:CG | 4:B:569:ASP:O | 2.58 | 0.41 |
| 4:B:589:GLY:O | 4:B:614:LYS:HD2 | 2.20 | 0.41 |
| 4:C:329:LYS:CG | 4:C:445:THR:HG23 | 2.50 | 0.41 |
| 4:C:452:ILE:HG13 | 4:C:456:GLY:CA | 2.50 | 0.41 |
| 4:C:620:TRP:NE1 | 4:C:677:MET:HB2 | 2.36 | 0.41 |
| 4:C:827:ALA:O | 4:C:828:VAL:C | 2.54 | 0.41 |
| 4:D:455:GLU:HA | 4:D:455:GLU:OE1 | 2.19 | 0.41 |
| 4:D:642:LYS:HB3 | 4:D:682:TRP:CH2 | 2.56 | 0.41 |
| 4:D:724:ALA:HA | 4:D:774:GLN:NE2 | 2.35 | 0.41 |
| 4:D:778:ILE:CG2 | 4:D:779:ALA:H | 2.30 | 0.41 |
| 4:A:112:GLU:N | 4:A:112:GLU:CD | 2.74 | 0.41 |
| 4:A:454:LYS:HA | 4:A:526:LEU:HD21 | 2.01 | 0.41 |
| 4:A:588:ASN:HD22 | 4:A:588:ASN:N | 2.19 | 0.41 |
| 4:A:632:ARG:O | 4:A:636:THR:HG23 | 2.20 | 0.41 |
| 4:B:329:LYS:O | 4:B:329:LYS:HG3 | 2.20 | 0.41 |
| 4:B:612:GLY:O | 4:B:613:THR:C | 2.58 | 0.41 |
| 4:B:615:ALA:O | 4:B:616:LEU:C | 2.58 | 0.41 |
| 4:B:771:ALA:O | 4:B:772:HIS:C | 2.57 | 0.41 |
| 4:B:845:PHE:O | 4:B:845:PHE:CD1 | 2.73 | 0.41 |
| 4:C:135:GLN:OE1 | 4:C:210:ILE:HG21 | 2.21 | 0.41 |
| 4:C:137:VAL:O | 4:C:141:ILE:HG13 | 2.20 | 0.41 |
| 4:C:158:GLU:HA | 4:C:195:LEU:CD1 | 2.43 | 0.41 |
| 4:C:176:HIS:O | 4:C:179:LYS:HB2 | 2.20 | 0.41 |
| 4:C:337:VAL:HG21 | 4:C:512:LEU:CD2 | 2.45 | 0.41 |
| 4:C:336:ALA:O | 4:C:337:VAL:O | 2.38 | 0.41 |
| 4:C:416:PHE:HA | 4:C:417:PRO:HD2 | 1.99 | 0.41 |
| 4:C:486:HIS:O | 4:C:489:ILE:HB | 2.20 | 0.41 |
| 4:C:543:ILE:O | 4:C:544:GLN:O | 2.39 | 0.41 |
| 4:C:557:ARG:HB3 | 4:C:557:ARG:NH1 | 2.33 | 0.41 |
| 4:C:559:VAL:O | 4:C:560:ASN:HB2 | 2.21 | 0.41 |
| 4:C:534:LEU:HD12 | 4:C:818:PRO:HA | 2.03 | 0.41 |
| 4:D:125:CYS:HB3 | 4:D:137:VAL:HG22 | 2.02 | 0.41 |
| 4:D:133:THR:C | 4:D:135:GLN:H | 2.22 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:420:MET:HG2 | 4:D:425:ARG:O | 2.20 | 0.41 |
| 4:D:646:PHE:HD1 | 4:D:649:GLN:OE1 | 2.03 | 0.41 |
| 4:D:829:ARG:CG | 4:D:829:ARG:HH11 | 2.25 | 0.41 |
| 4:A:14:ILE:HG23 | 4:A:288:ALA:HB1 | 2.02 | 0.41 |
| 4:A:384:VAL:HG12 | 4:A:384:VAL:O | 2.20 | 0.41 |
| 4:A:544:GLN:O | 4:A:547:SER:N | 2.54 | 0.41 |
| 4:A:78:LEU:HA | 4:A:78:LEU:HD12 | 1.83 | 0.41 |
| 4:A:825:PHE:HE1 | 4:A:829:ARG:CZ | 2.26 | 0.41 |
| 4:B:114:VAL:HG13 | 4:B:145:ILE:HD12 | 2.03 | 0.41 |
| 4:B:233:ASN:HB2 | 4:B:239:GLN:O | 2.21 | 0.41 |
| 4:B:474:PRO:HA | 4:B:880:PHE:CE1 | 2.56 | 0.41 |
| 4:B:475:PHE:C | 4:B:477:GLU:N | 2.74 | 0.41 |
| 4:B:477:GLU:O | 4:B:480:LYS:HB3 | 2.20 | 0.41 |
| 4:B:505:GLN:NE2 | 4:B:505:GLN:CA | 2.79 | 0.41 |
| 4:B:817:ILE:HG13 | 4:B:820:ASP:HB2 | 2.02 | 0.41 |
| 4:C:557:ARG:O | 4:C:557:ARG:HG2 | 2.19 | 0.41 |
| 4:C:556:GLY:O | 4:C:561:LEU:HB2 | 2.21 | 0.41 |
| 4:C:446:LEU:CD1 | 4:C:817:ILE:HG23 | 2.50 | 0.41 |
| 4:D:21:PHE:O | 4:D:21:PHE:HD1 | 2.03 | 0.41 |
| 4:D:254:ILE:HG13 | 4:D:254:ILE:H | 1.70 | 0.41 |
| 4:D:304:ALA:HA | 4:D:307:ARG:HG3 | 2.03 | 0.41 |
| 4:D:416:PHE:HA | 4:D:417:PRO:HD2 | 1.80 | 0.41 |
| 4:D:440:THR:C | 4:D:442:GLY:N | 2.74 | 0.41 |
| 4:D:732:GLY:O | 4:D:734:PRO:HD3 | 2.19 | 0.41 |
| 4:D:744:GLN:CG | 4:D:756:ARG:HB3 | 2.46 | 0.41 |
| 4:D:828:VAL:CB | 4:D:883:ALA:HA | 2.40 | 0.41 |
| 4:D:92:VAL:HG11 | 4:D:103:PHE:CD1 | 2.54 | 0.41 |
| 1:K:6:DT:H2'' | 1:K:7:DC:OP2 | 2.20 | 0.41 |
| 1:N:9:DA:N6 | 3:P:1:DG:N2 | 2.68 | 0.41 |
| 4:A:257:ARG:CD | 4:A:261:LEU:HD13 | 2.49 | 0.41 |
| 4:A:290:GLY:C | 4:A:292:ARG:H | 2.24 | 0.41 |
| 4:A:511:PHE:CD2 | 4:A:511:PHE:C | 2.93 | 0.41 |
| 4:A:457:TYR:CD1 | 4:A:521:VAL:HG11 | 2.55 | 0.41 |
| 4:A:635:MET:CE | 6:A:2000:APC:H2' | 2.51 | 0.41 |
| 4:A:709:GLU:HB2 | 4:A:722:ARG:NE | 2.35 | 0.41 |
| 4:A:792:ARG:CG | 4:A:792:ARG:HH11 | 2.30 | 0.41 |
| 4:B:268:PHE:CD1 | 4:B:286:TYR:CE2 | 3.09 | 0.41 |
| 4:B:461:LYS:HD3 | 4:B:483:GLU:OE2 | 2.21 | 0.41 |
| 4:B:57:ARG:O | 4:B:60:LYS:HB3 | 2.21 | 0.41 |
| 4:B:633:SER:O | 4:B:634:VAL:C | 2.54 | 0.41 |
| 4:B:676:TYR:CD1 | 4:B:680:LEU:HD11 | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:B:730:PRO:HD3 | 7:B:3081:HOH:O | 2.21 | 0.41 |
| 4:B:323:ALA:HB1 | 4:B:809:LEU:HD11 | 2.02 | 0.41 |
| 4:C:272:VAL:HG13 | 4:C:411:HIS:CD2 | 2.55 | 0.41 |
| 4:C:322:ILE:O | 4:C:323:ALA:C | 2.59 | 0.41 |
| 4:C:393:SER:C | 4:C:395:ARG:H | 2.24 | 0.41 |
| 4:C:619:GLN:NE2 | 4:C:668:THR:H | 2.19 | 0.41 |
| 4:C:711:LYS:HG3 | 4:C:718:ILE:HA | 2.03 | 0.41 |
| 4:C:297:VAL:CG2 | 4:C:733:PHE:HZ | 2.34 | 0.41 |
| 4:D:282:THR:OG1 | 4:D:283:GLY:N | 2.52 | 0.41 |
| 4:D:439:MET:HE3 | 4:D:443:LEU:HD11 | 2.02 | 0.41 |
| 4:D:678:ALA:O | 4:D:679:LYS:C | 2.59 | 0.41 |
| 4:D:702:ALA:O | 4:D:704:LYS:N | 2.54 | 0.41 |
| 1:N:17:DG:P | 4:D:57:ARG:HH12 | 2.44 | 0.41 |
| 4:A:308:TYR:HH | 4:A:733:PHE:HE2 | 1.68 | 0.41 |
| 4:A:374:LEU:C | 4:A:376:ALA:N | 2.74 | 0.41 |
| 4:A:559:VAL:CG1 | 7:A:3104:HOH:O | 2.68 | 0.41 |
| 4:A:678:ALA:O | 4:A:679:LYS:C | 2.59 | 0.41 |
| 4:A:715:THR:HG21 | 4:A:717:GLU:OE2 | 2.21 | 0.41 |
| 4:A:794:THR:HG21 | 4:A:828:VAL:HG13 | 2.02 | 0.41 |
| 4:B:105:PHE:CE1 | 4:B:208:ASP:HB3 | 2.55 | 0.41 |
| 4:B:569:ASP:OD1 | 4:B:572:GLY:N | 2.50 | 0.41 |
| 4:B:619:GLN:HE22 | 4:B:668:THR:H | 1.68 | 0.41 |
| 4:B:673:ALA:O | 4:B:676:TYR:HB3 | 2.20 | 0.41 |
| 4:B:705:LEU:C | 4:B:707:ALA:N | 2.75 | 0.41 |
| 4:B:805:GLU:HB2 | 7:B:3030:HOH:O | 2.21 | 0.41 |
| 4:C:199:GLU:HG2 | 4:C:201:TRP:CD1 | 2.55 | 0.41 |
| 4:C:632:ARG:CZ | 6:C:2002:APC:N7 | 2.84 | 0.41 |
| 4:C:269:GLN:O | 4:C:430:SER:CB | 2.65 | 0.41 |
| 4:C:36:GLN:NE2 | 4:C:271:CYS:HB3 | 2.35 | 0.41 |
| 4:C:445:THR:OG1 | 4:C:532:LEU:HA | 2.21 | 0.41 |
| 4:C:576:LYS:HB3 | 7:C:3018:HOH:O | 2.19 | 0.41 |
| 4:C:617:ALA:O | 4:C:618:GLY:C | 2.58 | 0.41 |
| 4:C:698:TRP:HE3 | 4:C:699:LEU:HG | 1.85 | 0.41 |
| 4:C:702:ALA:O | 4:C:703:ALA:C | 2.56 | 0.41 |
| 4:C:308:TYR:CE2 | 4:C:736:TRP:HZ3 | 2.38 | 0.41 |
| 4:C:699:LEU:HD22 | 4:C:782:PHE:CG | 2.56 | 0.41 |
| 4:D:6:ILE:HB | 4:D:11:PHE:CE2 | 2.55 | 0.41 |
| 4:D:150:ARG:HH21 | 4:D:187:GLU:CD | 2.22 | 0.41 |
| 4:D:323:ALA:O | 4:D:324:GLN:C | 2.55 | 0.41 |
| 4:D:400:PHE:O | 4:D:404:GLN:HB2 | 2.21 | 0.41 |
| 4:D:570:ILE:O | 4:D:573:ILE:HG22 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:A:110:LYS:O | 4:A:114:VAL:HG23 | 2.21 | 0.41 |
| 4:A:437:ASN:O | 4:A:438:ASP:O | 2.39 | 0.41 |
| 4:A:514:PHE:O | 4:A:517:GLU:N | 2.45 | 0.41 |
| 4:A:630:THR:CA | 7:A:3199:HOH:O | 2.62 | 0.41 |
| 4:A:701:SER:O | 4:A:702:ALA:C | 2.59 | 0.41 |
| 4:B:335:LEU:HG | 4:B:339:ASN:ND2 | 2.36 | 0.41 |
| 4:B:581:ILE:O | 4:B:584:ALA:N | 2.50 | 0.41 |
| 4:B:636:THR:O | 4:B:637:LEU:C | 2.59 | 0.41 |
| 4:B:700:LYS:HE3 | 4:B:775:GLU:HG2 | 2.03 | 0.41 |
| 4:C:301:SER:O | 4:C:302:LYS:C | 2.59 | 0.41 |
| 4:C:385:TYR:O | 4:C:388:ASP:N | 2.54 | 0.41 |
| 4:C:395:ARG:O | 4:C:396:ILE:C | 2.58 | 0.41 |
| 4:C:729:THR:OG1 | 4:C:733:PHE:HB3 | 2.21 | 0.41 |
| 4:C:696:MET:HG2 | 4:C:779:ALA:HB1 | 2.02 | 0.41 |
| 4:C:78:LEU:HD11 | 4:C:115:ALA:CB | 2.51 | 0.41 |
| 4:D:12:SER:O | 4:D:13:ASP:C | 2.59 | 0.41 |
| 4:D:457:TYR:HH | 4:D:518:TYR:HE2 | 1.67 | 0.41 |
| 4:D:582:LEU:CD2 | 4:D:620:TRP:HB2 | 2.49 | 0.41 |
| 4:D:840:ASP:C | 4:D:842:LEU:H | 2.23 | 0.41 |
| 4:D:843:ALA:HB2 | 4:D:864:LEU:HD21 | 2.03 | 0.41 |
| 1:K:12:DT:O4' | 4:C:423:ARG:NH2 | 2.54 | 0.41 |
| 4:A:103:PHE:CE2 | 7:A:3227:HOH:O | 2.57 | 0.41 |
| 4:A:199:GLU:O | 4:A:201:TRP:N | 2.44 | 0.41 |
| 4:A:341:ILE:O | 4:A:342:THR:C | 2.58 | 0.41 |
| 4:A:505:GLN:C | 4:A:507:SER:N | 2.71 | 0.41 |
| 4:A:705:LEU:O | 4:A:708:ALA:HB3 | 2.21 | 0.41 |
| 4:A:727:TRP:O | 4:A:734:PRO:HA | 2.21 | 0.41 |
| 4:A:734:PRO:O | 4:A:734:PRO:CG | 2.68 | 0.41 |
| 4:A:825:PHE:C | 4:A:825:PHE:HD1 | 2.22 | 0.41 |
| 4:B:634:VAL:O | 4:B:634:VAL:CG2 | 2.69 | 0.41 |
| 4:B:678:ALA:O | 4:B:681:ILE:N | 2.54 | 0.41 |
| 4:C:106:LEU:HG | 4:C:212:VAL:CG1 | 2.51 | 0.41 |
| 4:C:3:THR:HG23 | 4:C:258:ALA:HB3 | 2.02 | 0.41 |
| 4:C:397:SER:O | 4:C:400:PHE:N | 2.44 | 0.41 |
| 4:C:421:ASP:O | 4:C:424:GLY:N | 2.48 | 0.41 |
| 4:C:11:PHE:CE1 | 4:C:44:TYR:HB3 | 2.56 | 0.41 |
| 4:C:452:ILE:HG13 | 4:C:456:GLY:C | 2.41 | 0.41 |
| 4:C:733:PHE:HB2 | 4:C:792:ARG:HH21 | 1.86 | 0.41 |
| 4:D:133:THR:HG22 | 4:D:243:THR:HG22 | 2.03 | 0.41 |
| 4:D:201:TRP:HA | 4:D:204:TRP:CD1 | 2.51 | 0.41 |
| 4:D:77:LEU:HD21 | 4:D:226:MET:HB2 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:36:GLN:HG2 | 4:D:272:VAL:HB | 2.02 | 0.41 |
| 4:D:402:LEU:HD23 | 4:D:402:LEU:HA | 1.59 | 0.41 |
| 4:D:482:ILE:HD12 | 4:D:514:PHE:CZ | 2.55 | 0.41 |
| 4:D:619:GLN:CG | 4:D:666:MET:O | 2.68 | 0.41 |
| 4:D:698:TRP:CZ3 | 4:D:699:LEU:HD23 | 2.56 | 0.41 |
| 4:D:448:LYS:HD2 | 4:D:806:SER:HB3 | 2.03 | 0.41 |
| 4:D:827:ALA:O | 4:D:828:VAL:C | 2.59 | 0.41 |
| 4:D:563:PRO:HB3 | 4:D:877:GLU:C | 2.42 | 0.41 |
| 1:E:12:DT:C2' | 1:E:13:DC:H6 | 2.33 | 0.41 |
| 4:A:19:ILE:CG2 | 4:A:20:PRO:N | 2.84 | 0.40 |
| 4:A:646:PHE:CD1 | 4:A:646:PHE:N | 2.88 | 0.40 |
| 4:A:658:ALA:O | 4:A:661:SER:HB2 | 2.21 | 0.40 |
| 4:A:741:LYS:HB3 | 4:A:741:LYS:HE2 | 1.82 | 0.40 |
| 4:B:150:ARG:C | 4:B:152:GLY:H | 2.23 | 0.40 |
| 4:B:341:ILE:N | 4:B:341:ILE:HD12 | 2.36 | 0.40 |
| 4:B:502:TRP:CE3 | 4:B:512:LEU:HD22 | 2.56 | 0.40 |
| 4:B:645:GLY:O | 4:B:646:PHE:C | 2.59 | 0.40 |
| 4:B:646:PHE:O | 4:B:647:ARG:O | 2.39 | 0.40 |
| 4:B:797:TRP:CH2 | 4:B:801:LYS:HG3 | 2.56 | 0.40 |
| 4:C:834:ASP:O | 4:C:837:GLU:HB2 | 2.21 | 0.40 |
| 4:D:347:CYS:HB3 | 4:D:350:GLU:CG | 2.50 | 0.40 |
| 4:D:417:PRO:C | 4:D:429:VAL:HG23 | 2.40 | 0.40 |
| 4:D:437:ASN:ND2 | 4:D:437:ASN:C | 2.75 | 0.40 |
| 4:D:349:VAL:HG13 | 4:D:503:ALA:HB1 | 2.03 | 0.40 |
| 4:D:588:ASN:HB3 | 4:D:589:GLY:H | 1.65 | 0.40 |
| 4:D:642:LYS:O | 4:D:646:PHE:CD2 | 2.74 | 0.40 |
| 2:I:4:G:H4' | 4:B:389:LYS:HE3 | 2.03 | 0.40 |
| 1:K:12:DT:H4' | 4:C:423:ARG:NH1 | 2.36 | 0.40 |
| 1:N:15:DC:N3 | 1:N:16:DC:C5 | 2.89 | 0.40 |
| 4:A:103:PHE:CD2 | 4:A:107:GLN:NE2 | 2.89 | 0.40 |
| 4:A:126:LEU:HD23 | 4:A:132:THR:HG23 | 2.03 | 0.40 |
| 4:A:304:ALA:C | 4:A:307:ARG:HG3 | 2.36 | 0.40 |
| 4:A:433:ASN:CB | 4:A:434:PRO:HD2 | 2.50 | 0.40 |
| 4:A:620:TRP:HZ3 | 4:A:623:TYR:HD2 | 1.69 | 0.40 |
| 4:A:74:ILE:HG22 | 4:A:74:ILE:O | 2.21 | 0.40 |
| 4:A:816:THR:HG21 | 4:A:820:ASP:HB2 | 2.03 | 0.40 |
| 4:A:867:LYS:N | 4:A:867:LYS:HD2 | 2.36 | 0.40 |
| 4:B:230:HIS:CE1 | 4:B:232:GLN:HE21 | 2.39 | 0.40 |
| 4:B:418:TYR:CD2 | 4:B:427:TYR:O | 2.67 | 0.40 |
| 4:B:329:LYS:CD | 4:B:447:ALA:HA | 2.45 | 0.40 |
| 4:B:680:LEU:CD1 | 4:B:680:LEU:N | 2.80 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:C:13:ASP:CB | 7:C:3077:HOH:O | 2.69 | 0.40 |
| 4:C:281:ILE:HA | 4:C:281:ILE:HD12 | 1.83 | 0.40 |
| 4:C:425:ARG:HB2 | 4:C:427:TYR:HE1 | 1.86 | 0.40 |
| 4:C:402:LEU:CD1 | 4:C:439:MET:HE3 | 2.51 | 0.40 |
| 4:C:720:ARG:HG2 | 4:C:720:ARG:HH11 | 1.85 | 0.40 |
| 4:C:563:PRO:CD | 4:C:874:ASP:HB3 | 2.48 | 0.40 |
| 4:D:296:LEU:HG | 4:D:296:LEU:O | 2.21 | 0.40 |
| 4:D:327:ALA:HB2 | 4:D:415:TRP:CE2 | 2.56 | 0.40 |
| 4:D:439:MET:HG3 | 4:D:509:PHE:CE2 | 2.56 | 0.40 |
| 4:D:539:SER:HB3 | 4:D:559:VAL:HG12 | 2.02 | 0.40 |
| 4:D:733:PHE:HB2 | 4:D:792:ARG:NH2 | 2.37 | 0.40 |
| 4:D:735:VAL:CG2 | 4:D:736:TRP:N | 2.85 | 0.40 |
| 4:D:827:ALA:O | 4:D:831:THR:HG22 | 2.21 | 0.40 |
| 1:H:15:DC:C5' | 7:H:642:HOH:O | 2.69 | 0.40 |
| 4:A:51:PHE:CD2 | 4:A:262:ALA:HB2 | 2.56 | 0.40 |
| 4:A:386:ARG:HE | 4:A:386:ARG:HB2 | 1.20 | 0.40 |
| 4:A:58:GLN:HG3 | 4:A:67:ASN:ND2 | 2.36 | 0.40 |
| 4:B:105:PHE:C | 4:B:107:GLN:N | 2.75 | 0.40 |
| 4:B:779:ALA:O | 4:B:783:VAL:CG2 | 2.69 | 0.40 |
| 4:C:491:ALA:O | 4:C:494:LYS:N | 2.55 | 0.40 |
| 4:C:576:LYS:HD3 | 7:C:3018:HOH:O | 2.21 | 0.40 |
| 4:C:712:ASP:O | 4:C:716:GLY:N | 2.55 | 0.40 |
| 4:C:730:PRO:CD | 4:C:786:GLN:NE2 | 2.84 | 0.40 |
| 4:C:729:THR:HA | 4:C:730:PRO:HD3 | 1.88 | 0.40 |
| 4:D:236:VAL:CB | 4:D:239:GLN:HB2 | 2.51 | 0.40 |
| 4:D:274:PRO:HA | 4:D:275:PRO:HD3 | 1.93 | 0.40 |
| 4:D:571:TYR:CD1 | 4:D:634:VAL:CG1 | 3.04 | 0.40 |
| 4:D:744:GLN:HE21 | 4:D:756:ARG:N | 2.18 | 0.40 |
| 4:D:737:GLN:HG2 | 4:D:774:GLN:OE1 | 2.20 | 0.40 |
| 1:K:5:DA:H1' | 7:K:712:HOH:O | 2.20 | 0.40 |
| 2:L:6:G:C6 | 2:L:7:A:N7 | 2.89 | 0.40 |
| 3:M:7:DT:H2'' | 3:M:8:DC:C6 | 2.56 | 0.40 |
| 4:A:635:MET:HE1 | 6:A:2000:APC:H2' | 2.03 | 0.40 |
| 4:A:39:LEU:O | 4:A:40:GLU:C | 2.60 | 0.40 |
| 4:A:404:GLN:HG2 | 4:A:432:PHE:CD2 | 2.55 | 0.40 |
| 4:A:56:GLU:HG3 | 7:A:3057:HOH:O | 2.20 | 0.40 |
| 4:A:704:LYS:HE3 | 4:A:860:LYS:HZ1 | 1.83 | 0.40 |
| 4:A:550:LEU:HD21 | 4:A:865:PRO:HG2 | 2.04 | 0.40 |
| 4:B:108:GLU:HA | 4:B:108:GLU:OE2 | 2.21 | 0.40 |
| 4:B:109:ILE:H | 4:B:109:ILE:CD1 | 2.33 | 0.40 |
| 4:B:220:LEU:O | 4:B:222:GLU:N | 2.54 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:B:252:GLU:O | 4:B:253:ALA:C | 2.58 | 0.40 |
| 4:B:572:GLY:O | 4:B:575:ALA:HB3 | 2.21 | 0.40 |
| 4:B:643:GLU:O | 4:B:645:GLY:N | 2.54 | 0.40 |
| 4:B:577:LYS:HB3 | 4:B:684:SER:HB3 | 2.03 | 0.40 |
| 4:B:116:TYR:CE2 | 4:B:752:LEU:HD13 | 2.56 | 0.40 |
| 4:B:790:HIS:HD1 | 4:B:790:HIS:C | 2.24 | 0.40 |
| 4:B:810:ILE:HB | 4:B:813:SER:HB2 | 2.03 | 0.40 |
| 4:B:88:TRP:O | 4:B:92:VAL:HG23 | 2.22 | 0.40 |
| 4:C:84:ARG:CB | 4:C:223:SER:HB3 | 2.49 | 0.40 |
| 4:C:463:HIS:HE1 | 4:C:532:LEU:HD11 | 1.86 | 0.40 |
| 4:C:540:CYS:HB2 | 4:C:559:VAL:HG12 | 2.04 | 0.40 |
| 4:C:59:LEU:HA | 4:C:64:VAL:HG22 | 2.03 | 0.40 |
| 4:D:141:ILE:O | 4:D:145:ILE:CG1 | 2.66 | 0.40 |
| 4:D:294:LEU:HD13 | 4:D:419:ASN:HD21 | 1.86 | 0.40 |
| 4:D:508:PRO:C | 4:D:510:CYS:N | 2.73 | 0.40 |
| 4:D:726:HIS:CD2 | 4:D:735:VAL:O | 2.74 | 0.40 |
| 3:J:6:DT:C2' | 3:J:7:DT:H71 | 2.50 | 0.40 |
| 3:M:4:DG:H2'' | 3:M:5:DA:C8 | 2.57 | 0.40 |
| 2:O:6:G:H3' | 7:O:144:HOH:O | 2.20 | 0.40 |
| 4:A:24:LEU:HD21 | 4:A:287:TRP:CD2 | 2.56 | 0.40 |
| 4:A:868:GLY:N | 7:A:3164:HOH:O | 2.54 | 0.40 |
| 4:A:868:GLY:C | 4:A:869:ASN:HD22 | 2.25 | 0.40 |
| 4:B:185:VAL:O | 4:B:188:ALA:HB3 | 2.22 | 0.40 |
| 4:B:215:ARG:O | 4:B:219:MET:HE3 | 2.21 | 0.40 |
| 4:B:229:LEU:HD11 | 4:B:242:GLU:CG | 2.42 | 0.40 |
| 4:B:306:MET:O | 4:B:309:GLU:N | 2.51 | 0.40 |
| 4:C:261:LEU:HA | 4:C:261:LEU:HD12 | 1.82 | 0.40 |
| 4:C:483:GLU:O | 4:C:486:HIS:N | 2.52 | 0.40 |
| 4:C:523:HIS:N | 4:C:523:HIS:CD2 | 2.90 | 0.40 |
| 4:C:525:GLY:C | 4:C:527:SER:H | 2.24 | 0.40 |
| 4:C:551:ARG:HE | 4:C:872:LEU:CG | 2.34 | 0.40 |
| 4:C:749:LEU:CD1 | 4:C:750:MET:HG2 | 2.46 | 0.40 |
| 4:C:756:ARG:CG | 7:C:3143:HOH:O | 2.70 | 0.40 |
| 4:C:786:GLN:C | 4:C:788:GLY:N | 2.75 | 0.40 |
| 4:C:817:ILE:HD12 | 4:C:819:ALA:HB3 | 2.04 | 0.40 |
| 4:D:22:ASN:HA | 4:D:25:ALA:HB3 | 2.03 | 0.40 |
| 4:D:549:MET:HE3 | 4:D:836:TYR:HE1 | 1.86 | 0.40 |
| 4:D:702:ALA:HB2 | 4:D:861:MET:HE1 | 2.03 | 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 | |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 4 | A | 851/883 (96%) | 570 (67%) | 198 (23%) | 83 (10%) | 1 | 4 |
| 4 | B | 851/883 (96%) | 578 (68%) | 188 (22%) | 85 (10%) | 1 | 4 |
| 4 | C | 851/883 (96%) | 608 (71%) | 178 (21%) | 65 (8%) | 1 | 8 |
| 4 | D | 851/883 (96%) | 623 (73%) | 174 (20%) | 54 (6%) | 1 | 12 |
| All | All | 3404/3532 (96%) | 2379 (70%) | 738 (22%) | 287 (8%) | 1 | 6 |

All (287) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | A | 7 | ALA |
| 4 | A | 194 | GLY |
| 4 | A | 199 | GLU |
| 4 | A | 281 | ILE |
| 4 | A | 288 | ALA |
| 4 | A | 309 | GLU |
| 4 | A | 353 | PRO |
| 4 | A | 387 | LYS |
| 4 | A | 391 | ARG |
| 4 | A | 402 | LEU |
| 4 | A | 430 | SER |
| 4 | A | 506 | ASP |
| 4 | A | 508 | PRO |
| 4 | A | 526 | LEU |
| 4 | A | 549 | MET |
| 4 | A | 592 | ASN |
| 4 | A | 631 | LYS |
| 4 | A | 686 | SER |
| 4 | A | 708 | ALA |
| 4 | A | 721 | LYS |
| 4 | A | 744 | GLN |
| 4 | A | 745 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | A | 746 | ARG |
| 4 | A | 755 | PHE |
| 4 | A | 803 | GLY |
| 4 | A | 850 | ALA |
| 4 | B | 262 | ALA |
| 4 | B | 274 | PRO |
| 4 | B | 293 | PRO |
| 4 | B | 391 | ARG |
| 4 | B | 452 | ILE |
| 4 | B | 539 | SER |
| 4 | B | 610 | LYS |
| 4 | B | 611 | LEU |
| 4 | B | 646 | PHE |
| 4 | B | 647 | ARG |
| 4 | B | 663 | LYS |
| 4 | B | 690 | VAL |
| 4 | B | 706 | LEU |
| 4 | B | 755 | PHE |
| 4 | B | 784 | HIS |
| 4 | B | 785 | SER |
| 4 | B | 796 | VAL |
| 4 | B | 804 | ILE |
| 4 | B | 841 | VAL |
| 4 | B | 851 | ASP |
| 4 | C | 68 | ALA |
| 4 | C | 106 | LEU |
| 4 | C | 240 | ASP |
| 4 | C | 288 | ALA |
| 4 | C | 309 | GLU |
| 4 | C | 337 | VAL |
| 4 | C | 422 | TRP |
| 4 | C | 503 | ALA |
| 4 | C | 508 | PRO |
| 4 | C | 526 | LEU |
| 4 | C | 539 | SER |
| 4 | C | 631 | LYS |
| 4 | C | 744 | GLN |
| 4 | C | 745 | THR |
| 4 | C | 755 | PHE |
| 4 | C | 771 | ALA |
| 4 | C | 841 | VAL |
| 4 | D | 307 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | D | 324 | GLN |
| 4 | D | 353 | PRO |
| 4 | D | 508 | PRO |
| 4 | D | 539 | SER |
| 4 | D | 541 | SER |
| 4 | D | 592 | ASN |
| 4 | D | 647 | ARG |
| 4 | D | 663 | LYS |
| 4 | D | 755 | PHE |
| 4 | D | 841 | VAL |
| 4 | A | 60 | LYS |
| 4 | A | 106 | LEU |
| 4 | A | 177 | VAL |
| 4 | A | 200 | ALA |
| 4 | A | 332 | LYS |
| 4 | A | 375 | THR |
| 4 | A | 384 | VAL |
| 4 | A | 401 | MET |
| 4 | A | 422 | TRP |
| 4 | A | 438 | ASP |
| 4 | A | 474 | PRO |
| 4 | A | 544 | GLN |
| 4 | A | 632 | ARG |
| 4 | A | 641 | SER |
| 4 | A | 678 | ALA |
| 4 | A | 771 | ALA |
| 4 | A | 811 | HIS |
| 4 | A | 882 | PHE |
| 4 | B | 14 | ILE |
| 4 | B | 36 | GLN |
| 4 | B | 106 | LEU |
| 4 | B | 167 | GLU |
| 4 | B | 176 | HIS |
| 4 | B | 194 | GLY |
| 4 | B | 298 | ARG |
| 4 | B | 307 | ARG |
| 4 | B | 314 | PRO |
| 4 | B | 315 | GLU |
| 4 | B | 412 | LYS |
| 4 | B | 430 | SER |
| 4 | B | 431 | MET |
| 4 | B | 470 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | B | 526 | LEU |
| 4 | B | 542 | GLY |
| 4 | B | 589 | GLY |
| 4 | B | 592 | ASN |
| 4 | B | 641 | SER |
| 4 | B | 721 | LYS |
| 4 | B | 746 | ARG |
| 4 | B | 865 | PRO |
| 4 | B | 873 | ARG |
| 4 | B | 876 | LEU |
| 4 | C | 7 | ALA |
| 4 | C | 162 | PHE |
| 4 | C | 307 | ARG |
| 4 | C | 314 | PRO |
| 4 | C | 339 | ASN |
| 4 | C | 443 | LEU |
| 4 | C | 474 | PRO |
| 4 | C | 544 | GLN |
| 4 | C | 686 | SER |
| 4 | C | 690 | VAL |
| 4 | C | 796 | VAL |
| 4 | C | 811 | HIS |
| 4 | C | 882 | PHE |
| 4 | D | 7 | ALA |
| 4 | D | 119 | ILE |
| 4 | D | 167 | GLU |
| 4 | D | 259 | GLY |
| 4 | D | 292 | ARG |
| 4 | D | 422 | TRP |
| 4 | D | 443 | LEU |
| 4 | D | 452 | ILE |
| 4 | D | 593 | GLU |
| 4 | D | 648 | GLN |
| 4 | D | 745 | THR |
| 4 | D | 882 | PHE |
| 4 | A | 100 | PRO |
| 4 | A | 262 | ALA |
| 4 | A | 277 | PRO |
| 4 | A | 460 | LEU |
| 4 | A | 511 | PHE |
| 4 | A | 525 | GLY |
| 4 | A | 541 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | A | 542 | GLY |
| 4 | A | 647 | ARG |
| 4 | A | 660 | ASP |
| 4 | A | 734 | PRO |
| 4 | A | 797 | TRP |
| 4 | A | 825 | PHE |
| 4 | A | 872 | LEU |
| 4 | B | 7 | ALA |
| 4 | B | 68 | ALA |
| 4 | B | 150 | ARG |
| 4 | B | 199 | GLU |
| 4 | B | 200 | ALA |
| 4 | B | 260 | ALA |
| 4 | B | 348 | PRO |
| 4 | B | 382 | ALA |
| 4 | B | 505 | GLN |
| 4 | B | 508 | PRO |
| 4 | B | 551 | ARG |
| 4 | B | 593 | GLU |
| 4 | B | 617 | ALA |
| 4 | B | 627 | ARG |
| 4 | B | 628 | SER |
| 4 | B | 678 | ALA |
| 4 | B | 810 | ILE |
| 4 | B | 862 | PRO |
| 4 | C | 98 | LYS |
| 4 | C | 140 | ALA |
| 4 | C | 199 | GLU |
| 4 | C | 206 | LYS |
| 4 | C | 262 | ALA |
| 4 | C | 549 | MET |
| 4 | C | 647 | ARG |
| 4 | C | 850 | ALA |
| 4 | C | 851 | ASP |
| 4 | D | 240 | ASP |
| 4 | D | 288 | ALA |
| 4 | D | 309 | GLU |
| 4 | D | 314 | PRO |
| 4 | D | 348 | PRO |
| 4 | D | 405 | ALA |
| 4 | D | 544 | GLN |
| 4 | D | 589 | GLY |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | A | 160 | LYS |
| 4 | A | 204 | TRP |
| 4 | A | 274 | PRO |
| 4 | A | 345 | LYS |
| 4 | A | 425 | ARG |
| 4 | A | 464 | GLY |
| 4 | A | 611 | LEU |
| 4 | A | 670 | PRO |
| 4 | A | 677 | MET |
| 4 | A | 796 | VAL |
| 4 | B | 50 | ARG |
| 4 | B | 160 | LYS |
| 4 | B | 277 | PRO |
| 4 | B | 395 | ARG |
| 4 | B | 396 | ILE |
| 4 | B | 476 | PRO |
| 4 | B | 580 | GLU |
| 4 | B | 631 | LYS |
| 4 | B | 648 | GLN |
| 4 | B | 705 | LEU |
| 4 | B | 752 | LEU |
| 4 | B | 811 | HIS |
| 4 | B | 824 | LEU |
| 4 | B | 850 | ALA |
| 4 | C | 200 | ALA |
| 4 | C | 353 | PRO |
| 4 | C | 476 | PRO |
| 4 | C | 592 | ASN |
| 4 | C | 787 | ASP |
| 4 | D | 65 | ALA |
| 4 | D | 260 | ALA |
| 4 | D | 631 | LYS |
| 4 | D | 722 | ARG |
| 4 | A | 4 | ILE |
| 4 | A | 313 | MET |
| 4 | A | 348 | PRO |
| 4 | A | 383 | ALA |
| 4 | A | 560 | ASN |
| 4 | A | 690 | VAL |
| 4 | B | 115 | ALA |
| 4 | B | 265 | SER |
| 4 | B | 342 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | B | 557 | ARG |
| 4 | B | 780 | PRO |
| 4 | C | 102 | ALA |
| 4 | C | 348 | PRO |
| 4 | C | 541 | SER |
| 4 | C | 542 | GLY |
| 4 | C | 632 | ARG |
| 4 | C | 663 | LYS |
| 4 | C | 701 | SER |
| 4 | C | 832 | MET |
| 4 | D | 63 | GLU |
| 4 | D | 162 | PHE |
| 4 | D | 467 | CYS |
| 4 | D | 474 | PRO |
| 4 | D | 691 | ALA |
| 4 | D | 704 | LYS |
| 4 | D | 744 | GLN |
| 4 | A | 292 | ARG |
| 4 | A | 593 | GLU |
| 4 | B | 254 | ILE |
| 4 | C | 4 | ILE |
| 4 | C | 211 | HIS |
| 4 | C | 235 | GLY |
| 4 | C | 341 | ILE |
| 4 | C | 648 | GLN |
| 4 | C | 872 | LEU |
| 4 | D | 275 | PRO |
| 4 | D | 336 | ALA |
| 4 | D | 715 | THR |
| 4 | D | 811 | HIS |
| 4 | D | 850 | ALA |
| 4 | D | 860 | LYS |
| 4 | A | 710 | VAL |
| 4 | B | 270 | PRO |
| 4 | B | 479 | ILE |
| 4 | C | 804 | ILE |
| 4 | D | 114 | VAL |
| 4 | D | 194 | GLY |
| 4 | D | 693 | VAL |
| 4 | A | 533 | PRO |
| 4 | A | 650 | VAL |
| 4 | C | 19 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | C | 141 | ILE |
| 4 | C | 322 | ILE |
| 4 | C | 567 | VAL |
| 4 | A | 841 | VAL |
| 4 | B | 353 | PRO |
| 4 | C | 194 | GLY |
| 4 | C | 833 | VAL |
| 4 | D | 337 | VAL |
| 4 | A | 270 | PRO |
| 4 | A | 567 | VAL |
| 4 | A | 669 | GLN |
| 4 | D | 97 | GLY |
| 4 | D | 4 | 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 | |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 4 | A | 703/729 (96%) | 573 (82%) | 130 (18%) | 2 | 9 |
| 4 | B | 703/729 (96%) | 573 (82%) | 130 (18%) | 2 | 9 |
| 4 | C | 703/729 (96%) | 594 (84%) | 109 (16%) | 3 | 14 |
| 4 | D | 703/729 (96%) | 598 (85%) | 105 (15%) | 3 | 16 |
| All | All | 2812/2916 (96%) | 2338 (83%) | 474 (17%) | 2 | 11 |

All (474) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | A | 8 | LYS |
| 4 | A | 16 | LEU |
| 4 | A | 19 | ILE |
| 4 | A | 23 | THR |
| 4 | A | 27 | HIS |
| 4 | A | 36 | GLN |
| 4 | A | 50 | ARG |
| 4 | A | 53 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | A | 56 | GLU |
| 4 | A | 57 | ARG |
| 4 | A | 60 | LYS |
| 4 | A | 77 | LEU |
| 4 | A | 81 | MET |
| 4 | A | 84 | ARG |
| 4 | A | 86 | ASN |
| 4 | A | 96 | ARG |
| 4 | A | 101 | THR |
| 4 | A | 104 | GLN |
| 4 | A | 121 | THR |
| 4 | A | 130 | ASP |
| 4 | A | 143 | ARG |
| 4 | A | 145 | ILE |
| 4 | A | 155 | ARG |
| 4 | A | 157 | LEU |
| 4 | A | 165 | ASN |
| 4 | A | 170 | LEU |
| 4 | A | 183 | MET |
| 4 | A | 190 | MET |
| 4 | A | 206 | LYS |
| 4 | A | 207 | GLU |
| 4 | A | 208 | ASP |
| 4 | A | 230 | HIS |
| 4 | A | 248 | PRO |
| 4 | A | 257 | ARG |
| 4 | A | 261 | LEU |
| 4 | A | 282 | THR |
| 4 | A | 293 | PRO |
| 4 | A | 299 | THR |
| 4 | A | 301 | SER |
| 4 | A | 307 | ARG |
| 4 | A | 309 | GLU |
| 4 | A | 330 | ILE |
| 4 | A | 333 | LYS |
| 4 | A | 343 | LYS |
| 4 | A | 388 | ASP |
| 4 | A | 393 | SER |
| 4 | A | 395 | ARG |
| 4 | A | 401 | MET |
| 4 | A | 402 | LEU |
| 4 | A | 403 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | A | 404 | GLN |
| 4 | A | 410 | ASN |
| 4 | A | 418 | TYR |
| 4 | A | 422 | TRP |
| 4 | A | 423 | ARG |
| 4 | A | 429 | VAL |
| 4 | A | 430 | SER |
| 4 | A | 433 | ASN |
| 4 | A | 440 | THR |
| 4 | A | 448 | LYS |
| 4 | A | 451 | PRO |
| 4 | A | 452 | ILE |
| 4 | A | 454 | LYS |
| 4 | A | 457 | TYR |
| 4 | A | 462 | ILE |
| 4 | A | 470 | VAL |
| 4 | A | 472 | LYS |
| 4 | A | 473 | VAL |
| 4 | A | 475 | PHE |
| 4 | A | 495 | SER |
| 4 | A | 510 | CYS |
| 4 | A | 514 | PHE |
| 4 | A | 516 | PHE |
| 4 | A | 517 | GLU |
| 4 | A | 531 | SER |
| 4 | A | 540 | CYS |
| 4 | A | 543 | ILE |
| 4 | A | 550 | LEU |
| 4 | A | 559 | VAL |
| 4 | A | 561 | LEU |
| 4 | A | 565 | GLU |
| 4 | A | 573 | ILE |
| 4 | A | 574 | VAL |
| 4 | A | 613 | THR |
| 4 | A | 620 | TRP |
| 4 | A | 626 | THR |
| 4 | A | 627 | ARG |
| 4 | A | 632 | ARG |
| 4 | A | 634 | VAL |
| 4 | A | 641 | SER |
| 4 | A | 643 | GLU |
| 4 | A | 647 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | A | 651 | LEU |
| 4 | A | 656 | GLN |
| 4 | A | 660 | ASP |
| 4 | A | 666 | MET |
| 4 | A | 670 | PRO |
| 4 | A | 688 | THR |
| 4 | A | 730 | PRO |
| 4 | A | 734 | PRO |
| 4 | A | 744 | GLN |
| 4 | A | 746 | ARG |
| 4 | A | 749 | LEU |
| 4 | A | 751 | PHE |
| 4 | A | 752 | LEU |
| 4 | A | 755 | PHE |
| 4 | A | 766 | ASP |
| 4 | A | 776 | SER |
| 4 | A | 778 | ILE |
| 4 | A | 786 | GLN |
| 4 | A | 787 | ASP |
| 4 | A | 791 | LEU |
| 4 | A | 796 | VAL |
| 4 | A | 801 | LYS |
| 4 | A | 802 | TYR |
| 4 | A | 806 | SER |
| 4 | A | 814 | PHE |
| 4 | A | 816 | THR |
| 4 | A | 820 | ASP |
| 4 | A | 828 | VAL |
| 4 | A | 829 | ARG |
| 4 | A | 832 | MET |
| 4 | A | 839 | CYS |
| 4 | A | 841 | VAL |
| 4 | A | 846 | TYR |
| 4 | A | 851 | ASP |
| 4 | A | 860 | LYS |
| 4 | A | 869 | ASN |
| 4 | A | 879 | ASP |
| 4 | A | 882 | PHE |
| 4 | B | 13 | ASP |
| 4 | B | 15 | GLU |
| 4 | B | 16 | LEU |
| 4 | B | 19 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | B | 21 | PHE |
| 4 | B | 22 | ASN |
| 4 | B | 24 | LEU |
| 4 | B | 27 | HIS |
| 4 | B | 32 | LEU |
| 4 | B | 36 | GLN |
| 4 | B | 39 | LEU |
| 4 | B | 50 | ARG |
| 4 | B | 56 | GLU |
| 4 | B | 66 | ASP |
| 4 | B | 71 | LYS |
| 4 | B | 84 | ARG |
| 4 | B | 86 | ASN |
| 4 | B | 96 | ARG |
| 4 | B | 99 | ARG |
| 4 | B | 101 | THR |
| 4 | B | 120 | LYS |
| 4 | B | 123 | LEU |
| 4 | B | 132 | THR |
| 4 | B | 143 | ARG |
| 4 | B | 164 | LYS |
| 4 | B | 166 | VAL |
| 4 | B | 168 | GLU |
| 4 | B | 172 | LYS |
| 4 | B | 184 | GLN |
| 4 | B | 206 | LYS |
| 4 | B | 207 | GLU |
| 4 | B | 209 | SER |
| 4 | B | 214 | VAL |
| 4 | B | 224 | THR |
| 4 | B | 252 | GLU |
| 4 | B | 256 | THR |
| 4 | B | 257 | ARG |
| 4 | B | 261 | LEU |
| 4 | B | 264 | ILE |
| 4 | B | 267 | MET |
| 4 | B | 272 | VAL |
| 4 | B | 273 | VAL |
| 4 | B | 277 | PRO |
| 4 | B | 279 | THR |
| 4 | B | 291 | ARG |
| 4 | B | 299 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | B | 305 | LEU |
| 4 | B | 314 | PRO |
| 4 | B | 332 | LYS |
| 4 | B | 337 | VAL |
| 4 | B | 343 | LYS |
| 4 | B | 349 | VAL |
| 4 | B | 351 | ASP |
| 4 | B | 378 | LYS |
| 4 | B | 379 | ARG |
| 4 | B | 388 | ASP |
| 4 | B | 394 | ARG |
| 4 | B | 397 | SER |
| 4 | B | 402 | LEU |
| 4 | B | 404 | GLN |
| 4 | B | 408 | PHE |
| 4 | B | 419 | ASN |
| 4 | B | 422 | TRP |
| 4 | B | 423 | ARG |
| 4 | B | 437 | ASN |
| 4 | B | 441 | LYS |
| 4 | B | 452 | ILE |
| 4 | B | 454 | LYS |
| 4 | B | 461 | LYS |
| 4 | B | 472 | LYS |
| 4 | B | 483 | GLU |
| 4 | B | 492 | CYS |
| 4 | B | 494 | LYS |
| 4 | B | 495 | SER |
| 4 | B | 497 | LEU |
| 4 | B | 500 | THR |
| 4 | B | 512 | LEU |
| 4 | B | 514 | PHE |
| 4 | B | 527 | SER |
| 4 | B | 532 | LEU |
| 4 | B | 540 | CYS |
| 4 | B | 552 | ASP |
| 4 | B | 560 | ASN |
| 4 | B | 567 | VAL |
| 4 | B | 569 | ASP |
| 4 | B | 582 | LEU |
| 4 | B | 592 | ASN |
| 4 | B | 621 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | B | 626 | THR |
| 4 | B | 627 | ARG |
| 4 | B | 633 | SER |
| 4 | B | 643 | GLU |
| 4 | B | 651 | LEU |
| 4 | B | 654 | THR |
| 4 | B | 656 | GLN |
| 4 | B | 666 | MET |
| 4 | B | 668 | THR |
| 4 | B | 683 | GLU |
| 4 | B | 690 | VAL |
| 4 | B | 693 | VAL |
| 4 | B | 697 | ASN |
| 4 | B | 722 | ARG |
| 4 | B | 731 | ASP |
| 4 | B | 734 | PRO |
| 4 | B | 735 | VAL |
| 4 | B | 744 | GLN |
| 4 | B | 749 | LEU |
| 4 | B | 752 | LEU |
| 4 | B | 769 | ILE |
| 4 | B | 770 | ASP |
| 4 | B | 776 | SER |
| 4 | B | 780 | PRO |
| 4 | B | 783 | VAL |
| 4 | B | 785 | SER |
| 4 | B | 786 | GLN |
| 4 | B | 790 | HIS |
| 4 | B | 801 | LYS |
| 4 | B | 809 | LEU |
| 4 | B | 813 | SER |
| 4 | B | 828 | VAL |
| 4 | B | 832 | MET |
| 4 | B | 841 | VAL |
| 4 | B | 842 | LEU |
| 4 | B | 849 | PHE |
| 4 | B | 859 | ASP |
| 4 | B | 860 | LYS |
| 4 | B | 867 | LYS |
| 4 | B | 869 | ASN |
| 4 | B | 870 | LEU |
| 4 | B | 877 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | C | 2 | ASN |
| 4 | C | 3 | THR |
| 4 | C | 9 | ASN |
| 4 | C | 16 | LEU |
| 4 | C | 26 | ASP |
| 4 | C | 32 | LEU |
| 4 | C | 36 | GLN |
| 4 | C | 37 | LEU |
| 4 | C | 40 | GLU |
| 4 | C | 50 | ARG |
| 4 | C | 64 | VAL |
| 4 | C | 66 | ASP |
| 4 | C | 84 | ARG |
| 4 | C | 96 | ARG |
| 4 | C | 99 | ARG |
| 4 | C | 107 | GLN |
| 4 | C | 119 | ILE |
| 4 | C | 120 | LYS |
| 4 | C | 143 | ARG |
| 4 | C | 170 | LEU |
| 4 | C | 183 | MET |
| 4 | C | 195 | LEU |
| 4 | C | 208 | ASP |
| 4 | C | 214 | VAL |
| 4 | C | 227 | VAL |
| 4 | C | 230 | HIS |
| 4 | C | 244 | ILE |
| 4 | C | 256 | THR |
| 4 | C | 257 | ARG |
| 4 | C | 267 | MET |
| 4 | C | 281 | ILE |
| 4 | C | 282 | THR |
| 4 | C | 291 | ARG |
| 4 | C | 294 | LEU |
| 4 | C | 301 | SER |
| 4 | C | 305 | LEU |
| 4 | C | 313 | MET |
| 4 | C | 325 | ASN |
| 4 | C | 335 | LEU |
| 4 | C | 343 | LYS |
| 4 | C | 347 | CYS |
| 4 | C | 350 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | C | 377 | TRP |
| 4 | C | 378 | LYS |
| 4 | C | 379 | ARG |
| 4 | C | 397 | SER |
| 4 | C | 403 | GLU |
| 4 | C | 404 | GLN |
| 4 | C | 412 | LYS |
| 4 | C | 415 | TRP |
| 4 | C | 422 | TRP |
| 4 | C | 423 | ARG |
| 4 | C | 434 | PRO |
| 4 | C | 437 | ASN |
| 4 | C | 467 | CYS |
| 4 | C | 470 | VAL |
| 4 | C | 471 | ASP |
| 4 | C | 472 | LYS |
| 4 | C | 473 | VAL |
| 4 | C | 509 | PHE |
| 4 | C | 510 | CYS |
| 4 | C | 514 | PHE |
| 4 | C | 517 | GLU |
| 4 | C | 531 | SER |
| 4 | C | 532 | LEU |
| 4 | C | 544 | GLN |
| 4 | C | 551 | ARG |
| 4 | C | 553 | GLU |
| 4 | C | 559 | VAL |
| 4 | C | 565 | GLU |
| 4 | C | 573 | ILE |
| 4 | C | 577 | LYS |
| 4 | C | 588 | ASN |
| 4 | C | 601 | ASN |
| 4 | C | 614 | LYS |
| 4 | C | 636 | THR |
| 4 | C | 659 | ILE |
| 4 | C | 661 | SER |
| 4 | C | 663 | LYS |
| 4 | C | 666 | MET |
| 4 | C | 700 | LYS |
| 4 | C | 711 | LYS |
| 4 | C | 722 | ARG |
| 4 | C | 729 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | C | 733 | PHE |
| 4 | C | 734 | PRO |
| 4 | C | 744 | GLN |
| 4 | C | 749 | LEU |
| 4 | C | 750 | MET |
| 4 | C | 751 | PHE |
| 4 | C | 754 | GLN |
| 4 | C | 755 | PHE |
| 4 | C | 768 | GLU |
| 4 | C | 783 | VAL |
| 4 | C | 786 | GLN |
| 4 | C | 787 | ASP |
| 4 | C | 789 | SER |
| 4 | C | 801 | LYS |
| 4 | C | 814 | PHE |
| 4 | C | 817 | ILE |
| 4 | C | 831 | THR |
| 4 | C | 832 | MET |
| 4 | C | 838 | SER |
| 4 | C | 841 | VAL |
| 4 | C | 842 | LEU |
| 4 | C | 860 | LYS |
| 4 | C | 869 | ASN |
| 4 | C | 880 | PHE |
| 4 | C | 882 | PHE |
| 4 | D | 13 | ASP |
| 4 | D | 16 | LEU |
| 4 | D | 19 | ILE |
| 4 | D | 22 | ASN |
| 4 | D | 27 | HIS |
| 4 | D | 36 | GLN |
| 4 | D | 39 | LEU |
| 4 | D | 48 | GLU |
| 4 | D | 50 | ARG |
| 4 | D | 56 | GLU |
| 4 | D | 59 | LEU |
| 4 | D | 84 | ARG |
| 4 | D | 95 | LYS |
| 4 | D | 101 | THR |
| 4 | D | 109 | ILE |
| 4 | D | 120 | LYS |
| 4 | D | 131 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | D | 143 | ARG |
| 4 | D | 145 | ILE |
| 4 | D | 171 | ASN |
| 4 | D | 183 | MET |
| 4 | D | 190 | MET |
| 4 | D | 206 | LYS |
| 4 | D | 215 | ARG |
| 4 | D | 219 | MET |
| 4 | D | 232 | GLN |
| 4 | D | 236 | VAL |
| 4 | D | 257 | ARG |
| 4 | D | 269 | GLN |
| 4 | D | 271 | CYS |
| 4 | D | 281 | ILE |
| 4 | D | 282 | THR |
| 4 | D | 289 | ASN |
| 4 | D | 299 | THR |
| 4 | D | 305 | LEU |
| 4 | D | 335 | LEU |
| 4 | D | 341 | ILE |
| 4 | D | 348 | PRO |
| 4 | D | 350 | GLU |
| 4 | D | 351 | ASP |
| 4 | D | 378 | LYS |
| 4 | D | 391 | ARG |
| 4 | D | 394 | ARG |
| 4 | D | 398 | LEU |
| 4 | D | 403 | GLU |
| 4 | D | 412 | LYS |
| 4 | D | 419 | ASN |
| 4 | D | 422 | TRP |
| 4 | D | 425 | ARG |
| 4 | D | 435 | GLN |
| 4 | D | 437 | ASN |
| 4 | D | 441 | LYS |
| 4 | D | 444 | LEU |
| 4 | D | 448 | LYS |
| 4 | D | 450 | LYS |
| 4 | D | 452 | ILE |
| 4 | D | 467 | CYS |
| 4 | D | 472 | LYS |
| 4 | D | 477 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | D | 492 | CYS |
| 4 | D | 495 | SER |
| 4 | D | 497 | LEU |
| 4 | D | 499 | ASN |
| 4 | D | 510 | CYS |
| 4 | D | 514 | PHE |
| 4 | D | 518 | TYR |
| 4 | D | 530 | CYS |
| 4 | D | 540 | CYS |
| 4 | D | 559 | VAL |
| 4 | D | 571 | TYR |
| 4 | D | 601 | ASN |
| 4 | D | 606 | SER |
| 4 | D | 632 | ARG |
| 4 | D | 652 | GLU |
| 4 | D | 656 | GLN |
| 4 | D | 661 | SER |
| 4 | D | 666 | MET |
| 4 | D | 700 | LYS |
| 4 | D | 705 | LEU |
| 4 | D | 718 | ILE |
| 4 | D | 720 | ARG |
| 4 | D | 721 | LYS |
| 4 | D | 722 | ARG |
| 4 | D | 723 | CYS |
| 4 | D | 730 | PRO |
| 4 | D | 734 | PRO |
| 4 | D | 735 | VAL |
| 4 | D | 749 | LEU |
| 4 | D | 750 | MET |
| 4 | D | 752 | LEU |
| 4 | D | 776 | SER |
| 4 | D | 783 | VAL |
| 4 | D | 786 | GLN |
| 4 | D | 787 | ASP |
| 4 | D | 791 | LEU |
| 4 | D | 801 | LYS |
| 4 | D | 812 | ASP |
| 4 | D | 813 | SER |
| 4 | D | 820 | ASP |
| 4 | D | 828 | VAL |
| 4 | D | 842 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | D | 851 | ASP |
| 4 | D | 857 | GLN |
| 4 | D | 860 | LYS |
| 4 | D | 882 | PHE |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (125) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | A | 5 | ASN |
| 4 | A | 41 | HIS |
| 4 | A | 86 | ASN |
| 4 | A | 171 | ASN |
| 4 | A | 184 | GLN |
| 4 | A | 205 | HIS |
| 4 | A | 211 | HIS |
| 4 | A | 230 | HIS |
| 4 | A | 232 | GLN |
| 4 | A | 239 | GLN |
| 4 | A | 269 | GLN |
| 4 | A | 289 | ASN |
| 4 | A | 404 | GLN |
| 4 | A | 410 | ASN |
| 4 | A | 419 | ASN |
| 4 | A | 435 | GLN |
| 4 | A | 437 | ASN |
| 4 | A | 466 | ASN |
| 4 | A | 486 | HIS |
| 4 | A | 488 | ASN |
| 4 | A | 545 | HIS |
| 4 | A | 588 | ASN |
| 4 | A | 649 | GLN |
| 4 | A | 656 | GLN |
| 4 | A | 669 | GLN |
| 4 | A | 672 | GLN |
| 4 | A | 748 | ASN |
| 4 | A | 754 | GLN |
| 4 | A | 781 | ASN |
| 4 | A | 823 | ASN |
| 4 | A | 848 | GLN |
| 4 | A | 854 | HIS |
| 4 | A | 857 | GLN |
| 4 | A | 869 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | A | 871 | ASN |
| 4 | B | 5 | ASN |
| 4 | B | 22 | ASN |
| 4 | B | 86 | ASN |
| 4 | B | 107 | GLN |
| 4 | B | 161 | HIS |
| 4 | B | 169 | GLN |
| 4 | B | 171 | ASN |
| 4 | B | 205 | HIS |
| 4 | B | 232 | GLN |
| 4 | B | 233 | ASN |
| 4 | B | 239 | GLN |
| 4 | B | 269 | GLN |
| 4 | B | 324 | GLN |
| 4 | B | 404 | GLN |
| 4 | B | 419 | ASN |
| 4 | B | 435 | GLN |
| 4 | B | 437 | ASN |
| 4 | B | 499 | ASN |
| 4 | B | 505 | GLN |
| 4 | B | 529 | ASN |
| 4 | B | 544 | GLN |
| 4 | B | 545 | HIS |
| 4 | B | 560 | ASN |
| 4 | B | 588 | ASN |
| 4 | B | 619 | GLN |
| 4 | B | 656 | GLN |
| 4 | B | 672 | GLN |
| 4 | B | 726 | HIS |
| 4 | B | 748 | ASN |
| 4 | B | 772 | HIS |
| 4 | B | 774 | GLN |
| 4 | B | 781 | ASN |
| 4 | B | 786 | GLN |
| 4 | B | 823 | ASN |
| 4 | B | 848 | GLN |
| 4 | B | 869 | ASN |
| 4 | C | 5 | ASN |
| 4 | C | 58 | GLN |
| 4 | C | 86 | ASN |
| 4 | C | 104 | GLN |
| 4 | C | 107 | GLN |

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Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | C | 169 | GLN |
| 4 | C | 171 | ASN |
| 4 | C | 230 | HIS |
| 4 | C | 232 | GLN |
| 4 | C | 269 | GLN |
| 4 | C | 289 | ASN |
| 4 | C | 324 | GLN |
| 4 | C | 339 | ASN |
| 4 | C | 410 | ASN |
| 4 | C | 435 | GLN |
| 4 | C | 437 | ASN |
| 4 | C | 523 | HIS |
| 4 | C | 560 | ASN |
| 4 | C | 588 | ASN |
| 4 | C | 656 | GLN |
| 4 | C | 669 | GLN |
| 4 | C | 726 | HIS |
| 4 | C | 737 | GLN |
| 4 | C | 744 | GLN |
| 4 | C | 754 | GLN |
| 4 | C | 781 | ASN |
| 4 | C | 786 | GLN |
| 4 | C | 799 | HIS |
| 4 | D | 22 | ASN |
| 4 | D | 41 | HIS |
| 4 | D | 86 | ASN |
| 4 | D | 107 | GLN |
| 4 | D | 161 | HIS |
| 4 | D | 239 | GLN |
| 4 | D | 289 | ASN |
| 4 | D | 331 | ASN |
| 4 | D | 410 | ASN |
| 4 | D | 419 | ASN |
| 4 | D | 435 | GLN |
| 4 | D | 437 | ASN |
| 4 | D | 499 | ASN |
| 4 | D | 544 | GLN |
| 4 | D | 619 | GLN |
| 4 | D | 669 | GLN |
| 4 | D | 726 | HIS |
| 4 | D | 737 | GLN |
| 4 | D | 744 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | D | 748 | ASN |
| 4 | D | 754 | GLN |
| 4 | D | 790 | HIS |
| 4 | D | 823 | ASN |
| 4 | D | 854 | HIS |
| 4 | D | 857 | GLN |
| 4 | D | 871 | ASN |

5.3.3 RNA [i](#)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-------------|-------------------|-----------------|
| 2 | F | 7/12 (58%) | 0 | 0 |
| 2 | I | 7/12 (58%) | 1 (14%) | 0 |
| 2 | L | 7/12 (58%) | 0 | 0 |
| 2 | O | 7/12 (58%) | 0 | 0 |
| All | All | 28/48 (58%) | 1 (3%) | 0 |

All (1) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | I | 8 | U |

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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 | APC | A | 2000 | 5 | 28,33,33 | 1.99 | 6 (21%) | 28,52,52 | 1.59 | 7 (25%) |
| 6 | APC | B | 2001 | 5 | 28,33,33 | 2.07 | 8 (28%) | 28,52,52 | 1.78 | 6 (21%) |
| 6 | APC | C | 2002 | 5 | 28,33,33 | 2.20 | 7 (25%) | 28,52,52 | 1.35 | 5 (17%) |
| 6 | APC | D | 2003 | 5 | 28,33,33 | 1.98 | 5 (17%) | 28,52,52 | 1.43 | 5 (17%) |

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 | APC | A | 2000 | 5 | - | 0/15/38/38 | 0/3/3/3 |
| 6 | APC | B | 2001 | 5 | - | 0/15/38/38 | 0/3/3/3 |
| 6 | APC | C | 2002 | 5 | - | 0/15/38/38 | 0/3/3/3 |
| 6 | APC | D | 2003 | 5 | - | 0/15/38/38 | 0/3/3/3 |

All (26) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 6 | B | 2001 | APC | PB-O2B | -2.77 | 1.49 | 1.56 |
| 6 | B | 2001 | APC | PA-O2A | -2.51 | 1.50 | 1.56 |
| 6 | C | 2002 | APC | PA-O2A | -2.48 | 1.50 | 1.56 |
| 6 | A | 2000 | APC | C8-N7 | -2.33 | 1.30 | 1.34 |
| 6 | A | 2000 | APC | PB-O2B | -2.24 | 1.50 | 1.56 |
| 6 | C | 2002 | APC | PB-O2B | -2.09 | 1.51 | 1.56 |
| 6 | D | 2003 | APC | PA-O2A | -2.05 | 1.51 | 1.56 |
| 6 | C | 2002 | APC | C2-N1 | 2.27 | 1.38 | 1.33 |
| 6 | B | 2001 | APC | C5'-C4' | 2.32 | 1.58 | 1.51 |
| 6 | B | 2001 | APC | PG-O3B | 2.59 | 1.64 | 1.60 |
| 6 | D | 2003 | APC | PG-O3B | 2.76 | 1.64 | 1.60 |
| 6 | C | 2002 | APC | PG-O3B | 3.01 | 1.64 | 1.60 |
| 6 | A | 2000 | APC | C2-N3 | 3.03 | 1.37 | 1.32 |
| 6 | B | 2001 | APC | O4'-C1' | 3.30 | 1.45 | 1.41 |
| 6 | C | 2002 | APC | C2-N3 | 3.31 | 1.37 | 1.32 |
| 6 | D | 2003 | APC | PA-O5' | 3.40 | 1.61 | 1.57 |
| 6 | B | 2001 | APC | C2-N3 | 3.49 | 1.38 | 1.32 |
| 6 | D | 2003 | APC | C2-N3 | 3.53 | 1.38 | 1.32 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|------|-------------|----------|
| 6 | A | 2000 | APC | PG-O3B | 3.71 | 1.66 | 1.60 |
| 6 | A | 2000 | APC | PA-O5' | 3.94 | 1.61 | 1.57 |
| 6 | B | 2001 | APC | PB-O3B | 4.50 | 1.63 | 1.58 |
| 6 | C | 2002 | APC | PB-O3B | 5.50 | 1.64 | 1.58 |
| 6 | B | 2001 | APC | PA-O5' | 6.13 | 1.64 | 1.57 |
| 6 | A | 2000 | APC | PB-O3B | 6.55 | 1.65 | 1.58 |
| 6 | D | 2003 | APC | PB-O3B | 7.14 | 1.66 | 1.58 |
| 6 | C | 2002 | APC | PA-O5' | 7.28 | 1.65 | 1.57 |

All (23) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 6 | B | 2001 | APC | O1A-PA-C3A | -4.75 | 97.24 | 108.97 |
| 6 | B | 2001 | APC | PG-O3B-PB | -3.40 | 120.37 | 132.38 |
| 6 | A | 2000 | APC | PG-O3B-PB | -2.65 | 123.02 | 132.38 |
| 6 | C | 2002 | APC | PG-O3B-PB | -2.23 | 124.51 | 132.38 |
| 6 | D | 2003 | APC | O2B-PB-C3A | 2.06 | 115.31 | 106.54 |
| 6 | B | 2001 | APC | O2A-PA-C3A | 2.06 | 115.32 | 106.54 |
| 6 | A | 2000 | APC | C2'-C3'-C4' | 2.14 | 106.78 | 102.62 |
| 6 | A | 2000 | APC | O4'-C4'-C3' | 2.19 | 109.53 | 105.17 |
| 6 | D | 2003 | APC | C2'-C3'-C4' | 2.24 | 106.97 | 102.62 |
| 6 | C | 2002 | APC | C5-C6-N6 | 2.29 | 125.14 | 120.47 |
| 6 | B | 2001 | APC | O2A-PA-O1A | 2.51 | 118.51 | 110.09 |
| 6 | A | 2000 | APC | C1'-N9-C4 | 2.54 | 131.02 | 126.64 |
| 6 | D | 2003 | APC | O2'-C2'-C3' | 2.55 | 119.99 | 111.83 |
| 6 | A | 2000 | APC | O2B-PB-O1B | 2.81 | 119.50 | 110.09 |
| 6 | B | 2001 | APC | O2B-PB-O1B | 2.89 | 119.77 | 110.09 |
| 6 | C | 2002 | APC | O2A-PA-O1A | 2.90 | 119.80 | 110.09 |
| 6 | A | 2000 | APC | O2A-PA-O1A | 2.90 | 119.80 | 110.09 |
| 6 | C | 2002 | APC | C2'-C3'-C4' | 2.97 | 108.40 | 102.62 |
| 6 | D | 2003 | APC | O2A-PA-O1A | 3.03 | 120.24 | 110.09 |
| 6 | C | 2002 | APC | O2B-PB-O1B | 3.05 | 120.31 | 110.09 |
| 6 | D | 2003 | APC | O2B-PB-O1B | 3.22 | 120.85 | 110.09 |
| 6 | B | 2001 | APC | C2'-C3'-C4' | 3.39 | 109.23 | 102.62 |
| 6 | A | 2000 | APC | O1A-PA-C3A | 3.80 | 118.37 | 108.97 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 48 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 6 | A | 2000 | APC | 16 | 0 |
| 6 | B | 2001 | APC | 9 | 0 |
| 6 | C | 2002 | APC | 16 | 0 |
| 6 | D | 2003 | APC | 7 | 0 |

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---|-----------------------|-------|
| 1 | E | 17/18 (94%) | -0.23 | 0 100 100 | 19, 58, 179, 181 | 0 |
| 1 | H | 17/18 (94%) | 0.16 | 1 (5%) 23 13 | 21, 75, 158, 171 | 0 |
| 1 | K | 17/18 (94%) | 0.10 | 0 100 100 | 48, 94, 157, 159 | 0 |
| 1 | N | 17/18 (94%) | 0.10 | 0 100 100 | 51, 102, 172, 173 | 0 |
| 2 | F | 8/12 (66%) | -0.48 | 0 100 100 | 17, 23, 83, 93 | 0 |
| 2 | I | 8/12 (66%) | -0.03 | 0 100 100 | 17, 38, 82, 93 | 0 |
| 2 | L | 8/12 (66%) | 0.18 | 0 100 100 | 47, 53, 113, 118 | 0 |
| 2 | O | 8/12 (66%) | 0.13 | 0 100 100 | 51, 80, 132, 144 | 0 |
| 3 | G | 9/10 (90%) | 0.97 | 2 (22%) 1 1 | 146, 153, 176, 183 | 0 |
| 3 | J | 9/10 (90%) | 0.03 | 1 (11%) 6 4 | 130, 138, 162, 163 | 0 |
| 3 | M | 9/10 (90%) | -0.17 | 0 100 100 | 134, 146, 155, 158 | 0 |
| 3 | P | 9/10 (90%) | 1.29 | 1 (11%) 6 4 | 157, 167, 172, 172 | 0 |
| 4 | A | 857/883 (97%) | -0.30 | 35 (4%) 38 25 | 15, 76, 141, 153 | 0 |
| 4 | B | 857/883 (97%) | -0.42 | 15 (1%) 69 55 | 10, 69, 131, 150 | 0 |
| 4 | C | 857/883 (97%) | -0.31 | 18 (2%) 64 49 | 47, 93, 134, 160 | 0 |
| 4 | D | 857/883 (97%) | -0.06 | 26 (3%) 51 35 | 41, 102, 144, 156 | 0 |
| All | All | 3564/3692 (96%) | -0.26 | 99 (2%) 53 39 | 10, 89, 142, 183 | 0 |

All (99) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3 | P | 1 | DG | 8.1 |
| 4 | D | 235 | GLY | 7.0 |
| 3 | G | 1 | DG | 6.6 |
| 4 | A | 235 | GLY | 6.1 |
| 4 | A | 601 | ASN | 5.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 4 | D | 238 | GLY | 5.0 |
| 4 | C | 372 | GLU | 4.7 |
| 4 | B | 17 | ALA | 4.6 |
| 4 | B | 129 | ALA | 4.5 |
| 4 | D | 237 | VAL | 4.3 |
| 4 | A | 236 | VAL | 4.2 |
| 4 | B | 16 | LEU | 4.2 |
| 4 | D | 226 | MET | 4.1 |
| 4 | A | 752 | LEU | 3.8 |
| 4 | B | 94 | ALA | 3.8 |
| 4 | C | 375 | THR | 3.7 |
| 4 | A | 753 | GLY | 3.7 |
| 4 | A | 98 | LYS | 3.6 |
| 4 | A | 116 | TYR | 3.5 |
| 4 | B | 243 | THR | 3.5 |
| 4 | D | 169 | GLN | 3.5 |
| 4 | A | 168 | GLU | 3.4 |
| 4 | D | 603 | GLY | 3.4 |
| 4 | D | 816 | THR | 3.3 |
| 4 | D | 601 | ASN | 3.3 |
| 4 | C | 16 | LEU | 3.3 |
| 4 | D | 110 | LYS | 3.3 |
| 4 | A | 226 | MET | 3.3 |
| 4 | B | 18 | ALA | 3.3 |
| 4 | A | 608 | LYS | 3.3 |
| 4 | A | 239 | GLN | 3.3 |
| 4 | B | 372 | GLU | 3.3 |
| 4 | A | 242 | GLU | 3.2 |
| 4 | C | 237 | VAL | 3.2 |
| 4 | A | 234 | ALA | 3.2 |
| 4 | A | 598 | THR | 3.1 |
| 4 | B | 374 | LEU | 3.1 |
| 4 | B | 237 | VAL | 3.1 |
| 4 | C | 376 | ALA | 3.1 |
| 4 | A | 596 | THR | 3.0 |
| 4 | B | 130 | ASP | 3.0 |
| 4 | A | 67 | ASN | 3.0 |
| 4 | D | 606 | SER | 3.0 |
| 4 | A | 231 | ARG | 3.0 |
| 4 | C | 354 | ALA | 3.0 |
| 4 | A | 70 | ALA | 2.9 |
| 4 | C | 226 | MET | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 4 | D | 752 | LEU | 2.8 |
| 4 | C | 374 | LEU | 2.8 |
| 4 | C | 860 | LYS | 2.8 |
| 4 | D | 354 | ALA | 2.8 |
| 4 | C | 355 | ILE | 2.7 |
| 4 | A | 243 | THR | 2.7 |
| 4 | B | 230 | HIS | 2.7 |
| 4 | A | 600 | GLU | 2.7 |
| 4 | B | 594 | VAL | 2.7 |
| 4 | A | 237 | VAL | 2.6 |
| 4 | A | 607 | GLU | 2.6 |
| 4 | A | 602 | THR | 2.6 |
| 4 | C | 18 | ALA | 2.6 |
| 4 | C | 234 | ALA | 2.6 |
| 4 | A | 158 | GLU | 2.6 |
| 4 | A | 228 | SER | 2.6 |
| 4 | D | 746 | ARG | 2.5 |
| 4 | A | 751 | PHE | 2.4 |
| 4 | A | 229 | LEU | 2.4 |
| 4 | D | 602 | THR | 2.4 |
| 4 | B | 242 | GLU | 2.4 |
| 4 | A | 130 | ASP | 2.4 |
| 4 | A | 593 | GLU | 2.3 |
| 4 | D | 609 | VAL | 2.3 |
| 4 | A | 261 | LEU | 2.3 |
| 3 | J | 1 | DG | 2.3 |
| 4 | A | 754 | GLN | 2.3 |
| 4 | C | 17 | ALA | 2.3 |
| 4 | D | 65 | ALA | 2.3 |
| 4 | D | 530 | CYS | 2.3 |
| 4 | A | 238 | GLY | 2.3 |
| 1 | H | 2 | DG | 2.3 |
| 4 | C | 603 | GLY | 2.2 |
| 4 | D | 234 | ALA | 2.2 |
| 4 | D | 229 | LEU | 2.2 |
| 4 | B | 203 | SER | 2.2 |
| 4 | C | 15 | GLU | 2.2 |
| 4 | A | 9 | ASN | 2.2 |
| 4 | C | 161 | HIS | 2.1 |
| 4 | D | 594 | VAL | 2.1 |
| 3 | G | 2 | DT | 2.1 |
| 4 | C | 565 | GLU | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 4 | D | 883 | ALA | 2.1 |
| 4 | D | 86 | ASN | 2.1 |
| 4 | A | 594 | VAL | 2.1 |
| 4 | C | 602 | THR | 2.1 |
| 4 | B | 226 | MET | 2.1 |
| 4 | D | 244 | ILE | 2.1 |
| 4 | A | 68 | ALA | 2.1 |
| 4 | D | 90 | GLU | 2.0 |
| 4 | D | 89 | PHE | 2.0 |
| 4 | D | 216 | CYS | 2.0 |

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|----------------------------|-------|
| 6 | APC | B | 2001 | 31/31 | 0.94 | 0.22 | 1.24 | 28,47,63,68 | 0 |
| 6 | APC | A | 2000 | 31/31 | 0.95 | 0.20 | 1.19 | 34,58,80,82 | 0 |
| 6 | APC | C | 2002 | 31/31 | 0.93 | 0.24 | 0.47 | 65,70,77,78 | 0 |
| 6 | APC | D | 2003 | 31/31 | 0.94 | 0.17 | -0.82 | 48,57,61,63 | 0 |
| 5 | MG | D | 3004 | 1/1 | 0.70 | 0.31 | - | 79,79,79,79 | 0 |
| 5 | MG | B | 3002 | 1/1 | 0.95 | 0.55 | - | 65,65,65,65 | 0 |
| 5 | MG | C | 3007 | 1/1 | 0.99 | 0.18 | - | 46,46,46,46 | 0 |
| 5 | MG | F | 3005 | 1/1 | 0.96 | 0.16 | - | 18,18,18,18 | 0 |
| 5 | MG | C | 3003 | 1/1 | 0.99 | 0.27 | - | 41,41,41,41 | 0 |
| 5 | MG | D | 3008 | 1/1 | 0.97 | 0.18 | - | 16,16,16,16 | 0 |
| 5 | MG | B | 3006 | 1/1 | 0.98 | 0.17 | - | 34,34,34,34 | 0 |
| 5 | MG | A | 3001 | 1/1 | 0.94 | 0.13 | - | 22,22,22,22 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.