



## Full wwPDB EM Validation Report ⓘ

Jun 26, 2024 – 10:35 AM JST

PDB ID : 7YE2  
EMDB ID : EMD-33762  
Title : The cryo-EM structure of C. crescentus GcrA-TACdown  
Authors : Wu, X.X.; Zhang, Y.  
Deposited on : 2022-07-05  
Resolution : 3.80 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev92  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

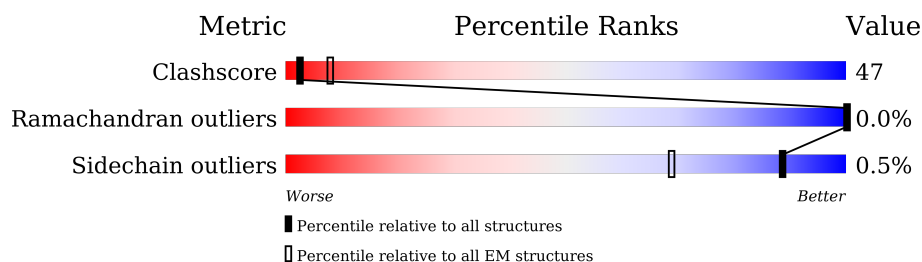
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 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<br>(#Entries) | EM structures<br>(#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore            | 158937                      | 4297                        |
| Ramachandran outliers | 154571                      | 4023                        |
| Sidechain outliers    | 154315                      | 3826                        |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 338    |                  |
| 1   | B     | 338    |                  |
| 2   | C     | 1356   |                  |
| 3   | D     | 1396   |                  |
| 4   | E     | 119    |                  |
| 5   | F     | 652    |                  |
| 6   | H     | 90     |                  |
| 7   | I     | 90     |                  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 8   | G     | 173    | <div><div><div></div><div></div><div></div><div></div></div><div>6%19%12%69%</div></div> |

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 28925 atoms, of which 12 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1   | A     | 306      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2054  | 1300 | 353 | 397 | 4 |         |       |
| 1   | B     | 220      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1633  | 1044 | 274 | 311 | 4 |         |       |

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

| Mol | Chain | Residues | Atoms |      |    |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|----|------|------|----|---------|-------|
| 2   | C     | 1303     | Total | C    | H  | N    | O    | S  | 0       | 0     |
|     |       |          | 9603  | 6112 | 12 | 1598 | 1841 | 40 |         |       |

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 3   | D     | 1140     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 8691  | 5586 | 1432 | 1630 | 43 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|-------|
| 4   | E     | 69       | Total | C   | N  | O   | S | 0       | 0     |
|     |       |          | 510   | 323 | 85 | 101 | 1 |         |       |

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5   | F     | 497      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3266  | 2049 | 576 | 631 | 10 |         |       |

- Molecule 6 is a DNA chain called DNA (90-MER)-non template.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 6   | H     | 68       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1396  | 663 | 257 | 408 | 68 |         |       |

- Molecule 7 is a DNA chain called DNA (90-MER)-template.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 7   | I     | 68       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1396  | 663 | 257 | 408 | 68 |         |       |

- Molecule 8 is a protein called Cell cycle regulatory protein GcrA.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 8   | G     | 53       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 372   | 237 | 61 | 70 | 4 |         |       |

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 9   | D     | 2        | Total | Zn | 0       |
|     |       |          | 2     | 2  |         |
| 9   | G     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

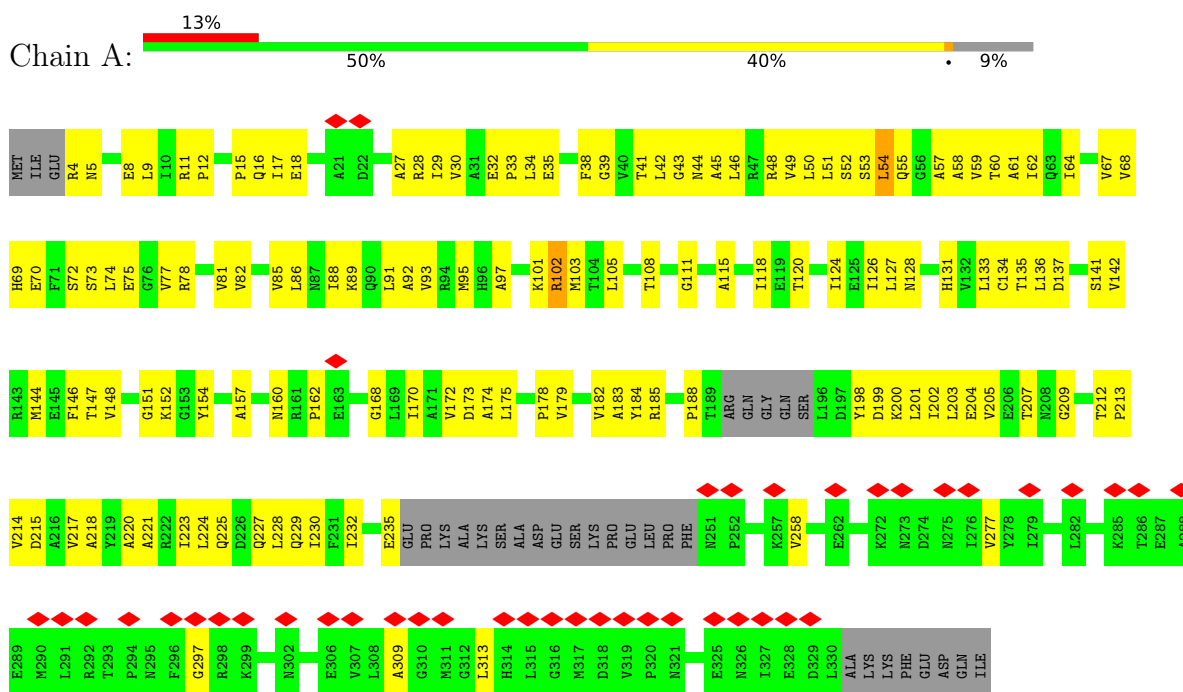
- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 10  | D     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

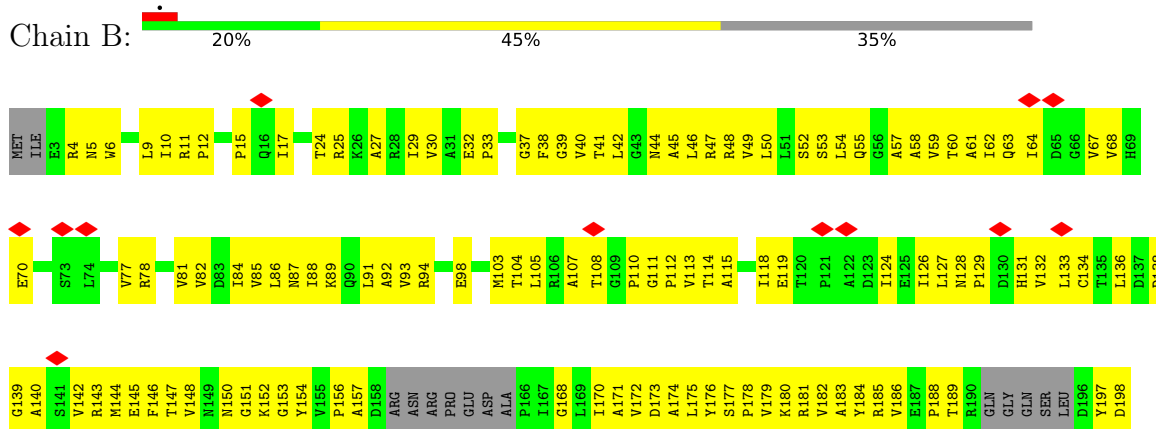
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DNA-directed RNA polymerase subunit alpha



- Molecule 1: DNA-directed RNA polymerase subunit alpha

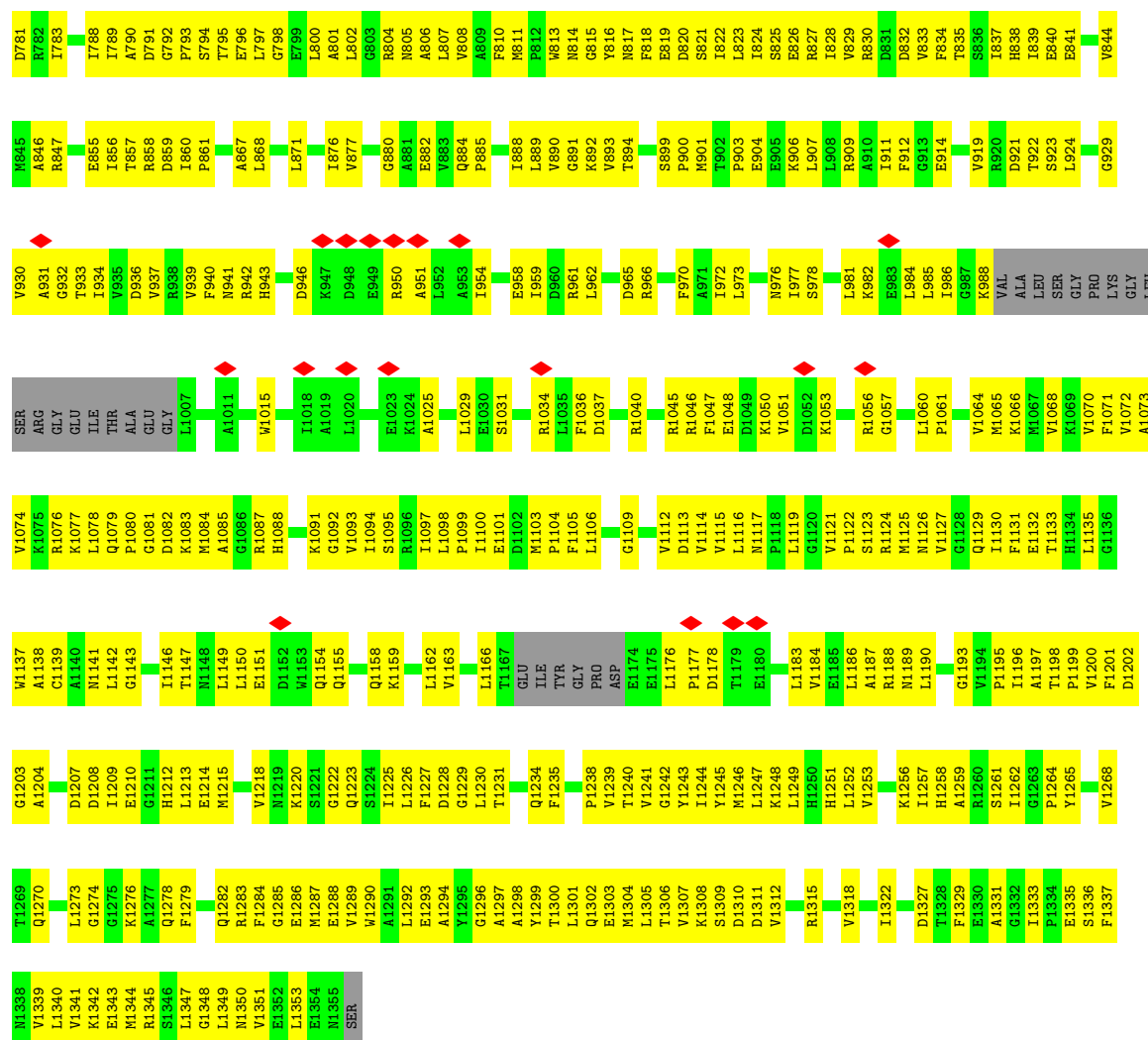


|      |     |
|------|-----|
| K199 | ASP |
| L200 | GLU |
| I201 | LEU |
| L202 | GLU |
| E203 | LEU |
| V204 | SER |
| E205 | VAL |
| T206 | ARG |
| N207 | SER |
| A208 | ALA |
| A209 | ASN |
| V210 | CYS |
| T211 | LEU |
| P212 | LYS |
| V213 | ASN |
| D214 | ASP |
| A215 | ASN |
| V216 | ILE |
| A217 | VAL |
| Y218 | TYR |
| A219 | ILE |
| A220 | GLY |
| R221 | ASP |
| L222 | LEU |
| L223 | ILE |
| Q224 | GLN |
| D225 | LYS |
| Q226 | THR |
| L227 | GLU |
| Q228 | ALA |
| I229 | GLU |
| F230 | MET |
| I231 | LEU |
| T232 | ARG |
| F233 | THR |
| E234 | PRO |
| GLU  | ASN |
| PRO  | PHE |
| LYS  | GLY |
| ALA  | ARG |
| LYS  | LYS |
| SER  | SER |
| ALA  | LEU |
| ASP  | ASN |
| GLU  | GLU |
| SER  | ILE |
| LYS  | LYS |
| PRO  | PRO |
| GLU  | VAL |
| LEU  | LEU |
| PRO  | ALA |
| PHE  | GLY |
| ASN  | MET |
| PRO  | GLY |
| ALA  | LEU |
| LEU  | HIS |
| LYS  | LEU |
| LYS  | GLY |
| VAL  | MET |
| ASP  | ASP |

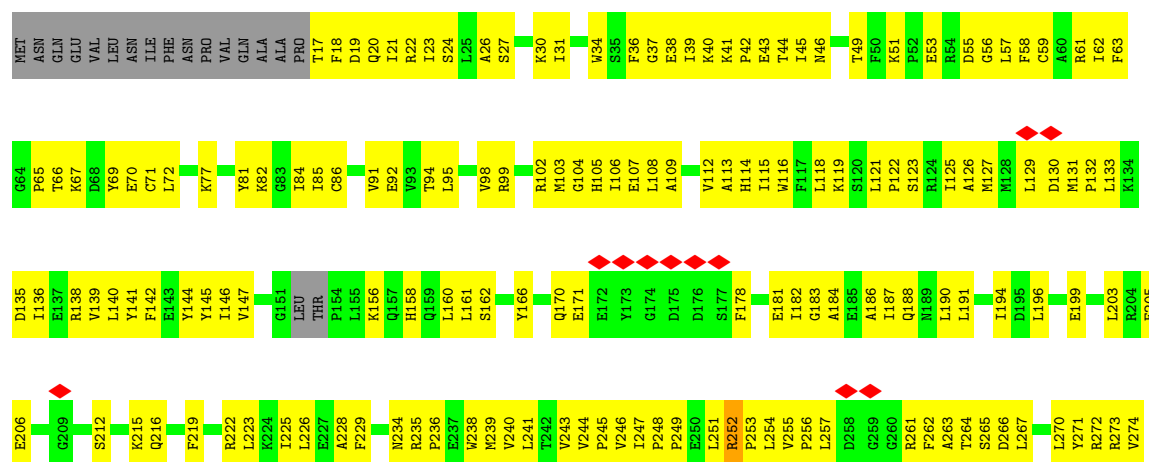
• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain C:  6% 39% 57%

|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| MET  | ALA  | Q3   | S4   | F5   | K8   | K9   | I10  | I11  | R12  | K13  | S14  | F15  | G16  | R17  | E20  | A21  | Q23  | N24  | P25  | N26  | L27  | I28  | E29  | R32  | Y35  | E36  | Q37  | F38  | L39  | T43  | R44  | P45  | G46  | L47  | R48  | E54  | F57  | K58  | S59  | V60  | F61  | P62  | L63  | K64  | D65  | F66  | A70  | V71  | L72  | E73  |      |      |      |      |      |      |      |      |      |      |      |      |
| Y74  | Y77  | E78  | F79  | Y84  | D85  | Y86  | E87  | E88  | C89  | I90  | M94  | T95  | F96  | A97  | A98  | F99  | K100 | K101 | V102 | K103 | L104 | R105 | L106 | I107 | V108 | T111 | E112 | E113 | E114 | T115 | G116 | A117 | R118 | S119 | D122 | Q126 | D127 | V128 | Y129 | M130 | G131 | D132 | I133 | P134 | L135 | M136 | T137 | D138 | K139 | G140 | T141 | F142 | I143 |      |      |      |      |      |      |      |      |      |
| V144 | N145 | G146 | T147 | E148 | R149 | V150 | I151 | V152 | S153 | Q154 | M155 | S158 | P159 | G160 | V161 | F162 | D166 | A172 | L176 | L177 | F178 | A179 | R180 | R181 | V182 | I183 | P184 | S188 | V189 | L190 | D191 | F192 | E193 | F194 | D195 | A196 | T199 | V200 | Y201 | V202 | R203 | T204 | D205 | R206 | R207 | R208 | R209 | P211 | A212 | T213 | T214 | F215 |      |      |      |      |      |      |      |      |      |      |
| L216 | Y217 | A218 | L219 | D222 | E225 | I226 | L227 | Y231 | P235 | K238 | R239 | S240 | G242 | W243 | P246 | Y247 | W252 | R253 | K256 | P260 | L261 | V262 | D263 | A264 | D265 | L266 | Q267 | E268 | E269 | V270 | A271 | P272 | T275 | T278 | A282 | K283 | K284 | F285 | A286 | D287 | G288 | L293 | LEU  | LEU  | ALA  |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
| PRO  | GLU  | ALA  | L300 | A309 | VAL  | ASN  | MET  | ALA  | THR  | GLY  | E316 | A321 | G322 | D323 | E324 | L325 | D326 | V327 | T328 | S329 | D335 | GLN  | GLY  | PHE  | SER  | THR  | ILE  | ASP  | VAL  | LEU  | ASP  | ILE  | ASP  | HIS  | VAL  | T350 | A353 | Y354 | M355 | R356 | N357 | T358 | L359 | R360 | V361 | D362 | K363 | N364 | A365 | I366 | R367 | E368 | D369 | A370 | L371 |      |      |      |      |      |      |      |
| F372 | D373 | I374 | V377 | M378 | G381 | A389 | R462 | S463 | V464 | K394 | S395 | L396 | F397 | F398 | D399 | Y403 | D404 | L405 | S406 | S407 | V408 | G409 | R410 | V411 | K412 | M413 | R414 | M415 | R416 | L417 | S422 | V425 | R426 | I427 | L428 | R429 | K430 | E431 | D432 | V433 | L434 | A435 | V436 | L437 | L440 | V441 | G442 | L443 | D444 | D445 | G446 | R447 |      |      |      |      |      |      |      |      |      |      |
| D451 | D452 | N455 | L456 | G457 | N458 | R469 | R460 | V461 | R462 | S463 | V464 | L467 | L468 | A469 | N470 | Q471 | Y472 | R473 | L477 | M478 | M479 | E480 | I483 | K484 | E485 | R486 | M487 | D491 | I492 | D493 | P497 | H498 | D499 | L500 | I501 | N502 | A503 | K504 | P505 | A506 | V510 | F513 | F514 | S517 | Q518 | L519 | S520 | F521 | F522 | M523 |      |      |      |      |      |      |      |      |      |      |      |      |
| D524 | Q525 | T526 | N527 | P528 | L529 | S530 | E531 | I532 | H534 | K535 | R536 | R537 | L538 | S539 | R540 | L541 | G542 | P543 | L546 | T547 | R548 | E549 | R550 | A551 | G552 | F553 | E554 | V555 | R556 | D557 | V558 | H559 | P560 | T561 | H562 | Y563 | G564 | R565 | I566 | C567 | P568 | I569 | T570 | G571 | L571 | L572 | L573 | L574 | L575 | L576 | L577 | L578 | L579 | L580 | R581 | S582 | L583 | A584 |      |      |      |      |
| T585 | H586 | A587 | N590 | K591 | L592 | I595 | E596 | S597 | V598 | P599 | R600 | R601 | V602 | L603 | D604 | P607 | V611 | M614 | S615 | A616 | V623 | I624 | A625 | E626 | S627 | N628 | I629 | A632 | E633 | G634 | E635 | I636 | D639 | L640 | V641 | P642 | G643 | R644 | I645 | R646 | G647 | E648 | T650 | L651 | L652 | Q653 | K654 | S655 | V656 | T657 | V657 |      |      |      |      |      |      |      |      |      |      |      |
| D658 | L659 | M660 | D661 | S662 | G663 | P664 | R665 | Q666 | V667 | V668 | S669 | V670 | R671 | A672 | A673 | L674 | I675 | P676 | F677 | L678 | E679 | N680 | D681 | D682 | A683 | N684 | R685 | A686 | L687 | Q688 | S689 | A690 | M691 | M692 | Q693 | R694 | Q695 | A696 | V697 | P698 | L699 | V700 | Q701 | S702 | D703 | A704 | P705 | L706 | L707 | G708 | T709 | G710 | M711 | L712 | R713 | V714 | L715 | A716 | K717 | V718 | V719 | G720 |
| D718 | S719 | A721 | V722 | V723 | A724 | A725 | K726 | R727 | T728 | G729 | V730 | V731 | E732 | Q733 | Q734 | D735 | R738 | I739 | V740 | I741 | R742 | A743 | T744 | E745 | E746 | T747 | D748 | P749 | A750 | R751 | S752 | I756 | Y757 | R758 | M759 | S760 | K761 | F762 | Q763 | R764 | S765 | N766 | Q767 | S768 | T769 | C770 | I771 | N772 | Q773 | R774 | P775 | L776 | V777 | K778 | V779 | G780 |      |      |      |      |      |      |

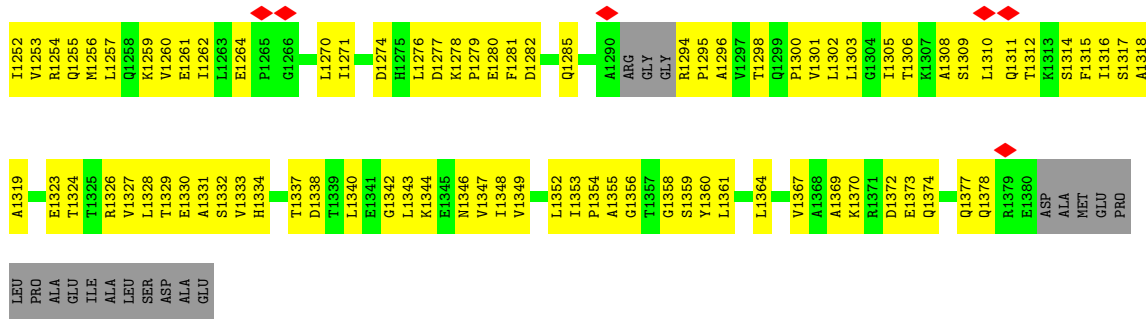


• Molecule 3: DNA-directed RNA polymerase subunit beta'

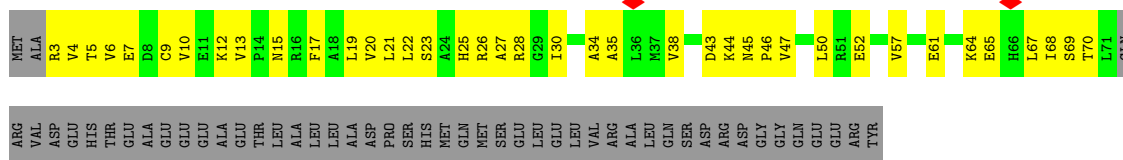
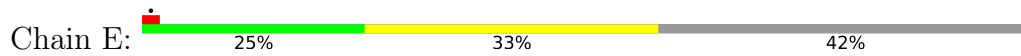




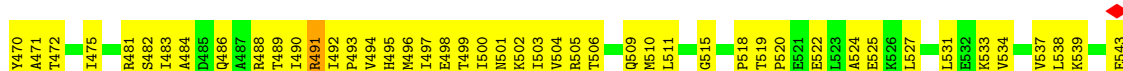
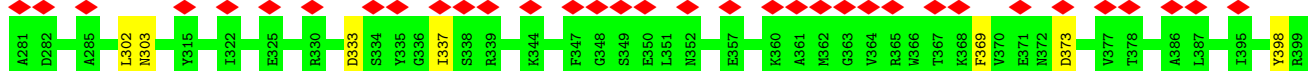
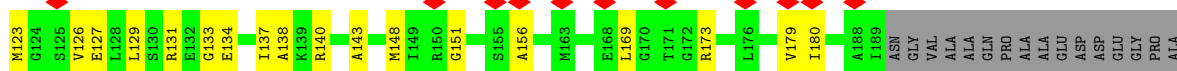
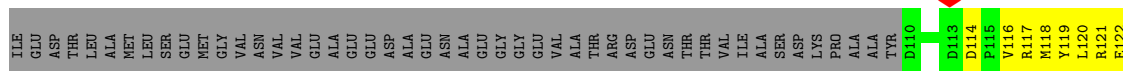
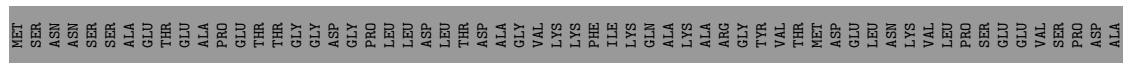
|     |     |     |     |     |     |     |     |      |      |      |     |      |       |      |      |      |      |  |
|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|-----|------|-------|------|------|------|------|--|
| VAL | GLU | GLY | ASP | THR | ARG | VAL | GLN | V872 | V806 | R740 | GLY | L604 | GLS33 | D464 | V403 | R339 | I275 |  |
| GLU | THR | ASP | ASP | THR | THR | LYS | VAL | V873 | E907 | G741 | LEU | I605 | E534  | Q467 | E404 | F340 | R276 |  |
| LEU | ALA | ALA | GLU | ALA | ASP | ASP | ALA | I673 | E908 | L742 | ASP | D906 | I535  | M468 | R406 | R341 | R277 |  |
| ILE | THR | THR | GLN | GLN | GLN | GLY | GLN | E677 | C910 | M743 | ASP | V809 | E536  | A469 | Q407 | N342 | N278 |  |
| PRO | GLY | ASP | ASP | ASP | ASP | LEU | ASP | K678 | T812 | K745 | THR | R610 | A538  | V470 | P408 | N343 | R280 |  |
| LYS | ASP | ASP | THR | THR | THR | VAL | PHE | Y679 | T813 | P746 | ASP | H611 | M539  | H471 | V410 | L344 | L281 |  |
| GLY | ASP | ASP | THR | THR | THR | VAL | THR | H680 | S747 | S747 | ASP | P473 | V543  | P472 | W411 | G346 | K282 |  |
| THR | ASP | ASP | THR | THR | THR | VAL | THR | K681 | Q614 | I751 | THR | L474 | L546  | L474 | D412 | K347 | R283 |  |
| LEU | THR | THR | THR | THR | THR | VAL | THR | V682 | K615 | E752 | THR | L476 | L546  | L476 | D413 | R348 | L284 |  |
| ARG | THR | THR | THR | THR | THR | VAL | THR | V683 | A616 | E753 | THR | L477 | L546  | L477 | D414 | V349 | L287 |  |
| THR | THR | THR | THR | THR | THR | VAL | THR | D684 | T617 | I754 | THR | E477 | H547  | E477 | E415 | D350 | E288 |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A685 | V618 | I755 | THR | I619 | A548  | I619 | E416 | Y351 | L289 |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A686 | I619 | I756 | THR | I619 | A548  | I619 | E416 | S352 | A289 |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A687 | I619 | I757 | THR | I619 | A548  | I619 | E416 | P290 | P290 |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A688 | I619 | I758 | THR | I619 | A548  | I619 | E416 | G353 | P290 |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A689 | I619 | I759 | THR | I619 | A548  | I619 | E416 | R354 | D291 |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A690 | I619 | I760 | THR | I619 | A548  | I619 | E416 | S355 | I292 |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A691 | I619 | I761 | THR | I619 | A548  | I619 | E416 | V356 | I293 |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A692 | I619 | I762 | THR | I619 | A548  | I619 | E416 | I357 | I294 |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A693 | I619 | I763 | THR | I619 | A548  | I619 | E416 | V358 | R295 |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A694 | I619 | I764 | THR | I619 | A548  | I619 | E416 | V359 | I296 |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A695 | I619 | I765 | THR | I619 | A548  | I619 | E416 | P361 | K298 |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A696 | I619 | I766 | THR | I619 | A548  | I619 | E416 | E362 | R299 |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A697 | I619 | I767 | THR | I619 | A548  | I619 | E416 | L363 | M300 |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A698 | I619 | I768 | THR | I619 | A548  | I619 | E416 | K364 | L301 |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A699 | I619 | I769 | THR | I619 | A548  | I619 | E416 | L365 | Q302 |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A700 | I619 | I770 | THR | I619 | A548  | I619 | E416 | H366 | V305 |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A701 | I619 | I771 | THR | I619 | A548  | I619 | E416 | E367 | D306 |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A702 | I619 | I772 | THR | I619 | A548  | I619 | E416 | G368 | A307 |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A703 | I619 | I773 | THR | I619 | A548  | I619 | E416 | L370 | L308 |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A704 | I619 | I774 | THR | I619 | A548  | I619 | E416 | P371 | F309 |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A705 | I619 | I775 | THR | I619 | A548  | I619 | E416 | K372 | D310 |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A706 | I619 | I776 | THR | I619 | A548  | I619 | E416 | M374 | N311 |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A707 | I619 | I777 | THR | I619 | A548  | I619 | E416 | G312 | G312 |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A708 | I619 | I778 | THR | I619 | A548  | I619 | E416 | R313 | R314 |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A709 | I619 | I779 | THR | I619 | A548  | I619 | E416 | E377 | I318 |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A710 | I619 | I780 | THR | I619 | A548  | I619 | E416 | L378 | T319 |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A711 | I619 | I781 | THR | I619 | A548  | I619 | E416 | G320 | G320 |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A712 | I619 | I782 | THR | I619 | A548  | I619 | E416 | N322 | A321 |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A713 | I619 | I783 | THR | I619 | A548  | I619 | E416 | R324 | R324 |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A714 | I619 | I784 | THR | I619 | A548  | I619 | E416 | L387 | P325 |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A715 | I619 | I785 | THR | I619 | A548  | I619 | E416 | L392 | L326 |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A716 | I619 | I786 | THR | I619 | A548  | I619 | E416 | K327 | K327 |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A717 | I619 | I787 | THR | I619 | A548  | I619 | E416 | S328 | S328 |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A718 | I619 | I788 | THR | I619 | A548  | I619 | E416 | L329 | L329 |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A719 | I619 | I789 | THR | I619 | A548  | I619 | E416 | T395 | T395 |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A720 | I619 | I790 | THR | I619 | A548  | I619 | E416 | D330 | D330 |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A721 | I619 | I791 | THR | I619 | A548  | I619 | E416 | M332 | M332 |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A722 | I619 | I792 | THR | I619 | A548  | I619 | E416 | L333 | L333 |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A723 | I619 | I793 | THR | I619 | A548  | I619 | E416 | K334 | K334 |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A724 | I619 | I794 | THR | I619 | A548  | I619 | E416 | G335 | G335 |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A725 | I619 | I795 | THR | I619 | A548  | I619 | E416 | R401 | R401 |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A726 | I619 | I796 | THR | I619 | A548  | I619 | E416 | M402 | M402 |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A727 | I619 | I797 | THR | I619 | A548  | I619 | E416 |      |      |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A728 | I619 | I798 | THR | I619 | A548  | I619 | E416 |      |      |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A729 | I619 | I799 | THR | I619 | A548  | I619 | E416 |      |      |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A730 | I619 | I800 | THR | I619 | A548  | I619 | E416 |      |      |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A731 | I619 | I801 | THR | I619 | A548  | I619 | E416 |      |      |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A732 | I619 | I802 | THR | I619 | A548  | I619 | E416 |      |      |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A733 | I619 | I803 | THR | I619 | A548  | I619 | E416 |      |      |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A734 | I619 | I804 | THR | I619 | A548  | I619 | E416 |      |      |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A735 | I619 | I805 | THR | I619 | A548  | I619 | E416 |      |      |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A736 | I619 | I806 | THR | I619 | A548  | I619 | E416 |      |      |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A737 | I619 | I807 | THR | I619 | A548  | I619 | E416 |      |      |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A738 | I619 | I808 | THR | I619 | A548  | I619 | E416 |      |      |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A739 | I619 | I809 | THR | I619 | A548  | I619 | E416 |      |      |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A740 | I619 | I810 | THR | I619 | A548  | I619 | E416 |      |      |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A741 | I619 | I811 | THR | I619 | A548  | I619 | E416 |      |      |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A742 | I619 | I812 | THR | I619 | A548  | I619 | E416 |      |      |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A743 | I619 | I813 | THR | I619 | A548  | I619 | E416 |      |      |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A744 | I619 | I814 | THR | I619 | A548  | I619 | E416 |      |      |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A745 | I619 | I815 | THR | I619 | A548  | I619 | E416 |      |      |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A746 | I619 | I816 | THR | I619 | A548  | I619 | E416 |      |      |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A747 | I619 | I817 | THR | I619 | A548  | I619 | E416 |      |      |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A748 | I619 | I818 | THR | I619 | A548  | I619 | E416 |      |      |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A749 | I619 | I819 | THR | I619 | A548  | I619 | E416 |      |      |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A750 | I619 | I820 | THR | I619 | A548  | I619 | E416 |      |      |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A751 | I619 | I821 | THR | I619 | A548  | I619 | E416 |      |      |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A752 | I619 | I822 | THR | I619 | A548  | I619 | E416 |      |      |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A753 | I619 | I823 | THR | I619 | A548  | I619 | E416 |      |      |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A754 | I619 | I824 | THR | I619 | A548  | I619 | E416 |      |      |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A755 | I619 | I825 | THR | I619 | A548  | I619 | E416 |      |      |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A756 | I619 | I826 | THR | I619 | A548  | I619 | E416 |      |      |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A757 | I619 | I827 | THR | I619 | A548  | I619 | E416 |      |      |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A758 | I619 | I828 | THR | I619 | A548  | I619 | E416 |      |      |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A759 | I619 | I829 | THR | I619 | A548  | I619 | E416 |      |      |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A760 | I619 | I830 | THR | I619 | A548  | I619 | E416 |      |      |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A761 | I619 | I831 | THR | I619 | A548  | I619 | E416 |      |      |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A762 | I619 | I832 | THR | I619 | A548  | I619 | E416 |      |      |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A763 | I619 | I833 | THR | I619 | A548  | I619 | E416 |      |      |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A764 | I619 | I834 | THR | I619 | A548  | I619 | E416 |      |      |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A765 | I619 | I835 | THR | I619 | A548  | I619 | E416 |      |      |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A766 | I619 | I836 | THR | I619 | A548  | I619 | E416 |      |      |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A767 | I619 | I837 | THR | I619 | A548  | I619 | E416 |      |      |  |
| ALA | THR | THR | THR | THR | THR | VAL | THR | A768 | I619 | I838 | THR | I619 | A548  | I619 | E416 |      |      |  |
| ALA | THR | THR | THR | THR | THR |     |     |      |      |      |     |      |       |      |      |      |      |  |

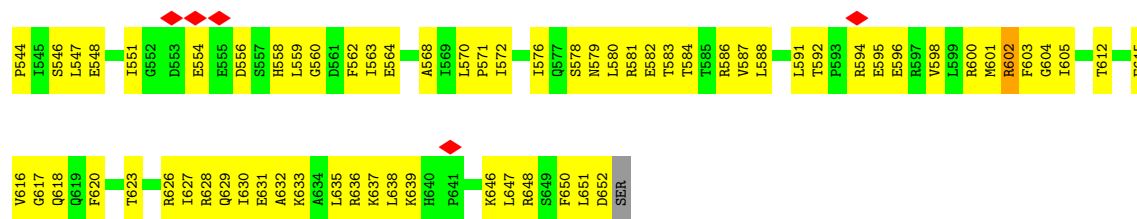


• Molecule 4: DNA-directed RNA polymerase subunit omega

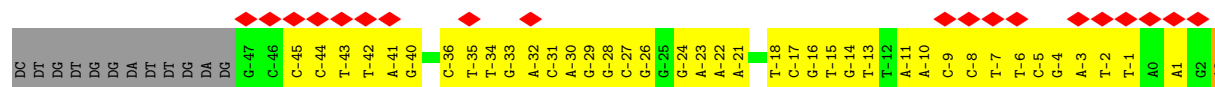
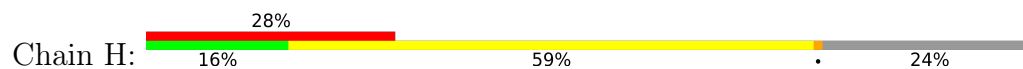


• Molecule 5: RNA polymerase sigma factor RpoD

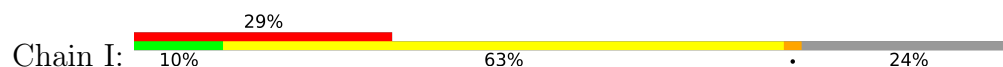




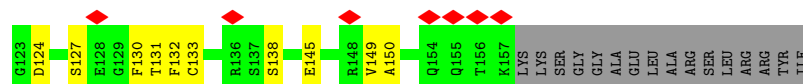
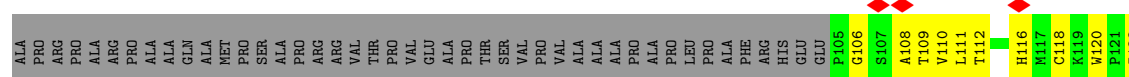
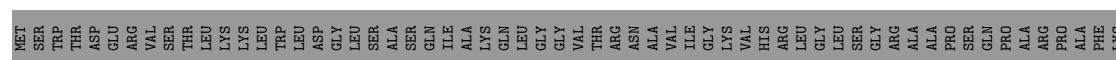
• Molecule 6: DNA (90-MER)-non template



• Molecule 7: DNA (90-MER)-template



• Molecule 8: Cell cycle regulatory protein GcrA



## 4 Experimental information

| Property                             | Value               | Source    |
|--------------------------------------|---------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE     | Depositor |
| Imposed symmetry                     | POINT, Not provided |           |
| Number of particles used             | 109869              | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF   | Depositor |
| CTF correction method                | PHASE FLIPPING ONLY | Depositor |
| Microscope                           | FEI TITAN KRIOS     | Depositor |
| Voltage (kV)                         | 300                 | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 60.8                | Depositor |
| Minimum defocus (nm)                 | 1200                | Depositor |
| Maximum defocus (nm)                 | 2200                | Depositor |
| Magnification                        | Not provided        |           |
| Image detector                       | GATAN K3 (6k x 4k)  | Depositor |
| Maximum map value                    | 0.121               | Depositor |
| Minimum map value                    | -0.083              | Depositor |
| Average map value                    | 0.000               | Depositor |
| Map value standard deviation         | 0.003               | Depositor |
| Recommended contour level            | 0.01                | Depositor |
| Map size ( $\text{\AA}$ )            | 300.0, 300.0, 300.0 | wwPDB     |
| Map dimensions                       | 300, 300, 300       | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0    | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.0, 1.0, 1.0       | Depositor |

## 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: 6MA, ZN, 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   | A     | 0.24         | 0/2078      | 0.41        | 0/2838      |
| 1   | B     | 0.23         | 0/1657      | 0.42        | 0/2249      |
| 2   | C     | 0.24         | 0/9735      | 0.40        | 0/13133     |
| 3   | D     | 0.24         | 0/8829      | 0.39        | 0/11870     |
| 4   | E     | 0.23         | 0/514       | 0.39        | 0/695       |
| 5   | F     | 0.23         | 0/3294      | 0.38        | 0/4467      |
| 6   | H     | 0.49         | 0/1513      | 0.88        | 0/2328      |
| 7   | I     | 0.52         | 0/1513      | 0.89        | 0/2328      |
| 8   | G     | 0.24         | 0/384       | 0.39        | 0/522       |
| All | All   | 0.28         | 0/29517     | 0.48        | 0/40430     |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2054  | 0        | 1816     | 216     | 0            |
| 1   | B     | 1633  | 0        | 1618     | 203     | 0            |
| 2   | C     | 9591  | 12       | 9110     | 1038    | 0            |
| 3   | D     | 8691  | 0        | 8727     | 1024    | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | E     | 510   | 0        | 505      | 57      | 0            |
| 5   | F     | 3266  | 0        | 2751     | 248     | 0            |
| 6   | H     | 1396  | 0        | 768      | 82      | 0            |
| 7   | I     | 1396  | 0        | 768      | 87      | 0            |
| 8   | G     | 372   | 0        | 325      | 14      | 0            |
| 9   | D     | 2     | 0        | 0        | 0       | 0            |
| 9   | G     | 1     | 0        | 0        | 0       | 0            |
| 10  | D     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 28913 | 12       | 26388    | 2614    | 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 47.

All (2614) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:45:ALA:O      | 1:A:49:VAL:HG12   | 1.48                     | 1.11              |
| 1:A:50:LEU:HB2    | 1:A:220:ALA:CB    | 1.84                     | 1.07              |
| 5:F:123:MET:HE2   | 5:F:123:MET:HA    | 1.34                     | 1.04              |
| 1:A:51:LEU:HD21   | 2:C:1100:ILE:HG13 | 1.40                     | 1.04              |
| 3:D:504:PRO:HB3   | 3:D:508:ILE:HB    | 1.39                     | 1.04              |
| 3:D:1134:GLU:HG2  | 3:D:1139:ARG:HD2  | 1.38                     | 1.03              |
| 2:C:1092:GLY:HA2  | 3:D:464:ASP:HA    | 1.39                     | 1.03              |
| 2:C:26:ASN:HB3    | 2:C:29:GLU:HB2    | 1.38                     | 1.02              |
| 1:B:30:VAL:HG13   | 1:B:201:ILE:HG22  | 1.41                     | 1.02              |
| 1:B:50:LEU:HB3    | 1:B:179:VAL:HG21  | 1.42                     | 1.01              |
| 3:D:432:HIS:HA    | 3:D:917:GLN:HB3   | 1.41                     | 1.01              |
| 1:B:77:VAL:HA     | 1:B:136:LEU:HD12  | 1.39                     | 1.00              |
| 3:D:228:ALA:HB1   | 3:D:1334:HIS:HA   | 1.41                     | 1.00              |
| 3:D:527:LYS:HB3   | 3:D:550:ILE:HD11  | 1.43                     | 1.00              |
| 1:A:50:LEU:HD13   | 1:A:220:ALA:HB2   | 1.38                     | 0.99              |
| 3:D:359:VAL:HG12  | 3:D:361:PRO:HD3   | 1.42                     | 0.99              |
| 1:A:48:ARG:HD2    | 1:B:41:THR:HB     | 1.46                     | 0.98              |
| 2:C:208:ARG:HD3   | 2:C:377:VAL:HG22  | 1.43                     | 0.98              |
| 2:C:1262:ILE:HD11 | 5:F:572:ILE:HG13  | 1.46                     | 0.98              |
| 2:C:199:ILE:HG13  | 2:C:358:THR:HG22  | 1.43                     | 0.97              |
| 2:C:939:VAL:HG12  | 2:C:1068:VAL:HG22 | 1.44                     | 0.97              |
| 2:C:1294:ALA:HA   | 3:D:910:ALA:HB3   | 1.46                     | 0.96              |
| 5:F:129:LEU:HD11  | 6:H:-7:DT:C2      | 2.00                     | 0.96              |
| 3:D:822:VAL:HG12  | 3:D:827:VAL:HA    | 1.47                     | 0.96              |
| 3:D:67:LYS:HB2    | 3:D:70:GLU:HB2    | 1.47                     | 0.96              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:931:ALA:HA    | 2:C:1074:VAL:HG22 | 1.46                     | 0.96              |
| 1:B:179:VAL:HA    | 1:B:206:THR:HA    | 1.48                     | 0.95              |
| 2:C:1287:MET:HB3  | 7:I:0:DT:H4'      | 1.48                     | 0.94              |
| 3:D:790:GLY:HA3   | 7:I:-1:DT:H1'     | 1.48                     | 0.94              |
| 3:D:203:LEU:HD22  | 3:D:223:LEU:HB2   | 1.50                     | 0.94              |
| 1:A:182:VAL:HG22  | 1:A:205:VAL:HG23  | 1.48                     | 0.94              |
| 1:A:188:PRO:HA    | 1:A:199:ASP:HA    | 1.46                     | 0.94              |
| 7:I:-11:DT:H2''   | 7:I:-10:DC:H5''   | 1.50                     | 0.94              |
| 2:C:12:ARG:HG2    | 2:C:1195:PRO:HB2  | 1.50                     | 0.93              |
| 1:A:49:VAL:HG11   | 1:A:224:LEU:HG    | 1.51                     | 0.93              |
| 1:A:64:ILE:HG12   | 1:A:144:MET:HG2   | 1.47                     | 0.93              |
| 2:C:655:GLU:HG2   | 2:C:656:THR:HG23  | 1.50                     | 0.93              |
| 3:D:371:PRO:HG2   | 3:D:374:MET:HB3   | 1.49                     | 0.93              |
| 1:A:50:LEU:HB2    | 1:A:220:ALA:HB2   | 1.49                     | 0.93              |
| 3:D:548:ALA:HA    | 3:D:572:PRO:HD2   | 1.51                     | 0.93              |
| 3:D:403:VAL:HG12  | 3:D:410:VAL:HG21  | 1.50                     | 0.92              |
| 1:B:108:THR:HG23  | 1:B:140:ALA:HB2   | 1.52                     | 0.92              |
| 3:D:686:TRP:HB3   | 3:D:742:LEU:HD21  | 1.48                     | 0.92              |
| 2:C:738:ARG:HD2   | 2:C:756:ILE:HD11  | 1.51                     | 0.92              |
| 1:A:74:LEU:HD13   | 1:A:142:VAL:HG11  | 1.50                     | 0.92              |
| 5:F:137:ILE:HG21  | 5:F:419:MET:HB2   | 1.51                     | 0.92              |
| 3:D:37:GLY:HA3    | 3:D:62:ILE:HD12   | 1.51                     | 0.91              |
| 2:C:770:CYS:HB3   | 2:C:837:ILE:HB    | 1.52                     | 0.91              |
| 1:B:231:ILE:HG22  | 1:B:232:THR:HG23  | 1.52                     | 0.91              |
| 2:C:734:ILE:HG22  | 2:C:739:ILE:HG22  | 1.53                     | 0.91              |
| 3:D:212:SER:HB2   | 3:D:216:GLN:HB2   | 1.53                     | 0.91              |
| 1:A:67:VAL:HG21   | 1:A:81:VAL:HG21   | 1.51                     | 0.90              |
| 3:D:820:ALA:HB2   | 3:D:831:LEU:HB2   | 1.53                     | 0.90              |
| 1:A:46:LEU:HD21   | 1:A:217:VAL:HG13  | 1.53                     | 0.90              |
| 2:C:1213:LEU:HD22 | 2:C:1218:VAL:HG11 | 1.54                     | 0.89              |
| 2:C:551:ALA:HB2   | 2:C:579:LEU:HD21  | 1.55                     | 0.89              |
| 3:D:369:GLY:HA3   | 3:D:450:GLN:HB2   | 1.51                     | 0.89              |
| 1:B:115:ALA:HB3   | 1:B:129:PRO:HA    | 1.51                     | 0.89              |
| 1:B:60:THR:HA     | 1:B:172:VAL:HB    | 1.55                     | 0.89              |
| 1:A:50:LEU:CD1    | 1:A:220:ALA:HB2   | 2.02                     | 0.88              |
| 1:A:50:LEU:CD1    | 1:A:54:LEU:HD21   | 2.02                     | 0.88              |
| 2:C:1283:ARG:HA   | 3:D:348:ARG:HA    | 1.54                     | 0.88              |
| 2:C:1199:PRO:HD2  | 2:C:1203:GLY:HA2  | 1.56                     | 0.88              |
| 1:A:52:SER:HG     | 1:B:38:PHE:HE1    | 1.19                     | 0.88              |
| 3:D:270:LEU:HD23  | 3:D:308:LEU:HA    | 1.56                     | 0.88              |
| 2:C:128:VAL:HG11  | 2:C:501:ILE:HD13  | 1.55                     | 0.88              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:824:ILE:HG23  | 2:C:1097:ILE:HA   | 1.54                     | 0.88              |
| 3:D:145:TYR:HA    | 3:D:182:ILE:HD13  | 1.55                     | 0.88              |
| 5:F:524:ALA:HA    | 5:F:534:VAL:HG21  | 1.55                     | 0.88              |
| 1:B:105:LEU:HB3   | 1:B:144:MET:HG3   | 1.56                     | 0.88              |
| 3:D:821:VAL:HG22  | 3:D:829:VAL:HG12  | 1.57                     | 0.87              |
| 1:B:77:VAL:HG21   | 1:B:134:CYS:HB3   | 1.57                     | 0.87              |
| 2:C:150:VAL:HG21  | 2:C:535:LYS:HG2   | 1.57                     | 0.87              |
| 2:C:408:VAL:HG23  | 2:C:592:TYR:HB3   | 1.57                     | 0.87              |
| 2:C:1304:MET:HG3  | 3:D:349:VAL:HG21  | 1.55                     | 0.86              |
| 1:B:179:VAL:HG12  | 1:B:206:THR:HG22  | 1.57                     | 0.86              |
| 1:B:182:VAL:HG23  | 1:B:204:VAL:HG12  | 1.57                     | 0.86              |
| 3:D:85:ILE:HG22   | 3:D:92:GLU:HB3    | 1.55                     | 0.86              |
| 3:D:1262:ILE:HA   | 3:D:1298:THR:HG22 | 1.55                     | 0.86              |
| 5:F:441:PHE:CZ    | 6:H:-5:DC:C6      | 2.64                     | 0.85              |
| 1:A:93:VAL:HG12   | 1:A:126:ILE:HA    | 1.59                     | 0.85              |
| 3:D:290:PRO:HB3   | 5:F:417:LYS:HG3   | 1.58                     | 0.85              |
| 2:C:1141:ASN:HD22 | 2:C:1218:VAL:HG22 | 1.41                     | 0.85              |
| 2:C:1225:ILE:HD11 | 2:C:1234:GLN:HG3  | 1.59                     | 0.84              |
| 1:A:51:LEU:HD21   | 2:C:1100:ILE:CG1  | 2.07                     | 0.84              |
| 2:C:1137:TRP:HB2  | 2:C:1242:GLY:HA2  | 1.58                     | 0.84              |
| 3:D:26:ALA:HB1    | 3:D:31:ILE:HD11   | 1.59                     | 0.84              |
| 3:D:365:LEU:HD23  | 3:D:618:VAL:HG23  | 1.56                     | 0.84              |
| 4:E:12:LYS:HB3    | 4:E:57:VAL:HG21   | 1.59                     | 0.84              |
| 1:A:52:SER:HB3    | 2:C:1101:GLU:CD   | 1.97                     | 0.84              |
| 2:C:43:THR:HG23   | 2:C:45:PRO:HD2    | 1.57                     | 0.84              |
| 2:C:1308:LYS:HE3  | 3:D:474:LEU:HD13  | 1.59                     | 0.84              |
| 2:C:1283:ARG:HB2  | 3:D:348:ARG:HD3   | 1.59                     | 0.84              |
| 2:C:1347:LEU:HD11 | 3:D:329:LEU:HB3   | 1.59                     | 0.84              |
| 5:F:416:LYS:HG3   | 5:F:456:VAL:HG11  | 1.59                     | 0.84              |
| 1:A:9:LEU:HD21    | 1:A:33:PRO:HB2    | 1.57                     | 0.83              |
| 2:C:200:VAL:HG12  | 2:C:358:THR:HG21  | 1.59                     | 0.83              |
| 3:D:515:LEU:HD11  | 3:D:631:GLU:HG3   | 1.60                     | 0.83              |
| 2:C:216:LEU:HB3   | 2:C:222:ASP:HB2   | 1.61                     | 0.83              |
| 3:D:693:VAL:HG11  | 3:D:739:MET:HB2   | 1.61                     | 0.83              |
| 3:D:420:GLU:HG3   | 4:E:47:VAL:HG11   | 1.60                     | 0.83              |
| 3:D:800:ALA:HA    | 3:D:1255:GLN:HG3  | 1.57                     | 0.83              |
| 5:F:441:PHE:CE1   | 6:H:-5:DC:C5      | 2.67                     | 0.83              |
| 3:D:310:ASP:HA    | 3:D:330:ALA:HB3   | 1.60                     | 0.83              |
| 5:F:444:LEU:HD21  | 5:F:483:ILE:HD11  | 1.60                     | 0.83              |
| 6:H:8:DC:H3'      | 6:H:9:DT:H71      | 1.61                     | 0.83              |
| 1:A:61:ALA:HB3    | 1:A:147:THR:HB    | 1.61                     | 0.83              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:823:LEU:HD21  | 2:C:1098:LEU:HD12 | 1.59                     | 0.83              |
| 3:D:512:LEU:HD23  | 3:D:596:LEU:HD21  | 1.61                     | 0.83              |
| 2:C:788:ILE:HD13  | 2:C:798:GLY:HA2   | 1.60                     | 0.82              |
| 2:C:1138:ALA:HB2  | 2:C:1213:LEU:HD23 | 1.61                     | 0.82              |
| 3:D:489:THR:HG22  | 3:D:618:VAL:HG21  | 1.61                     | 0.82              |
| 1:A:52:SER:HB3    | 2:C:1101:GLU:OE1  | 1.79                     | 0.82              |
| 3:D:745:LYS:HE3   | 3:D:746:PRO:HD2   | 1.61                     | 0.82              |
| 1:A:45:ALA:O      | 1:A:49:VAL:CG1    | 2.27                     | 0.82              |
| 3:D:418:ILE:HD12  | 3:D:443:LEU:HD21  | 1.60                     | 0.82              |
| 6:H:-14:DG:H5''   | 6:H:-13:DT:H71    | 1.61                     | 0.82              |
| 3:D:926:LEU:HD23  | 3:D:1240:GLN:HG2  | 1.59                     | 0.82              |
| 5:F:120:LEU:HD12  | 6:H:-6:DT:O2      | 1.80                     | 0.82              |
| 3:D:112:VAL:HG23  | 3:D:302:GLN:HG2   | 1.60                     | 0.82              |
| 2:C:180:ALA:HB2   | 2:C:440:LEU:HD13  | 1.60                     | 0.82              |
| 3:D:1343:LEU:HD12 | 3:D:1354:PRO:HG2  | 1.60                     | 0.82              |
| 1:A:50:LEU:CB     | 1:A:220:ALA:HB2   | 2.10                     | 0.81              |
| 2:C:598:PRO:HB2   | 2:C:662:VAL:HG21  | 1.60                     | 0.81              |
| 3:D:683:VAL:HA    | 3:D:687:ALA:HB3   | 1.62                     | 0.81              |
| 3:D:1168:ILE:HG22 | 3:D:1170:PRO:HD3  | 1.62                     | 0.81              |
| 1:B:86:LEU:HD21   | 3:D:528:ILE:HB    | 1.62                     | 0.81              |
| 2:C:743:ALA:HB1   | 2:C:747:THR:HG21  | 1.62                     | 0.81              |
| 2:C:1119:LEU:HD13 | 3:D:506:GLN:HB3   | 1.63                     | 0.81              |
| 5:F:426:LEU:CD2   | 5:F:430:ILE:HD12  | 2.10                     | 0.81              |
| 5:F:116:VAL:O     | 5:F:120:LEU:HD23  | 1.78                     | 0.81              |
| 3:D:654:VAL:HG11  | 3:D:756:VAL:HG21  | 1.62                     | 0.81              |
| 6:H:-3:DA:H2''    | 6:H:-2:DT:H2'     | 1.60                     | 0.81              |
| 1:A:183:ALA:HB3   | 1:A:204:GLU:HB2   | 1.62                     | 0.81              |
| 1:A:50:LEU:HB2    | 1:A:220:ALA:HB1   | 1.61                     | 0.81              |
| 1:B:103:MET:HB2   | 1:B:146:PHE:HB2   | 1.60                     | 0.81              |
| 2:C:78:GLU:HG3    | 2:C:101:LYS:HB2   | 1.62                     | 0.81              |
| 2:C:1293:GLU:HG2  | 3:D:1343:LEU:HD23 | 1.61                     | 0.81              |
| 1:B:91:LEU:HD21   | 1:B:126:ILE:HD12  | 1.63                     | 0.81              |
| 2:C:9:LYS:HG3     | 2:C:797:LEU:HD13  | 1.61                     | 0.81              |
| 7:I:22:DT:H2''    | 7:I:23:DT:H71     | 1.62                     | 0.81              |
| 1:A:49:VAL:HG11   | 1:A:224:LEU:CG    | 2.11                     | 0.81              |
| 3:D:854:VAL:HG21  | 3:D:868:ILE:HD11  | 1.64                     | 0.80              |
| 8:G:124:ASP:HB3   | 8:G:127:SER:HB3   | 1.61                     | 0.80              |
| 2:C:664:PRO:HB2   | 2:C:1201:PHE:HB2  | 1.63                     | 0.80              |
| 2:C:847:ARG:HG2   | 2:C:1064:VAL:HB   | 1.62                     | 0.80              |
| 4:E:13:VAL:HG22   | 4:E:57:VAL:HG13   | 1.61                     | 0.80              |
| 2:C:1123:SER:HB2  | 3:D:727:ARG:HB3   | 1.64                     | 0.80              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:I:27:DG:H1'     | 7:I:28:DC:H5'     | 1.64                     | 0.80              |
| 2:C:1285:GLY:HA2  | 3:D:346:GLY:HA2   | 1.64                     | 0.80              |
| 3:D:434:LEU:HD22  | 3:D:491:ASN:HB3   | 1.61                     | 0.80              |
| 3:D:1353:ILE:HG22 | 3:D:1355:ALA:H    | 1.48                     | 0.79              |
| 1:B:115:ALA:HB1   | 1:B:126:ILE:HG21  | 1.64                     | 0.79              |
| 3:D:1253:VAL:HA   | 3:D:1256:MET:HE2  | 1.65                     | 0.79              |
| 3:D:840:THR:HG23  | 3:D:860:ILE:HD11  | 1.64                     | 0.79              |
| 3:D:112:VAL:HG23  | 3:D:302:GLN:HA    | 1.65                     | 0.78              |
| 3:D:292:ILE:HD12  | 5:F:123:MET:HE1   | 1.66                     | 0.78              |
| 2:C:822:ILE:HG12  | 2:C:1116:LEU:HD22 | 1.65                     | 0.78              |
| 3:D:328:SER:H     | 3:D:331:ASP:HB2   | 1.48                     | 0.78              |
| 2:C:844:VAL:HG11  | 2:C:890:VAL:HG21  | 1.64                     | 0.78              |
| 3:D:1360:TYR:HD2  | 4:E:21:LEU:HD12   | 1.49                     | 0.78              |
| 5:F:452:LEU:HB2   | 5:F:475:ILE:HD11  | 1.66                     | 0.78              |
| 2:C:698:PRO:HA    | 2:C:794:SER:HB3   | 1.65                     | 0.78              |
| 2:C:1339:VAL:HG23 | 3:D:251:LEU:HD13  | 1.64                     | 0.78              |
| 3:D:112:VAL:HG21  | 3:D:305:VAL:HB    | 1.64                     | 0.78              |
| 3:D:1128:GLY:HA2  | 3:D:1236:VAL:HG13 | 1.65                     | 0.78              |
| 5:F:580:LEU:HA    | 5:F:583:THR:HG22  | 1.65                     | 0.78              |
| 2:C:456:LEU:HD11  | 2:C:595:ILE:HD12  | 1.65                     | 0.78              |
| 2:C:1327:ASP:HB2  | 3:D:476:LEU:HB2   | 1.66                     | 0.78              |
| 3:D:428:ALA:HB3   | 3:D:429:PRO:HD3   | 1.66                     | 0.78              |
| 1:B:184:TYR:HA    | 1:B:202:LEU:HA    | 1.67                     | 0.77              |
| 5:F:481:ARG:HD3   | 5:F:494:VAL:HG11  | 1.64                     | 0.77              |
| 1:A:17:ILE:HG12   | 1:A:214:VAL:HG23  | 1.66                     | 0.77              |
| 1:A:85:VAL:HG13   | 1:A:172:VAL:HG23  | 1.65                     | 0.77              |
| 3:D:926:LEU:HA    | 3:D:1240:GLN:HG2  | 1.65                     | 0.77              |
| 1:B:40:VAL:HG21   | 2:C:1230:LEU:HG   | 1.66                     | 0.77              |
| 2:C:1162:LEU:HD23 | 2:C:1166:LEU:HD23 | 1.65                     | 0.77              |
| 5:F:129:LEU:HD22  | 6:H:-7:DT:H2'     | 1.65                     | 0.77              |
| 2:C:683:ALA:HB1   | 3:D:772:THR:HA    | 1.65                     | 0.77              |
| 1:A:108:THR:HB    | 1:A:141:SER:HB2   | 1.66                     | 0.77              |
| 8:G:109:THR:HG22  | 8:G:112:THR:HG22  | 1.67                     | 0.77              |
| 1:A:51:LEU:CD2    | 2:C:1100:ILE:HG13 | 2.15                     | 0.77              |
| 1:A:179:VAL:HG12  | 1:A:207:THR:HB    | 1.67                     | 0.77              |
| 2:C:155:MET:HG2   | 2:C:461:VAL:HG23  | 1.66                     | 0.77              |
| 1:B:157:ALA:HB1   | 1:B:171:ALA:HB1   | 1.65                     | 0.76              |
| 2:C:1340:LEU:HD22 | 3:D:339:ARG:HG3   | 1.65                     | 0.76              |
| 3:D:510:LEU:HD21  | 3:D:637:ILE:HG21  | 1.65                     | 0.76              |
| 1:A:88:ILE:HD13   | 1:A:133:LEU:HD22  | 1.66                     | 0.76              |
| 3:D:558:THR:HG23  | 3:D:559:PRO:HD3   | 1.68                     | 0.76              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:674:LEU:HD13  | 2:C:712:GLU:HG2   | 1.67                     | 0.76              |
| 2:C:371:LEU:HD13  | 2:C:390:GLU:HB2   | 1.67                     | 0.76              |
| 2:C:769:THR:HA    | 2:C:838:HIS:HA    | 1.67                     | 0.76              |
| 5:F:123:MET:HE2   | 5:F:123:MET:CA    | 2.15                     | 0.76              |
| 2:C:111:THR:HA    | 2:C:118:ARG:HH21  | 1.50                     | 0.76              |
| 3:D:427:ARG:HD2   | 3:D:461:ALA:HB2   | 1.68                     | 0.76              |
| 2:C:847:ARG:HA    | 2:C:1064:VAL:HA   | 1.67                     | 0.76              |
| 1:B:47:ARG:HG3    | 1:B:182:VAL:HG13  | 1.67                     | 0.75              |
| 3:D:1294:ARG:HH11 | 3:D:1295:PRO:HD2  | 1.50                     | 0.75              |
| 2:C:79:PHE:HE1    | 2:C:133:ILE:HD11  | 1.50                     | 0.75              |
| 2:C:538:LEU:HD11  | 2:C:583:LEU:HD13  | 1.68                     | 0.75              |
| 3:D:427:ARG:HG2   | 3:D:429:PRO:HD2   | 1.67                     | 0.75              |
| 1:A:64:ILE:HB     | 1:A:67:VAL:HG12   | 1.67                     | 0.75              |
| 2:C:204:ILE:HD11  | 2:C:396:LEU:HD21  | 1.69                     | 0.75              |
| 2:C:1344:MET:HE3  | 3:D:339:ARG:HH12  | 1.51                     | 0.75              |
| 3:D:661:ALA:HA    | 3:D:681:LYS:HD2   | 1.68                     | 0.75              |
| 2:C:823:LEU:HD11  | 2:C:1098:LEU:HD11 | 1.69                     | 0.75              |
| 2:C:877:VAL:HG11  | 2:C:889:LEU:HD12  | 1.66                     | 0.75              |
| 5:F:617:GLY:HA2   | 5:F:627:ILE:HG13  | 1.69                     | 0.75              |
| 7:I:-5:6MA:H2'    | 7:I:-4:DC:H5      | 1.51                     | 0.75              |
| 2:C:456:LEU:HD22  | 2:C:562:HIS:HA    | 1.66                     | 0.75              |
| 2:C:939:VAL:HG21  | 2:C:951:ALA:HB1   | 1.68                     | 0.75              |
| 3:D:899:LEU:HD21  | 3:D:1245:ASN:HD22 | 1.52                     | 0.74              |
| 2:C:158:SER:HB2   | 2:C:460:ARG:HB3   | 1.68                     | 0.74              |
| 1:B:186:VAL:HG13  | 1:B:198:ASP:HB3   | 1.67                     | 0.74              |
| 2:C:696:ALA:HB2   | 2:C:1247:LEU:HD23 | 1.68                     | 0.74              |
| 2:C:835:THR:HG22  | 2:C:1077:LYS:HA   | 1.70                     | 0.74              |
| 3:D:1260:VAL:HG12 | 3:D:1300:PRO:HA   | 1.68                     | 0.74              |
| 1:B:61:ALA:HB3    | 1:B:146:PHE:HA    | 1.68                     | 0.74              |
| 1:B:200:LEU:HD21  | 1:B:202:LEU:HD22  | 1.68                     | 0.74              |
| 2:C:44:ARG:HA     | 2:C:47:LEU:HD12   | 1.69                     | 0.74              |
| 2:C:857:THR:HG22  | 2:C:893:VAL:HG21  | 1.67                     | 0.74              |
| 2:C:397:PHE:HB3   | 2:C:428:LEU:HD21  | 1.69                     | 0.74              |
| 2:C:1308:LYS:HE2  | 3:D:351:TYR:HB2   | 1.69                     | 0.74              |
| 3:D:98:VAL:HG22   | 3:D:102:ARG:HG3   | 1.69                     | 0.74              |
| 3:D:849:THR:HG23  | 3:D:851:GLU:HG2   | 1.68                     | 0.74              |
| 2:C:670:VAL:HG13  | 2:C:711:MET:HE3   | 1.70                     | 0.74              |
| 2:C:696:ALA:HB3   | 2:C:802:LEU:HD12  | 1.69                     | 0.74              |
| 5:F:426:LEU:HD21  | 5:F:430:ILE:HD12  | 1.69                     | 0.74              |
| 2:C:892:LYS:HE3   | 2:C:922:THR:HG22  | 1.70                     | 0.73              |
| 1:B:12:PRO:HB3    | 1:B:33:PRO:HD2    | 1.69                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:819:GLU:HB2   | 3:D:463:PHE:HD2   | 1.52                     | 0.73              |
| 2:C:28:ILE:HD12   | 2:C:32:ARG:HD2    | 1.69                     | 0.73              |
| 3:D:1257:LEU:HD21 | 3:D:1302:LEU:HD12 | 1.69                     | 0.73              |
| 1:B:27:ALA:HB3    | 1:B:212:PRO:HB2   | 1.69                     | 0.73              |
| 2:C:814:ASN:H     | 3:D:633:ALA:HB2   | 1.53                     | 0.73              |
| 3:D:292:ILE:CD1   | 5:F:123:MET:HE1   | 2.19                     | 0.73              |
| 5:F:422:ALA:O     | 5:F:423:ASN:ND2   | 2.22                     | 0.73              |
| 1:B:127:LEU:HD13  | 1:B:209:ALA:HB2   | 1.71                     | 0.73              |
| 2:C:10:ARG:HG3    | 2:C:1195:PRO:HG2  | 1.70                     | 0.73              |
| 5:F:488:ARG:HG3   | 5:F:492:ILE:HD12  | 1.71                     | 0.73              |
| 2:C:1262:ILE:HG21 | 5:F:571:PRO:HG2   | 1.69                     | 0.73              |
| 3:D:255:VAL:HG11  | 5:F:563:ILE:HG12  | 1.71                     | 0.73              |
| 3:D:357:ILE:HG21  | 3:D:468:MET:HG3   | 1.71                     | 0.73              |
| 2:C:548:ARG:HD3   | 2:C:575:PRO:HB2   | 1.70                     | 0.73              |
| 3:D:319:THR:HB    | 3:D:326:LEU:HD21  | 1.69                     | 0.73              |
| 3:D:882:LEU:HD23  | 3:D:1254:ARG:HB2  | 1.70                     | 0.73              |
| 3:D:65:PRO:HG2    | 3:D:94:THR:H      | 1.54                     | 0.72              |
| 1:B:127:LEU:HD22  | 1:B:209:ALA:HA    | 1.71                     | 0.72              |
| 2:C:904:GLU:HB3   | 5:F:580:LEU:HG    | 1.71                     | 0.72              |
| 3:D:108:LEU:HD13  | 3:D:301:LEU:HD21  | 1.71                     | 0.72              |
| 1:A:55:GLN:HB2    | 1:B:5:ASN:HB3     | 1.71                     | 0.72              |
| 2:C:699:LEU:HD11  | 2:C:1248:LYS:HB3  | 1.72                     | 0.72              |
| 7:I:0:DT:H71      | 7:I:1:DA:H62      | 1.55                     | 0.72              |
| 1:A:70:GLU:HB3    | 1:A:170:ILE:HG23  | 1.70                     | 0.72              |
| 2:C:461:VAL:HG21  | 2:C:538:LEU:HD22  | 1.71                     | 0.72              |
| 5:F:618:GLN:HE21  | 5:F:623:THR:HG21  | 1.55                     | 0.72              |
| 1:A:105:LEU:HD13  | 1:A:118:ILE:HG12  | 1.71                     | 0.72              |
| 1:B:67:VAL:HB     | 1:B:168:GLY:HA2   | 1.72                     | 0.72              |
| 2:C:740:VAL:HG11  | 2:C:972:ILE:HG12  | 1.70                     | 0.72              |
| 2:C:808:VAL:HG11  | 2:C:1244:ILE:HB   | 1.71                     | 0.72              |
| 3:D:422:PRO:HB2   | 3:D:438:ALA:HB1   | 1.72                     | 0.72              |
| 2:C:22:VAL:HG21   | 2:C:611:VAL:HG21  | 1.70                     | 0.71              |
| 2:C:675:ILE:HB    | 2:C:678:LEU:HD12  | 1.72                     | 0.71              |
| 3:D:507:ASP:HB3   | 3:D:629:PHE:HE1   | 1.54                     | 0.71              |
| 5:F:524:ALA:HB1   | 5:F:531:LEU:HA    | 1.71                     | 0.71              |
| 2:C:150:VAL:H     | 2:C:523:MET:HB2   | 1.55                     | 0.71              |
| 2:C:151:ILE:HB    | 2:C:464:VAL:HB    | 1.71                     | 0.71              |
| 5:F:602:ARG:HG2   | 5:F:616:VAL:HG11  | 1.70                     | 0.71              |
| 1:A:53:SER:O      | 1:A:54:LEU:HG     | 1.90                     | 0.71              |
| 2:C:636:ILE:HG13  | 2:C:654:LYS:HG3   | 1.73                     | 0.71              |
| 2:C:652:LEU:HD12  | 2:C:657:VAL:HG22  | 1.71                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:841:GLU:HA    | 2:C:1071:PHE:HA   | 1.70                     | 0.71              |
| 2:C:1131:PHE:HZ   | 3:D:760:LYS:HG3   | 1.55                     | 0.71              |
| 2:C:1257:ILE:HG13 | 3:D:355:SER:HB3   | 1.71                     | 0.71              |
| 2:C:1048:GLU:HA   | 2:C:1051:VAL:HG12 | 1.73                     | 0.71              |
| 3:D:1217:LEU:HB2  | 3:D:1225:LEU:HD12 | 1.73                     | 0.71              |
| 6:H:-29:DG:N2     | 7:I:30:DT:O2      | 2.23                     | 0.71              |
| 2:C:623:VAL:HG23  | 2:C:645:ILE:HG22  | 1.73                     | 0.71              |
| 3:D:908:GLY:O     | 3:D:1356:GLY:N    | 2.24                     | 0.71              |
| 1:B:113:VAL:HG12  | 1:B:134:CYS:HB2   | 1.72                     | 0.71              |
| 2:C:813:TRP:HB2   | 2:C:1115:VAL:HG11 | 1.72                     | 0.71              |
| 7:I:-13:6MA:H5''  | 7:I:-13:6MA:H8    | 1.73                     | 0.71              |
| 1:A:50:LEU:HD12   | 1:A:54:LEU:HD21   | 1.72                     | 0.71              |
| 2:C:1226:LEU:HD13 | 2:C:1241:VAL:HG21 | 1.73                     | 0.71              |
| 5:F:469:THR:HB    | 6:H:-9:DC:OP1     | 1.91                     | 0.71              |
| 3:D:336:LYS:O     | 3:D:342:GLN:N     | 2.24                     | 0.70              |
| 3:D:550:ILE:HG22  | 3:D:572:PRO:HD3   | 1.73                     | 0.70              |
| 3:D:645:ILE:HG22  | 3:D:701:LEU:HD13  | 1.72                     | 0.70              |
| 1:A:41:THR:HG22   | 1:B:48:ARG:HD3    | 1.73                     | 0.70              |
| 5:F:612:THR:HG22  | 5:F:615:GLU:HG2   | 1.73                     | 0.70              |
| 2:C:1270:GLN:HE22 | 5:F:568:ALA:HB2   | 1.55                     | 0.70              |
| 2:C:1305:LEU:HB2  | 3:D:347:LYS:HD2   | 1.72                     | 0.70              |
| 1:B:178:PRO:HB2   | 1:B:210:VAL:HG11  | 1.72                     | 0.70              |
| 2:C:166:ASP:HB2   | 2:C:177:LEU:HB2   | 1.74                     | 0.70              |
| 5:F:129:LEU:CD2   | 6:H:-7:DT:H2'     | 2.22                     | 0.70              |
| 3:D:844:VAL:HG12  | 3:D:854:VAL:HB    | 1.73                     | 0.70              |
| 1:A:58:ALA:HB3    | 1:A:174:ALA:HB1   | 1.74                     | 0.70              |
| 2:C:937:VAL:HG22  | 2:C:1070:VAL:HG23 | 1.72                     | 0.70              |
| 3:D:39:ILE:HD11   | 3:D:246:VAL:HG11  | 1.71                     | 0.70              |
| 7:I:-5:6MA:H2'    | 7:I:-4:DC:C5      | 2.27                     | 0.70              |
| 2:C:882:GLU:HA    | 2:C:933:THR:HA    | 1.74                     | 0.70              |
| 3:D:844:VAL:HB    | 3:D:876:VAL:HG23  | 1.72                     | 0.70              |
| 5:F:471:ALA:O     | 5:F:475:ILE:HG12  | 1.91                     | 0.70              |
| 2:C:381:GLY:O     | 5:F:121:ARG:CZ    | 2.40                     | 0.69              |
| 2:C:817:ASN:O     | 2:C:1117:ASN:ND2  | 2.25                     | 0.69              |
| 1:A:200:LYS:HE3   | 1:A:202:ILE:HD11  | 1.73                     | 0.69              |
| 2:C:816:TYR:HB2   | 2:C:823:LEU:HD12  | 1.74                     | 0.69              |
| 2:C:860:ILE:HD12  | 2:C:861:PRO:HD2   | 1.72                     | 0.69              |
| 3:D:375:ALA:HB3   | 3:D:414:LEU:HD21  | 1.74                     | 0.69              |
| 1:A:27:ALA:H      | 1:A:213:PRO:HG2   | 1.57                     | 0.69              |
| 1:B:63:GLN:HG3    | 1:B:143:ARG:HB2   | 1.74                     | 0.69              |
| 1:B:170:ILE:HG23  | 1:B:172:VAL:HG23  | 1.74                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1352:LEU:HD21 | 3:D:1358:GLY:HA2  | 1.73                     | 0.69              |
| 1:A:51:LEU:O      | 1:A:51:LEU:HD23   | 1.91                     | 0.69              |
| 1:B:46:LEU:HD13   | 1:B:216:VAL:HG13  | 1.75                     | 0.69              |
| 3:D:438:ALA:N     | 3:D:486:MET:O     | 2.24                     | 0.69              |
| 3:D:1217:LEU:HD22 | 3:D:1302:LEU:HB2  | 1.75                     | 0.69              |
| 5:F:503:ILE:HD12  | 5:F:537:VAL:HG11  | 1.74                     | 0.69              |
| 1:B:94:ARG:HD2    | 1:B:209:ALA:HB1   | 1.74                     | 0.69              |
| 1:B:154:TYR:HD1   | 1:B:175:LEU:HB3   | 1.56                     | 0.69              |
| 3:D:495:PRO:O     | 3:D:1248:HIS:NE2  | 2.26                     | 0.69              |
| 3:D:818:LEU:HD12  | 3:D:878:VAL:HG21  | 1.74                     | 0.69              |
| 5:F:123:MET:HA    | 5:F:123:MET:CE    | 2.19                     | 0.69              |
| 1:A:44:ASN:ND2    | 2:C:1231:THR:O    | 2.26                     | 0.69              |
| 2:C:1270:GLN:HB2  | 2:C:1335:GLU:HG2  | 1.73                     | 0.69              |
| 2:C:1298:ALA:HB3  | 3:D:1358:GLY:H    | 1.57                     | 0.69              |
| 3:D:439:PHE:HZ    | 3:D:455:VAL:HG21  | 1.58                     | 0.69              |
| 6:H:-8:DC:H2"     | 6:H:-7:DT:OP1     | 1.92                     | 0.69              |
| 1:A:60:THR:OG1    | 1:A:160:ASN:ND2   | 2.24                     | 0.69              |
| 2:C:61:PHE:HD2    | 2:C:74:TYR:HB2    | 1.57                     | 0.69              |
| 2:C:1310:ASP:O    | 2:C:1335:GLU:N    | 2.22                     | 0.69              |
| 2:C:1349:LEU:HD11 | 3:D:116:TRP:HZ3   | 1.56                     | 0.69              |
| 1:A:50:LEU:HD11   | 1:A:54:LEU:HD21   | 1.75                     | 0.69              |
| 2:C:1259:ALA:HB2  | 3:D:374:MET:HG3   | 1.73                     | 0.69              |
| 3:D:1158:LYS:H    | 3:D:1161:LYS:HE2  | 1.58                     | 0.69              |
| 1:A:78:ARG:HG3    | 2:C:775:PRO:HG2   | 1.74                     | 0.68              |
| 3:D:372:LYS:HG2   | 3:D:443:LEU:HD12  | 1.75                     | 0.68              |
| 3:D:477:GLU:O     | 3:D:481:GLU:N     | 2.23                     | 0.68              |
| 6:H:-35:DT:H1'    | 6:H:-34:DT:H5"    | 1.75                     | 0.68              |
| 1:A:53:SER:OG     | 1:B:38:PHE:CZ     | 2.46                     | 0.68              |
| 2:C:776:LEU:HD11  | 2:C:791:ASP:HB3   | 1.74                     | 0.68              |
| 3:D:434:LEU:HD11  | 3:D:494:SER:HA    | 1.76                     | 0.68              |
| 3:D:718:ILE:HA    | 3:D:721:MET:HE3   | 1.73                     | 0.68              |
| 5:F:426:LEU:C     | 5:F:426:LEU:HD23  | 2.14                     | 0.68              |
| 1:B:60:THR:HG23   | 1:B:147:THR:HB    | 1.75                     | 0.68              |
| 1:A:35:GLU:HB2    | 1:A:38:PHE:HB3    | 1.76                     | 0.68              |
| 2:C:674:LEU:HD11  | 2:C:715:VAL:HG11  | 1.74                     | 0.68              |
| 3:D:668:TYR:HB2   | 3:D:677:GLU:HG3   | 1.74                     | 0.68              |
| 1:A:50:LEU:CD1    | 1:A:54:LEU:HD11   | 2.24                     | 0.68              |
| 1:B:175:LEU:HD13  | 1:B:177:SER:HB3   | 1.74                     | 0.68              |
| 3:D:140:LEU:HD21  | 3:D:187:ILE:HG21  | 1.75                     | 0.68              |
| 3:D:333:LEU:HB3   | 3:D:1324:THR:HG21 | 1.76                     | 0.68              |
| 6:H:3:6MA:H2      | 7:I:-3:DT:H3      | 1.59                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:62:ILE:HB     | 1:A:170:ILE:HB    | 1.75                     | 0.68              |
| 1:A:218:ALA:HB1   | 1:B:233:PHE:HE2   | 1.58                     | 0.68              |
| 2:C:734:ILE:HG12  | 2:C:779:VAL:HG22  | 1.76                     | 0.68              |
| 5:F:506:THR:HG21  | 5:F:527:LEU:HD21  | 1.76                     | 0.68              |
| 3:D:123:SER:HB3   | 3:D:126:ALA:HB3   | 1.75                     | 0.67              |
| 3:D:683:VAL:O     | 3:D:688:LYS:N     | 2.27                     | 0.67              |
| 1:A:137:ASP:HB2   | 2:C:733:GLN:HB2   | 1.77                     | 0.67              |
| 2:C:748:ASP:HB2   | 2:C:751:ARG:HB2   | 1.76                     | 0.67              |
| 1:B:58:ALA:HB1    | 1:B:174:ALA:HB3   | 1.74                     | 0.67              |
| 3:D:383:ILE:HD11  | 3:D:414:LEU:HA    | 1.75                     | 0.67              |
| 3:D:1319:ALA:HA   | 3:D:1327:VAL:HG11 | 1.76                     | 0.67              |
| 3:D:483:ARG:HA    | 3:D:487:MET:HG2   | 1.75                     | 0.67              |
| 2:C:63:ILE:HG21   | 2:C:480:GLU:HG3   | 1.77                     | 0.67              |
| 2:C:1081:GLY:H    | 2:C:1094:ILE:HG22 | 1.58                     | 0.67              |
| 3:D:559:PRO:HD3   | 3:D:563:LEU:HD22  | 1.77                     | 0.67              |
| 2:C:1078:LEU:HD13 | 2:C:1084:MET:HE1  | 1.77                     | 0.67              |
| 2:C:1119:LEU:HD21 | 3:D:510:LEU:HD12  | 1.74                     | 0.67              |
| 5:F:426:LEU:HD23  | 5:F:430:ILE:HD12  | 1.77                     | 0.67              |
| 3:D:797:VAL:HG13  | 3:D:913:VAL:HG13  | 1.76                     | 0.67              |
| 1:B:44:ASN:ND2    | 2:C:1231:THR:O    | 2.28                     | 0.67              |
| 1:B:59:VAL:HG21   | 1:B:88:ILE:HG22   | 1.76                     | 0.67              |
| 2:C:973:LEU:HA    | 2:C:976:ASN:HD21  | 1.59                     | 0.67              |
| 2:C:161:VAL:HA    | 2:C:182:VAL:HA    | 1.77                     | 0.67              |
| 2:C:529:LEU:HB2   | 2:C:800:LEU:HD21  | 1.76                     | 0.67              |
| 3:D:834:ARG:NE    | 3:D:1246:ASP:OD2  | 2.28                     | 0.67              |
| 7:I:33:DC:H2'     | 7:I:34:DA:C8      | 2.29                     | 0.67              |
| 7:I:34:DA:H2'     | 7:I:35:DA:C8      | 2.29                     | 0.67              |
| 1:A:111:GLY:HA2   | 1:A:136:LEU:HB2   | 1.77                     | 0.66              |
| 2:C:28:ILE:HG22   | 2:C:535:LYS:HD2   | 1.76                     | 0.66              |
| 3:D:69:TYR:HE1    | 3:D:82:LYS:HG3    | 1.59                     | 0.66              |
| 3:D:261:ARG:NE    | 5:F:543:GLU:O     | 2.25                     | 0.66              |
| 3:D:359:VAL:HG13  | 3:D:453:PRO:HG3   | 1.76                     | 0.66              |
| 5:F:436:ASN:O     | 7:I:9:DG:N2       | 2.27                     | 0.66              |
| 5:F:419:MET:SD    | 5:F:423:ASN:OD1   | 2.54                     | 0.66              |
| 2:C:532:ILE:HD11  | 2:C:719:SER:HB2   | 1.78                     | 0.66              |
| 3:D:614:GLN:H     | 4:E:7:GLU:HG2     | 1.59                     | 0.66              |
| 3:D:637:ILE:HG23  | 3:D:720:MET:HE3   | 1.77                     | 0.66              |
| 5:F:600:ARG:HG3   | 5:F:605:ILE:HG12  | 1.78                     | 0.66              |
| 1:B:53:SER:HB3    | 1:B:152:LYS:HB3   | 1.77                     | 0.66              |
| 2:C:571:THR:HG21  | 2:C:578:GLY:H     | 1.61                     | 0.66              |
| 2:C:1210:GLU:OE1  | 3:D:641:LYS:NZ    | 2.29                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:57:LEU:HD22   | 3:D:271:TYR:HB3   | 1.77                     | 0.66              |
| 3:D:1152:GLY:O    | 3:D:1200:ILE:N    | 2.27                     | 0.66              |
| 2:C:590:ASN:ND2   | 2:C:615:SER:OG    | 2.29                     | 0.66              |
| 2:C:1257:ILE:HD12 | 3:D:447:LYS:HB3   | 1.78                     | 0.66              |
| 2:C:104:LEU:HB2   | 2:C:126:GLN:HB2   | 1.76                     | 0.66              |
| 2:C:569:ILE:HD11  | 2:C:672:ALA:HB1   | 1.78                     | 0.66              |
| 2:C:813:TRP:HB3   | 2:C:823:LEU:HD13  | 1.78                     | 0.66              |
| 3:D:129:LEU:HD12  | 3:D:190:LEU:HG    | 1.77                     | 0.66              |
| 5:F:554:GLU:HG2   | 5:F:556:ASP:H     | 1.61                     | 0.66              |
| 7:I:30:DT:H2''    | 7:I:31:DG:H5''    | 1.76                     | 0.66              |
| 1:A:228:LEU:HB3   | 1:B:220:ALA:HB1   | 1.77                     | 0.65              |
| 2:C:885:PRO:HB3   | 2:C:929:GLY:H     | 1.61                     | 0.65              |
| 3:D:792:LEU:HA    | 3:D:795:ARG:HE    | 1.61                     | 0.65              |
| 3:D:906:ASN:ND2   | 4:E:15:ASN:O      | 2.28                     | 0.65              |
| 2:C:1292:LEU:HB2  | 2:C:1301:LEU:HD21 | 1.78                     | 0.65              |
| 2:C:1293:GLU:HG3  | 3:D:1353:ILE:HD13 | 1.79                     | 0.65              |
| 3:D:121:LEU:HB2   | 3:D:122:PRO:HD3   | 1.78                     | 0.65              |
| 3:D:366:HIS:HB3   | 3:D:489:THR:HG23  | 1.78                     | 0.65              |
| 6:H:-31:DC:H2''   | 6:H:-30:DA:H5'    | 1.77                     | 0.65              |
| 2:C:366:ILE:HG23  | 2:C:369:ASP:H     | 1.60                     | 0.65              |
| 2:C:817:ASN:ND2   | 2:C:1115:VAL:O    | 2.29                     | 0.65              |
| 2:C:528:PRO:HG2   | 2:C:800:LEU:HD13  | 1.79                     | 0.65              |
| 3:D:365:LEU:HD11  | 3:D:502:ILE:HD11  | 1.77                     | 0.65              |
| 3:D:804:ILE:HD12  | 3:D:910:ALA:HA    | 1.77                     | 0.65              |
| 3:D:1278:LYS:HB2  | 3:D:1279:PRO:HD3  | 1.79                     | 0.65              |
| 7:I:34:DA:H2'     | 7:I:35:DA:H8      | 1.62                     | 0.65              |
| 1:B:12:PRO:HA     | 1:B:33:PRO:HG2    | 1.77                     | 0.65              |
| 2:C:765:SER:HB2   | 2:C:771:ILE:HG12  | 1.78                     | 0.65              |
| 2:C:943:HIS:ND1   | 2:C:1056:ARG:O    | 2.30                     | 0.65              |
| 2:C:1210:GLU:O    | 2:C:1214:GLU:HG3  | 1.97                     | 0.65              |
| 3:D:423:VAL:HG22  | 3:D:441:PRO:HG3   | 1.78                     | 0.65              |
| 1:A:59:VAL:HG13   | 1:A:146:PHE:HB3   | 1.76                     | 0.65              |
| 2:C:951:ALA:HA    | 2:C:954:ILE:HD13  | 1.78                     | 0.65              |
| 3:D:432:HIS:CE1   | 3:D:434:LEU:HB2   | 2.32                     | 0.65              |
| 2:C:692:MET:SD    | 2:C:695:GLN:NE2   | 2.70                     | 0.65              |
| 3:D:339:ARG:HD3   | 3:D:1348:ILE:HD13 | 1.78                     | 0.65              |
| 1:A:52:SER:OG     | 1:B:38:PHE:HE1    | 1.79                     | 0.65              |
| 3:D:267:LEU:HD22  | 3:D:329:LEU:HD22  | 1.79                     | 0.65              |
| 3:D:434:LEU:HD13  | 3:D:501:ILE:HG21  | 1.77                     | 0.65              |
| 5:F:180:ILE:HA    | 5:F:302:LEU:HA    | 1.79                     | 0.65              |
| 5:F:548:GLU:O     | 5:F:558:HIS:ND1   | 2.30                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:161:VAL:HG21  | 2:C:417:LEU:HD22  | 1.79                     | 0.65              |
| 1:A:11:ARG:N      | 1:B:226:GLN:OE1   | 2.29                     | 0.65              |
| 2:C:27:LEU:HD12   | 2:C:532:ILE:HD13  | 1.78                     | 0.64              |
| 5:F:426:LEU:HD21  | 5:F:430:ILE:CD1   | 2.27                     | 0.64              |
| 1:B:103:MET:HE1   | 1:B:126:ILE:HD11  | 1.79                     | 0.64              |
| 2:C:179:ALA:HA    | 2:C:193:GLU:HA    | 1.78                     | 0.64              |
| 2:C:835:THR:HG21  | 2:C:1077:LYS:HD3  | 1.79                     | 0.64              |
| 3:D:701:LEU:HG    | 3:D:719:TYR:HB2   | 1.78                     | 0.64              |
| 2:C:795:THR:HG22  | 2:C:800:LEU:HA    | 1.78                     | 0.64              |
| 2:C:1309:SER:HB3  | 3:D:349:VAL:HA    | 1.79                     | 0.64              |
| 3:D:273:ARG:O     | 3:D:277:ARG:HG2   | 1.97                     | 0.64              |
| 5:F:434:TYR:HA    | 5:F:437:ARG:HD2   | 1.80                     | 0.64              |
| 2:C:565:ARG:HA    | 2:C:587:ALA:HB2   | 1.79                     | 0.64              |
| 6:H:-29:DG:H4'    | 6:H:-28:DG:OP1    | 1.98                     | 0.64              |
| 2:C:893:VAL:CG1   | 2:C:919:VAL:HG21  | 2.27                     | 0.64              |
| 3:D:574:ARG:HG2   | 3:D:592:ILE:HG22  | 1.78                     | 0.64              |
| 2:C:822:ILE:HD13  | 2:C:1246:MET:HE3  | 1.78                     | 0.64              |
| 2:C:868:LEU:HD12  | 2:C:871:LEU:HD22  | 1.79                     | 0.64              |
| 2:C:940:PHE:HB3   | 2:C:1060:LEU:HD21 | 1.78                     | 0.64              |
| 2:C:1292:LEU:HD21 | 3:D:436:ILE:HG21  | 1.79                     | 0.64              |
| 3:D:647:PRO:HG2   | 3:D:650:LYS:HB2   | 1.79                     | 0.64              |
| 2:C:455:ASN:HB3   | 2:C:458:ASN:HB2   | 1.79                     | 0.64              |
| 2:C:811:MET:HE1   | 2:C:1104:PRO:HB3  | 1.80                     | 0.64              |
| 2:C:1106:LEU:HD13 | 2:C:1241:VAL:HG11 | 1.78                     | 0.64              |
| 5:F:116:VAL:HG22  | 5:F:442:LEU:HB2   | 1.79                     | 0.64              |
| 2:C:771:ILE:HD12  | 2:C:793:PRO:HG3   | 1.80                     | 0.64              |
| 2:C:1239:VAL:HA   | 3:D:638:SER:HB2   | 1.80                     | 0.64              |
| 3:D:351:TYR:HE2   | 3:D:381:PRO:HG3   | 1.61                     | 0.64              |
| 1:A:225:GLN:O     | 1:B:224:GLN:NE2   | 2.31                     | 0.64              |
| 2:C:707:VAL:HG11  | 2:C:1132:GLU:HG2  | 1.80                     | 0.64              |
| 6:H:9:DT:H2'      | 6:H:10:DG:C8      | 2.33                     | 0.64              |
| 2:C:824:ILE:HB    | 2:C:1094:ILE:HD11 | 1.79                     | 0.63              |
| 3:D:925:GLN:O     | 3:D:1240:GLN:NE2  | 2.30                     | 0.63              |
| 2:C:411:VAL:O     | 2:C:415:MET:HG2   | 1.98                     | 0.63              |
| 2:C:674:LEU:HD11  | 2:C:800:LEU:HD23  | 1.80                     | 0.63              |
| 3:D:801:GLN:NE2   | 3:D:1317:SER:OG   | 2.31                     | 0.63              |
| 5:F:426:LEU:CD1   | 5:F:471:ALA:HB3   | 2.27                     | 0.63              |
| 1:B:32:GLU:HB3    | 1:B:33:PRO:HD3    | 1.81                     | 0.63              |
| 3:D:196:LEU:HD21  | 3:D:236:PRO:HG3   | 1.80                     | 0.63              |
| 1:B:4:ARG:NH2     | 1:B:234:GLU:OE2   | 2.32                     | 0.63              |
| 2:C:151:ILE:HD12  | 2:C:520:SER:HB2   | 1.80                     | 0.63              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:D:1136:PHE:HB3 | 3:D:1305:ILE:HD13 | 1.79                     | 0.63              |
| 6:H:19:DC:H2''   | 6:H:20:DG:H5''    | 1.79                     | 0.63              |
| 1:B:29:ILE:HD12  | 1:B:216:VAL:HG21  | 1.80                     | 0.63              |
| 1:B:57:ALA:HB3   | 1:B:93:VAL:HG13   | 1.79                     | 0.63              |
| 2:C:395:SER:HA   | 2:C:399:ASP:HB2   | 1.79                     | 0.63              |
| 2:C:673:ALA:HB3  | 2:C:711:MET:HG2   | 1.80                     | 0.63              |
| 2:C:699:LEU:HD23 | 2:C:834:PHE:HA    | 1.81                     | 0.63              |
| 2:C:856:ILE:HG22 | 2:C:950:ARG:HD2   | 1.79                     | 0.63              |
| 2:C:1293:GLU:OE1 | 3:D:1343:LEU:HB3  | 1.98                     | 0.63              |
| 3:D:1147:ILE:HA  | 3:D:1205:TYR:HB3  | 1.79                     | 0.63              |
| 8:G:109:THR:HG23 | 8:G:111:LEU:H     | 1.63                     | 0.63              |
| 3:D:493:LEU:HA   | 3:D:500:PRO:HA    | 1.81                     | 0.63              |
| 5:F:441:PHE:CZ   | 6:H:-5:DC:C5      | 2.86                     | 0.63              |
| 1:B:103:MET:O    | 1:B:146:PHE:N     | 2.32                     | 0.63              |
| 1:B:175:LEU:HD21 | 1:B:180:LYS:HD3   | 1.81                     | 0.63              |
| 3:D:800:ALA:HB2  | 3:D:1252:ILE:HD13 | 1.81                     | 0.63              |
| 3:D:835:VAL:HG23 | 3:D:878:VAL:HG21  | 1.79                     | 0.63              |
| 3:D:118:LEU:HB2  | 3:D:125:ILE:HD12  | 1.80                     | 0.63              |
| 1:A:50:LEU:O     | 1:A:54:LEU:HG     | 1.99                     | 0.62              |
| 2:C:1290:TRP:CH2 | 3:D:794:ARG:HA    | 2.34                     | 0.62              |
| 1:A:50:LEU:HD13  | 1:A:220:ALA:CB    | 2.23                     | 0.62              |
| 2:C:139:LYS:HE3  | 2:C:141:THR:HG21  | 1.80                     | 0.62              |
| 2:C:201:TYR:HD1  | 2:C:211:PRO:HA    | 1.62                     | 0.62              |
| 2:C:687:LEU:HD22 | 3:D:779:LEU:HD21  | 1.81                     | 0.62              |
| 2:C:804:ARG:HB2  | 2:C:834:PHE:HE1   | 1.64                     | 0.62              |
| 3:D:482:ALA:HA   | 3:D:486:MET:HB2   | 1.79                     | 0.62              |
| 5:F:600:ARG:HD3  | 5:F:605:ILE:HB    | 1.80                     | 0.62              |
| 2:C:1300:THR:O   | 2:C:1304:MET:N    | 2.32                     | 0.62              |
| 7:I:-19:DG:H2''  | 7:I:-18:DT:H5'    | 1.82                     | 0.62              |
| 2:C:807:LEU:HD11 | 2:C:1241:VAL:HG12 | 1.81                     | 0.62              |
| 3:D:1129:LEU:HB3 | 3:D:1130:PRO:HD3  | 1.82                     | 0.62              |
| 5:F:426:LEU:HD11 | 5:F:471:ALA:HB3   | 1.80                     | 0.62              |
| 6:H:-28:DG:N2    | 7:I:29:DC:O2      | 2.31                     | 0.62              |
| 1:B:112:PRO:HB3  | 1:B:133:LEU:HB3   | 1.79                     | 0.62              |
| 2:C:1123:SER:O   | 3:D:732:GLN:NE2   | 2.32                     | 0.62              |
| 7:I:37:DG:H2'    | 7:I:38:DG:C8      | 2.34                     | 0.62              |
| 2:C:22:VAL:HB    | 2:C:662:VAL:HG11  | 1.81                     | 0.62              |
| 2:C:211:PRO:HG2  | 2:C:214:THR:HG23  | 1.82                     | 0.62              |
| 2:C:1261:SER:HA  | 3:D:351:TYR:HA    | 1.81                     | 0.62              |
| 1:A:64:ILE:HG21  | 1:A:74:LEU:HD21   | 1.80                     | 0.62              |
| 1:B:92:ALA:H     | 1:B:128:ASN:HD21  | 1.48                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:1150:LEU:HD13 | 2:C:1187:ALA:HB3  | 1.82                     | 0.62              |
| 2:C:1256:LYS:HE3  | 7:I:3:DT:H4'      | 1.82                     | 0.62              |
| 3:D:1259:LYS:HD3  | 3:D:1303:LEU:HD21 | 1.81                     | 0.62              |
| 2:C:9:LYS:HB2     | 2:C:1189:ASN:HD22 | 1.65                     | 0.62              |
| 2:C:1296:GLY:HA2  | 3:D:1356:GLY:HA3  | 1.82                     | 0.62              |
| 3:D:646:ILE:HG22  | 3:D:758:ASN:HD21  | 1.64                     | 0.62              |
| 2:C:1284:PHE:HE2  | 2:C:1289:VAL:HG23 | 1.65                     | 0.62              |
| 5:F:156:ALA:HB1   | 5:F:398:TYR:HD1   | 1.65                     | 0.62              |
| 2:C:222:ASP:HA    | 2:C:226:ILE:HB    | 1.81                     | 0.62              |
| 2:C:707:VAL:HG23  | 2:C:1135:LEU:HD23 | 1.82                     | 0.62              |
| 2:C:1273:LEU:HD13 | 2:C:1278:GLN:HE21 | 1.64                     | 0.62              |
| 3:D:550:ILE:H     | 3:D:572:PRO:HD3   | 1.65                     | 0.62              |
| 3:D:1145:ALA:HA   | 3:D:1207:ILE:HD13 | 1.81                     | 0.62              |
| 1:B:200:LEU:CD2   | 1:B:202:LEU:HD22  | 2.29                     | 0.61              |
| 2:C:323:ASP:O     | 2:C:360:ARG:NH2   | 2.33                     | 0.61              |
| 2:C:692:MET:HB3   | 2:C:1249:LEU:HD21 | 1.82                     | 0.61              |
| 3:D:494:SER:HB2   | 3:D:501:ILE:HB    | 1.82                     | 0.61              |
| 5:F:495:HIS:O     | 5:F:498:GLU:HG2   | 2.00                     | 0.61              |
| 3:D:94:THR:HG22   | 3:D:95:LEU:HD23   | 1.81                     | 0.61              |
| 3:D:116:TRP:HE1   | 3:D:330:ALA:HB2   | 1.63                     | 0.61              |
| 3:D:528:ILE:HG22  | 3:D:551:LYS:HD2   | 1.82                     | 0.61              |
| 7:I:21:DT:H2'     | 7:I:22:DT:H71     | 1.82                     | 0.61              |
| 2:C:823:LEU:HA    | 2:C:1095:SER:HB3  | 1.80                     | 0.61              |
| 5:F:404:THR:HA    | 5:F:407:LYS:HD2   | 1.82                     | 0.61              |
| 2:C:1149:LEU:HD22 | 2:C:1159:LYS:HB2  | 1.82                     | 0.61              |
| 3:D:792:LEU:HD11  | 3:D:1136:PHE:HD2  | 1.64                     | 0.61              |
| 2:C:353:ALA:O     | 2:C:357:ASN:ND2   | 2.32                     | 0.61              |
| 2:C:846:ALA:H     | 2:C:1064:VAL:HG23 | 1.65                     | 0.61              |
| 3:D:109:ALA:HB3   | 3:D:281:LEU:HG    | 1.82                     | 0.61              |
| 5:F:402:VAL:HA    | 5:F:405:VAL:HG12  | 1.81                     | 0.61              |
| 7:I:-10:DC:H2'    | 7:I:-9:DA:C8      | 2.35                     | 0.61              |
| 2:C:1121:VAL:HB   | 2:C:1122:PRO:HD3  | 1.81                     | 0.61              |
| 2:C:1285:GLY:HA2  | 3:D:346:GLY:CA    | 2.30                     | 0.61              |
| 3:D:99:ARG:HG2    | 3:D:249:PRO:HG2   | 1.83                     | 0.61              |
| 3:D:141:TYR:HD2   | 5:F:118:MET:HE1   | 1.66                     | 0.61              |
| 3:D:644:ILE:HG23  | 3:D:760:LYS:HD2   | 1.82                     | 0.61              |
| 1:B:37:GLY:N      | 1:B:198:ASP:OD2   | 2.28                     | 0.61              |
| 2:C:532:ILE:HG21  | 2:C:670:VAL:HG11  | 1.82                     | 0.61              |
| 3:D:653:ILE:O     | 3:D:656:GLU:HG3   | 2.01                     | 0.61              |
| 7:I:5:DG:H2''     | 7:I:6:DA:O4'      | 2.01                     | 0.61              |
| 2:C:27:LEU:HD11   | 2:C:711:MET:HE1   | 1.82                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:597:SER:HB2   | 2:C:666:GLN:HE21  | 1.66                     | 0.61              |
| 3:D:319:THR:HB    | 3:D:326:LEU:HD11  | 1.82                     | 0.61              |
| 3:D:598:LYS:N     | 3:D:724:SER:O     | 2.29                     | 0.61              |
| 1:A:5:ASN:HA      | 1:B:222:ILE:HD11  | 1.83                     | 0.61              |
| 2:C:70:ALA:HB2    | 2:C:492:ILE:HD13  | 1.83                     | 0.61              |
| 2:C:911:ILE:HD13  | 5:F:638:LEU:HD11  | 1.82                     | 0.61              |
| 2:C:527:ASN:HB2   | 2:C:528:PRO:HD2   | 1.83                     | 0.60              |
| 2:C:1095:SER:HA   | 3:D:358:VAL:CG1   | 2.31                     | 0.60              |
| 3:D:274:VAL:HG21  | 3:D:308:LEU:HD13  | 1.82                     | 0.60              |
| 6:H:-15:DT:H3'    | 6:H:-14:DG:H8     | 1.64                     | 0.60              |
| 2:C:1351:VAL:HG22 | 3:D:23:ILE:HG22   | 1.82                     | 0.60              |
| 1:A:27:ALA:HB3    | 1:A:213:PRO:HB2   | 1.83                     | 0.60              |
| 2:C:394:LYS:HA    | 2:C:398:PHE:HB2   | 1.83                     | 0.60              |
| 2:C:958:GLU:O     | 2:C:961:ARG:HG3   | 2.01                     | 0.60              |
| 1:B:17:ILE:HB     | 1:B:30:VAL:HB     | 1.83                     | 0.60              |
| 2:C:203:ARG:HG2   | 2:C:206:ARG:HA    | 1.82                     | 0.60              |
| 2:C:709:THR:HG22  | 2:C:711:MET:H     | 1.67                     | 0.60              |
| 2:C:1135:LEU:HD22 | 2:C:1209:ILE:HD11 | 1.82                     | 0.60              |
| 3:D:854:VAL:HG22  | 3:D:864:ILE:HG23  | 1.83                     | 0.60              |
| 3:D:1246:ASP:O    | 3:D:1250:GLU:HG2  | 2.02                     | 0.60              |
| 2:C:860:ILE:CD1   | 2:C:861:PRO:HD2   | 2.32                     | 0.60              |
| 2:C:1290:TRP:CG   | 3:D:797:VAL:HG11  | 2.37                     | 0.60              |
| 5:F:489:THR:HB    | 5:F:544:PRO:HG3   | 1.84                     | 0.60              |
| 5:F:493:PRO:HG2   | 5:F:496:MET:HB3   | 1.83                     | 0.60              |
| 1:B:204:VAL:HG23  | 1:B:212:PRO:HB3   | 1.83                     | 0.60              |
| 2:C:568:PRO:HG2   | 3:D:772:THR:HG21  | 1.84                     | 0.60              |
| 2:C:877:VAL:HG13  | 2:C:889:LEU:O     | 2.01                     | 0.60              |
| 3:D:116:TRP:HB3   | 3:D:1329:THR:CG2  | 2.31                     | 0.60              |
| 2:C:222:ASP:N     | 2:C:225:GLU:OE2   | 2.33                     | 0.60              |
| 2:C:739:ILE:HD12  | 2:C:789:ILE:HG21  | 1.83                     | 0.60              |
| 7:I:-19:DG:H5''   | 7:I:-19:DG:H8     | 1.66                     | 0.60              |
| 2:C:856:ILE:HG21  | 2:C:1066:LYS:HD3  | 1.84                     | 0.60              |
| 2:C:1343:GLU:HG2  | 3:D:247:ILE:HD12  | 1.82                     | 0.60              |
| 1:A:228:LEU:HD21  | 1:B:42:LEU:HD22   | 1.82                     | 0.59              |
| 2:C:154:GLN:O     | 2:C:462:ARG:N     | 2.28                     | 0.59              |
| 2:C:1045:ARG:HA   | 2:C:1048:GLU:OE1  | 2.02                     | 0.59              |
| 3:D:591:LEU:HD13  | 3:D:607:ILE:HG21  | 1.84                     | 0.59              |
| 6:H:-34:DT:H1'    | 6:H:-33:DG:H5'    | 1.84                     | 0.59              |
| 3:D:371:PRO:HB3   | 3:D:447:LYS:HA    | 1.84                     | 0.59              |
| 3:D:722:ALA:HA    | 3:D:728:GLY:HA3   | 1.83                     | 0.59              |
| 5:F:524:ALA:CB    | 5:F:531:LEU:HA    | 2.32                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:50:LEU:CB     | 1:A:220:ALA:CB    | 2.69                     | 0.59              |
| 3:D:504:PRO:CB    | 3:D:508:ILE:HB    | 2.26                     | 0.59              |
| 6:H:19:DC:H4'     | 6:H:20:DG:OP1     | 2.02                     | 0.59              |
| 1:B:189:THR:HG21  | 1:B:199:LYS:HD3   | 1.84                     | 0.59              |
| 2:C:688:MET:O     | 2:C:692:MET:HG2   | 2.03                     | 0.59              |
| 2:C:1262:ILE:CD1  | 5:F:572:ILE:HG13  | 2.28                     | 0.59              |
| 3:D:85:ILE:HA     | 3:D:92:GLU:HA     | 1.84                     | 0.59              |
| 3:D:529:PHE:CD2   | 3:D:535:ILE:HG13  | 2.37                     | 0.59              |
| 3:D:791:TYR:CE2   | 3:D:795:ARG:HD3   | 2.37                     | 0.59              |
| 3:D:512:LEU:HD22  | 3:D:601:ILE:CD1   | 2.32                     | 0.59              |
| 3:D:643:ASP:O     | 3:D:716:ASN:ND2   | 2.30                     | 0.59              |
| 3:D:926:LEU:HD12  | 3:D:1129:LEU:HD13 | 1.85                     | 0.59              |
| 3:D:1247:LYS:O    | 3:D:1251:THR:HG23 | 2.02                     | 0.59              |
| 8:G:110:VAL:HG12  | 8:G:132:PHE:HE2   | 1.66                     | 0.59              |
| 1:A:51:LEU:HD23   | 1:A:51:LEU:C      | 2.23                     | 0.59              |
| 2:C:142:PHE:HB3   | 2:C:514:PHE:HE2   | 1.65                     | 0.59              |
| 2:C:1288:GLU:OE1  | 3:D:426:ASN:ND2   | 2.24                     | 0.59              |
| 2:C:1353:LEU:HD13 | 3:D:18:PHE:CD2    | 2.37                     | 0.59              |
| 3:D:480:LEU:HD21  | 4:E:23:SER:HB2    | 1.84                     | 0.59              |
| 3:D:614:GLN:HB3   | 4:E:7:GLU:HB2     | 1.84                     | 0.59              |
| 3:D:1343:LEU:HG   | 3:D:1353:ILE:HG23 | 1.83                     | 0.59              |
| 2:C:1079:GLN:HE21 | 2:C:1253:VAL:HG12 | 1.68                     | 0.59              |
| 3:D:529:PHE:HD2   | 3:D:535:ILE:HG13  | 1.68                     | 0.59              |
| 3:D:751:ILE:CG2   | 3:D:753:THR:HG22  | 2.33                     | 0.59              |
| 5:F:423:ASN:O     | 5:F:426:LEU:HB3   | 2.03                     | 0.59              |
| 5:F:493:PRO:HG2   | 5:F:496:MET:CB    | 2.32                     | 0.59              |
| 1:A:228:LEU:HD11  | 1:B:223:LEU:HD23  | 1.83                     | 0.59              |
| 1:A:59:VAL:O      | 1:A:174:ALA:HB2   | 2.03                     | 0.59              |
| 2:C:86:VAL:HG23   | 2:C:143:ILE:HD12  | 1.85                     | 0.59              |
| 3:D:557:MET:H     | 3:D:563:LEU:HD23  | 1.68                     | 0.59              |
| 3:D:800:ALA:O     | 3:D:912:GLY:HA3   | 2.03                     | 0.59              |
| 3:D:841:ALA:HB3   | 3:D:877:LYS:HG3   | 1.84                     | 0.59              |
| 2:C:676:PRO:HG2   | 2:C:1132:GLU:HG3  | 1.84                     | 0.58              |
| 2:C:876:ILE:HG22  | 2:C:890:VAL:HG12  | 1.84                     | 0.58              |
| 3:D:405:ARG:HG3   | 3:D:407:GLN:HG3   | 1.84                     | 0.58              |
| 3:D:653:ILE:HD11  | 3:D:693:VAL:HG23  | 1.85                     | 0.58              |
| 4:E:30:ILE:HA     | 4:E:34:ALA:HB3    | 1.84                     | 0.58              |
| 6:H:-5:DC:H2''    | 6:H:-4:DG:H5'     | 1.85                     | 0.58              |
| 7:I:-18:DT:H2''   | 7:I:-17:DC:C6     | 2.37                     | 0.58              |
| 1:A:88:ILE:HD11   | 1:A:133:LEU:HD13  | 1.85                     | 0.58              |
| 2:C:27:LEU:HD13   | 2:C:670:VAL:HG11  | 1.85                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:670:VAL:HG13  | 2:C:711:MET:CE    | 2.33                     | 0.58              |
| 2:C:810:PHE:CZ    | 2:C:1116:LEU:HD12 | 2.38                     | 0.58              |
| 3:D:363:LEU:HD22  | 3:D:442:LYS:HD3   | 1.83                     | 0.58              |
| 3:D:422:PRO:HG2   | 3:D:482:ALA:HB3   | 1.85                     | 0.58              |
| 3:D:426:ASN:O     | 3:D:469:ALA:N     | 2.35                     | 0.58              |
| 3:D:793:THR:O     | 3:D:797:VAL:HG23  | 2.03                     | 0.58              |
| 3:D:881:VAL:HG21  | 3:D:1251:THR:HA   | 1.83                     | 0.58              |
| 2:C:60:VAL:HG13   | 2:C:477:LEU:HD23  | 1.84                     | 0.58              |
| 2:C:394:LYS:HG2   | 2:C:398:PHE:HB2   | 1.85                     | 0.58              |
| 2:C:537:ARG:HG2   | 2:C:580:ILE:HG22  | 1.85                     | 0.58              |
| 3:D:897:ARG:HE    | 3:D:902:GLY:HA2   | 1.69                     | 0.58              |
| 5:F:594:ARG:HD3   | 5:F:620:PHE:HE1   | 1.66                     | 0.58              |
| 1:A:50:LEU:CG     | 1:A:220:ALA:HB2   | 2.32                     | 0.58              |
| 1:A:185:ARG:HB2   | 1:A:202:ILE:HB    | 1.85                     | 0.58              |
| 2:C:570:GLU:HG3   | 2:C:671:ALA:HB3   | 1.84                     | 0.58              |
| 2:C:1337:PHE:HZ   | 3:D:21:ILE:HD12   | 1.69                     | 0.58              |
| 3:D:56:GLY:N      | 3:D:59:CYS:SG     | 2.68                     | 0.58              |
| 2:C:559:HIS:H     | 2:C:562:HIS:HD2   | 1.51                     | 0.58              |
| 2:C:626:GLN:HE22  | 3:D:764:THR:HG21  | 1.67                     | 0.58              |
| 2:C:856:ILE:HD13  | 2:C:1066:LYS:HE3  | 1.86                     | 0.58              |
| 3:D:855:PRO:HG2   | 3:D:858:THR:OG1   | 2.03                     | 0.58              |
| 3:D:1343:LEU:HD11 | 3:D:1355:ALA:HB2  | 1.84                     | 0.58              |
| 1:B:105:LEU:HD13  | 1:B:118:ILE:HA    | 1.85                     | 0.58              |
| 2:C:828:ILE:HG23  | 2:C:1078:LEU:HD12 | 1.84                     | 0.58              |
| 2:C:1306:THR:O    | 2:C:1311:ASP:HB2  | 2.04                     | 0.58              |
| 2:C:1342:LYS:HB2  | 3:D:251:LEU:HD11  | 1.84                     | 0.58              |
| 3:D:95:LEU:O      | 3:D:98:VAL:HG12   | 2.04                     | 0.58              |
| 3:D:418:ILE:HG21  | 3:D:441:PRO:HB2   | 1.85                     | 0.58              |
| 3:D:568:ILE:HB    | 3:D:570:THR:HG23  | 1.84                     | 0.58              |
| 3:D:751:ILE:HG22  | 3:D:753:THR:HG22  | 1.86                     | 0.58              |
| 3:D:1233:ILE:HG21 | 3:D:1249:ILE:HD12 | 1.85                     | 0.58              |
| 2:C:150:VAL:HG12  | 2:C:523:MET:HG3   | 1.86                     | 0.58              |
| 2:C:676:PRO:HG2   | 2:C:1088:HIS:HE1  | 1.68                     | 0.58              |
| 2:C:1301:LEU:HD12 | 3:D:1353:ILE:HD12 | 1.85                     | 0.58              |
| 3:D:71:CYS:SG     | 3:D:86:CYS:HB2    | 2.43                     | 0.58              |
| 3:D:637:ILE:HD12  | 3:D:720:MET:HE1   | 1.85                     | 0.58              |
| 1:A:103:MET:HB2   | 1:A:146:PHE:HB2   | 1.85                     | 0.58              |
| 2:C:825:SER:HB2   | 2:C:1103:MET:HG3  | 1.84                     | 0.58              |
| 2:C:1080:PRO:HA   | 2:C:1094:ILE:HG23 | 1.85                     | 0.58              |
| 1:A:58:ALA:CB     | 1:A:174:ALA:HB1   | 2.33                     | 0.58              |
| 1:A:179:VAL:HA    | 1:A:207:THR:HA    | 1.86                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:1286:GLU:HA   | 2:C:1289:VAL:HG12 | 1.84                     | 0.58              |
| 2:C:1294:ALA:HB1  | 3:D:914:ILE:CG1   | 2.34                     | 0.58              |
| 3:D:272:ARG:HE    | 5:F:489:THR:HA    | 1.69                     | 0.58              |
| 3:D:424:LEU:HB2   | 3:D:471:HIS:HB2   | 1.86                     | 0.58              |
| 6:H:8:DC:H2'      | 6:H:9:DT:C6       | 2.39                     | 0.58              |
| 1:B:77:VAL:HG23   | 1:B:78:ARG:H      | 1.69                     | 0.58              |
| 2:C:571:THR:O     | 2:C:691:ASN:ND2   | 2.35                     | 0.58              |
| 2:C:651:LEU:HD11  | 3:D:754:PRO:HD3   | 1.86                     | 0.58              |
| 3:D:515:LEU:HD21  | 3:D:631:GLU:HB3   | 1.84                     | 0.58              |
| 3:D:646:ILE:HG23  | 3:D:760:LYS:HD3   | 1.86                     | 0.58              |
| 1:A:49:VAL:HG11   | 1:A:224:LEU:CD1   | 2.34                     | 0.57              |
| 3:D:550:ILE:HG22  | 3:D:572:PRO:CD    | 2.33                     | 0.57              |
| 3:D:780:ALA:O     | 3:D:784:LEU:N     | 2.36                     | 0.57              |
| 3:D:789:SER:OG    | 3:D:923:GLY:HA3   | 2.04                     | 0.57              |
| 3:D:1163:LYS:HG3  | 3:D:1190:LYS:HE2  | 1.85                     | 0.57              |
| 2:C:825:SER:O     | 2:C:828:ILE:HG22  | 2.04                     | 0.57              |
| 3:D:686:TRP:CZ2   | 3:D:754:PRO:HB3   | 2.40                     | 0.57              |
| 1:B:53:SER:CB     | 1:B:152:LYS:HB3   | 2.34                     | 0.57              |
| 2:C:128:VAL:HB    | 2:C:498:HIS:HB2   | 1.86                     | 0.57              |
| 2:C:172:ALA:HB2   | 2:C:196:ALA:HB2   | 1.86                     | 0.57              |
| 2:C:607:PRO:HD2   | 2:C:635:GLU:HA    | 1.86                     | 0.57              |
| 2:C:1084:MET:HG3  | 2:C:1247:LEU:O    | 2.04                     | 0.57              |
| 2:C:1214:GLU:HG2  | 2:C:1220:LYS:HG3  | 1.86                     | 0.57              |
| 2:C:61:PHE:HB3    | 2:C:62:PRO:HD3    | 1.86                     | 0.57              |
| 2:C:216:LEU:HG    | 2:C:226:ILE:HD12  | 1.86                     | 0.57              |
| 2:C:547:THR:HG23  | 2:C:550:ARG:H     | 1.69                     | 0.57              |
| 2:C:565:ARG:HG2   | 2:C:597:SER:HB3   | 1.86                     | 0.57              |
| 2:C:154:GLN:N     | 2:C:462:ARG:O     | 2.36                     | 0.57              |
| 2:C:487:MET:HE2   | 2:C:500:LEU:HD11  | 1.86                     | 0.57              |
| 3:D:1145:ALA:CA   | 3:D:1207:ILE:HD13 | 2.35                     | 0.57              |
| 1:A:50:LEU:HD12   | 1:A:54:LEU:CD2    | 2.35                     | 0.57              |
| 1:B:59:VAL:HG11   | 1:B:88:ILE:HG22   | 1.87                     | 0.57              |
| 2:C:467:LEU:CD2   | 2:C:519:LEU:HG    | 2.34                     | 0.57              |
| 3:D:395:THR:HG23  | 3:D:398:GLN:H     | 1.68                     | 0.57              |
| 3:D:679:TYR:HA    | 3:D:682:VAL:HG12  | 1.87                     | 0.57              |
| 5:F:519:THR:HG23  | 5:F:522:GLU:H     | 1.70                     | 0.57              |
| 5:F:617:GLY:CA    | 5:F:627:ILE:HG13  | 2.35                     | 0.57              |
| 1:B:154:TYR:HE2   | 3:D:543:VAL:HG11  | 1.69                     | 0.57              |
| 2:C:930:VAL:O     | 2:C:1074:VAL:HG13 | 2.05                     | 0.57              |
| 2:C:1239:VAL:HG13 | 3:D:638:SER:OG    | 2.04                     | 0.57              |
| 3:D:444:ILE:HG21  | 3:D:450:GLN:HG2   | 1.86                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:819:ARG:CB    | 3:D:875:SER:HB3   | 2.35                     | 0.57              |
| 5:F:151:GLY:O     | 5:F:401:ILE:HG23  | 2.05                     | 0.57              |
| 1:A:221:ALA:HB1   | 1:B:227:LEU:HG    | 1.87                     | 0.57              |
| 2:C:1087:ARG:HD2  | 2:C:1245:TYR:HB3  | 1.87                     | 0.57              |
| 3:D:425:LEU:HB3   | 3:D:468:MET:HE3   | 1.87                     | 0.57              |
| 3:D:604:LEU:HA    | 3:D:607:ILE:HG22  | 1.87                     | 0.57              |
| 5:F:628:ARG:CZ    | 5:F:632:ALA:HB2   | 2.34                     | 0.57              |
| 1:A:203:LEU:HD23  | 1:A:205:VAL:H     | 1.70                     | 0.57              |
| 2:C:72:LEU:HA     | 2:C:106:LEU:HD23  | 1.87                     | 0.57              |
| 2:C:703:ASP:OD1   | 2:C:804:ARG:HD2   | 2.05                     | 0.57              |
| 2:C:705:PRO:HG2   | 2:C:708:GLY:HA3   | 1.86                     | 0.57              |
| 1:A:51:LEU:HD21   | 2:C:1100:ILE:CD1  | 2.35                     | 0.57              |
| 1:A:52:SER:HB3    | 2:C:1101:GLU:OE2  | 2.05                     | 0.57              |
| 2:C:807:LEU:HD23  | 2:C:1112:VAL:HA   | 1.86                     | 0.57              |
| 2:C:815:GLY:O     | 3:D:359:VAL:HG11  | 2.05                     | 0.57              |
| 3:D:554:HIS:HB3   | 3:D:568:ILE:HD11  | 1.87                     | 0.57              |
| 5:F:138:ALA:HB2   | 5:F:459:PHE:CE2   | 2.39                     | 0.57              |
| 6:H:-2:DT:H1'     | 6:H:-1:DT:C2      | 2.40                     | 0.57              |
| 1:A:43:GLY:CA     | 1:A:201:LEU:HD11  | 2.34                     | 0.56              |
| 4:E:22:LEU:HD22   | 4:E:61:GLU:HA     | 1.85                     | 0.56              |
| 4:E:43:ASP:HB3    | 4:E:47:VAL:HG13   | 1.86                     | 0.56              |
| 6:H:3:6MA:H2      | 7:I:-3:DT:N3      | 2.20                     | 0.56              |
| 6:H:13:DT:H2'     | 6:H:14:DC:C6      | 2.40                     | 0.56              |
| 1:A:137:ASP:HB3   | 2:C:734:ILE:O     | 2.05                     | 0.56              |
| 2:C:820:ASP:HB3   | 3:D:464:ASP:HB3   | 1.88                     | 0.56              |
| 2:C:1135:LEU:HD11 | 2:C:1196:ILE:HD12 | 1.87                     | 0.56              |
| 2:C:1333:ILE:HG23 | 2:C:1337:PHE:HD2  | 1.70                     | 0.56              |
| 3:D:59:CYS:HB2    | 3:D:62:ILE:HB     | 1.86                     | 0.56              |
| 3:D:480:LEU:HD21  | 4:E:23:SER:CB     | 2.34                     | 0.56              |
| 3:D:678:LYS:O     | 3:D:682:VAL:HG12  | 2.05                     | 0.56              |
| 3:D:1139:ARG:HD3  | 6:H:4:DG:O3'      | 2.06                     | 0.56              |
| 4:E:25:HIS:HE1    | 4:E:67:LEU:HD13   | 1.70                     | 0.56              |
| 1:B:178:PRO:O     | 1:B:207:ASN:N     | 2.28                     | 0.56              |
| 2:C:35:TYR:HE1    | 2:C:464:VAL:HG22  | 1.70                     | 0.56              |
| 2:C:62:PRO:HA     | 2:C:72:LEU:O      | 2.05                     | 0.56              |
| 2:C:810:PHE:O     | 3:D:638:SER:HA    | 2.05                     | 0.56              |
| 2:C:911:ILE:O     | 5:F:639:LYS:HE2   | 2.05                     | 0.56              |
| 2:C:1159:LYS:HE3  | 2:C:1187:ALA:HB2  | 1.85                     | 0.56              |
| 2:C:1285:GLY:N    | 7:I:1:DA:OP1      | 2.35                     | 0.56              |
| 2:C:1288:GLU:HA   | 3:D:430:THR:HG21  | 1.87                     | 0.56              |
| 3:D:141:TYR:CD2   | 5:F:118:MET:HE1   | 2.40                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:805:ILE:HG22  | 3:D:909:GLU:O     | 2.05                     | 0.56              |
| 3:D:815:GLY:HA2   | 3:D:883:THR:HG21  | 1.88                     | 0.56              |
| 5:F:469:THR:O     | 5:F:472:THR:HG22  | 2.05                     | 0.56              |
| 5:F:505:ARG:HA    | 7:I:11:DT:H73     | 1.87                     | 0.56              |
| 6:H:-27:DC:H6     | 6:H:-27:DC:H5''   | 1.71                     | 0.56              |
| 1:A:35:GLU:HB2    | 1:A:38:PHE:CB     | 2.34                     | 0.56              |
| 2:C:639:ASP:O     | 2:C:640:LEU:HD22  | 2.05                     | 0.56              |
| 2:C:687:LEU:HD13  | 3:D:779:LEU:HD23  | 1.88                     | 0.56              |
| 2:C:813:TRP:CZ2   | 2:C:1230:LEU:HB2  | 2.41                     | 0.56              |
| 2:C:813:TRP:HH2   | 2:C:1230:LEU:HD13 | 1.69                     | 0.56              |
| 2:C:1297:ALA:HA   | 3:D:481:GLU:HG2   | 1.87                     | 0.56              |
| 3:D:281:LEU:HA    | 3:D:297:GLU:HG2   | 1.86                     | 0.56              |
| 3:D:701:LEU:CG    | 3:D:719:TYR:HB2   | 2.36                     | 0.56              |
| 1:B:142:VAL:HG23  | 1:B:143:ARG:H     | 1.70                     | 0.56              |
| 2:C:17:ARG:HG2    | 2:C:1202:ASP:OD1  | 2.05                     | 0.56              |
| 2:C:664:PRO:HA    | 3:D:765:VAL:HG21  | 1.87                     | 0.56              |
| 2:C:664:PRO:HG3   | 2:C:1202:ASP:HB2  | 1.86                     | 0.56              |
| 3:D:21:ILE:CG2    | 3:D:1338:ASP:HB3  | 2.36                     | 0.56              |
| 3:D:158:HIS:CE1   | 3:D:190:LEU:HD11  | 2.41                     | 0.56              |
| 1:A:86:LEU:HD11   | 2:C:832:ASP:HB3   | 1.88                     | 0.56              |
| 2:C:152:VAL:O     | 2:C:519:LEU:HD12  | 2.06                     | 0.56              |
| 2:C:1053:LYS:HA   | 2:C:1056:ARG:HG2  | 1.88                     | 0.56              |
| 2:C:1256:LYS:HD2  | 3:D:467:GLN:HE22  | 1.71                     | 0.56              |
| 3:D:438:ALA:CB    | 3:D:482:ALA:HB1   | 2.35                     | 0.56              |
| 3:D:895:TYR:HD2   | 3:D:905:VAL:HG21  | 1.70                     | 0.56              |
| 3:D:351:TYR:CZ    | 3:D:474:LEU:HD21  | 2.40                     | 0.56              |
| 3:D:512:LEU:HD22  | 3:D:601:ILE:HD12  | 1.88                     | 0.56              |
| 3:D:616:ALA:HA    | 3:D:619:ILE:HG22  | 1.87                     | 0.56              |
| 3:D:768:TYR:O     | 3:D:772:THR:HG22  | 2.06                     | 0.56              |
| 4:E:7:GLU:HA      | 4:E:10:VAL:HG12   | 1.86                     | 0.56              |
| 6:H:14:DC:H2'     | 6:H:15:DG:C8      | 2.41                     | 0.56              |
| 2:C:456:LEU:HD21  | 2:C:565:ARG:HB2   | 1.87                     | 0.56              |
| 2:C:673:ALA:HA    | 2:C:1200:VAL:HG21 | 1.87                     | 0.56              |
| 2:C:677:PHE:HZ    | 2:C:1209:ILE:HD11 | 1.70                     | 0.56              |
| 2:C:751:ARG:HD2   | 2:C:752:SER:OG    | 2.06                     | 0.56              |
| 2:C:808:VAL:HG23  | 2:C:1116:LEU:HG   | 1.86                     | 0.56              |
| 2:C:1131:PHE:CZ   | 3:D:760:LYS:HG3   | 2.39                     | 0.56              |
| 3:D:392:LEU:HD21  | 3:D:409:GLN:OE1   | 2.06                     | 0.56              |
| 3:D:1135:LEU:HD12 | 3:D:1229:LEU:HD23 | 1.87                     | 0.56              |
| 3:D:1217:LEU:HB2  | 3:D:1225:LEU:CD1  | 2.34                     | 0.56              |
| 3:D:1261:GLU:HG3  | 3:D:1301:VAL:HB   | 1.88                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:65:ASP:HB2    | 2:C:70:ALA:H      | 1.71                     | 0.56              |
| 2:C:134:PRO:HD3   | 2:C:510:VAL:HG21  | 1.88                     | 0.56              |
| 2:C:180:ALA:HB3   | 2:C:440:LEU:HD22  | 1.87                     | 0.56              |
| 2:C:479:MET:CE    | 2:C:506:ALA:HB2   | 2.34                     | 0.56              |
| 3:D:407:GLN:O     | 3:D:410:VAL:HG12  | 2.06                     | 0.56              |
| 3:D:480:LEU:HD13  | 4:E:46:PRO:HB3    | 1.88                     | 0.56              |
| 2:C:10:ARG:HD3    | 2:C:704:ALA:HB3   | 1.88                     | 0.56              |
| 2:C:11:ILE:HG12   | 2:C:1186:LEU:HD11 | 1.87                     | 0.56              |
| 7:I:-19:DG:H2'    | 7:I:-18:DT:C6     | 2.41                     | 0.56              |
| 1:A:57:ALA:HB3    | 1:A:93:VAL:O      | 2.05                     | 0.55              |
| 2:C:702:SER:O     | 2:C:796:GLU:HB2   | 2.06                     | 0.55              |
| 2:C:1105:PHE:N    | 2:C:1227:PHE:O    | 2.39                     | 0.55              |
| 2:C:1348:GLY:O    | 3:D:26:ALA:N      | 2.38                     | 0.55              |
| 3:D:552:ALA:HB3   | 3:D:575:MET:SD    | 2.46                     | 0.55              |
| 4:E:30:ILE:CD1    | 4:E:35:ALA:HB2    | 2.35                     | 0.55              |
| 2:C:137:THR:HG22  | 2:C:138:ASP:OD1   | 2.06                     | 0.55              |
| 2:C:699:LEU:HD11  | 2:C:1248:LYS:CB   | 2.36                     | 0.55              |
| 2:C:1351:VAL:HG22 | 3:D:23:ILE:CG2    | 2.35                     | 0.55              |
| 3:D:554:HIS:HB3   | 3:D:568:ILE:CD1   | 2.36                     | 0.55              |
| 3:D:881:VAL:O     | 3:D:1254:ARG:HD2  | 2.06                     | 0.55              |
| 1:B:103:MET:CE    | 1:B:126:ILE:HD11  | 2.35                     | 0.55              |
| 1:B:175:LEU:HD23  | 3:D:534:GLU:OE2   | 2.07                     | 0.55              |
| 2:C:147:THR:HB    | 2:C:766:ASN:OD1   | 2.07                     | 0.55              |
| 2:C:893:VAL:HG13  | 2:C:919:VAL:HG21  | 1.88                     | 0.55              |
| 3:D:135:ASP:HB3   | 3:D:160:LEU:CD1   | 2.36                     | 0.55              |
| 3:D:366:HIS:HB2   | 3:D:487:MET:CE    | 2.36                     | 0.55              |
| 3:D:425:LEU:HB3   | 3:D:468:MET:CE    | 2.36                     | 0.55              |
| 3:D:539:MET:HE1   | 3:D:546:LEU:HD13  | 1.88                     | 0.55              |
| 3:D:555:THR:HG22  | 3:D:565:ARG:HG2   | 1.87                     | 0.55              |
| 3:D:1356:GLY:HA2  | 4:E:17:PHE:CZ     | 2.41                     | 0.55              |
| 2:C:126:GLN:CG    | 2:C:497:PRO:HB3   | 2.37                     | 0.55              |
| 3:D:746:PRO:HD3   | 3:D:773:HIS:CE1   | 2.42                     | 0.55              |
| 3:D:1262:ILE:HB   | 3:D:1270:LEU:O    | 2.07                     | 0.55              |
| 5:F:441:PHE:CE1   | 5:F:445:ILE:HD11  | 2.41                     | 0.55              |
| 1:A:55:GLN:HG3    | 1:B:5:ASN:HA      | 1.88                     | 0.55              |
| 1:A:118:ILE:HD13  | 1:A:146:PHE:HE2   | 1.72                     | 0.55              |
| 1:B:64:ILE:H      | 1:B:64:ILE:HD12   | 1.71                     | 0.55              |
| 2:C:526:THR:OG1   | 2:C:767:GLN:HG3   | 2.07                     | 0.55              |
| 2:C:536:ARG:HD3   | 2:C:670:VAL:HG21  | 1.89                     | 0.55              |
| 2:C:708:GLY:HA2   | 2:C:1087:ARG:CZ   | 2.37                     | 0.55              |
| 3:D:311:ASN:HB2   | 3:D:328:SER:OG    | 2.07                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:F:420:VAL:O     | 5:F:424:LEU:HG    | 2.06                     | 0.55              |
| 2:C:86:VAL:HG23   | 2:C:143:ILE:CD1   | 2.37                     | 0.55              |
| 2:C:573:GLU:HG2   | 2:C:688:MET:SD    | 2.46                     | 0.55              |
| 2:C:942:ARG:O     | 2:C:946:ASP:HB3   | 2.07                     | 0.55              |
| 2:C:1306:THR:HG22 | 2:C:1331:ALA:CB   | 2.37                     | 0.55              |
| 3:D:563:LEU:HD12  | 3:D:564:LEU:H     | 1.70                     | 0.55              |
| 3:D:736:LEU:O     | 3:D:758:ASN:HB2   | 2.05                     | 0.55              |
| 3:D:915:ALA:HB1   | 3:D:1248:HIS:O    | 2.06                     | 0.55              |
| 5:F:420:VAL:HG13  | 5:F:452:LEU:HD22  | 1.88                     | 0.55              |
| 1:A:78:ARG:N      | 1:A:135:THR:O     | 2.26                     | 0.55              |
| 1:B:185:ARG:HE    | 1:B:201:ILE:HD11  | 1.72                     | 0.55              |
| 2:C:483:ILE:HD11  | 2:C:501:ILE:HG13  | 1.87                     | 0.55              |
| 2:C:1240:THR:H    | 3:D:638:SER:HB3   | 1.72                     | 0.55              |
| 2:C:1283:ARG:HB2  | 3:D:348:ARG:CD    | 2.32                     | 0.55              |
| 1:A:49:VAL:HG23   | 1:B:38:PHE:CE1    | 2.42                     | 0.55              |
| 1:B:151:GLY:HA3   | 1:B:176:TYR:CD2   | 2.42                     | 0.55              |
| 1:B:156:PRO:HA    | 1:B:173:ASP:HB2   | 1.87                     | 0.55              |
| 2:C:471:GLN:OE1   | 2:C:513:PHE:HB2   | 2.07                     | 0.55              |
| 2:C:651:LEU:HD11  | 3:D:754:PRO:CD    | 2.36                     | 0.55              |
| 2:C:716:ALA:HB2   | 2:C:800:LEU:HB2   | 1.89                     | 0.55              |
| 2:C:838:HIS:CE1   | 2:C:1252:LEU:HD11 | 2.42                     | 0.55              |
| 2:C:1138:ALA:HB2  | 2:C:1213:LEU:CD2  | 2.35                     | 0.55              |
| 3:D:188:GLN:HB2   | 3:D:240:VAL:HG11  | 1.87                     | 0.55              |
| 3:D:485:LEU:HD21  | 4:E:17:PHE:HE1    | 1.71                     | 0.55              |
| 3:D:614:GLN:HB3   | 4:E:7:GLU:CB      | 2.36                     | 0.55              |
| 3:D:926:LEU:HA    | 3:D:1240:GLN:CG   | 2.34                     | 0.55              |
| 3:D:1132:VAL:HG23 | 3:D:1236:VAL:HG11 | 1.89                     | 0.55              |
| 1:A:309:ALA:HA    | 1:A:313:LEU:O     | 2.06                     | 0.55              |
| 1:B:114:THR:HB    | 1:B:129:PRO:O     | 2.07                     | 0.55              |
| 2:C:825:SER:HB3   | 2:C:1113:ASP:HA   | 1.89                     | 0.55              |
| 2:C:894:THR:O     | 2:C:919:VAL:HG23  | 2.07                     | 0.55              |
| 3:D:330:ALA:O     | 3:D:334:LYS:HG3   | 2.07                     | 0.55              |
| 1:B:27:ALA:CB     | 1:B:212:PRO:HB2   | 2.37                     | 0.55              |
| 2:C:159:PRO:O     | 2:C:409:GLY:HA2   | 2.07                     | 0.55              |
| 2:C:354:TYR:O     | 2:C:358:THR:HG23  | 2.07                     | 0.55              |
| 2:C:629:ILE:HG21  | 2:C:641:VAL:HG23  | 1.89                     | 0.55              |
| 2:C:1119:LEU:HD13 | 3:D:506:GLN:CB    | 2.36                     | 0.55              |
| 2:C:1282:GLN:CD   | 3:D:354:ARG:HB2   | 2.28                     | 0.55              |
| 2:C:1287:MET:HE3  | 3:D:793:THR:HG21  | 1.89                     | 0.55              |
| 2:C:1350:ASN:N    | 3:D:24:SER:O      | 2.40                     | 0.55              |
| 3:D:589:HIS:O     | 3:D:593:GLU:HG2   | 2.08                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:698:MET:HG3   | 3:D:730:GLN:HE22  | 1.71                     | 0.55              |
| 2:C:162:PHE:N     | 2:C:181:ARG:O     | 2.39                     | 0.54              |
| 2:C:607:PRO:CD    | 2:C:635:GLU:HA    | 2.37                     | 0.54              |
| 3:D:39:ILE:CD1    | 3:D:246:VAL:HG11  | 2.36                     | 0.54              |
| 3:D:576:LYS:O     | 3:D:580:LEU:HD13  | 2.06                     | 0.54              |
| 5:F:601:MET:HB2   | 5:F:616:VAL:HG23  | 1.89                     | 0.54              |
| 2:C:652:LEU:HD23  | 2:C:652:LEU:H     | 1.72                     | 0.54              |
| 2:C:693:GLN:NE2   | 2:C:1087:ARG:O    | 2.40                     | 0.54              |
| 2:C:701:GLN:O     | 2:C:804:ARG:HD3   | 2.08                     | 0.54              |
| 2:C:890:VAL:CG2   | 2:C:924:LEU:HB3   | 2.38                     | 0.54              |
| 2:C:970:PHE:HE1   | 2:C:1040:ARG:HD3  | 1.71                     | 0.54              |
| 2:C:1196:ILE:HD11 | 2:C:1212:HIS:CE1  | 2.41                     | 0.54              |
| 3:D:366:HIS:HB3   | 3:D:489:THR:CG2   | 2.37                     | 0.54              |
| 3:D:437:GLN:HG2   | 3:D:491:ASN:HD22  | 1.71                     | 0.54              |
| 2:C:443:LEU:HA    | 2:C:446:GLY:O     | 2.07                     | 0.54              |
| 2:C:732:GLU:HB3   | 2:C:740:VAL:HG23  | 1.89                     | 0.54              |
| 2:C:892:LYS:HE3   | 2:C:922:THR:CG2   | 2.38                     | 0.54              |
| 2:C:1344:MET:HB3  | 2:C:1351:VAL:HG21 | 1.90                     | 0.54              |
| 3:D:181:GLU:HG3   | 3:D:186:ALA:CB    | 2.38                     | 0.54              |
| 5:F:424:LEU:O     | 5:F:428:ILE:HG13  | 2.06                     | 0.54              |
| 1:B:105:LEU:HD23  | 1:B:144:MET:SD    | 2.47                     | 0.54              |
| 2:C:184:PRO:HD2   | 2:C:189:TRP:CD1   | 2.43                     | 0.54              |
| 2:C:1341:VAL:HG23 | 2:C:1351:VAL:CG1  | 2.38                     | 0.54              |
| 3:D:38:GLU:OE1    | 3:D:107:GLU:HB2   | 2.08                     | 0.54              |
| 5:F:119:TYR:O     | 5:F:123:MET:HG2   | 2.08                     | 0.54              |
| 5:F:122:GLU:O     | 5:F:126:VAL:HB    | 2.06                     | 0.54              |
| 5:F:156:ALA:HB2   | 5:F:401:ILE:HD12  | 1.89                     | 0.54              |
| 5:F:450:ILE:HA    | 5:F:453:MET:CE    | 2.38                     | 0.54              |
| 1:A:18:GLU:HG3    | 1:A:28:ARG:HG3    | 1.89                     | 0.54              |
| 2:C:644:ARG:HB3   | 2:C:649:PRO:HA    | 1.88                     | 0.54              |
| 3:D:114:HIS:CD2   | 3:D:116:TRP:HB2   | 2.42                     | 0.54              |
| 3:D:745:LYS:HB3   | 3:D:746:PRO:HD2   | 1.90                     | 0.54              |
| 3:D:880:SER:O     | 3:D:894:CYS:HB3   | 2.08                     | 0.54              |
| 1:A:157:ALA:N     | 1:A:173:ASP:HB3   | 2.22                     | 0.54              |
| 2:C:533:THR:HG21  | 2:C:694:ARG:CB    | 2.37                     | 0.54              |
| 2:C:709:THR:HG23  | 2:C:1198:THR:O    | 2.07                     | 0.54              |
| 2:C:804:ARG:HB2   | 2:C:834:PHE:CE1   | 2.42                     | 0.54              |
| 2:C:893:VAL:HG12  | 2:C:919:VAL:HG21  | 1.89                     | 0.54              |
| 3:D:456:CYS:HB2   | 3:D:461:ALA:O     | 2.08                     | 0.54              |
| 3:D:1237:TYR:HB3  | 3:D:1242:VAL:O    | 2.06                     | 0.54              |
| 7:I:35:DA:H2'     | 7:I:36:DG:C8      | 2.42                     | 0.54              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 8:G:145:GLU:O     | 8:G:149:VAL:HG13 | 2.07                     | 0.54              |
| 2:C:526:THR:O     | 2:C:698:PRO:HD3  | 2.08                     | 0.54              |
| 2:C:733:GLN:HG2   | 2:C:740:VAL:CG2  | 2.38                     | 0.54              |
| 2:C:1149:LEU:HD11 | 2:C:1158:GLN:OE1 | 2.08                     | 0.54              |
| 3:D:853:VAL:HG13  | 3:D:854:VAL:HG23 | 1.89                     | 0.54              |
| 5:F:502:LYS:HD2   | 5:F:527:LEU:HD13 | 1.89                     | 0.54              |
| 1:A:61:ALA:HB3    | 1:A:147:THR:CB   | 2.35                     | 0.54              |
| 2:C:70:ALA:HB1    | 2:C:492:ILE:HG21 | 1.90                     | 0.54              |
| 3:D:1135:LEU:HD12 | 3:D:1229:LEU:CD2 | 2.38                     | 0.54              |
| 7:I:17:DG:H2''    | 7:I:18:DA:C8     | 2.43                     | 0.54              |
| 2:C:639:ASP:HA    | 2:C:654:LYS:HB2  | 1.90                     | 0.54              |
| 2:C:859:ASP:OD2   | 2:C:868:LEU:HD13 | 2.07                     | 0.54              |
| 3:D:56:GLY:H      | 3:D:59:CYS:HG    | 1.54                     | 0.54              |
| 3:D:257:LEU:HD11  | 5:F:559:LEU:HD21 | 1.89                     | 0.54              |
| 3:D:512:LEU:HB3   | 3:D:596:LEU:HG   | 1.90                     | 0.54              |
| 3:D:701:LEU:CD2   | 3:D:719:TYR:HB2  | 2.37                     | 0.54              |
| 3:D:1252:ILE:O    | 3:D:1256:MET:HG3 | 2.08                     | 0.54              |
| 1:A:108:THR:HA    | 1:A:136:LEU:CD1  | 2.39                     | 0.53              |
| 1:B:199:LYS:O     | 1:B:201:ILE:HG23 | 2.08                     | 0.53              |
| 2:C:79:PHE:CE2    | 2:C:135:LEU:HD12 | 2.44                     | 0.53              |
| 2:C:712:GLU:HA    | 2:C:715:VAL:HG12 | 1.89                     | 0.53              |
| 2:C:860:ILE:HD11  | 2:C:919:VAL:HG13 | 1.90                     | 0.53              |
| 2:C:890:VAL:HG22  | 2:C:924:LEU:HB3  | 1.88                     | 0.53              |
| 2:C:1351:VAL:CG1  | 3:D:21:ILE:HD11  | 2.38                     | 0.53              |
| 3:D:297:GLU:HA    | 5:F:446:GLN:OE1  | 2.07                     | 0.53              |
| 3:D:400:LYS:O     | 3:D:404:GLU:HB2  | 2.08                     | 0.53              |
| 3:D:1155:GLU:O    | 3:D:1164:ARG:NH2 | 2.41                     | 0.53              |
| 3:D:1260:VAL:HG21 | 3:D:1279:PRO:HG2 | 1.89                     | 0.53              |
| 5:F:580:LEU:HD13  | 5:F:650:PHE:CE1  | 2.43                     | 0.53              |
| 7:I:7:DA:H2'      | 7:I:7:DA:N3      | 2.22                     | 0.53              |
| 2:C:626:GLN:HA    | 2:C:661:ASP:OD2  | 2.08                     | 0.53              |
| 2:C:748:ASP:HB3   | 2:C:749:PRO:HD2  | 1.89                     | 0.53              |
| 2:C:1322:ILE:CG2  | 3:D:381:PRO:HB2  | 2.38                     | 0.53              |
| 3:D:158:HIS:HE1   | 3:D:190:LEU:HD11 | 1.72                     | 0.53              |
| 3:D:196:LEU:CD2   | 3:D:236:PRO:HG3  | 2.37                     | 0.53              |
| 5:F:570:LEU:HG    | 5:F:571:PRO:HD2  | 1.90                     | 0.53              |
| 6:H:-11:DA:H2''   | 6:H:-10:DA:OP1   | 2.08                     | 0.53              |
| 7:I:37:DG:H2''    | 7:I:38:DG:H5'    | 1.90                     | 0.53              |
| 2:C:150:VAL:HG21  | 2:C:535:LYS:CG   | 2.34                     | 0.53              |
| 2:C:396:LEU:O     | 2:C:403:TYR:HB2  | 2.08                     | 0.53              |
| 2:C:500:LEU:HD23  | 2:C:500:LEU:H    | 1.73                     | 0.53              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:523:MET:O    | 2:C:767:GLN:NE2   | 2.41                     | 0.53              |
| 2:C:532:ILE:HD12 | 2:C:715:VAL:HG23  | 1.90                     | 0.53              |
| 3:D:357:ILE:HD13 | 3:D:468:MET:HG3   | 1.90                     | 0.53              |
| 3:D:365:LEU:HD23 | 3:D:618:VAL:CG2   | 2.36                     | 0.53              |
| 3:D:550:ILE:HG22 | 3:D:572:PRO:CG    | 2.37                     | 0.53              |
| 3:D:840:THR:CG2  | 3:D:860:ILE:HD11  | 2.34                     | 0.53              |
| 3:D:859:TYR:CZ   | 3:D:897:ARG:HB2   | 2.44                     | 0.53              |
| 3:D:899:LEU:HD21 | 3:D:1247:LYS:HD2  | 1.89                     | 0.53              |
| 5:F:430:ILE:CD1  | 5:F:472:THR:HA    | 2.38                     | 0.53              |
| 6:H:8:DC:C3'     | 6:H:9:DT:H71      | 2.37                     | 0.53              |
| 2:C:15:PHE:CE2   | 2:C:1196:ILE:HD13 | 2.44                     | 0.53              |
| 2:C:61:PHE:CD2   | 2:C:74:TYR:HB2    | 2.43                     | 0.53              |
| 2:C:180:ALA:HB3  | 2:C:192:PHE:HB2   | 1.89                     | 0.53              |
| 2:C:184:PRO:HB3  | 2:C:403:TYR:CZ    | 2.44                     | 0.53              |
| 2:C:203:ARG:CG   | 2:C:206:ARG:HA    | 2.39                     | 0.53              |
| 2:C:541:LEU:HA   | 2:C:546:LEU:O     | 2.08                     | 0.53              |
| 2:C:856:ILE:CG2  | 2:C:950:ARG:HD2   | 2.38                     | 0.53              |
| 2:C:857:THR:HG22 | 2:C:893:VAL:CG2   | 2.38                     | 0.53              |
| 2:C:909:ARG:HG3  | 2:C:914:GLU:O     | 2.08                     | 0.53              |
| 2:C:977:ILE:HD13 | 2:C:1036:PHE:HB3  | 1.90                     | 0.53              |
| 3:D:246:VAL:HA   | 3:D:271:TYR:CE1   | 2.44                     | 0.53              |
| 3:D:359:VAL:CG1  | 3:D:453:PRO:HG3   | 2.38                     | 0.53              |
| 6:H:-27:DC:H1'   | 6:H:-26:DG:H5'    | 1.89                     | 0.53              |
| 2:C:166:ASP:O    | 2:C:176:LEU:HD22  | 2.08                     | 0.53              |
| 2:C:556:ARG:HG2  | 2:C:577:ILE:O     | 2.08                     | 0.53              |
| 2:C:632:ALA:N    | 2:C:635:GLU:O     | 2.39                     | 0.53              |
| 2:C:822:ILE:HD13 | 2:C:1246:MET:CE   | 2.37                     | 0.53              |
| 2:C:1282:GLN:HG2 | 3:D:352:SER:OG    | 2.08                     | 0.53              |
| 3:D:387:LEU:CD2  | 3:D:413:ILE:HG13  | 2.38                     | 0.53              |
| 3:D:581:LEU:CD2  | 3:D:604:LEU:HD11  | 2.39                     | 0.53              |
| 7:I:21:DT:C2'    | 7:I:22:DT:H71     | 2.38                     | 0.53              |
| 1:A:5:ASN:HA     | 1:B:222:ILE:CD1   | 2.39                     | 0.53              |
| 1:B:54:LEU:O     | 1:B:152:LYS:HA    | 2.07                     | 0.53              |
| 2:C:9:LYS:HB2    | 2:C:1189:ASN:ND2  | 2.23                     | 0.53              |
| 2:C:551:ALA:HB1  | 2:C:579:LEU:HD11  | 1.90                     | 0.53              |
| 2:C:600:ARG:N    | 2:C:660:MET:O     | 2.42                     | 0.53              |
| 2:C:776:LEU:HD13 | 2:C:797:LEU:HA    | 1.89                     | 0.53              |
| 3:D:63:PHE:O     | 3:D:99:ARG:HA     | 2.09                     | 0.53              |
| 3:D:104:GLY:HA3  | 3:D:246:VAL:HG22  | 1.91                     | 0.53              |
| 3:D:702:GLN:HG2  | 3:D:719:TYR:CZ    | 2.44                     | 0.53              |
| 5:F:626:ARG:O    | 5:F:630:ILE:HG23  | 2.09                     | 0.53              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:I:40:DC:H2'    | 7:I:41:DT:H71     | 1.90                     | 0.53              |
| 1:A:108:THR:HA   | 1:A:136:LEU:HD12  | 1.89                     | 0.53              |
| 1:B:38:PHE:HA    | 1:B:41:THR:HG22   | 1.91                     | 0.53              |
| 2:C:5:PHE:HE2    | 2:C:777:VAL:HG12  | 1.73                     | 0.53              |
| 2:C:759:MET:HG2  | 2:C:773:GLN:HB2   | 1.91                     | 0.53              |
| 3:D:92:GLU:OE1   | 3:D:94:THR:OG1    | 2.27                     | 0.53              |
| 3:D:693:VAL:HG11 | 3:D:739:MET:HE2   | 1.91                     | 0.53              |
| 3:D:796:LEU:HA   | 3:D:799:VAL:HG12  | 1.91                     | 0.53              |
| 6:H:-31:DC:H2''  | 6:H:-30:DA:C5'    | 2.38                     | 0.53              |
| 1:A:67:VAL:HG23  | 1:A:72:SER:HB3    | 1.90                     | 0.53              |
| 2:C:161:VAL:HG13 | 2:C:413:MET:HG2   | 1.91                     | 0.53              |
| 2:C:519:LEU:CD2  | 2:C:543:PRO:HD2   | 2.39                     | 0.53              |
| 2:C:859:ASP:HB2  | 2:C:868:LEU:HD13  | 1.89                     | 0.53              |
| 2:C:942:ARG:N    | 2:C:1065:MET:O    | 2.41                     | 0.53              |
| 2:C:1274:GLY:HA3 | 3:D:348:ARG:CZ    | 2.39                     | 0.53              |
| 3:D:145:TYR:CZ   | 3:D:182:ILE:HG21  | 2.44                     | 0.53              |
| 3:D:419:ARG:HB3  | 4:E:44:LYS:HZ3    | 1.73                     | 0.53              |
| 3:D:555:THR:CG2  | 3:D:565:ARG:HG2   | 2.38                     | 0.53              |
| 3:D:804:ILE:CD1  | 3:D:910:ALA:HA    | 2.39                     | 0.53              |
| 5:F:134:GLU:OE2  | 5:F:467:PHE:N     | 2.29                     | 0.53              |
| 5:F:426:LEU:HD13 | 5:F:471:ALA:CB    | 2.38                     | 0.53              |
| 5:F:430:ILE:HD13 | 5:F:472:THR:HA    | 1.90                     | 0.53              |
| 5:F:592:THR:HB   | 5:F:595:GLU:CB    | 2.39                     | 0.53              |
| 1:A:12:PRO:HD3   | 1:A:33:PRO:HG2    | 1.90                     | 0.53              |
| 1:B:154:TYR:CE2  | 3:D:543:VAL:HG11  | 2.44                     | 0.53              |
| 2:C:546:LEU:HD13 | 2:C:551:ALA:HA    | 1.89                     | 0.53              |
| 2:C:972:ILE:O    | 2:C:976:ASN:ND2   | 2.42                     | 0.53              |
| 2:C:1299:TYR:CZ  | 3:D:1361:LEU:HD22 | 2.44                     | 0.53              |
| 2:C:1303:GLU:HA  | 2:C:1307:VAL:HG12 | 1.90                     | 0.53              |
| 3:D:112:VAL:HG21 | 3:D:305:VAL:CB    | 2.38                     | 0.53              |
| 3:D:859:TYR:CE1  | 3:D:897:ARG:HB2   | 2.43                     | 0.53              |
| 1:B:199:LYS:HG2  | 1:B:201:ILE:CG2   | 2.39                     | 0.53              |
| 2:C:525:GLN:HG3  | 2:C:531:GLU:HG2   | 1.91                     | 0.53              |
| 2:C:700:VAL:HG22 | 2:C:835:THR:O     | 2.08                     | 0.53              |
| 2:C:705:PRO:HB3  | 2:C:1245:TYR:CD1  | 2.43                     | 0.53              |
| 2:C:1122:PRO:HG2 | 3:D:721:MET:SD    | 2.49                     | 0.53              |
| 2:C:1315:ARG:HG2 | 5:F:571:PRO:HG3   | 1.91                     | 0.53              |
| 3:D:112:VAL:CG2  | 3:D:302:GLN:HA    | 2.37                     | 0.53              |
| 3:D:292:ILE:HD12 | 5:F:123:MET:CE    | 2.36                     | 0.53              |
| 3:D:493:LEU:HB2  | 3:D:900:ALA:O     | 2.09                     | 0.53              |
| 5:F:551:ILE:HD11 | 5:F:559:LEU:HB2   | 1.89                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:104:THR:HA    | 1:B:145:GLU:HA    | 1.90                     | 0.52              |
| 2:C:884:GLN:HB3   | 2:C:885:PRO:HD2   | 1.91                     | 0.52              |
| 2:C:1159:LYS:O    | 2:C:1163:VAL:HG23 | 2.09                     | 0.52              |
| 3:D:44:THR:HB     | 3:D:58:PHE:CD1    | 2.44                     | 0.52              |
| 3:D:354:ARG:NE    | 3:D:467:GLN:OE1   | 2.33                     | 0.52              |
| 3:D:492:ILE:HG23  | 3:D:502:ILE:CG2   | 2.39                     | 0.52              |
| 3:D:837:GLY:CA    | 3:D:897:ARG:HB3   | 2.39                     | 0.52              |
| 3:D:1192:ILE:HG22 | 3:D:1194:VAL:H    | 1.74                     | 0.52              |
| 4:E:4:VAL:HG12    | 4:E:47:VAL:HG23   | 1.91                     | 0.52              |
| 4:E:27:ALA:HB1    | 4:E:45:ASN:HB3    | 1.90                     | 0.52              |
| 5:F:453:MET:O     | 5:F:456:VAL:HG12  | 2.09                     | 0.52              |
| 2:C:1127:VAL:HB   | 3:D:736:LEU:HD11  | 1.91                     | 0.52              |
| 2:C:1213:LEU:HD13 | 2:C:1222:GLY:HA2  | 1.91                     | 0.52              |
| 3:D:490:ASN:OD1   | 3:D:614:GLN:NE2   | 2.29                     | 0.52              |
| 3:D:792:LEU:O     | 3:D:796:LEU:HG    | 2.09                     | 0.52              |
| 3:D:839:PHE:HB2   | 3:D:893:ALA:O     | 2.10                     | 0.52              |
| 3:D:896:GLY:O     | 3:D:905:VAL:HG12  | 2.09                     | 0.52              |
| 2:C:225:GLU:OE1   | 2:C:225:GLU:N     | 2.42                     | 0.52              |
| 2:C:564:GLY:HA2   | 2:C:666:GLN:HG2   | 1.91                     | 0.52              |
| 2:C:705:PRO:HB3   | 2:C:1245:TYR:CG   | 2.44                     | 0.52              |
| 2:C:727:ARG:HB3   | 2:C:743:ALA:O     | 2.09                     | 0.52              |
| 2:C:876:ILE:HD12  | 2:C:937:VAL:CG1   | 2.39                     | 0.52              |
| 2:C:1099:PRO:HB2  | 2:C:1101:GLU:HG2  | 1.90                     | 0.52              |
| 2:C:1268:VAL:HG13 | 3:D:251:LEU:O     | 2.08                     | 0.52              |
| 2:C:1286:GLU:HB3  | 3:D:345:LEU:HD23  | 1.91                     | 0.52              |
| 2:C:1339:VAL:HG23 | 3:D:251:LEU:HD22  | 1.89                     | 0.52              |
| 3:D:104:GLY:CA    | 3:D:246:VAL:HG22  | 2.39                     | 0.52              |
| 3:D:654:VAL:CG1   | 3:D:756:VAL:HG21  | 2.38                     | 0.52              |
| 1:B:115:ALA:HB2   | 1:B:131:HIS:CE1   | 2.43                     | 0.52              |
| 1:B:175:LEU:HD12  | 1:B:177:SER:H     | 1.73                     | 0.52              |
| 1:B:206:THR:HG21  | 1:B:210:VAL:HG13  | 1.92                     | 0.52              |
| 2:C:538:LEU:HD11  | 2:C:583:LEU:CD1   | 2.38                     | 0.52              |
| 2:C:602:VAL:HB    | 2:C:607:PRO:HA    | 1.91                     | 0.52              |
| 2:C:777:VAL:CG1   | 2:C:789:ILE:HG23  | 2.39                     | 0.52              |
| 3:D:41:LYS:HB2    | 3:D:55:ASP:O      | 2.09                     | 0.52              |
| 3:D:85:ILE:HG22   | 3:D:92:GLU:CB     | 2.34                     | 0.52              |
| 3:D:131:MET:HE1   | 3:D:158:HIS:HB3   | 1.90                     | 0.52              |
| 3:D:529:PHE:HB2   | 3:D:552:ALA:CB    | 2.40                     | 0.52              |
| 3:D:548:ALA:CA    | 3:D:572:PRO:HD2   | 2.34                     | 0.52              |
| 3:D:922:PRO:HB3   | 3:D:1242:VAL:HG11 | 1.91                     | 0.52              |
| 3:D:1294:ARG:HD2  | 3:D:1295:PRO:HD2  | 1.90                     | 0.52              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:1309:SER:HB2  | 3:D:1318:ALA:CB  | 2.39                     | 0.52              |
| 4:E:3:ARG:HD3     | 4:E:43:ASP:OD2   | 2.10                     | 0.52              |
| 1:B:48:ARG:O      | 1:B:52:SER:HB3   | 2.10                     | 0.52              |
| 2:C:104:LEU:HD11  | 2:C:128:VAL:HG12 | 1.90                     | 0.52              |
| 2:C:155:MET:HG3   | 2:C:538:LEU:HB3  | 1.90                     | 0.52              |
| 2:C:191:ASP:HB2   | 2:C:203:ARG:O    | 2.10                     | 0.52              |
| 2:C:876:ILE:HD12  | 2:C:937:VAL:HG11 | 1.92                     | 0.52              |
| 2:C:962:LEU:HA    | 2:C:965:ASP:OD2  | 2.09                     | 0.52              |
| 2:C:1257:ILE:HD12 | 3:D:447:LYS:O    | 2.10                     | 0.52              |
| 3:D:81:TYR:HB3    | 3:D:84:ILE:CG1   | 2.40                     | 0.52              |
| 3:D:919:ILE:HG21  | 3:D:1136:PHE:HE2 | 1.72                     | 0.52              |
| 3:D:1312:THR:CG2  | 3:D:1318:ALA:HB2 | 2.39                     | 0.52              |
| 3:D:1372:ASP:OD1  | 4:E:69:SER:OG    | 2.28                     | 0.52              |
| 5:F:133:GLY:O     | 5:F:137:ILE:HG12 | 2.10                     | 0.52              |
| 5:F:398:TYR:O     | 5:F:402:VAL:HG12 | 2.10                     | 0.52              |
| 2:C:405:LEU:HD21  | 2:C:409:GLY:HA3  | 1.91                     | 0.52              |
| 2:C:650:THR:HG22  | 3:D:752:GLU:OE2  | 2.10                     | 0.52              |
| 2:C:739:ILE:HG13  | 2:C:757:TYR:HB2  | 1.91                     | 0.52              |
| 2:C:1298:ALA:HB3  | 3:D:1358:GLY:N   | 2.24                     | 0.52              |
| 3:D:166:TYR:HA    | 3:D:170:GLN:HB2  | 1.92                     | 0.52              |
| 3:D:529:PHE:HB2   | 3:D:552:ALA:HB2  | 1.91                     | 0.52              |
| 3:D:557:MET:N     | 3:D:563:LEU:HD23 | 2.25                     | 0.52              |
| 3:D:643:ASP:OD2   | 3:D:717:ALA:HB3  | 2.09                     | 0.52              |
| 1:A:108:THR:HB    | 1:A:141:SER:CB   | 2.38                     | 0.52              |
| 1:B:91:LEU:CD2    | 1:B:126:ILE:HD12 | 2.36                     | 0.52              |
| 2:C:104:LEU:CB    | 2:C:126:GLN:HB2  | 2.40                     | 0.52              |
| 2:C:761:LYS:HE2   | 2:C:761:LYS:HA   | 1.91                     | 0.52              |
| 2:C:988:LYS:HD3   | 2:C:1025:ALA:CB  | 2.40                     | 0.52              |
| 2:C:1343:GLU:HG2  | 3:D:247:ILE:CD1  | 2.40                     | 0.52              |
| 3:D:113:ALA:HB3   | 3:D:302:GLN:NE2  | 2.25                     | 0.52              |
| 1:A:12:PRO:HG3    | 1:A:33:PRO:HD2   | 1.92                     | 0.52              |
| 2:C:467:LEU:HD21  | 2:C:519:LEU:HG   | 1.92                     | 0.52              |
| 2:C:777:VAL:HG11  | 2:C:789:ILE:HG23 | 1.91                     | 0.52              |
| 2:C:1155:GLN:HE21 | 2:C:1184:VAL:HB  | 1.75                     | 0.52              |
| 2:C:1294:ALA:HB1  | 3:D:914:ILE:HG13 | 1.92                     | 0.52              |
| 3:D:605:ILE:HA    | 3:D:608:VAL:HG12 | 1.92                     | 0.52              |
| 3:D:637:ILE:HD12  | 3:D:720:MET:CE   | 2.40                     | 0.52              |
| 3:D:838:ARG:HD3   | 3:D:878:VAL:HG11 | 1.92                     | 0.52              |
| 5:F:131:ARG:N     | 8:G:150:ALA:O    | 2.43                     | 0.52              |
| 5:F:580:LEU:HA    | 5:F:583:THR:CG2  | 2.39                     | 0.52              |
| 2:C:134:PRO:HG2   | 2:C:514:PHE:CE1  | 2.45                     | 0.52              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:149:ARG:HA   | 2:C:523:MET:HB2   | 1.91                     | 0.52              |
| 2:C:614:MET:HG3  | 2:C:659:LEU:CD1   | 2.39                     | 0.52              |
| 2:C:649:PRO:HG3  | 3:D:770:ASN:HD21  | 1.75                     | 0.52              |
| 2:C:810:PHE:HZ   | 2:C:1244:ILE:HD12 | 1.73                     | 0.52              |
| 2:C:813:TRP:CH2  | 2:C:1230:LEU:HD13 | 2.45                     | 0.52              |
| 3:D:105:HIS:HB2  | 3:D:243:VAL:CG2   | 2.40                     | 0.52              |
| 3:D:658:ARG:O    | 3:D:662:GLU:HG2   | 2.10                     | 0.52              |
| 3:D:1259:LYS:HE2 | 3:D:1311:GLN:HB2  | 1.90                     | 0.52              |
| 2:C:844:VAL:HG12 | 2:C:1068:VAL:O    | 2.09                     | 0.52              |
| 3:D:1234:GLN:HB3 | 3:D:1238:ARG:CZ   | 2.40                     | 0.52              |
| 5:F:506:THR:O    | 5:F:510:MET:HG3   | 2.10                     | 0.52              |
| 6:H:-16:DG:H2'   | 6:H:-15:DT:H6     | 1.75                     | 0.52              |
| 7:I:15:DA:H2''   | 7:I:16:DC:C6      | 2.45                     | 0.52              |
| 1:A:103:MET:O    | 1:A:146:PHE:N     | 2.26                     | 0.51              |
| 1:B:82:VAL:HG23  | 3:D:528:ILE:CD1   | 2.40                     | 0.51              |
| 1:B:178:PRO:HB2  | 1:B:210:VAL:CG1   | 2.38                     | 0.51              |
| 2:C:216:LEU:HG   | 2:C:226:ILE:CD1   | 2.39                     | 0.51              |
| 2:C:698:PRO:HG2  | 2:C:770:CYS:SG    | 2.50                     | 0.51              |
| 3:D:351:TYR:CD2  | 3:D:474:LEU:HD11  | 2.45                     | 0.51              |
| 3:D:786:THR:HG1  | 7:I:-1:DT:H3      | 1.58                     | 0.51              |
| 3:D:808:GLU:HG3  | 3:D:809:ASP:OD1   | 2.10                     | 0.51              |
| 3:D:1158:LYS:HB2 | 3:D:1161:LYS:CD   | 2.40                     | 0.51              |
| 5:F:426:LEU:CD1  | 5:F:471:ALA:CB    | 2.88                     | 0.51              |
| 5:F:432:LYS:HA   | 5:F:441:PHE:HE2   | 1.75                     | 0.51              |
| 1:A:50:LEU:HD12  | 1:A:54:LEU:CG     | 2.40                     | 0.51              |
| 1:A:89:LYS:HZ2   | 2:C:832:ASP:HB2   | 1.76                     | 0.51              |
| 1:A:183:ALA:CB   | 1:A:204:GLU:HB2   | 2.37                     | 0.51              |
| 2:C:567:CYS:SG   | 2:C:570:GLU:HB3   | 2.50                     | 0.51              |
| 2:C:673:ALA:CB   | 2:C:711:MET:HG2   | 2.39                     | 0.51              |
| 2:C:931:ALA:HB1  | 2:C:1072:VAL:CG2  | 2.40                     | 0.51              |
| 2:C:1287:MET:HA  | 2:C:1290:TRP:CE3  | 2.45                     | 0.51              |
| 3:D:527:LYS:HB3  | 3:D:550:ILE:CD1   | 2.28                     | 0.51              |
| 3:D:558:THR:CG2  | 3:D:559:PRO:HD3   | 2.37                     | 0.51              |
| 3:D:598:LYS:HA   | 3:D:601:ILE:HG22  | 1.91                     | 0.51              |
| 3:D:837:GLY:O    | 3:D:897:ARG:N     | 2.38                     | 0.51              |
| 5:F:600:ARG:O    | 5:F:604:GLY:N     | 2.42                     | 0.51              |
| 6:H:-22:DA:H2''  | 6:H:-21:DA:C8     | 2.45                     | 0.51              |
| 6:H:-2:DT:H1'    | 6:H:-1:DT:N3      | 2.24                     | 0.51              |
| 8:G:106:GLY:HA3  | 8:G:132:PHE:O     | 2.10                     | 0.51              |
| 8:G:108:ALA:O    | 8:G:131:THR:HB    | 2.11                     | 0.51              |
| 1:A:29:ILE:N     | 1:A:203:LEU:O     | 2.43                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:50:LEU:HD11  | 1:A:54:LEU:HD11   | 1.92                     | 0.51              |
| 1:A:232:ILE:HG22 | 1:B:217:ALA:O     | 2.10                     | 0.51              |
| 2:C:207:ARG:NH1  | 2:C:378:MET:HA    | 2.26                     | 0.51              |
| 2:C:412:LYS:NZ   | 2:C:458:ASN:O     | 2.44                     | 0.51              |
| 2:C:699:LEU:CD2  | 2:C:834:PHE:HA    | 2.40                     | 0.51              |
| 2:C:1105:PHE:O   | 2:C:1227:PHE:N    | 2.44                     | 0.51              |
| 2:C:1163:VAL:HA  | 2:C:1166:LEU:CD2  | 2.41                     | 0.51              |
| 2:C:1303:GLU:HB3 | 2:C:1329:PHE:CZ   | 2.45                     | 0.51              |
| 2:C:1322:ILE:O   | 3:D:385:ALA:HB2   | 2.10                     | 0.51              |
| 3:D:423:VAL:CG2  | 3:D:441:PRO:HG3   | 2.39                     | 0.51              |
| 3:D:644:ILE:HD11 | 3:D:737:GLY:CA    | 2.41                     | 0.51              |
| 5:F:129:LEU:CD1  | 6:H:-7:DT:C2      | 2.86                     | 0.51              |
| 7:I:20:DG:H2''   | 7:I:21:DT:C5'     | 2.40                     | 0.51              |
| 1:A:232:ILE:HA   | 1:B:217:ALA:HB1   | 1.92                     | 0.51              |
| 1:B:40:VAL:HG21  | 2:C:1230:LEU:CG   | 2.39                     | 0.51              |
| 2:C:1257:ILE:CD1 | 3:D:447:LYS:HB3   | 2.41                     | 0.51              |
| 2:C:1308:LYS:HE3 | 3:D:474:LEU:CD1   | 2.37                     | 0.51              |
| 2:C:1337:PHE:CZ  | 3:D:21:ILE:HD12   | 2.46                     | 0.51              |
| 3:D:21:ILE:HG22  | 3:D:1338:ASP:HB3  | 1.93                     | 0.51              |
| 3:D:376:LEU:CD2  | 3:D:414:LEU:HD22  | 2.40                     | 0.51              |
| 3:D:557:MET:SD   | 3:D:562:VAL:HA    | 2.50                     | 0.51              |
| 3:D:797:VAL:CG1  | 3:D:913:VAL:HG13  | 2.41                     | 0.51              |
| 3:D:1364:LEU:HA  | 3:D:1367:VAL:HG12 | 1.92                     | 0.51              |
| 1:B:53:SER:HA    | 1:B:153:GLY:N     | 2.26                     | 0.51              |
| 1:B:113:VAL:O    | 1:B:132:VAL:HG13  | 2.10                     | 0.51              |
| 2:C:530:SER:HA   | 2:C:533:THR:HG22  | 1.92                     | 0.51              |
| 2:C:1349:LEU:O   | 3:D:26:ALA:HB2    | 2.11                     | 0.51              |
| 3:D:247:ILE:HG22 | 3:D:271:TYR:CE2   | 2.46                     | 0.51              |
| 3:D:375:ALA:CB   | 3:D:414:LEU:HD21  | 2.39                     | 0.51              |
| 3:D:1155:GLU:CG  | 3:D:1167:LYS:HB3  | 2.41                     | 0.51              |
| 5:F:114:ASP:O    | 5:F:118:MET:HG3   | 2.11                     | 0.51              |
| 5:F:333:ASP:HA   | 5:F:337:ILE:CB    | 2.40                     | 0.51              |
| 7:I:42:DA:H2''   | 7:I:43:DA:C8      | 2.46                     | 0.51              |
| 2:C:5:PHE:CE2    | 2:C:777:VAL:HG12  | 2.46                     | 0.51              |
| 2:C:13:LYS:HD2   | 2:C:1166:LEU:O    | 2.10                     | 0.51              |
| 2:C:394:LYS:HG2  | 2:C:398:PHE:CB    | 2.41                     | 0.51              |
| 2:C:1105:PHE:HB2 | 2:C:1227:PHE:HB2  | 1.93                     | 0.51              |
| 2:C:1214:GLU:HG2 | 2:C:1220:LYS:HE3  | 1.92                     | 0.51              |
| 4:E:38:VAL:HG12  | 4:E:52:GLU:HB3    | 1.92                     | 0.51              |
| 5:F:123:MET:CA   | 5:F:123:MET:CE    | 2.85                     | 0.51              |
| 7:I:24:DC:H4'    | 7:I:25:DC:OP1     | 2.10                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:60:VAL:CG1   | 2:C:477:LEU:HD23 | 2.41                     | 0.51              |
| 2:C:558:VAL:CG1  | 3:D:773:HIS:HA   | 2.40                     | 0.51              |
| 2:C:689:GLY:O    | 2:C:693:GLN:HG2  | 2.11                     | 0.51              |
| 2:C:1159:LYS:NZ  | 2:C:1183:LEU:HG  | 2.26                     | 0.51              |
| 2:C:1166:LEU:HA  | 2:C:1215:MET:CE  | 2.41                     | 0.51              |
| 2:C:586:HIS:HB3  | 2:C:598:PRO:CG   | 2.40                     | 0.51              |
| 2:C:903:PRO:HG2  | 2:C:904:GLU:OE2  | 2.11                     | 0.51              |
| 3:D:71:CYS:SG    | 3:D:72:LEU:N     | 2.84                     | 0.51              |
| 3:D:247:ILE:CG1  | 3:D:251:LEU:HD12 | 2.41                     | 0.51              |
| 3:D:257:LEU:HD21 | 5:F:563:ILE:HD13 | 1.92                     | 0.51              |
| 3:D:844:VAL:CG1  | 3:D:854:VAL:HB   | 2.41                     | 0.51              |
| 4:E:43:ASP:HB3   | 4:E:47:VAL:CG1   | 2.41                     | 0.51              |
| 1:A:86:LEU:CD1   | 2:C:832:ASP:HB3  | 2.41                     | 0.51              |
| 1:B:57:ALA:CB    | 1:B:93:VAL:HG13  | 2.41                     | 0.51              |
| 2:C:213:THR:HB   | 2:C:362:ASP:OD2  | 2.11                     | 0.51              |
| 2:C:408:VAL:HA   | 2:C:411:VAL:HG12 | 1.93                     | 0.51              |
| 2:C:569:ILE:CD1  | 2:C:678:LEU:HD11 | 2.41                     | 0.51              |
| 2:C:1204:ALA:HB1 | 2:C:1208:ASP:HB3 | 1.93                     | 0.51              |
| 3:D:402:MET:HG3  | 3:D:407:GLN:NE2  | 2.25                     | 0.51              |
| 3:D:423:VAL:HG12 | 3:D:472:VAL:HG22 | 1.93                     | 0.51              |
| 3:D:510:LEU:HD12 | 3:D:721:MET:HG2  | 1.92                     | 0.51              |
| 3:D:1158:LYS:HB2 | 3:D:1161:LYS:HD3 | 1.92                     | 0.51              |
| 3:D:1253:VAL:HA  | 3:D:1256:MET:CE  | 2.39                     | 0.51              |
| 5:F:492:ILE:HG23 | 5:F:493:PRO:HD2  | 1.93                     | 0.51              |
| 6:H:19:DC:H2''   | 6:H:20:DG:C5'    | 2.40                     | 0.51              |
| 2:C:602:VAL:O    | 2:C:658:ASP:HA   | 2.11                     | 0.51              |
| 2:C:808:VAL:CG2  | 2:C:1116:LEU:HG  | 2.40                     | 0.51              |
| 2:C:818:PHE:CE2  | 2:C:819:GLU:HG2  | 2.45                     | 0.51              |
| 2:C:1303:GLU:O   | 2:C:1308:LYS:HB2 | 2.11                     | 0.51              |
| 3:D:336:LYS:HE3  | 7:I:-2:DC:OP2    | 2.11                     | 0.51              |
| 3:D:365:LEU:HD21 | 3:D:502:ILE:HG12 | 1.93                     | 0.51              |
| 3:D:428:ALA:HB1  | 7:I:1:DA:C4      | 2.44                     | 0.51              |
| 3:D:484:VAL:HG12 | 3:D:485:LEU:HD12 | 1.93                     | 0.51              |
| 3:D:786:THR:OG1  | 3:D:924:THR:HG22 | 2.11                     | 0.51              |
| 3:D:1310:LEU:HB3 | 3:D:1311:GLN:OE1 | 2.10                     | 0.51              |
| 7:I:29:DC:H2''   | 7:I:30:DT:O5'    | 2.11                     | 0.51              |
| 1:A:38:PHE:CE2   | 1:A:42:LEU:HB2   | 2.46                     | 0.50              |
| 1:A:101:LYS:HG3  | 1:A:124:ILE:HG12 | 1.92                     | 0.50              |
| 1:B:29:ILE:HD12  | 1:B:216:VAL:CG2  | 2.41                     | 0.50              |
| 2:C:159:PRO:HG2  | 2:C:408:VAL:HG13 | 1.93                     | 0.50              |
| 2:C:546:LEU:HD13 | 2:C:551:ALA:CA   | 2.41                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:1137:TRP:HB2 | 2:C:1242:GLY:CA   | 2.34                     | 0.50              |
| 3:D:553:ARG:HD3  | 3:D:565:ARG:HB3   | 1.94                     | 0.50              |
| 3:D:677:GLU:O    | 3:D:681:LYS:HG2   | 2.09                     | 0.50              |
| 3:D:1372:ASP:OD2 | 4:E:70:THR:HG22   | 2.12                     | 0.50              |
| 5:F:441:PHE:O    | 5:F:445:ILE:HG13  | 2.10                     | 0.50              |
| 5:F:502:LYS:HD3  | 5:F:527:LEU:HD22  | 1.92                     | 0.50              |
| 2:C:77:TYR:CB    | 2:C:102:VAL:HG12  | 2.41                     | 0.50              |
| 2:C:455:ASN:HB3  | 2:C:458:ASN:CB    | 2.41                     | 0.50              |
| 2:C:473:ARG:O    | 2:C:477:LEU:HG    | 2.12                     | 0.50              |
| 2:C:614:MET:HG3  | 2:C:659:LEU:HD11  | 1.92                     | 0.50              |
| 2:C:936:ASP:O    | 2:C:1071:PHE:N    | 2.29                     | 0.50              |
| 3:D:265:SER:HA   | 5:F:547:LEU:HB3   | 1.92                     | 0.50              |
| 3:D:433:ARG:CZ   | 3:D:900:ALA:HB2   | 2.41                     | 0.50              |
| 3:D:439:PHE:CZ   | 3:D:455:VAL:HG21  | 2.44                     | 0.50              |
| 3:D:503:VAL:HA   | 3:D:605:ILE:HD12  | 1.92                     | 0.50              |
| 3:D:753:THR:O    | 3:D:755:ILE:HD12  | 2.10                     | 0.50              |
| 3:D:805:ILE:HG23 | 3:D:908:GLY:H     | 1.75                     | 0.50              |
| 3:D:1352:LEU:CD2 | 3:D:1361:LEU:HD23 | 2.41                     | 0.50              |
| 5:F:592:THR:HB   | 5:F:595:GLU:HB2   | 1.93                     | 0.50              |
| 2:C:84:TYR:HE1   | 2:C:1053:LYS:HD3  | 1.77                     | 0.50              |
| 2:C:190:LEU:HD11 | 2:C:397:PHE:CE1   | 2.47                     | 0.50              |
| 2:C:457:GLY:CA   | 2:C:616:ALA:HB3   | 2.41                     | 0.50              |
| 2:C:815:GLY:HA3  | 3:D:629:PHE:CD2   | 2.46                     | 0.50              |
| 2:C:1308:LYS:HB3 | 3:D:349:VAL:HG23  | 1.93                     | 0.50              |
| 3:D:21:ILE:O     | 3:D:1338:ASP:N    | 2.40                     | 0.50              |
| 3:D:272:ARG:NE   | 5:F:489:THR:HA    | 2.25                     | 0.50              |
| 3:D:355:SER:OG   | 3:D:449:ILE:HG13  | 2.12                     | 0.50              |
| 3:D:357:ILE:HG21 | 3:D:468:MET:CG    | 2.41                     | 0.50              |
| 3:D:1318:ALA:CB  | 3:D:1327:VAL:HG21 | 2.42                     | 0.50              |
| 3:D:1329:THR:O   | 3:D:1333:VAL:HG22 | 2.12                     | 0.50              |
| 5:F:576:ILE:HG23 | 5:F:650:PHE:CZ    | 2.47                     | 0.50              |
| 6:H:8:DC:H2'     | 6:H:9:DT:H6       | 1.75                     | 0.50              |
| 8:G:110:VAL:HG12 | 8:G:132:PHE:CE2   | 2.46                     | 0.50              |
| 1:A:43:GLY:HA3   | 1:A:184:TYR:CE1   | 2.47                     | 0.50              |
| 1:A:111:GLY:HA2  | 1:A:136:LEU:CB    | 2.42                     | 0.50              |
| 1:A:297:GLY:HA3  | 7:I:43:DA:O5'     | 2.11                     | 0.50              |
| 2:C:183:ILE:HG23 | 2:C:189:TRP:CE2   | 2.47                     | 0.50              |
| 2:C:623:VAL:HG11 | 2:C:656:THR:O     | 2.11                     | 0.50              |
| 2:C:1104:PRO:HG2 | 2:C:1112:VAL:HG22 | 1.92                     | 0.50              |
| 3:D:433:ARG:HG2  | 3:D:495:PRO:HG3   | 1.94                     | 0.50              |
| 3:D:795:ARG:HD2  | 3:D:1306:THR:HG22 | 1.92                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:F:426:LEU:CD2   | 5:F:430:ILE:CD1   | 2.85                     | 0.50              |
| 5:F:500:ILE:O     | 5:F:504:VAL:HG22  | 2.11                     | 0.50              |
| 5:F:533:LYS:O     | 5:F:537:VAL:HG23  | 2.11                     | 0.50              |
| 1:A:46:LEU:HD22   | 1:B:229:ILE:HD11  | 1.92                     | 0.50              |
| 2:C:378:MET:CE    | 2:C:396:LEU:HD22  | 2.41                     | 0.50              |
| 2:C:716:ALA:O     | 2:C:722:VAL:HG21  | 2.11                     | 0.50              |
| 3:D:17:THR:OG1    | 3:D:18:PHE:N      | 2.44                     | 0.50              |
| 3:D:129:LEU:HD13  | 3:D:158:HIS:CE1   | 2.45                     | 0.50              |
| 3:D:141:TYR:CD2   | 5:F:118:MET:CE    | 2.95                     | 0.50              |
| 3:D:427:ARG:CD    | 3:D:461:ALA:HB2   | 2.39                     | 0.50              |
| 3:D:706:LYS:HA    | 3:D:712:GLU:HA    | 1.94                     | 0.50              |
| 5:F:591:LEU:CD2   | 5:F:637:LYS:HD2   | 2.41                     | 0.50              |
| 1:A:78:ARG:CG     | 2:C:775:PRO:HG2   | 2.40                     | 0.50              |
| 2:C:183:ILE:HD12  | 2:C:189:TRP:CD2   | 2.46                     | 0.50              |
| 2:C:523:MET:O     | 2:C:766:ASN:ND2   | 2.44                     | 0.50              |
| 2:C:560:PRO:HB2   | 2:C:647:GLY:HA2   | 1.94                     | 0.50              |
| 3:D:234:ASN:HA    | 3:D:238:TRP:CZ3   | 2.47                     | 0.50              |
| 3:D:508:ILE:HD12  | 3:D:508:ILE:H     | 1.77                     | 0.50              |
| 3:D:847:PRO:HG3   | 3:D:874:GLN:HE22  | 1.77                     | 0.50              |
| 1:A:69:HIS:HB3    | 2:C:880:GLY:HA2   | 1.94                     | 0.50              |
| 1:A:230:ILE:HD12  | 1:B:12:PRO:HG2    | 1.93                     | 0.50              |
| 1:B:86:LEU:HD21   | 3:D:528:ILE:CB    | 2.37                     | 0.50              |
| 1:B:154:TYR:CD1   | 1:B:175:LEU:HB3   | 2.43                     | 0.50              |
| 2:C:826:GLU:HB3   | 2:C:1100:ILE:HG23 | 1.94                     | 0.50              |
| 2:C:860:ILE:HG21  | 2:C:921:ASP:CG    | 2.32                     | 0.50              |
| 3:D:166:TYR:HA    | 3:D:170:GLN:CB    | 2.42                     | 0.50              |
| 3:D:184:ALA:O     | 3:D:187:ILE:HG22  | 2.11                     | 0.50              |
| 3:D:518:ALA:HA    | 3:D:547:HIS:O     | 2.12                     | 0.50              |
| 5:F:148:MET:HG2   | 5:F:405:VAL:HG23  | 1.94                     | 0.50              |
| 5:F:469:THR:HG23  | 5:F:470:TYR:N     | 2.26                     | 0.50              |
| 2:C:111:THR:CG2   | 2:C:115:THR:HB    | 2.41                     | 0.50              |
| 2:C:973:LEU:HA    | 2:C:976:ASN:ND2   | 2.26                     | 0.50              |
| 3:D:129:LEU:HD13  | 3:D:158:HIS:HE1   | 1.77                     | 0.50              |
| 3:D:357:ILE:HD13  | 3:D:468:MET:CG    | 2.42                     | 0.50              |
| 3:D:444:ILE:HG12  | 3:D:450:GLN:HG3   | 1.94                     | 0.50              |
| 3:D:529:PHE:CE2   | 3:D:550:ILE:HD13  | 2.47                     | 0.50              |
| 3:D:1139:ARG:CZ   | 6:H:4:DG:H2"      | 2.42                     | 0.50              |
| 3:D:1207:ILE:HG13 | 3:D:1209:GLY:H    | 1.76                     | 0.50              |
| 2:C:192:PHE:CD2   | 2:C:202:VAL:HG22  | 2.47                     | 0.50              |
| 2:C:413:MET:O     | 2:C:417:LEU:HD23  | 2.11                     | 0.50              |
| 2:C:551:ALA:CB    | 2:C:579:LEU:HD11  | 2.42                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:692:MET:CG    | 2:C:1249:LEU:HD21 | 2.42                     | 0.50              |
| 2:C:1015:TRP:O    | 2:C:1029:LEU:HD21 | 2.10                     | 0.50              |
| 2:C:1114:VAL:HG21 | 2:C:1246:MET:SD   | 2.52                     | 0.50              |
| 3:D:46:ASN:HB2    | 3:D:49:THR:O      | 2.11                     | 0.50              |
| 3:D:138:ARG:HD3   | 3:D:144:TYR:CE2   | 2.47                     | 0.50              |
| 3:D:367:GLU:OE2   | 3:D:442:LYS:HB2   | 2.11                     | 0.50              |
| 3:D:396:VAL:HG23  | 5:F:579:ASN:HD22  | 1.76                     | 0.50              |
| 3:D:681:LYS:O     | 3:D:685:ALA:HB3   | 2.12                     | 0.50              |
| 5:F:127:GLU:HG3   | 5:F:421:GLU:HB3   | 1.93                     | 0.50              |
| 6:H:-18:DT:H2''   | 6:H:-17:DC:C6     | 2.47                     | 0.50              |
| 2:C:765:SER:HB2   | 2:C:771:ILE:CG1   | 2.42                     | 0.49              |
| 2:C:820:ASP:CB    | 3:D:464:ASP:HB3   | 2.42                     | 0.49              |
| 2:C:826:GLU:HB2   | 2:C:1099:PRO:HA   | 1.94                     | 0.49              |
| 2:C:877:VAL:HG21  | 2:C:934:ILE:HG13  | 1.94                     | 0.49              |
| 2:C:1135:LEU:HD11 | 2:C:1196:ILE:CD1  | 2.42                     | 0.49              |
| 2:C:1186:LEU:O    | 2:C:1190:LEU:HG   | 2.12                     | 0.49              |
| 2:C:1286:GLU:HB3  | 3:D:345:LEU:HB3   | 1.94                     | 0.49              |
| 3:D:433:ARG:N     | 3:D:917:GLN:OE1   | 2.45                     | 0.49              |
| 3:D:651:THR:O     | 3:D:655:GLU:HG2   | 2.12                     | 0.49              |
| 3:D:1354:PRO:O    | 3:D:1359:SER:HB2  | 2.11                     | 0.49              |
| 5:F:450:ILE:HA    | 5:F:453:MET:HE3   | 1.92                     | 0.49              |
| 1:A:48:ARG:CD     | 1:B:41:THR:HB     | 2.30                     | 0.49              |
| 1:A:101:LYS:CD    | 1:A:124:ILE:HD11  | 2.42                     | 0.49              |
| 2:C:24:MET:HB3    | 2:C:586:HIS:CE1   | 2.48                     | 0.49              |
| 2:C:28:ILE:CD1    | 2:C:32:ARG:HD2    | 2.40                     | 0.49              |
| 2:C:111:THR:HA    | 2:C:118:ARG:NH2   | 2.24                     | 0.49              |
| 2:C:366:ILE:HG13  | 2:C:368:GLU:H     | 1.76                     | 0.49              |
| 2:C:378:MET:SD    | 2:C:396:LEU:HD22  | 2.52                     | 0.49              |
| 2:C:1147:THR:O    | 2:C:1151:GLU:HG3  | 2.11                     | 0.49              |
| 3:D:444:ILE:HG21  | 3:D:450:GLN:CG    | 2.42                     | 0.49              |
| 3:D:805:ILE:HD13  | 3:D:905:VAL:HG22  | 1.94                     | 0.49              |
| 3:D:1164:ARG:HH21 | 3:D:1167:LYS:HE2  | 1.77                     | 0.49              |
| 3:D:1257:LEU:CD2  | 3:D:1302:LEU:HD12 | 2.41                     | 0.49              |
| 3:D:1262:ILE:O    | 3:D:1271:ILE:HA   | 2.11                     | 0.49              |
| 4:E:30:ILE:CA     | 4:E:34:ALA:HB3    | 2.41                     | 0.49              |
| 5:F:116:VAL:HA    | 5:F:442:LEU:HD12  | 1.94                     | 0.49              |
| 6:H:-16:DG:H2'    | 6:H:-15:DT:C6     | 2.47                     | 0.49              |
| 1:A:232:ILE:HA    | 1:B:217:ALA:CB    | 2.43                     | 0.49              |
| 2:C:547:THR:HG22  | 2:C:550:ARG:HB2   | 1.93                     | 0.49              |
| 2:C:834:PHE:HB2   | 2:C:1078:LEU:HD11 | 1.93                     | 0.49              |
| 3:D:41:LYS:O      | 3:D:56:GLY:HA2    | 2.12                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:458:ALA:HB2   | 3:D:501:ILE:HG23  | 1.94                     | 0.49              |
| 3:D:609:TYR:HD2   | 3:D:617:THR:HG21  | 1.76                     | 0.49              |
| 3:D:844:VAL:HB    | 3:D:876:VAL:CG2   | 2.39                     | 0.49              |
| 7:I:-8:DG:H2'     | 7:I:-7:DC:C6      | 2.47                     | 0.49              |
| 1:A:229:GLN:HG3   | 1:B:224:GLN:HE22  | 1.76                     | 0.49              |
| 1:B:59:VAL:HG11   | 1:B:88:ILE:CG2    | 2.42                     | 0.49              |
| 1:B:94:ARG:HB3    | 1:B:209:ALA:HB1   | 1.93                     | 0.49              |
| 1:B:230:PHE:HB2   | 1:B:233:PHE:CE2   | 2.46                     | 0.49              |
| 2:C:159:PRO:HB2   | 2:C:409:GLY:HA3   | 1.94                     | 0.49              |
| 2:C:188:SER:HB2   | 2:C:396:LEU:HD11  | 1.95                     | 0.49              |
| 2:C:200:VAL:CG1   | 2:C:358:THR:HG21  | 2.35                     | 0.49              |
| 2:C:540:ALA:N     | 2:C:579:LEU:O     | 2.30                     | 0.49              |
| 2:C:668:VAL:HG11  | 2:C:1200:VAL:HG11 | 1.94                     | 0.49              |
| 3:D:360:GLY:N     | 3:D:451:LEU:O     | 2.46                     | 0.49              |
| 3:D:396:VAL:H     | 5:F:579:ASN:HD22  | 1.60                     | 0.49              |
| 3:D:764:THR:HG22  | 3:D:767:GLU:OE2   | 2.12                     | 0.49              |
| 3:D:1201:THR:O    | 3:D:1204:GLU:HG2  | 2.12                     | 0.49              |
| 1:B:127:LEU:O     | 1:B:129:PRO:HD3   | 2.11                     | 0.49              |
| 2:C:27:LEU:CD1    | 2:C:532:ILE:HD13  | 2.42                     | 0.49              |
| 2:C:38:PHE:O      | 2:C:39:LEU:HD23   | 2.12                     | 0.49              |
| 2:C:202:VAL:HG23  | 2:C:212:ALA:HA    | 1.94                     | 0.49              |
| 2:C:840:GLU:HB2   | 2:C:1072:VAL:CG1  | 2.42                     | 0.49              |
| 2:C:911:ILE:CD1   | 5:F:638:LEU:HD11  | 2.42                     | 0.49              |
| 2:C:1341:VAL:HG23 | 2:C:1351:VAL:HG12 | 1.94                     | 0.49              |
| 3:D:19:ASP:OD1    | 3:D:20:GLN:N      | 2.45                     | 0.49              |
| 3:D:66:THR:HG23   | 3:D:67:LYS:HG2    | 1.95                     | 0.49              |
| 3:D:1326:ARG:NE   | 3:D:1330:GLU:OE2  | 2.39                     | 0.49              |
| 5:F:129:LEU:HD22  | 6:H:-7:DT:C2'     | 2.40                     | 0.49              |
| 1:A:45:ALA:O      | 1:A:224:LEU:HD11  | 2.12                     | 0.49              |
| 2:C:43:THR:O      | 2:C:47:LEU:HG     | 2.13                     | 0.49              |
| 2:C:1083:LYS:O    | 2:C:1249:LEU:HB2  | 2.13                     | 0.49              |
| 3:D:1352:LEU:HD22 | 3:D:1361:LEU:HD23 | 1.94                     | 0.49              |
| 3:D:1369:ALA:O    | 3:D:1373:GLU:HG2  | 2.13                     | 0.49              |
| 7:I:41:DT:H2''    | 7:I:42:DA:C5'     | 2.43                     | 0.49              |
| 1:A:72:SER:OG     | 1:A:73:SER:N      | 2.45                     | 0.49              |
| 2:C:10:ARG:CG     | 2:C:1195:PRO:HG2  | 2.42                     | 0.49              |
| 2:C:10:ARG:NH2    | 2:C:796:GLU:OE1   | 2.45                     | 0.49              |
| 2:C:806:ALA:HB1   | 2:C:1113:ASP:HB2  | 1.93                     | 0.49              |
| 2:C:1119:LEU:HD23 | 3:D:721:MET:HG2   | 1.95                     | 0.49              |
| 3:D:196:LEU:CD1   | 3:D:229:PHE:HB3   | 2.43                     | 0.49              |
| 3:D:484:VAL:O     | 4:E:6:VAL:HG21    | 2.13                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:799:VAL:HG23  | 3:D:1308:ALA:CB   | 2.43                     | 0.49              |
| 3:D:806:VAL:HG23  | 3:D:807:GLU:HG3   | 1.94                     | 0.49              |
| 3:D:919:ILE:HD12  | 3:D:1252:ILE:HG13 | 1.94                     | 0.49              |
| 6:H:5:DT:H2'      | 6:H:6:DC:C6       | 2.47                     | 0.49              |
| 7:I:9:DG:H2''     | 7:I:10:DT:O2      | 2.12                     | 0.49              |
| 1:A:46:LEU:HD23   | 1:A:203:LEU:HD13  | 1.95                     | 0.49              |
| 1:B:87:ASN:ND2    | 1:B:131:HIS:O     | 2.43                     | 0.49              |
| 2:C:683:ALA:HB2   | 3:D:771:SER:OG    | 2.13                     | 0.49              |
| 2:C:1119:LEU:HB3  | 3:D:727:ARG:HG3   | 1.93                     | 0.49              |
| 2:C:1339:VAL:HG23 | 3:D:251:LEU:CD1   | 2.39                     | 0.49              |
| 3:D:81:TYR:HB3    | 3:D:84:ILE:HG12   | 1.93                     | 0.49              |
| 3:D:804:ILE:HD11  | 3:D:1343:LEU:HD22 | 1.95                     | 0.49              |
| 1:B:86:LEU:HD22   | 3:D:529:PHE:O     | 2.13                     | 0.49              |
| 2:C:623:VAL:CG2   | 2:C:645:ILE:HG22  | 2.41                     | 0.49              |
| 2:C:1258:HIS:CE1  | 2:C:1276:LYS:HA   | 2.48                     | 0.49              |
| 2:C:1340:LEU:HD13 | 3:D:339:ARG:HB2   | 1.93                     | 0.49              |
| 3:D:118:LEU:HD22  | 3:D:140:LEU:HD13  | 1.94                     | 0.49              |
| 3:D:171:GLU:HG3   | 3:D:178:PHE:CG    | 2.48                     | 0.49              |
| 3:D:881:VAL:HA    | 3:D:884:CYS:SG    | 2.52                     | 0.49              |
| 3:D:891:CYS:SG    | 3:D:892:GLY:N     | 2.86                     | 0.49              |
| 3:D:1149:GLU:HB2  | 3:D:1219:ILE:HG23 | 1.95                     | 0.49              |
| 3:D:1278:LYS:O    | 3:D:1282:ASP:N    | 2.27                     | 0.49              |
| 6:H:-5:DC:H2''    | 6:H:-4:DG:C5'     | 2.43                     | 0.49              |
| 7:I:-1:DT:H3'     | 7:I:0:DT:H5''     | 1.95                     | 0.49              |
| 7:I:22:DT:C2'     | 7:I:23:DT:H71     | 2.36                     | 0.49              |
| 1:A:53:SER:HG     | 1:B:38:PHE:HZ     | 1.51                     | 0.49              |
| 2:C:15:PHE:CD2    | 2:C:1204:ALA:HB2  | 2.48                     | 0.49              |
| 2:C:397:PHE:O     | 2:C:427:ILE:HB    | 2.13                     | 0.49              |
| 2:C:405:LEU:HD23  | 2:C:406:SER:O     | 2.13                     | 0.49              |
| 2:C:824:ILE:HB    | 2:C:1094:ILE:CD1  | 2.41                     | 0.49              |
| 2:C:1085:ALA:HB1  | 2:C:1091:LYS:HG2  | 1.95                     | 0.49              |
| 2:C:1262:ILE:HD13 | 5:F:571:PRO:HB2   | 1.95                     | 0.49              |
| 2:C:1264:PRO:HD2  | 2:C:1279:PHE:HB2  | 1.93                     | 0.49              |
| 3:D:31:ILE:HD12   | 3:D:245:PRO:HG3   | 1.95                     | 0.49              |
| 3:D:919:ILE:HG21  | 3:D:1136:PHE:CE2  | 2.47                     | 0.49              |
| 3:D:1352:LEU:CD2  | 3:D:1358:GLY:HA2  | 2.43                     | 0.49              |
| 1:A:8:GLU:OE2     | 1:B:226:GLN:NE2   | 2.46                     | 0.48              |
| 1:A:34:LEU:HD23   | 1:A:39:GLY:HA2    | 1.94                     | 0.48              |
| 1:A:68:VAL:HG23   | 1:A:69:HIS:CD2    | 2.48                     | 0.48              |
| 1:A:75:GLU:O      | 2:C:735:ASP:HB2   | 2.13                     | 0.48              |
| 1:B:68:VAL:HG22   | 1:B:70:GLU:H      | 1.77                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:175:LEU:HD21  | 1:B:180:LYS:CD    | 2.42                     | 0.48              |
| 2:C:159:PRO:HA    | 2:C:183:ILE:O     | 2.13                     | 0.48              |
| 2:C:366:ILE:CG2   | 2:C:369:ASP:HB2   | 2.43                     | 0.48              |
| 2:C:829:VAL:HG23  | 2:C:1077:LYS:HB3  | 1.94                     | 0.48              |
| 2:C:1213:LEU:HD22 | 2:C:1218:VAL:CG1  | 2.36                     | 0.48              |
| 2:C:1286:GLU:CB   | 3:D:345:LEU:HD23  | 2.43                     | 0.48              |
| 3:D:45:ILE:HG13   | 5:F:490:ILE:HG23  | 1.94                     | 0.48              |
| 3:D:290:PRO:O     | 3:D:294:ILE:HG13  | 2.13                     | 0.48              |
| 3:D:508:ILE:HG13  | 3:D:629:PHE:CE1   | 2.48                     | 0.48              |
| 3:D:581:LEU:HD22  | 3:D:604:LEU:HD11  | 1.93                     | 0.48              |
| 4:E:22:LEU:HD11   | 4:E:61:GLU:HB2    | 1.94                     | 0.48              |
| 5:F:631:GLU:O     | 5:F:635:LEU:HD23  | 2.12                     | 0.48              |
| 1:A:67:VAL:CG2    | 1:A:72:SER:HB3    | 2.43                     | 0.48              |
| 1:A:85:VAL:HG13   | 1:A:172:VAL:CG2   | 2.39                     | 0.48              |
| 2:C:652:LEU:CD1   | 2:C:657:VAL:HG22  | 2.43                     | 0.48              |
| 2:C:914:GLU:OE1   | 5:F:651:LEU:HD21  | 2.13                     | 0.48              |
| 2:C:1133:THR:HG22 | 2:C:1242:GLY:HA3  | 1.94                     | 0.48              |
| 2:C:1143:GLY:HA2  | 2:C:1146:ILE:HG22 | 1.95                     | 0.48              |
| 2:C:1292:LEU:HD12 | 2:C:1301:LEU:HD21 | 1.94                     | 0.48              |
| 2:C:1294:ALA:HB1  | 3:D:914:ILE:HG12  | 1.94                     | 0.48              |
| 3:D:20:GLN:HA     | 3:D:1338:ASP:O    | 2.12                     | 0.48              |
| 3:D:1309:SER:HB2  | 3:D:1318:ALA:HA   | 1.96                     | 0.48              |
| 2:C:491:ASP:HB2   | 2:C:493:ASP:OD1   | 2.12                     | 0.48              |
| 2:C:682:ASP:HB2   | 2:C:1125:MET:O    | 2.13                     | 0.48              |
| 2:C:941:ASN:HB2   | 2:C:946:ASP:HB2   | 1.95                     | 0.48              |
| 3:D:181:GLU:OE2   | 3:D:186:ALA:HA    | 2.13                     | 0.48              |
| 3:D:246:VAL:HA    | 3:D:271:TYR:CZ    | 2.48                     | 0.48              |
| 3:D:358:VAL:HG23  | 3:D:448:ALA:HB1   | 1.93                     | 0.48              |
| 3:D:413:ILE:O     | 3:D:417:VAL:HG12  | 2.14                     | 0.48              |
| 3:D:492:ILE:HD13  | 3:D:617:THR:HG22  | 1.94                     | 0.48              |
| 3:D:814:LYS:HG3   | 3:D:883:THR:OG1   | 2.13                     | 0.48              |
| 3:D:822:VAL:CG1   | 3:D:827:VAL:HG12  | 2.43                     | 0.48              |
| 5:F:129:LEU:HD11  | 6:H:-7:DT:O2      | 2.12                     | 0.48              |
| 5:F:437:ARG:CZ    | 7:I:10:DT:H1'     | 2.43                     | 0.48              |
| 5:F:511:LEU:HA    | 5:F:515:GLY:O     | 2.13                     | 0.48              |
| 5:F:520:PRO:HB3   | 5:F:538:LEU:HD21  | 1.95                     | 0.48              |
| 7:I:-16:DG:C8     | 7:I:-16:DG:H5'    | 2.48                     | 0.48              |
| 1:A:95:MET:HE2    | 1:A:97:ALA:O      | 2.14                     | 0.48              |
| 2:C:26:ASN:HA     | 2:C:718:ASP:OD2   | 2.13                     | 0.48              |
| 2:C:104:LEU:CD1   | 2:C:128:VAL:HG12  | 2.43                     | 0.48              |
| 2:C:194:PHE:HE1   | 2:C:200:VAL:HB    | 1.77                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:456:LEU:CD2  | 2:C:565:ARG:HB2  | 2.43                     | 0.48              |
| 2:C:562:HIS:CE1  | 2:C:566:ILE:HD12 | 2.48                     | 0.48              |
| 2:C:859:ASP:HB2  | 2:C:868:LEU:CD1  | 2.42                     | 0.48              |
| 3:D:108:LEU:HA   | 3:D:278:ASN:ND2  | 2.27                     | 0.48              |
| 3:D:309:PHE:O    | 3:D:330:ALA:N    | 2.42                     | 0.48              |
| 5:F:546:SER:HB3  | 5:F:548:GLU:OE1  | 2.12                     | 0.48              |
| 2:C:461:VAL:CG2  | 2:C:538:LEU:HD22 | 2.40                     | 0.48              |
| 2:C:485:GLU:OE2  | 5:F:433:LYS:HD3  | 2.13                     | 0.48              |
| 2:C:966:ARG:HB2  | 2:C:1047:PHE:CD2 | 2.49                     | 0.48              |
| 2:C:1048:GLU:HA  | 2:C:1051:VAL:CG1 | 2.41                     | 0.48              |
| 2:C:1080:PRO:HA  | 2:C:1094:ILE:CG2 | 2.43                     | 0.48              |
| 2:C:1095:SER:HA  | 3:D:358:VAL:HG11 | 1.96                     | 0.48              |
| 3:D:69:TYR:CE2   | 3:D:95:LEU:HB3   | 2.49                     | 0.48              |
| 3:D:510:LEU:CD2  | 3:D:637:ILE:HG13 | 2.43                     | 0.48              |
| 3:D:661:ALA:O    | 3:D:681:LYS:HE2  | 2.14                     | 0.48              |
| 1:A:111:GLY:O    | 1:A:135:THR:HA   | 2.14                     | 0.48              |
| 2:C:21:ALA:HB3   | 2:C:662:VAL:HG13 | 1.96                     | 0.48              |
| 2:C:22:VAL:HB    | 2:C:662:VAL:CG1  | 2.43                     | 0.48              |
| 2:C:571:THR:CG2  | 2:C:578:GLY:H    | 2.27                     | 0.48              |
| 2:C:837:ILE:HG23 | 2:C:1073:ALA:HB1 | 1.96                     | 0.48              |
| 2:C:855:GLU:HB3  | 2:C:893:VAL:HB   | 1.94                     | 0.48              |
| 2:C:988:LYS:HD3  | 2:C:1025:ALA:HB1 | 1.95                     | 0.48              |
| 3:D:266:ASP:OD2  | 3:D:327:LYS:HB2  | 2.13                     | 0.48              |
| 3:D:437:GLN:HB2  | 3:D:459:PHE:CZ   | 2.49                     | 0.48              |
| 3:D:513:TYR:O    | 3:D:517:VAL:HG13 | 2.13                     | 0.48              |
| 3:D:805:ILE:HD11 | 3:D:892:GLY:HA2  | 1.94                     | 0.48              |
| 3:D:841:ALA:HB3  | 3:D:877:LYS:CG   | 2.43                     | 0.48              |
| 1:B:50:LEU:CD2   | 1:B:219:ALA:HB2  | 2.43                     | 0.48              |
| 2:C:128:VAL:HB   | 2:C:498:HIS:CB   | 2.44                     | 0.48              |
| 2:C:907:LEU:HB2  | 5:F:603:PHE:CD2  | 2.49                     | 0.48              |
| 3:D:271:TYR:CD1  | 3:D:308:LEU:HD11 | 2.48                     | 0.48              |
| 3:D:307:ALA:HA   | 3:D:311:ASN:HA   | 1.94                     | 0.48              |
| 3:D:508:ILE:HG12 | 3:D:625:MET:HA   | 1.95                     | 0.48              |
| 3:D:922:PRO:HB3  | 3:D:1242:VAL:CG1 | 2.43                     | 0.48              |
| 3:D:1315:PHE:CE1 | 3:D:1338:ASP:HB2 | 2.49                     | 0.48              |
| 5:F:432:LYS:HA   | 5:F:441:PHE:CE2  | 2.49                     | 0.48              |
| 5:F:491:ARG:O    | 5:F:491:ARG:NE   | 2.29                     | 0.48              |
| 5:F:584:THR:HA   | 5:F:587:VAL:HG22 | 1.96                     | 0.48              |
| 1:A:95:MET:HA    | 1:A:124:ILE:HA   | 1.96                     | 0.48              |
| 1:B:42:LEU:O     | 1:B:46:LEU:HG    | 2.14                     | 0.48              |
| 1:B:103:MET:CB   | 1:B:146:PHE:HB2  | 2.40                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:188:SER:CB    | 2:C:396:LEU:HD11  | 2.44                     | 0.48              |
| 2:C:452:ASP:N     | 2:C:452:ASP:OD1   | 2.47                     | 0.48              |
| 2:C:818:PHE:HE1   | 3:D:506:GLN:H     | 1.61                     | 0.48              |
| 2:C:912:PHE:CZ    | 5:F:648:ARG:HA    | 2.49                     | 0.48              |
| 2:C:1290:TRP:HH2  | 3:D:794:ARG:HG3   | 1.79                     | 0.48              |
| 3:D:339:ARG:HA    | 3:D:343:ASN:HB2   | 1.95                     | 0.48              |
| 3:D:351:TYR:CG    | 3:D:474:LEU:HD11  | 2.49                     | 0.48              |
| 3:D:563:LEU:HD12  | 3:D:564:LEU:N     | 2.29                     | 0.48              |
| 3:D:1131:ARG:O    | 3:D:1135:LEU:HD23 | 2.14                     | 0.48              |
| 3:D:1343:LEU:HG   | 3:D:1353:ILE:CG2  | 2.43                     | 0.48              |
| 5:F:495:HIS:CE1   | 6:H:-18:DT:H3'    | 2.49                     | 0.48              |
| 1:B:24:THR:O      | 1:B:212:PRO:HD3   | 2.14                     | 0.48              |
| 2:C:539:SER:HA    | 2:C:580:ILE:HA    | 1.95                     | 0.48              |
| 2:C:673:ALA:O     | 2:C:709:THR:HG21  | 2.14                     | 0.48              |
| 2:C:1273:LEU:HD21 | 5:F:563:ILE:O     | 2.13                     | 0.48              |
| 2:C:1292:LEU:HD21 | 3:D:436:ILE:CG2   | 2.43                     | 0.48              |
| 3:D:353:GLY:O     | 3:D:470:VAL:HG12  | 2.13                     | 0.48              |
| 3:D:655:GLU:OE1   | 3:D:658:ARG:HD3   | 2.12                     | 0.48              |
| 3:D:1161:LYS:HE3  | 3:D:1163:LYS:O    | 2.13                     | 0.48              |
| 1:B:87:ASN:ND2    | 1:B:132:VAL:HA    | 2.28                     | 0.48              |
| 1:B:92:ALA:HB2    | 1:B:207:ASN:O     | 2.14                     | 0.48              |
| 1:B:156:PRO:HB3   | 3:D:543:VAL:HG21  | 1.95                     | 0.48              |
| 2:C:71:VAL:CG1    | 2:C:107:ILE:HG12  | 2.44                     | 0.48              |
| 2:C:532:ILE:CD1   | 2:C:719:SER:HB2   | 2.43                     | 0.48              |
| 2:C:765:SER:HB3   | 2:C:769:THR:HG22  | 1.95                     | 0.48              |
| 5:F:417:LYS:O     | 5:F:421:GLU:HG3   | 2.13                     | 0.48              |
| 1:B:61:ALA:HB2    | 1:B:147:THR:OG1   | 2.13                     | 0.47              |
| 2:C:219:LEU:HD23  | 2:C:430:LYS:HA    | 1.96                     | 0.47              |
| 2:C:658:ASP:OD1   | 2:C:658:ASP:N     | 2.46                     | 0.47              |
| 2:C:844:VAL:CG1   | 2:C:1068:VAL:HB   | 2.44                     | 0.47              |
| 3:D:199:GLU:HB3   | 3:D:226:LEU:HD13  | 1.96                     | 0.47              |
| 3:D:376:LEU:HD23  | 3:D:414:LEU:HD22  | 1.95                     | 0.47              |
| 3:D:842:GLU:OE1   | 3:D:877:LYS:HG2   | 2.14                     | 0.47              |
| 3:D:1318:ALA:HB3  | 3:D:1327:VAL:HG21 | 1.96                     | 0.47              |
| 4:E:26:ARG:O      | 4:E:30:ILE:HG13   | 2.13                     | 0.47              |
| 6:H:-28:DG:H1'    | 6:H:-27:DC:C5     | 2.48                     | 0.47              |
| 6:H:-3:DA:H5''    | 6:H:-3:DA:C8      | 2.48                     | 0.47              |
| 2:C:160:GLY:HA2   | 2:C:413:MET:HG3   | 1.95                     | 0.47              |
| 2:C:741:ILE:HD12  | 2:C:783:ILE:HD11  | 1.96                     | 0.47              |
| 2:C:807:LEU:HD13  | 2:C:1243:TYR:CE1  | 2.49                     | 0.47              |
| 2:C:931:ALA:HB1   | 2:C:1072:VAL:HG22 | 1.96                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:977:ILE:O     | 2:C:981:LEU:HG    | 2.14                     | 0.47              |
| 2:C:1114:VAL:HG11 | 2:C:1246:MET:SD   | 2.55                     | 0.47              |
| 3:D:434:LEU:CD1   | 3:D:501:ILE:HG21  | 2.43                     | 0.47              |
| 5:F:425:ARG:HD2   | 6:H:-7:DT:H2''    | 1.96                     | 0.47              |
| 2:C:563:TYR:CE2   | 3:D:765:VAL:HG12  | 2.49                     | 0.47              |
| 2:C:674:LEU:CD1   | 2:C:800:LEU:HD23  | 2.43                     | 0.47              |
| 2:C:1163:VAL:HG12 | 2:C:1176:LEU:CD2  | 2.44                     | 0.47              |
| 2:C:1290:TRP:O    | 3:D:917:GLN:NE2   | 2.47                     | 0.47              |
| 2:C:1302:GLN:O    | 2:C:1306:THR:HB   | 2.14                     | 0.47              |
| 3:D:294:ILE:O     | 3:D:298:LYS:HG3   | 2.14                     | 0.47              |
| 3:D:434:LEU:O     | 3:D:437:GLN:HG3   | 2.15                     | 0.47              |
| 3:D:483:ARG:HA    | 3:D:487:MET:CG    | 2.44                     | 0.47              |
| 3:D:484:VAL:HA    | 4:E:6:VAL:CG2     | 2.45                     | 0.47              |
| 3:D:515:LEU:HD11  | 3:D:631:GLU:CG    | 2.40                     | 0.47              |
| 3:D:558:THR:HG22  | 3:D:563:LEU:CD2   | 2.45                     | 0.47              |
| 3:D:568:ILE:HD12  | 3:D:570:THR:HG21  | 1.95                     | 0.47              |
| 3:D:791:TYR:O     | 3:D:795:ARG:HG3   | 2.14                     | 0.47              |
| 5:F:134:GLU:CD    | 5:F:467:PHE:HB3   | 2.35                     | 0.47              |
| 5:F:499:THR:HG21  | 5:F:533:LYS:HZ3   | 1.79                     | 0.47              |
| 5:F:584:THR:O     | 5:F:588:LEU:HG    | 2.14                     | 0.47              |
| 6:H:-24:DG:H2''   | 6:H:-23:DA:C8     | 2.49                     | 0.47              |
| 1:A:30:VAL:HG13   | 1:A:200:LYS:HD2   | 1.97                     | 0.47              |
| 2:C:22:VAL:HG21   | 2:C:611:VAL:HG11  | 1.96                     | 0.47              |
| 2:C:77:TYR:HB3    | 2:C:102:VAL:HG12  | 1.96                     | 0.47              |
| 2:C:78:GLU:CG     | 2:C:101:LYS:HB2   | 2.40                     | 0.47              |
| 2:C:356:ARG:O     | 2:C:360:ARG:HD3   | 2.15                     | 0.47              |
| 2:C:679:GLU:HG2   | 2:C:680:ASN:OD1   | 2.14                     | 0.47              |
| 2:C:822:ILE:HD12  | 2:C:1084:MET:O    | 2.14                     | 0.47              |
| 2:C:1282:GLN:HA   | 7:I:2:DA:OP1      | 2.14                     | 0.47              |
| 3:D:287:LEU:O     | 3:D:287:LEU:HD23  | 2.14                     | 0.47              |
| 3:D:336:LYS:HA    | 3:D:340:PHE:HD2   | 1.79                     | 0.47              |
| 1:A:58:ALA:C      | 1:A:148:VAL:HG23  | 2.35                     | 0.47              |
| 2:C:172:ALA:HB2   | 2:C:196:ALA:CB    | 2.45                     | 0.47              |
| 2:C:217:TYR:HB3   | 2:C:367:ARG:HA    | 1.96                     | 0.47              |
| 2:C:565:ARG:HB3   | 2:C:595:ILE:CG2   | 2.44                     | 0.47              |
| 2:C:1284:PHE:CE2  | 2:C:1289:VAL:HG23 | 2.48                     | 0.47              |
| 3:D:427:ARG:HB2   | 3:D:468:MET:SD    | 2.55                     | 0.47              |
| 3:D:571:THR:HB    | 3:D:572:PRO:HD2   | 1.97                     | 0.47              |
| 3:D:637:ILE:CG2   | 3:D:720:MET:HE3   | 2.43                     | 0.47              |
| 3:D:800:ALA:HB1   | 3:D:912:GLY:CA    | 2.45                     | 0.47              |
| 4:E:25:HIS:CE1    | 4:E:67:LEU:HD13   | 2.48                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:H:-33:DG:H2''   | 6:H:-32:DA:N7     | 2.28                     | 0.47              |
| 6:H:9:DT:H2''     | 6:H:10:DG:H5'     | 1.97                     | 0.47              |
| 7:I:-8:DG:H2'     | 7:I:-7:DC:H6      | 1.79                     | 0.47              |
| 1:A:182:VAL:HA    | 1:A:205:VAL:HA    | 1.97                     | 0.47              |
| 1:B:25:ARG:HG2    | 1:B:208:GLY:HA2   | 1.95                     | 0.47              |
| 2:C:43:THR:CG2    | 2:C:45:PRO:HD2    | 2.37                     | 0.47              |
| 2:C:262:VAL:HA    | 2:C:268:GLU:O     | 2.14                     | 0.47              |
| 2:C:546:LEU:HD23  | 6:H:1:DA:C6       | 2.49                     | 0.47              |
| 2:C:629:ILE:HG21  | 2:C:641:VAL:CG2   | 2.45                     | 0.47              |
| 2:C:695:GLN:O     | 2:C:1249:LEU:HA   | 2.14                     | 0.47              |
| 2:C:1061:PRO:HD2  | 2:C:1064:VAL:HG13 | 1.97                     | 0.47              |
| 3:D:40:LYS:O      | 3:D:279:ASN:ND2   | 2.40                     | 0.47              |
| 3:D:57:LEU:HD11   | 3:D:272:ARG:HB2   | 1.97                     | 0.47              |
| 3:D:181:GLU:HG3   | 3:D:186:ALA:HA    | 1.96                     | 0.47              |
| 3:D:257:LEU:HB2   | 3:D:261:ARG:O     | 2.14                     | 0.47              |
| 3:D:354:ARG:HG2   | 3:D:467:GLN:HB3   | 1.96                     | 0.47              |
| 3:D:386:ARG:HG3   | 3:D:417:VAL:HB    | 1.96                     | 0.47              |
| 3:D:387:LEU:HD23  | 3:D:413:ILE:HG13  | 1.95                     | 0.47              |
| 3:D:735:GLN:HA    | 3:D:740:ARG:HA    | 1.96                     | 0.47              |
| 3:D:804:ILE:HG13  | 3:D:1343:LEU:CD1  | 2.45                     | 0.47              |
| 3:D:810:CYS:SG    | 3:D:812:THR:HG22  | 2.55                     | 0.47              |
| 1:B:136:LEU:HD22  | 1:B:139:GLY:CA    | 2.45                     | 0.47              |
| 2:C:57:PHE:CZ     | 2:C:102:VAL:HG11  | 2.50                     | 0.47              |
| 2:C:79:PHE:HE2    | 2:C:135:LEU:HD12  | 1.80                     | 0.47              |
| 2:C:84:TYR:HB3    | 2:C:88:GLU:OE2    | 2.14                     | 0.47              |
| 2:C:235:PRO:CB    | 2:C:247:TYR:HA    | 2.45                     | 0.47              |
| 2:C:367:ARG:O     | 2:C:371:LEU:HG    | 2.15                     | 0.47              |
| 2:C:456:LEU:CD2   | 2:C:562:HIS:HA    | 2.41                     | 0.47              |
| 2:C:519:LEU:HD23  | 2:C:543:PRO:HD2   | 1.97                     | 0.47              |
| 2:C:684:ASN:OD1   | 3:D:779:LEU:HD13  | 2.14                     | 0.47              |
| 2:C:839:ILE:HG12  | 2:C:1073:ALA:HB2  | 1.96                     | 0.47              |
| 2:C:1298:ALA:HB1  | 3:D:1353:ILE:HB   | 1.97                     | 0.47              |
| 3:D:43:GLU:HB2    | 3:D:53:GLU:HG3    | 1.97                     | 0.47              |
| 3:D:506:GLN:HA    | 3:D:726:ALA:HB1   | 1.95                     | 0.47              |
| 3:D:693:VAL:HG11  | 3:D:739:MET:CE    | 2.44                     | 0.47              |
| 3:D:805:ILE:CD1   | 3:D:892:GLY:HA2   | 2.45                     | 0.47              |
| 3:D:805:ILE:HG12  | 3:D:907:ILE:HA    | 1.96                     | 0.47              |
| 3:D:1262:ILE:HD11 | 3:D:1274:ASP:OD2  | 2.15                     | 0.47              |
| 5:F:400:ARG:O     | 5:F:404:THR:HG22  | 2.15                     | 0.47              |
| 5:F:484:ALA:HB1   | 5:F:497:ILE:HG13  | 1.97                     | 0.47              |
| 5:F:578:SER:O     | 5:F:582:GLU:HG3   | 2.15                     | 0.47              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 7:I:45:DG:H2'     | 7:I:46:DG:C8     | 2.50                     | 0.47              |
| 2:C:178:PHE:O     | 2:C:440:LEU:HD11 | 2.15                     | 0.47              |
| 2:C:417:LEU:HD23  | 2:C:417:LEU:H    | 1.80                     | 0.47              |
| 2:C:529:LEU:HD21  | 2:C:671:ALA:CB   | 2.45                     | 0.47              |
| 2:C:856:ILE:HG21  | 2:C:1066:LYS:CE  | 2.45                     | 0.47              |
| 2:C:1184:VAL:O    | 2:C:1188:ARG:HG2 | 2.14                     | 0.47              |
| 2:C:1302:GLN:HG3  | 3:D:1352:LEU:CA  | 2.44                     | 0.47              |
| 3:D:434:LEU:HB3   | 3:D:437:GLN:HE21 | 1.79                     | 0.47              |
| 5:F:497:ILE:O     | 5:F:500:ILE:HG22 | 2.15                     | 0.47              |
| 1:A:62:ILE:HD11   | 1:A:88:ILE:HG21  | 1.96                     | 0.47              |
| 2:C:558:VAL:HG13  | 3:D:773:HIS:HD1  | 1.80                     | 0.47              |
| 2:C:676:PRO:HG2   | 2:C:1088:HIS:CE1 | 2.49                     | 0.47              |
| 2:C:717:ARG:O     | 2:C:724:ILE:HD11 | 2.15                     | 0.47              |
| 2:C:837:ILE:HA    | 2:C:1074:VAL:O   | 2.15                     | 0.47              |
| 2:C:1261:SER:O    | 3:D:350:ASP:HB2  | 2.14                     | 0.47              |
| 2:C:1273:LEU:HD11 | 5:F:564:GLU:HA   | 1.97                     | 0.47              |
| 2:C:1306:THR:HG22 | 2:C:1331:ALA:HB3 | 1.95                     | 0.47              |
| 3:D:126:ALA:HB1   | 3:D:131:MET:O    | 2.14                     | 0.47              |
| 3:D:257:LEU:CD2   | 5:F:563:ILE:HD13 | 2.45                     | 0.47              |
| 3:D:689:ALA:HA    | 3:D:692:ARG:HB3  | 1.97                     | 0.47              |
| 4:E:45:ASN:HB2    | 4:E:46:PRO:HD3   | 1.97                     | 0.47              |
| 5:F:117:ARG:CZ    | 6:H:-4:DG:N2     | 2.78                     | 0.47              |
| 1:A:120:THR:HB    | 1:A:126:ILE:HD11 | 1.96                     | 0.47              |
| 2:C:32:ARG:N      | 2:C:136:MET:HE1  | 2.30                     | 0.47              |
| 2:C:373:ASP:O     | 2:C:377:VAL:HG23 | 2.16                     | 0.47              |
| 2:C:550:ARG:HG3   | 2:C:550:ARG:O    | 2.15                     | 0.47              |
| 2:C:1046:ARG:O    | 2:C:1050:LYS:HG2 | 2.15                     | 0.47              |
| 2:C:1265:TYR:CE2  | 5:F:570:LEU:HD12 | 2.50                     | 0.47              |
| 3:D:112:VAL:CG2   | 3:D:302:GLN:HG2  | 2.38                     | 0.47              |
| 3:D:254:LEU:HD23  | 3:D:254:LEU:O    | 2.15                     | 0.47              |
| 3:D:405:ARG:HD2   | 3:D:407:GLN:OE1  | 2.15                     | 0.47              |
| 1:A:12:PRO:CG     | 1:A:33:PRO:HD2   | 2.45                     | 0.46              |
| 1:A:93:VAL:CG1    | 1:A:126:ILE:HG23 | 2.45                     | 0.46              |
| 3:D:414:LEU:HA    | 3:D:417:VAL:HG12 | 1.97                     | 0.46              |
| 3:D:480:LEU:HB2   | 4:E:46:PRO:HB3   | 1.96                     | 0.46              |
| 3:D:610:ARG:HE    | 3:D:862:GLU:HG2  | 1.80                     | 0.46              |
| 3:D:619:ILE:O     | 3:D:623:LYS:HG2  | 2.14                     | 0.46              |
| 3:D:698:MET:O     | 3:D:702:GLN:HG3  | 2.16                     | 0.46              |
| 5:F:612:THR:HG22  | 5:F:615:GLU:CG   | 2.42                     | 0.46              |
| 7:I:35:DA:H2'     | 7:I:36:DG:H8     | 1.79                     | 0.46              |
| 1:A:92:ALA:O      | 1:A:127:LEU:HB2  | 2.16                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:93:VAL:HG12   | 1:A:126:ILE:HG23  | 1.97                     | 0.46              |
| 1:B:82:VAL:HG23   | 3:D:528:ILE:HD13  | 1.97                     | 0.46              |
| 2:C:408:VAL:CG2   | 2:C:592:TYR:HB3   | 2.37                     | 0.46              |
| 2:C:560:PRO:HB2   | 2:C:647:GLY:CA    | 2.45                     | 0.46              |
| 2:C:840:GLU:HB2   | 2:C:1072:VAL:HG13 | 1.97                     | 0.46              |
| 2:C:1130:ILE:HG13 | 3:D:639:PHE:CD1   | 2.50                     | 0.46              |
| 2:C:1284:PHE:O    | 3:D:346:GLY:HA2   | 2.15                     | 0.46              |
| 3:D:344:LEU:O     | 3:D:347:LYS:HG3   | 2.15                     | 0.46              |
| 3:D:548:ALA:HB1   | 3:D:571:THR:CB    | 2.46                     | 0.46              |
| 3:D:559:PRO:CD    | 3:D:563:LEU:HD22  | 2.44                     | 0.46              |
| 3:D:781:ASP:O     | 3:D:785:LYS:HB2   | 2.16                     | 0.46              |
| 3:D:913:VAL:HG12  | 3:D:917:GLN:NE2   | 2.29                     | 0.46              |
| 3:D:923:GLY:O     | 3:D:924:THR:OG1   | 2.31                     | 0.46              |
| 4:E:22:LEU:CD1    | 4:E:61:GLU:HB2    | 2.45                     | 0.46              |
| 1:A:74:LEU:CD1    | 1:A:77:VAL:HG21   | 2.45                     | 0.46              |
| 1:B:68:VAL:CG2    | 1:B:70:GLU:HG2    | 2.44                     | 0.46              |
| 2:C:521:GLN:OE1   | 2:C:521:GLN:N     | 2.47                     | 0.46              |
| 2:C:821:SER:HB2   | 3:D:463:PHE:CB    | 2.45                     | 0.46              |
| 2:C:1031:SER:O    | 2:C:1034:ARG:HG2  | 2.14                     | 0.46              |
| 2:C:1093:VAL:HG23 | 3:D:463:PHE:O     | 2.16                     | 0.46              |
| 2:C:1119:LEU:HB3  | 3:D:727:ARG:CG    | 2.45                     | 0.46              |
| 2:C:1343:GLU:O    | 2:C:1347:LEU:HD12 | 2.15                     | 0.46              |
| 3:D:538:ALA:HB1   | 3:D:543:VAL:HG13  | 1.97                     | 0.46              |
| 3:D:739:MET:SD    | 3:D:756:VAL:HG23  | 2.55                     | 0.46              |
| 4:E:12:LYS:HB3    | 4:E:57:VAL:CG2    | 2.39                     | 0.46              |
| 5:F:447:GLU:HG2   | 5:F:482:SER:OG    | 2.14                     | 0.46              |
| 6:H:-14:DG:H2'    | 6:H:-13:DT:C6     | 2.50                     | 0.46              |
| 7:I:40:DC:C2'     | 7:I:41:DT:H71     | 2.45                     | 0.46              |
| 8:G:120:TRP:CZ3   | 8:G:122:ILE:HG13  | 2.50                     | 0.46              |
| 2:C:104:LEU:O     | 2:C:126:GLN:N     | 2.48                     | 0.46              |
| 2:C:398:PHE:HA    | 2:C:427:ILE:HD12  | 1.98                     | 0.46              |
| 2:C:706:LEU:HD11  | 2:C:805:ASN:HD22  | 1.80                     | 0.46              |
| 2:C:1135:LEU:HD13 | 2:C:1209:ILE:CD1  | 2.46                     | 0.46              |
| 3:D:426:ASN:N     | 3:D:469:ALA:O     | 2.35                     | 0.46              |
| 3:D:509:VAL:HG13  | 3:D:726:ALA:HB2   | 1.97                     | 0.46              |
| 4:E:38:VAL:CG1    | 4:E:52:GLU:HB3    | 2.45                     | 0.46              |
| 6:H:-36:DC:H2''   | 6:H:-35:DT:H5'    | 1.95                     | 0.46              |
| 7:I:-13:6MA:H2'   | 7:I:-12:DC:C6     | 2.50                     | 0.46              |
| 1:A:59:VAL:HB     | 1:A:88:ILE:HG22   | 1.97                     | 0.46              |
| 1:A:223:ILE:HG12  | 1:B:6:TRP:HB3     | 1.96                     | 0.46              |
| 2:C:10:ARG:HB2    | 2:C:797:LEU:HD12  | 1.96                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:533:THR:HG21 | 2:C:694:ARG:HB3   | 1.97                     | 0.46              |
| 2:C:859:ASP:OD1  | 2:C:860:ILE:N     | 2.48                     | 0.46              |
| 2:C:891:GLY:HA2  | 2:C:923:SER:CB    | 2.45                     | 0.46              |
| 3:D:49:THR:HG21  | 3:D:51:LYS:HE2    | 1.96                     | 0.46              |
| 3:D:99:ARG:CG    | 3:D:249:PRO:HG2   | 2.46                     | 0.46              |
| 3:D:277:ARG:HD2  | 3:D:300:MET:HG2   | 1.97                     | 0.46              |
| 3:D:311:ASN:ND2  | 3:D:326:LEU:O     | 2.42                     | 0.46              |
| 3:D:515:LEU:CD1  | 3:D:577:ILE:HD11  | 2.45                     | 0.46              |
| 3:D:616:ALA:O    | 3:D:619:ILE:HG22  | 2.15                     | 0.46              |
| 3:D:693:VAL:CG1  | 3:D:739:MET:HB2   | 2.37                     | 0.46              |
| 3:D:1156:PHE:HA  | 3:D:1164:ARG:NH2  | 2.30                     | 0.46              |
| 3:D:1342:GLY:O   | 3:D:1346:ASN:ND2  | 2.47                     | 0.46              |
| 5:F:506:THR:O    | 5:F:509:GLN:HG2   | 2.16                     | 0.46              |
| 5:F:588:LEU:O    | 5:F:596:GLU:HG3   | 2.16                     | 0.46              |
| 1:B:154:TYR:HA   | 1:B:175:LEU:HA    | 1.98                     | 0.46              |
| 2:C:85:ASP:O     | 2:C:89:CYS:N      | 2.48                     | 0.46              |
| 2:C:180:ALA:CB   | 2:C:440:LEU:HD22  | 2.45                     | 0.46              |
| 2:C:1045:ARG:O   | 2:C:1048:GLU:HG2  | 2.15                     | 0.46              |
| 2:C:1103:MET:O   | 2:C:1229:GLY:HA3  | 2.15                     | 0.46              |
| 3:D:135:ASP:HB3  | 3:D:160:LEU:HD11  | 1.97                     | 0.46              |
| 3:D:215:LYS:HE3  | 3:D:219:PHE:CE2   | 2.51                     | 0.46              |
| 3:D:701:LEU:HD21 | 3:D:719:TYR:HB2   | 1.96                     | 0.46              |
| 3:D:1143:ASP:O   | 3:D:1207:ILE:HD11 | 2.16                     | 0.46              |
| 3:D:1374:GLN:O   | 3:D:1378:GLN:HG3  | 2.15                     | 0.46              |
| 2:C:16:GLY:HA2   | 2:C:1202:ASP:O    | 2.15                     | 0.46              |
| 2:C:27:LEU:HD13  | 2:C:532:ILE:HG21  | 1.97                     | 0.46              |
| 2:C:526:THR:HG22 | 2:C:697:VAL:HA    | 1.98                     | 0.46              |
| 2:C:1103:MET:HE3 | 2:C:1115:VAL:HG23 | 1.98                     | 0.46              |
| 3:D:114:HIS:HD2  | 3:D:116:TRP:HB2   | 1.81                     | 0.46              |
| 3:D:290:PRO:CB   | 5:F:417:LYS:HG3   | 2.40                     | 0.46              |
| 3:D:318:ILE:HG23 | 3:D:324:ARG:O     | 2.16                     | 0.46              |
| 3:D:497:ASN:HD21 | 3:D:1243:PRO:HG2  | 1.81                     | 0.46              |
| 3:D:615:LYS:HE2  | 4:E:5:THR:OG1     | 2.15                     | 0.46              |
| 3:D:1328:LEU:O   | 3:D:1332:SER:N    | 2.39                     | 0.46              |
| 1:A:78:ARG:HB3   | 1:A:135:THR:HB    | 1.98                     | 0.46              |
| 1:A:105:LEU:N    | 1:A:144:MET:O     | 2.37                     | 0.46              |
| 1:B:62:ILE:HG21  | 1:B:170:ILE:HB    | 1.97                     | 0.46              |
| 1:B:127:LEU:CD2  | 1:B:209:ALA:HA    | 2.44                     | 0.46              |
| 2:C:70:ALA:CB    | 2:C:492:ILE:HG21  | 2.46                     | 0.46              |
| 2:C:563:TYR:HE2  | 3:D:765:VAL:HG12  | 1.79                     | 0.46              |
| 2:C:807:LEU:HD11 | 2:C:1241:VAL:CG1  | 2.46                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:823:LEU:HD22  | 2:C:1115:VAL:HB   | 1.97                     | 0.46              |
| 3:D:532:LEU:HD22  | 3:D:579:ALA:CB    | 2.44                     | 0.46              |
| 3:D:882:LEU:HD13  | 3:D:1226:ALA:CB   | 2.46                     | 0.46              |
| 5:F:501:ASN:HA    | 5:F:504:VAL:HG22  | 1.98                     | 0.46              |
| 8:G:118:CYS:HB3   | 8:G:133:CYS:HB2   | 1.96                     | 0.46              |
| 1:A:128:ASN:HB3   | 1:A:131:HIS:HB2   | 1.98                     | 0.46              |
| 1:B:136:LEU:HD22  | 1:B:139:GLY:HA3   | 1.98                     | 0.46              |
| 1:B:211:THR:HG23  | 1:B:214:ASP:H     | 1.81                     | 0.46              |
| 2:C:707:VAL:HG23  | 2:C:1135:LEU:CD2  | 2.46                     | 0.46              |
| 2:C:934:ILE:HD13  | 2:C:1072:VAL:HG23 | 1.98                     | 0.46              |
| 3:D:244:VAL:HG23  | 3:D:309:PHE:HZ    | 1.81                     | 0.46              |
| 3:D:394:GLY:HA3   | 5:F:646:LYS:HG3   | 1.98                     | 0.46              |
| 3:D:453:PRO:HD2   | 3:D:625:MET:SD    | 2.55                     | 0.46              |
| 3:D:504:PRO:HG2   | 3:D:601:ILE:CD1   | 2.46                     | 0.46              |
| 3:D:664:TYR:HB2   | 3:D:681:LYS:NZ    | 2.31                     | 0.46              |
| 5:F:420:VAL:HG22  | 5:F:452:LEU:CD2   | 2.46                     | 0.46              |
| 1:A:235:GLU:HG2   | 1:B:218:TYR:CE1   | 2.51                     | 0.46              |
| 2:C:191:ASP:O     | 2:C:203:ARG:N     | 2.49                     | 0.46              |
| 2:C:417:LEU:HD12  | 2:C:435:ALA:CB    | 2.46                     | 0.46              |
| 2:C:422:SER:HB3   | 2:C:425:VAL:CG1   | 2.46                     | 0.46              |
| 2:C:729:GLY:N     | 2:C:744:THR:HA    | 2.31                     | 0.46              |
| 2:C:816:TYR:CB    | 2:C:823:LEU:HD12  | 2.43                     | 0.46              |
| 2:C:846:ALA:H     | 2:C:1064:VAL:CG2  | 2.29                     | 0.46              |
| 2:C:901:MET:SD    | 2:C:906:LYS:HD2   | 2.56                     | 0.46              |
| 2:C:1142:LEU:O    | 2:C:1146:ILE:HG22 | 2.16                     | 0.46              |
| 2:C:1166:LEU:HA   | 2:C:1215:MET:HE1  | 1.98                     | 0.46              |
| 3:D:203:LEU:O     | 3:D:203:LEU:HD23  | 2.16                     | 0.46              |
| 3:D:284:LEU:HD12  | 3:D:297:GLU:HG2   | 1.97                     | 0.46              |
| 3:D:354:ARG:HD3   | 7:I:2:DA:H4'      | 1.98                     | 0.46              |
| 3:D:476:LEU:CD1   | 4:E:46:PRO:HG3    | 2.46                     | 0.46              |
| 3:D:539:MET:CE    | 3:D:546:LEU:HD13  | 2.45                     | 0.46              |
| 3:D:1145:ALA:HB2  | 3:D:1207:ILE:HG12 | 1.97                     | 0.46              |
| 5:F:123:MET:O     | 5:F:127:GLU:HB2   | 2.16                     | 0.46              |
| 5:F:180:ILE:HA    | 5:F:303:ASN:N     | 2.31                     | 0.46              |
| 2:C:142:PHE:HB3   | 2:C:514:PHE:CE2   | 2.50                     | 0.45              |
| 2:C:759:MET:HE1   | 2:C:775:PRO:HB3   | 1.98                     | 0.45              |
| 2:C:882:GLU:HG3   | 2:C:932:GLY:CA    | 2.46                     | 0.45              |
| 2:C:1262:ILE:CD1  | 5:F:571:PRO:HB2   | 2.46                     | 0.45              |
| 2:C:1312:VAL:HG12 | 2:C:1335:GLU:OE2  | 2.16                     | 0.45              |
| 3:D:251:LEU:O     | 3:D:253:PRO:HD3   | 2.15                     | 0.45              |
| 3:D:481:GLU:OE1   | 4:E:20:VAL:HG21   | 2.16                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:882:LEU:HD13  | 3:D:1226:ALA:HB1  | 1.98                     | 0.45              |
| 4:E:30:ILE:CG1    | 4:E:34:ALA:HB3    | 2.46                     | 0.45              |
| 1:A:8:GLU:HA      | 1:B:152:LYS:HZ2   | 1.81                     | 0.45              |
| 1:B:45:ALA:HB1    | 1:B:223:LEU:HD22  | 1.97                     | 0.45              |
| 1:B:57:ALA:HB1    | 1:B:148:VAL:HG23  | 1.98                     | 0.45              |
| 1:B:110:PRO:HG3   | 1:B:138:ASP:H     | 1.82                     | 0.45              |
| 2:C:735:ASP:OD1   | 2:C:735:ASP:N     | 2.45                     | 0.45              |
| 2:C:834:PHE:HB3   | 2:C:1078:LEU:HD21 | 1.99                     | 0.45              |
| 2:C:1240:THR:H    | 3:D:638:SER:CB    | 2.30                     | 0.45              |
| 3:D:36:PHE:HB2    | 3:D:62:ILE:O      | 2.16                     | 0.45              |
| 3:D:452:HIS:NE2   | 3:D:625:MET:SD    | 2.89                     | 0.45              |
| 3:D:454:LEU:HD11  | 3:D:625:MET:HB2   | 1.97                     | 0.45              |
| 3:D:481:GLU:OE1   | 4:E:20:VAL:HG11   | 2.17                     | 0.45              |
| 3:D:655:GLU:O     | 3:D:658:ARG:HG2   | 2.17                     | 0.45              |
| 3:D:823:GLU:OE1   | 3:D:828:LEU:HB2   | 2.14                     | 0.45              |
| 3:D:1323:GLU:O    | 3:D:1327:VAL:HG12 | 2.16                     | 0.45              |
| 5:F:635:LEU:O     | 5:F:639:LYS:HE3   | 2.16                     | 0.45              |
| 2:C:35:TYR:CE1    | 2:C:464:VAL:HG22  | 2.48                     | 0.45              |
| 2:C:623:VAL:HG22  | 2:C:652:LEU:HD13  | 1.98                     | 0.45              |
| 2:C:856:ILE:HG21  | 2:C:1066:LYS:CD   | 2.47                     | 0.45              |
| 2:C:985:LEU:HD21  | 2:C:1029:LEU:CD1  | 2.46                     | 0.45              |
| 3:D:838:ARG:HB3   | 3:D:878:VAL:CG1   | 2.46                     | 0.45              |
| 7:I:-13:6MA:H8    | 7:I:-13:6MA:C5'   | 2.44                     | 0.45              |
| 1:A:88:ILE:CD1    | 1:A:133:LEU:HD13  | 2.45                     | 0.45              |
| 1:B:115:ALA:O     | 1:B:118:ILE:HG22  | 2.16                     | 0.45              |
| 2:C:139:LYS:HG3   | 2:C:141:THR:HG23  | 1.97                     | 0.45              |
| 2:C:565:ARG:CG    | 2:C:597:SER:HB3   | 2.46                     | 0.45              |
| 2:C:681:ASP:OD2   | 2:C:1088:HIS:HB3  | 2.16                     | 0.45              |
| 2:C:702:SER:HA    | 2:C:804:ARG:HG2   | 1.98                     | 0.45              |
| 2:C:723:VAL:HG22  | 2:C:790:ALA:HB3   | 1.99                     | 0.45              |
| 2:C:741:ILE:HG13  | 2:C:757:TYR:HE2   | 1.82                     | 0.45              |
| 2:C:834:PHE:CB    | 2:C:1078:LEU:HD11 | 2.46                     | 0.45              |
| 2:C:1037:ASP:HA   | 2:C:1040:ARG:HD2  | 1.98                     | 0.45              |
| 2:C:1286:GLU:O    | 2:C:1289:VAL:HG12 | 2.16                     | 0.45              |
| 3:D:423:VAL:O     | 3:D:438:ALA:HA    | 2.17                     | 0.45              |
| 3:D:702:GLN:HG2   | 3:D:719:TYR:CE1   | 2.51                     | 0.45              |
| 3:D:847:PRO:HG2   | 3:D:872:VAL:O     | 2.15                     | 0.45              |
| 3:D:1230:VAL:O    | 3:D:1234:GLN:HG2  | 2.16                     | 0.45              |
| 3:D:1262:ILE:HA   | 3:D:1298:THR:CG2  | 2.36                     | 0.45              |
| 3:D:1312:THR:HG23 | 3:D:1314:SER:O    | 2.17                     | 0.45              |
| 5:F:452:LEU:HB2   | 5:F:475:ILE:CD1   | 2.40                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:I:46:DG:H2''    | 7:I:47:DC:C6      | 2.52                     | 0.45              |
| 1:A:175:LEU:HD12  | 1:A:175:LEU:O     | 2.16                     | 0.45              |
| 2:C:150:VAL:HG12  | 2:C:523:MET:CG    | 2.46                     | 0.45              |
| 2:C:208:ARG:HB2   | 2:C:377:VAL:HG13  | 1.98                     | 0.45              |
| 2:C:214:THR:O     | 2:C:370:ALA:HB1   | 2.16                     | 0.45              |
| 2:C:984:LEU:HD11  | 2:C:988:LYS:HE3   | 1.98                     | 0.45              |
| 3:D:264:THR:HG22  | 5:F:544:PRO:HB2   | 1.97                     | 0.45              |
| 3:D:512:LEU:HD11  | 3:D:624:VAL:HG22  | 1.98                     | 0.45              |
| 3:D:797:VAL:HG22  | 3:D:916:ALA:HB3   | 1.97                     | 0.45              |
| 3:D:1353:ILE:HG23 | 3:D:1354:PRO:HD2  | 1.99                     | 0.45              |
| 1:A:258:VAL:N     | 1:A:277:VAL:O     | 2.49                     | 0.45              |
| 1:B:81:VAL:O      | 1:B:85:VAL:HG12   | 2.16                     | 0.45              |
| 1:B:181:ARG:O     | 1:B:205:GLU:N     | 2.46                     | 0.45              |
| 1:B:182:VAL:CG2   | 1:B:204:VAL:HG12  | 2.39                     | 0.45              |
| 2:C:32:ARG:HA     | 2:C:136:MET:SD    | 2.56                     | 0.45              |
| 2:C:667:VAL:HG11  | 3:D:765:VAL:HG13  | 1.99                     | 0.45              |
| 3:D:300:MET:SD    | 5:F:443:ASP:HA    | 2.57                     | 0.45              |
| 3:D:382:PHE:HZ    | 3:D:474:LEU:HA    | 1.82                     | 0.45              |
| 3:D:468:MET:HE3   | 3:D:468:MET:HB3   | 1.92                     | 0.45              |
| 3:D:507:ASP:HB3   | 3:D:629:PHE:CE1   | 2.43                     | 0.45              |
| 3:D:538:ALA:HB1   | 3:D:543:VAL:CG1   | 2.46                     | 0.45              |
| 3:D:1231:ASP:O    | 3:D:1235:GLU:HG3  | 2.17                     | 0.45              |
| 1:A:16:GLN:HG2    | 1:A:16:GLN:O      | 2.16                     | 0.45              |
| 1:A:30:VAL:CG1    | 1:A:200:LYS:HD2   | 2.47                     | 0.45              |
| 1:A:46:LEU:O      | 1:A:50:LEU:HB3    | 2.16                     | 0.45              |
| 1:A:91:LEU:HD11   | 1:A:115:ALA:HB1   | 1.97                     | 0.45              |
| 2:C:1256:LYS:HE3  | 7:I:3:DT:C4'      | 2.46                     | 0.45              |
| 2:C:1285:GLY:HA3  | 7:I:1:DA:P        | 2.56                     | 0.45              |
| 3:D:280:ARG:HB3   | 3:D:297:GLU:OE2   | 2.16                     | 0.45              |
| 3:D:661:ALA:HA    | 3:D:681:LYS:CD    | 2.44                     | 0.45              |
| 5:F:441:PHE:CE1   | 6:H:-5:DC:C4      | 3.04                     | 0.45              |
| 7:I:-16:DG:H2''   | 7:I:-15:DC:O5'    | 2.17                     | 0.45              |
| 7:I:1:DA:C2       | 7:I:2:DA:H1'      | 2.52                     | 0.45              |
| 1:B:10:ILE:CG2    | 1:B:33:PRO:HB2    | 2.47                     | 0.45              |
| 2:C:100:LEU:HD11  | 2:C:133:ILE:HD13  | 1.98                     | 0.45              |
| 2:C:912:PHE:HZ    | 5:F:648:ARG:HA    | 1.81                     | 0.45              |
| 2:C:1139:CYS:O    | 2:C:1193:GLY:HA2  | 2.16                     | 0.45              |
| 2:C:1296:GLY:HA3  | 4:E:17:PHE:CE1    | 2.52                     | 0.45              |
| 2:C:1348:GLY:H    | 3:D:114:HIS:CE1   | 2.34                     | 0.45              |
| 3:D:804:ILE:HG13  | 3:D:1343:LEU:HD13 | 1.98                     | 0.45              |
| 5:F:420:VAL:HG22  | 5:F:452:LEU:HD23  | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:F:547:LEU:HG    | 5:F:560:GLY:CA    | 2.47                     | 0.45              |
| 7:I:38:DG:H2''    | 7:I:39:DG:C8      | 2.52                     | 0.45              |
| 2:C:15:PHE:HE2    | 2:C:1135:LEU:HD21 | 1.82                     | 0.45              |
| 2:C:24:MET:CE     | 2:C:27:LEU:HD21   | 2.46                     | 0.45              |
| 2:C:89:CYS:SG     | 2:C:94:MET:HG3    | 2.57                     | 0.45              |
| 2:C:111:THR:HB    | 2:C:118:ARG:HE    | 1.82                     | 0.45              |
| 2:C:139:LYS:O     | 2:C:535:LYS:NZ    | 2.41                     | 0.45              |
| 2:C:636:ILE:CG1   | 2:C:654:LYS:HG3   | 2.43                     | 0.45              |
| 2:C:707:VAL:CG1   | 2:C:1132:GLU:HG2  | 2.46                     | 0.45              |
| 2:C:707:VAL:HG21  | 2:C:1135:LEU:HB3  | 1.98                     | 0.45              |
| 2:C:730:VAL:HG12  | 2:C:742:ARG:HE    | 1.81                     | 0.45              |
| 2:C:1163:VAL:HA   | 2:C:1166:LEU:HD21 | 1.99                     | 0.45              |
| 2:C:1308:LYS:HD3  | 3:D:349:VAL:CG2   | 2.47                     | 0.45              |
| 3:D:26:ALA:HA     | 3:D:30:LYS:NZ     | 2.32                     | 0.45              |
| 3:D:136:ILE:HA    | 3:D:139:VAL:HG12  | 1.98                     | 0.45              |
| 3:D:147:VAL:HG21  | 3:D:156:LYS:O     | 2.16                     | 0.45              |
| 3:D:372:LYS:HB3   | 3:D:411:TRP:CZ3   | 2.52                     | 0.45              |
| 3:D:416:GLU:O     | 4:E:44:LYS:NZ     | 2.46                     | 0.45              |
| 3:D:492:ILE:O     | 3:D:501:ILE:N     | 2.46                     | 0.45              |
| 3:D:548:ALA:C     | 3:D:571:THR:HB    | 2.37                     | 0.45              |
| 3:D:756:VAL:O     | 3:D:757:SER:OG    | 2.32                     | 0.45              |
| 5:F:595:GLU:HA    | 5:F:598:VAL:HG22  | 1.98                     | 0.45              |
| 7:I:20:DG:H2''    | 7:I:21:DT:H5'     | 1.97                     | 0.45              |
| 1:B:175:LEU:HD11  | 1:B:180:LYS:NZ    | 2.31                     | 0.45              |
| 2:C:118:ARG:HG2   | 2:C:119:SER:H     | 1.82                     | 0.45              |
| 2:C:140:GLY:O     | 2:C:535:LYS:HD3   | 2.17                     | 0.45              |
| 2:C:577:ILE:CD1   | 3:D:779:LEU:HG    | 2.47                     | 0.45              |
| 2:C:808:VAL:HB    | 2:C:1244:ILE:HG22 | 1.99                     | 0.45              |
| 2:C:821:SER:HB2   | 3:D:463:PHE:HB3   | 1.99                     | 0.45              |
| 2:C:824:ILE:HB    | 2:C:1094:ILE:CG1  | 2.47                     | 0.45              |
| 2:C:959:ILE:HD13  | 2:C:1051:VAL:HG23 | 1.99                     | 0.45              |
| 3:D:145:TYR:HB2   | 3:D:161:LEU:O     | 2.17                     | 0.45              |
| 3:D:337:GLN:HG2   | 5:F:558:HIS:HD2   | 1.82                     | 0.45              |
| 3:D:397:LYS:HE2   | 5:F:652:ASP:HB2   | 1.98                     | 0.45              |
| 3:D:639:PHE:CE2   | 3:D:718:ILE:HB    | 2.52                     | 0.45              |
| 3:D:745:LYS:HA    | 3:D:773:HIS:NE2   | 2.32                     | 0.45              |
| 3:D:823:GLU:OE1   | 3:D:823:GLU:N     | 2.50                     | 0.45              |
| 3:D:1312:THR:HG21 | 3:D:1318:ALA:HB2  | 1.98                     | 0.45              |
| 5:F:482:SER:HB2   | 5:F:486:GLN:NE2   | 2.32                     | 0.45              |
| 5:F:572:ILE:O     | 5:F:576:ILE:HD12  | 2.17                     | 0.45              |
| 6:H:-2:DT:H3'     | 6:H:-2:DT:OP2     | 2.17                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:I:30:DT:H2''    | 7:I:31:DG:C5'     | 2.46                     | 0.45              |
| 1:A:34:LEU:O      | 1:A:198:TYR:HB3   | 2.16                     | 0.44              |
| 1:A:89:LYS:NZ     | 2:C:832:ASP:HB2   | 2.31                     | 0.44              |
| 1:B:89:LYS:HG3    | 1:B:174:ALA:HB2   | 1.99                     | 0.44              |
| 1:B:230:PHE:HB2   | 1:B:233:PHE:CD2   | 2.53                     | 0.44              |
| 2:C:97:ALA:CB     | 2:C:132:ASP:HB2   | 2.47                     | 0.44              |
| 2:C:100:LEU:N     | 2:C:131:GLY:O     | 2.48                     | 0.44              |
| 2:C:405:LEU:HB3   | 2:C:426:ARG:O     | 2.17                     | 0.44              |
| 2:C:966:ARG:HB2   | 2:C:1047:PHE:CE2  | 2.52                     | 0.44              |
| 2:C:1081:GLY:C    | 2:C:1253:VAL:HB   | 2.37                     | 0.44              |
| 3:D:142:PHE:CE2   | 3:D:183:GLY:HA3   | 2.52                     | 0.44              |
| 3:D:396:VAL:H     | 5:F:579:ASN:ND2   | 2.14                     | 0.44              |
| 3:D:492:ILE:HG23  | 3:D:502:ILE:HG22  | 1.99                     | 0.44              |
| 7:I:24:DC:H2''    | 7:I:25:DC:C6      | 2.52                     | 0.44              |
| 1:B:40:VAL:CA     | 1:B:186:VAL:HG21  | 2.47                     | 0.44              |
| 2:C:1301:LEU:O    | 2:C:1305:LEU:HG   | 2.17                     | 0.44              |
| 3:D:22:ARG:HA     | 3:D:1337:THR:HA   | 1.98                     | 0.44              |
| 3:D:70:GLU:HA     | 3:D:77:LYS:HA     | 1.99                     | 0.44              |
| 3:D:112:VAL:HG12  | 3:D:241:LEU:O     | 2.18                     | 0.44              |
| 3:D:122:PRO:HG3   | 3:D:1326:ARG:NE   | 2.32                     | 0.44              |
| 3:D:265:SER:HA    | 5:F:547:LEU:CB    | 2.48                     | 0.44              |
| 3:D:424:LEU:HD23  | 3:D:436:ILE:HG21  | 1.98                     | 0.44              |
| 5:F:179:VAL:O     | 5:F:303:ASN:N     | 2.30                     | 0.44              |
| 5:F:442:LEU:HD21  | 5:F:446:GLN:NE2   | 2.33                     | 0.44              |
| 5:F:493:PRO:HG2   | 5:F:496:MET:HB2   | 2.00                     | 0.44              |
| 2:C:24:MET:HE1    | 2:C:585:THR:OG1   | 2.18                     | 0.44              |
| 2:C:572:PRO:HA    | 2:C:691:ASN:HD21  | 1.81                     | 0.44              |
| 2:C:723:VAL:CG2   | 2:C:790:ALA:HB3   | 2.48                     | 0.44              |
| 2:C:930:VAL:HG13  | 2:C:1074:VAL:CG1  | 2.47                     | 0.44              |
| 2:C:1176:LEU:HB3  | 2:C:1177:PRO:HD3  | 1.98                     | 0.44              |
| 2:C:1285:GLY:O    | 2:C:1289:VAL:N    | 2.47                     | 0.44              |
| 2:C:1306:THR:HG22 | 2:C:1331:ALA:HB1  | 2.00                     | 0.44              |
| 3:D:216:GLN:NE2   | 3:D:1271:ILE:HD13 | 2.32                     | 0.44              |
| 3:D:241:LEU:HD23  | 3:D:241:LEU:H     | 1.81                     | 0.44              |
| 3:D:353:GLY:O     | 3:D:470:VAL:N     | 2.34                     | 0.44              |
| 3:D:497:ASN:C     | 3:D:899:LEU:HD12  | 2.37                     | 0.44              |
| 3:D:831:LEU:O     | 3:D:835:VAL:HG12  | 2.18                     | 0.44              |
| 4:E:6:VAL:HG13    | 4:E:19:LEU:CD2    | 2.48                     | 0.44              |
| 7:I:-5:6MA:H8     | 7:I:-5:6MA:O5'    | 2.17                     | 0.44              |
| 7:I:16:DC:H2''    | 7:I:17:DG:H5''    | 1.98                     | 0.44              |
| 1:A:67:VAL:CG2    | 1:A:81:VAL:HG21   | 2.36                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:77:TYR:HA    | 2:C:102:VAL:HA    | 2.00                     | 0.44              |
| 2:C:536:ARG:O    | 2:C:582:SER:HB2   | 2.18                     | 0.44              |
| 2:C:692:MET:HG3  | 2:C:1249:LEU:HD21 | 2.00                     | 0.44              |
| 2:C:844:VAL:CG1  | 2:C:890:VAL:HG21  | 2.40                     | 0.44              |
| 2:C:1163:VAL:O   | 2:C:1166:LEU:HG   | 2.18                     | 0.44              |
| 3:D:142:PHE:CD2  | 3:D:295:ARG:HB2   | 2.52                     | 0.44              |
| 3:D:144:TYR:HD1  | 3:D:162:SER:HB3   | 1.83                     | 0.44              |
| 3:D:432:HIS:HE1  | 3:D:434:LEU:HB2   | 1.82                     | 0.44              |
| 3:D:512:LEU:HD11 | 3:D:624:VAL:CG2   | 2.48                     | 0.44              |
| 3:D:1370:LYS:O   | 3:D:1374:GLN:HG2  | 2.17                     | 0.44              |
| 5:F:420:VAL:HG13 | 5:F:452:LEU:CD2   | 2.46                     | 0.44              |
| 5:F:502:LYS:O    | 5:F:506:THR:HG23  | 2.18                     | 0.44              |
| 2:C:371:LEU:O    | 2:C:389:ALA:HB1   | 2.16                     | 0.44              |
| 2:C:685:ARG:CZ   | 2:C:1124:ARG:HD2  | 2.48                     | 0.44              |
| 2:C:860:ILE:HG21 | 2:C:921:ASP:OD1   | 2.17                     | 0.44              |
| 2:C:1098:LEU:HB2 | 2:C:1103:MET:SD   | 2.57                     | 0.44              |
| 2:C:1149:LEU:CD2 | 2:C:1159:LYS:HB2  | 2.45                     | 0.44              |
| 2:C:1302:GLN:HG3 | 3:D:1352:LEU:HA   | 2.00                     | 0.44              |
| 3:D:26:ALA:HB1   | 3:D:31:ILE:CD1    | 2.38                     | 0.44              |
| 3:D:266:ASP:HB3  | 5:F:548:GLU:OE1   | 2.18                     | 0.44              |
| 3:D:345:LEU:HD11 | 3:D:1344:LYS:HD2  | 2.00                     | 0.44              |
| 3:D:484:VAL:HA   | 4:E:6:VAL:HG21    | 1.98                     | 0.44              |
| 3:D:715:ILE:HD11 | 3:D:719:TYR:CD2   | 2.52                     | 0.44              |
| 3:D:792:LEU:HD11 | 3:D:1136:PHE:CD2  | 2.49                     | 0.44              |
| 5:F:432:LYS:HD2  | 6:H:-5:DC:H4'     | 1.98                     | 0.44              |
| 7:I:0:DT:C7      | 7:I:1:DA:H62      | 2.28                     | 0.44              |
| 1:B:112:PRO:HB3  | 1:B:133:LEU:CB    | 2.45                     | 0.44              |
| 2:C:1123:SER:HB2 | 3:D:727:ARG:CB    | 2.43                     | 0.44              |
| 3:D:130:ASP:HB2  | 3:D:222:ARG:CZ    | 2.47                     | 0.44              |
| 3:D:584:HIS:ND1  | 3:D:585:PRO:O     | 2.51                     | 0.44              |
| 3:D:635:ALA:CB   | 3:D:637:ILE:HD11  | 2.48                     | 0.44              |
| 3:D:683:VAL:HA   | 3:D:687:ALA:CB    | 2.41                     | 0.44              |
| 3:D:764:THR:CG2  | 3:D:767:GLU:HG2   | 2.47                     | 0.44              |
| 5:F:426:LEU:CD2  | 5:F:426:LEU:C     | 2.86                     | 0.44              |
| 6:H:-43:DT:H2''  | 6:H:-42:DT:C6     | 2.53                     | 0.44              |
| 1:A:62:ILE:HG13  | 1:A:172:VAL:HG11  | 1.99                     | 0.44              |
| 1:A:162:PRO:HB3  | 2:C:882:GLU:CD    | 2.37                     | 0.44              |
| 1:A:225:GLN:HE22 | 1:B:230:PHE:HE2   | 1.66                     | 0.44              |
| 2:C:71:VAL:HG12  | 2:C:107:ILE:HG12  | 2.00                     | 0.44              |
| 2:C:149:ARG:HA   | 2:C:523:MET:CB    | 2.47                     | 0.44              |
| 2:C:815:GLY:HA3  | 3:D:629:PHE:CG    | 2.52                     | 0.44              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:1322:ILE:HG22 | 3:D:381:PRO:HB2  | 1.98                     | 0.44              |
| 3:D:500:PRO:O     | 3:D:503:VAL:HG13 | 2.17                     | 0.44              |
| 3:D:819:ARG:HB2   | 3:D:875:SER:HB3  | 1.99                     | 0.44              |
| 3:D:1135:LEU:HG   | 3:D:1232:GLU:CD  | 2.38                     | 0.44              |
| 5:F:453:MET:HE3   | 5:F:453:MET:HB2  | 1.78                     | 0.44              |
| 5:F:481:ARG:CD    | 5:F:494:VAL:HG11 | 2.40                     | 0.44              |
| 8:G:116:HIS:HB3   | 8:G:138:SER:OG   | 2.18                     | 0.44              |
| 1:A:55:GLN:HA     | 1:A:151:GLY:O    | 2.18                     | 0.44              |
| 2:C:9:LYS:CG      | 2:C:797:LEU:HD13 | 2.40                     | 0.44              |
| 2:C:792:GLY:N     | 2:C:795:THR:OG1  | 2.50                     | 0.44              |
| 2:C:1053:LYS:HB2  | 2:C:1053:LYS:HE3 | 1.79                     | 0.44              |
| 3:D:332:MET:O     | 3:D:338:GLY:HA3  | 2.18                     | 0.44              |
| 3:D:679:TYR:HA    | 3:D:682:VAL:CG1  | 2.48                     | 0.44              |
| 3:D:1159:ASP:OD1  | 3:D:1159:ASP:N   | 2.46                     | 0.44              |
| 3:D:1276:LEU:O    | 3:D:1280:GLU:HG3 | 2.17                     | 0.44              |
| 2:C:142:PHE:CZ    | 2:C:464:VAL:HG11 | 2.53                     | 0.44              |
| 2:C:628:ASN:ND2   | 2:C:1202:ASP:OD1 | 2.51                     | 0.44              |
| 2:C:697:VAL:HG11  | 2:C:838:HIS:CE1  | 2.53                     | 0.44              |
| 2:C:722:VAL:HG12  | 2:C:792:GLY:N    | 2.33                     | 0.44              |
| 2:C:1087:ARG:HB2  | 2:C:1245:TYR:O   | 2.18                     | 0.44              |
| 2:C:1353:LEU:HD13 | 3:D:18:PHE:CG    | 2.52                     | 0.44              |
| 3:D:114:HIS:HB2   | 3:D:239:MET:O    | 2.17                     | 0.44              |
| 3:D:322:ASN:HD21  | 3:D:324:ARG:HD3  | 1.83                     | 0.44              |
| 3:D:548:ALA:CA    | 3:D:571:THR:HB   | 2.48                     | 0.44              |
| 3:D:663:GLU:HG3   | 3:D:664:TYR:CD2  | 2.53                     | 0.44              |
| 7:I:-19:DG:H2''   | 7:I:-18:DT:C5'   | 2.47                     | 0.44              |
| 1:A:8:GLU:HB2     | 1:B:152:LYS:HZ1  | 1.83                     | 0.43              |
| 1:A:48:ARG:HD2    | 1:B:41:THR:CB    | 2.34                     | 0.43              |
| 2:C:210:LEU:HD11  | 2:C:374:ILE:CD1  | 2.48                     | 0.43              |
| 2:C:834:PHE:O     | 2:C:1248:LYS:HD2 | 2.18                     | 0.43              |
| 2:C:1085:ALA:HA   | 2:C:1091:LYS:HA  | 1.98                     | 0.43              |
| 3:D:337:GLN:HA    | 3:D:342:GLN:CB   | 2.48                     | 0.43              |
| 3:D:626:GLY:O     | 3:D:630:LYS:HG3  | 2.18                     | 0.43              |
| 3:D:687:ALA:O     | 3:D:690:THR:HG22 | 2.18                     | 0.43              |
| 3:D:713:LYS:HG3   | 3:D:714:GLU:H    | 1.83                     | 0.43              |
| 3:D:895:TYR:CE2   | 3:D:911:VAL:HG13 | 2.53                     | 0.43              |
| 3:D:1164:ARG:NH2  | 3:D:1167:LYS:HE2 | 2.33                     | 0.43              |
| 4:E:3:ARG:HG2     | 4:E:47:VAL:HG21  | 2.00                     | 0.43              |
| 5:F:369:PHE:HA    | 5:F:373:ASP:CB   | 2.47                     | 0.43              |
| 5:F:627:ILE:O     | 5:F:630:ILE:HG12 | 2.18                     | 0.43              |
| 1:B:68:VAL:HG22   | 1:B:70:GLU:HG2   | 2.00                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:98:GLU:OE1    | 1:B:150:ASN:HB3   | 2.18                     | 0.43              |
| 2:C:158:SER:HB3   | 2:C:412:LYS:HZ3   | 1.83                     | 0.43              |
| 2:C:201:TYR:CD1   | 2:C:211:PRO:HA    | 2.48                     | 0.43              |
| 2:C:527:ASN:ND2   | 2:C:802:LEU:HD11  | 2.32                     | 0.43              |
| 2:C:1127:VAL:HG12 | 3:D:759:PHE:HB3   | 1.99                     | 0.43              |
| 2:C:1132:GLU:OE1  | 2:C:1244:ILE:HG13 | 2.17                     | 0.43              |
| 3:D:182:ILE:N     | 3:D:186:ALA:HB2   | 2.33                     | 0.43              |
| 3:D:743:MET:CE    | 3:D:771:SER:HA    | 2.47                     | 0.43              |
| 3:D:835:VAL:HG23  | 3:D:878:VAL:CG2   | 2.47                     | 0.43              |
| 4:E:30:ILE:HG12   | 4:E:34:ALA:HB3    | 1.99                     | 0.43              |
| 5:F:551:ILE:HG21  | 5:F:562:PHE:HE2   | 1.82                     | 0.43              |
| 5:F:588:LEU:HB3   | 5:F:596:GLU:CG    | 2.48                     | 0.43              |
| 5:F:600:ARG:CD    | 5:F:605:ILE:HB    | 2.46                     | 0.43              |
| 1:A:28:ARG:HA     | 1:A:204:GLU:HA    | 2.01                     | 0.43              |
| 1:A:51:LEU:CD2    | 1:A:51:LEU:C      | 2.87                     | 0.43              |
| 1:A:77:VAL:HG21   | 1:A:142:VAL:HG11  | 2.00                     | 0.43              |
| 2:C:891:GLY:HA2   | 2:C:923:SER:HB2   | 2.00                     | 0.43              |
| 2:C:1163:VAL:HG12 | 2:C:1176:LEU:HD22 | 2.00                     | 0.43              |
| 2:C:1292:LEU:HD12 | 2:C:1301:LEU:CD2  | 2.49                     | 0.43              |
| 3:D:71:CYS:SG     | 3:D:91:VAL:HG13   | 2.58                     | 0.43              |
| 3:D:139:VAL:HG21  | 3:D:146:ILE:HB    | 2.00                     | 0.43              |
| 3:D:289:ALA:O     | 3:D:294:ILE:HD11  | 2.17                     | 0.43              |
| 3:D:366:HIS:HA    | 3:D:488:SER:OG    | 2.18                     | 0.43              |
| 3:D:512:LEU:HG    | 3:D:577:ILE:HG12  | 2.00                     | 0.43              |
| 3:D:882:LEU:CD1   | 3:D:1226:ALA:HB1  | 2.49                     | 0.43              |
| 3:D:1155:GLU:HG2  | 3:D:1167:LYS:HB3  | 2.01                     | 0.43              |
| 3:D:1233:ILE:HG21 | 3:D:1249:ILE:CD1  | 2.48                     | 0.43              |
| 5:F:143:ALA:HB2   | 8:G:130:PHE:CE2   | 2.53                     | 0.43              |
| 6:H:-24:DG:H2"    | 6:H:-23:DA:H8     | 1.83                     | 0.43              |
| 1:A:152:LYS:HZ3   | 1:B:9:LEU:HA      | 1.84                     | 0.43              |
| 1:A:230:ILE:HD13  | 1:B:11:ARG:CG     | 2.48                     | 0.43              |
| 2:C:38:PHE:CD2    | 2:C:39:LEU:HG     | 2.54                     | 0.43              |
| 2:C:54:GLU:O      | 2:C:58:LYS:HG2    | 2.19                     | 0.43              |
| 2:C:192:PHE:CE2   | 2:C:437:LEU:HD21  | 2.53                     | 0.43              |
| 2:C:820:ASP:O     | 2:C:1092:GLY:HA3  | 2.17                     | 0.43              |
| 2:C:1082:ASP:OD1  | 2:C:1252:LEU:HD22 | 2.18                     | 0.43              |
| 2:C:1085:ALA:HB3  | 2:C:1249:LEU:CD1  | 2.48                     | 0.43              |
| 2:C:1315:ARG:O    | 2:C:1318:VAL:HG12 | 2.19                     | 0.43              |
| 3:D:277:ARG:HD2   | 3:D:300:MET:CE    | 2.48                     | 0.43              |
| 3:D:310:ASP:OD2   | 3:D:313:ARG:HD3   | 2.18                     | 0.43              |
| 3:D:915:ALA:O     | 3:D:919:ILE:HG13  | 2.18                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1150:MET:SD   | 3:D:1154:VAL:HG23 | 2.58                     | 0.43              |
| 3:D:1158:LYS:N    | 3:D:1161:LYS:HE2  | 2.29                     | 0.43              |
| 3:D:1259:LYS:HZ1  | 3:D:1312:THR:HA   | 1.83                     | 0.43              |
| 4:E:30:ILE:HD13   | 4:E:35:ALA:HB2    | 1.99                     | 0.43              |
| 5:F:140:ARG:HD2   | 5:F:411:GLU:OE1   | 2.19                     | 0.43              |
| 1:A:127:LEU:HG    | 1:A:209:GLY:C     | 2.39                     | 0.43              |
| 2:C:27:LEU:HD13   | 2:C:670:VAL:CG1   | 2.47                     | 0.43              |
| 2:C:39:LEU:HD11   | 2:C:133:ILE:HD12  | 1.99                     | 0.43              |
| 2:C:162:PHE:O     | 2:C:181:ARG:N     | 2.48                     | 0.43              |
| 2:C:194:PHE:CE1   | 2:C:200:VAL:HB    | 2.53                     | 0.43              |
| 2:C:442:GLY:O     | 2:C:447:ARG:HB3   | 2.18                     | 0.43              |
| 2:C:678:LEU:HB3   | 2:C:1200:VAL:HG13 | 2.00                     | 0.43              |
| 2:C:1301:LEU:HD12 | 3:D:1353:ILE:CD1  | 2.49                     | 0.43              |
| 3:D:37:GLY:CA     | 3:D:62:ILE:HG23   | 2.49                     | 0.43              |
| 3:D:42:PRO:HB2    | 3:D:272:ARG:HG2   | 2.00                     | 0.43              |
| 3:D:106:ILE:HG21  | 3:D:275:ILE:HD13  | 2.01                     | 0.43              |
| 3:D:368:CYS:HB3   | 3:D:439:PHE:CG    | 2.53                     | 0.43              |
| 3:D:485:LEU:HD21  | 4:E:17:PHE:CE1    | 2.50                     | 0.43              |
| 3:D:788:ASN:HB2   | 3:D:1129:LEU:HD21 | 1.99                     | 0.43              |
| 3:D:1340:LEU:HD21 | 3:D:1349:VAL:HG11 | 2.00                     | 0.43              |
| 5:F:493:PRO:HG3   | 6:H:-17:DC:OP2    | 2.18                     | 0.43              |
| 6:H:-23:DA:H2''   | 6:H:-22:DA:O5'    | 2.17                     | 0.43              |
| 1:A:68:VAL:HG23   | 1:A:69:HIS:HD2    | 1.82                     | 0.43              |
| 1:A:230:ILE:O     | 1:B:15:PRO:HG3    | 2.19                     | 0.43              |
| 1:B:199:LYS:HG2   | 1:B:201:ILE:HG23  | 2.00                     | 0.43              |
| 2:C:205:ASP:OD1   | 2:C:207:ARG:HB2   | 2.18                     | 0.43              |
| 2:C:811:MET:HB3   | 3:D:638:SER:OG    | 2.17                     | 0.43              |
| 2:C:889:LEU:CD2   | 2:C:1070:VAL:HG11 | 2.48                     | 0.43              |
| 2:C:892:LYS:H     | 2:C:923:SER:HA    | 1.84                     | 0.43              |
| 2:C:899:SER:HB2   | 2:C:900:PRO:HD2   | 1.99                     | 0.43              |
| 2:C:943:HIS:HA    | 2:C:1057:GLY:HA3  | 2.00                     | 0.43              |
| 5:F:554:GLU:OE1   | 5:F:554:GLU:N     | 2.47                     | 0.43              |
| 1:A:32:GLU:HB3    | 1:A:33:PRO:HD3    | 2.01                     | 0.43              |
| 1:B:39:GLY:O      | 1:B:200:LEU:HD12  | 2.18                     | 0.43              |
| 2:C:937:VAL:HA    | 2:C:1070:VAL:HA   | 2.00                     | 0.43              |
| 3:D:515:LEU:CD2   | 3:D:546:LEU:HD21  | 2.48                     | 0.43              |
| 3:D:558:THR:HG22  | 3:D:563:LEU:HD22  | 2.00                     | 0.43              |
| 3:D:694:ALA:O     | 3:D:698:MET:HG2   | 2.18                     | 0.43              |
| 3:D:841:ALA:HA    | 3:D:879:ARG:HG3   | 1.99                     | 0.43              |
| 5:F:582:GLU:O     | 5:F:586:ARG:HG3   | 2.19                     | 0.43              |
| 5:F:588:LEU:HB3   | 5:F:596:GLU:HG3   | 2.00                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:101:LYS:HE3  | 1:A:124:ILE:HD11  | 2.00                     | 0.43              |
| 1:A:101:LYS:O    | 1:A:102:ARG:HD2   | 2.19                     | 0.43              |
| 1:A:203:LEU:HD22 | 1:A:217:VAL:CG2   | 2.48                     | 0.43              |
| 1:B:127:LEU:HD22 | 1:B:208:GLY:O     | 2.19                     | 0.43              |
| 2:C:366:ILE:HG23 | 2:C:369:ASP:HB2   | 2.01                     | 0.43              |
| 2:C:504:LYS:HB3  | 7:I:9:DG:C3'      | 2.49                     | 0.43              |
| 2:C:569:ILE:HD12 | 2:C:678:LEU:HD11  | 2.00                     | 0.43              |
| 2:C:730:VAL:HG23 | 2:C:781:ASP:C     | 2.39                     | 0.43              |
| 2:C:748:ASP:CB   | 2:C:751:ARG:HB2   | 2.48                     | 0.43              |
| 2:C:791:ASP:HB2  | 2:C:795:THR:OG1   | 2.19                     | 0.43              |
| 2:C:867:ALA:HB1  | 2:C:888:ILE:HG12  | 2.01                     | 0.43              |
| 2:C:877:VAL:CG1  | 2:C:889:LEU:HD12  | 2.42                     | 0.43              |
| 2:C:1159:LYS:NZ  | 2:C:1183:LEU:O    | 2.45                     | 0.43              |
| 3:D:112:VAL:HG11 | 3:D:305:VAL:HG11  | 2.01                     | 0.43              |
| 3:D:763:LEU:HA   | 3:D:767:GLU:OE1   | 2.19                     | 0.43              |
| 3:D:799:VAL:HG11 | 3:D:1305:ILE:HG22 | 2.00                     | 0.43              |
| 3:D:809:ASP:OD2  | 3:D:893:ALA:HB2   | 2.19                     | 0.43              |
| 3:D:815:GLY:O    | 3:D:877:LYS:HE2   | 2.18                     | 0.43              |
| 3:D:1281:PHE:O   | 3:D:1285:GLN:HG2  | 2.18                     | 0.43              |
| 5:F:583:THR:O    | 5:F:587:VAL:HG13  | 2.19                     | 0.43              |
| 6:H:-42:DT:H2''  | 6:H:-41:DA:C8     | 2.53                     | 0.43              |
| 6:H:-41:DA:H2''  | 6:H:-40:DG:C8     | 2.54                     | 0.43              |
| 1:A:15:PRO:O     | 1:A:17:ILE:HD12   | 2.19                     | 0.43              |
| 1:A:50:LEU:HG    | 1:A:54:LEU:HD11   | 2.00                     | 0.43              |
| 1:B:38:PHE:HA    | 1:B:41:THR:CG2    | 2.48                     | 0.43              |
| 1:B:181:ARG:HD2  | 3:D:536:GLU:OE2   | 2.19                     | 0.43              |
| 1:B:231:ILE:HG22 | 1:B:232:THR:CG2   | 2.37                     | 0.43              |
| 2:C:207:ARG:HH21 | 6:H:-1:DT:H73     | 1.83                     | 0.43              |
| 2:C:260:PRO:O    | 2:C:293:LEU:HA    | 2.19                     | 0.43              |
| 2:C:463:SER:O    | 2:C:467:LEU:HD13  | 2.19                     | 0.43              |
| 2:C:524:ASP:HA   | 2:C:767:GLN:NE2   | 2.34                     | 0.43              |
| 2:C:553:PHE:CZ   | 3:D:777:LYS:HG3   | 2.53                     | 0.43              |
| 2:C:586:HIS:HB3  | 2:C:598:PRO:HG3   | 2.00                     | 0.43              |
| 2:C:675:ILE:CB   | 2:C:678:LEU:HD12  | 2.44                     | 0.43              |
| 2:C:708:GLY:O    | 2:C:1198:THR:HG22 | 2.18                     | 0.43              |
| 2:C:822:ILE:HG21 | 2:C:1246:MET:HE1  | 1.99                     | 0.43              |
| 2:C:1083:LYS:NZ  | 3:D:464:ASP:O     | 2.52                     | 0.43              |
| 2:C:1264:PRO:HG2 | 2:C:1273:LEU:HD12 | 2.01                     | 0.43              |
| 3:D:160:LEU:O    | 3:D:160:LEU:HD23  | 2.19                     | 0.43              |
| 3:D:205:GLU:OE2  | 3:D:206:GLU:HG3   | 2.19                     | 0.43              |
| 3:D:367:GLU:HG3  | 3:D:440:GLU:O     | 2.19                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:368:CYS:CB    | 3:D:425:LEU:HD11  | 2.48                     | 0.43              |
| 3:D:607:ILE:HG13  | 3:D:611:HIS:CE1   | 2.54                     | 0.43              |
| 3:D:880:SER:C     | 3:D:894:CYS:HB3   | 2.39                     | 0.43              |
| 3:D:881:VAL:HG21  | 3:D:1251:THR:CA   | 2.48                     | 0.43              |
| 3:D:1145:ALA:HB2  | 3:D:1207:ILE:CG1  | 2.49                     | 0.43              |
| 3:D:1276:LEU:O    | 3:D:1279:PRO:HD2  | 2.19                     | 0.43              |
| 6:H:5:DT:H2'      | 6:H:6:DC:C5       | 2.53                     | 0.43              |
| 2:C:3:GLN:O       | 2:C:8:LYS:HE2     | 2.19                     | 0.43              |
| 2:C:63:ILE:CG2    | 2:C:480:GLU:HG3   | 2.47                     | 0.43              |
| 2:C:822:ILE:HG23  | 2:C:1116:LEU:HD23 | 2.01                     | 0.43              |
| 2:C:857:THR:CG2   | 2:C:893:VAL:HG21  | 2.44                     | 0.43              |
| 2:C:1300:THR:HA   | 2:C:1303:GLU:HG3  | 2.01                     | 0.43              |
| 2:C:1307:VAL:HG11 | 2:C:1329:PHE:CD2  | 2.54                     | 0.43              |
| 3:D:417:VAL:HG13  | 3:D:418:ILE:HG13  | 2.01                     | 0.43              |
| 3:D:476:LEU:HD23  | 4:E:28:ARG:CG     | 2.49                     | 0.43              |
| 3:D:769:PHE:HA    | 3:D:772:THR:HG22  | 2.01                     | 0.43              |
| 3:D:876:VAL:HG13  | 3:D:878:VAL:HG23  | 2.01                     | 0.43              |
| 5:F:425:ARG:NH1   | 5:F:425:ARG:HB2   | 2.34                     | 0.43              |
| 5:F:539:LYS:HE2   | 5:F:539:LYS:HB3   | 1.89                     | 0.43              |
| 6:H:-30:DA:H5'    | 6:H:-30:DA:C8     | 2.54                     | 0.43              |
| 6:H:7:DG:H2'      | 6:H:8:DC:C6       | 2.54                     | 0.43              |
| 7:I:33:DC:H2'     | 7:I:34:DA:H8      | 1.79                     | 0.43              |
| 2:C:86:VAL:O      | 2:C:90:ILE:HG13   | 2.19                     | 0.42              |
| 2:C:523:MET:HB3   | 2:C:766:ASN:HD22  | 1.83                     | 0.42              |
| 2:C:537:ARG:CG    | 2:C:580:ILE:HG22  | 2.49                     | 0.42              |
| 2:C:697:VAL:HG22  | 2:C:1248:LYS:O    | 2.19                     | 0.42              |
| 2:C:733:GLN:HG2   | 2:C:740:VAL:HG21  | 2.01                     | 0.42              |
| 2:C:824:ILE:HD12  | 2:C:1094:ILE:HG12 | 2.01                     | 0.42              |
| 3:D:132:PRO:HG2   | 3:D:135:ASP:OD2   | 2.19                     | 0.42              |
| 3:D:247:ILE:HG13  | 3:D:251:LEU:HD12  | 2.01                     | 0.42              |
| 3:D:267:LEU:CD2   | 3:D:329:LEU:HD22  | 2.47                     | 0.42              |
| 3:D:383:ILE:HG21  | 3:D:403:VAL:HG11  | 2.00                     | 0.42              |
| 3:D:519:ARG:HG2   | 3:D:712:GLU:CD    | 2.39                     | 0.42              |
| 3:D:919:ILE:CD1   | 3:D:1249:ILE:HD13 | 2.49                     | 0.42              |
| 3:D:1131:ARG:HG2  | 3:D:1232:GLU:OE2  | 2.19                     | 0.42              |
| 3:D:1154:VAL:HB   | 3:D:1200:ILE:HG21 | 2.01                     | 0.42              |
| 5:F:427:VAL:HG22  | 5:F:475:ILE:HG13  | 2.01                     | 0.42              |
| 5:F:493:PRO:HB2   | 5:F:495:HIS:HD1   | 1.83                     | 0.42              |
| 6:H:12:DG:C8      | 6:H:13:DT:H72     | 2.54                     | 0.42              |
| 7:I:1:DA:H2'      | 7:I:2:DA:O4'      | 2.19                     | 0.42              |
| 1:A:54:LEU:HB3    | 1:A:178:PRO:CD    | 2.49                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:68:VAL:O     | 1:A:168:GLY:HA2   | 2.20                     | 0.42              |
| 2:C:24:MET:SD    | 2:C:714:VAL:HG11  | 2.59                     | 0.42              |
| 2:C:114:GLU:OE1  | 2:C:114:GLU:N     | 2.52                     | 0.42              |
| 2:C:215:PHE:CE1  | 2:C:433:VAL:HG11  | 2.55                     | 0.42              |
| 2:C:687:LEU:HD13 | 3:D:779:LEU:CD2   | 2.49                     | 0.42              |
| 2:C:807:LEU:HG   | 2:C:1112:VAL:HG12 | 2.00                     | 0.42              |
| 2:C:985:LEU:HD11 | 2:C:1029:LEU:CD1  | 2.49                     | 0.42              |
| 2:C:1287:MET:HG2 | 3:D:430:THR:HG23  | 2.00                     | 0.42              |
| 3:D:109:ALA:HB2  | 3:D:282:LYS:CD    | 2.49                     | 0.42              |
| 3:D:257:LEU:CD1  | 3:D:263:ALA:HB2   | 2.49                     | 0.42              |
| 3:D:807:GLU:O    | 3:D:892:GLY:N     | 2.51                     | 0.42              |
| 3:D:838:ARG:HB3  | 3:D:878:VAL:HG13  | 2.00                     | 0.42              |
| 3:D:1156:PHE:HA  | 3:D:1164:ARG:HH21 | 1.84                     | 0.42              |
| 3:D:1229:LEU:O   | 3:D:1233:ILE:HG12 | 2.18                     | 0.42              |
| 4:E:22:LEU:CD2   | 4:E:61:GLU:HA     | 2.49                     | 0.42              |
| 7:I:-16:DG:H5'   | 7:I:-16:DG:H8     | 1.84                     | 0.42              |
| 7:I:44:DG:H2''   | 7:I:45:DG:C8      | 2.53                     | 0.42              |
| 1:A:74:LEU:HD13  | 1:A:142:VAL:CG1   | 2.36                     | 0.42              |
| 1:A:154:TYR:HB2  | 2:C:830:ARG:HD3   | 2.00                     | 0.42              |
| 1:A:212:THR:CG2  | 1:A:215:ASP:HB2   | 2.50                     | 0.42              |
| 1:A:227:GLN:OE1  | 1:B:9:LEU:HD11    | 2.19                     | 0.42              |
| 1:A:235:GLU:HG2  | 1:B:218:TYR:HE1   | 1.84                     | 0.42              |
| 2:C:97:ALA:HB3   | 2:C:132:ASP:HB2   | 2.01                     | 0.42              |
| 2:C:146:GLY:O    | 2:C:147:THR:OG1   | 2.33                     | 0.42              |
| 2:C:525:GLN:H    | 2:C:767:GLN:HE21  | 1.68                     | 0.42              |
| 2:C:567:CYS:HA   | 2:C:667:VAL:O     | 2.19                     | 0.42              |
| 2:C:623:VAL:CG2  | 2:C:652:LEU:HD13  | 2.49                     | 0.42              |
| 2:C:723:VAL:HG23 | 2:C:790:ALA:H     | 1.85                     | 0.42              |
| 2:C:841:GLU:HA   | 2:C:1070:VAL:O    | 2.20                     | 0.42              |
| 2:C:922:THR:HG22 | 2:C:922:THR:O     | 2.18                     | 0.42              |
| 2:C:1159:LYS:HZ1 | 2:C:1183:LEU:HG   | 1.83                     | 0.42              |
| 2:C:1342:LYS:HA  | 2:C:1342:LYS:HE2  | 2.02                     | 0.42              |
| 3:D:361:PRO:HB3  | 3:D:629:PHE:CE2   | 2.54                     | 0.42              |
| 3:D:1147:ILE:HB  | 3:D:1219:ILE:HG13 | 2.01                     | 0.42              |
| 5:F:120:LEU:HD13 | 5:F:428:ILE:HD13  | 2.01                     | 0.42              |
| 5:F:499:THR:HG21 | 5:F:533:LYS:NZ    | 2.35                     | 0.42              |
| 1:A:203:LEU:HD21 | 1:A:205:VAL:HB    | 1.99                     | 0.42              |
| 2:C:217:TYR:CD1  | 2:C:222:ASP:HB3   | 2.54                     | 0.42              |
| 2:C:551:ALA:O    | 2:C:555:VAL:HG12  | 2.19                     | 0.42              |
| 2:C:725:ALA:HB2  | 2:C:789:ILE:HD11  | 2.01                     | 0.42              |
| 2:C:807:LEU:HD12 | 2:C:1242:GLY:O    | 2.19                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:235:ARG:HB2   | 3:D:238:TRP:CE2   | 2.54                     | 0.42              |
| 3:D:256:PRO:HB3   | 3:D:262:PHE:CE1   | 2.55                     | 0.42              |
| 3:D:481:GLU:OE2   | 3:D:485:LEU:HB2   | 2.20                     | 0.42              |
| 3:D:552:ALA:HB3   | 3:D:575:MET:CE    | 2.50                     | 0.42              |
| 3:D:1155:GLU:O    | 3:D:1167:LYS:HG2  | 2.19                     | 0.42              |
| 5:F:484:ALA:O     | 5:F:497:ILE:HG13  | 2.19                     | 0.42              |
| 1:A:230:ILE:CD1   | 1:B:12:PRO:HG2    | 2.50                     | 0.42              |
| 2:C:11:ILE:HD13   | 2:C:1176:LEU:HD13 | 2.02                     | 0.42              |
| 2:C:1121:VAL:HA   | 2:C:1126:ASN:OD1  | 2.19                     | 0.42              |
| 2:C:1129:GLN:HE21 | 2:C:1244:ILE:CD1  | 2.32                     | 0.42              |
| 2:C:1292:LEU:HB2  | 2:C:1301:LEU:HD11 | 2.01                     | 0.42              |
| 3:D:187:ILE:O     | 3:D:191:LEU:HG    | 2.19                     | 0.42              |
| 3:D:515:LEU:O     | 3:D:573:GLY:HA3   | 2.19                     | 0.42              |
| 3:D:810:CYS:N     | 3:D:891:CYS:SG    | 2.92                     | 0.42              |
| 5:F:427:VAL:HG22  | 5:F:475:ILE:CD1   | 2.49                     | 0.42              |
| 5:F:551:ILE:HG21  | 5:F:562:PHE:CE2   | 2.54                     | 0.42              |
| 1:A:49:VAL:HG13   | 1:A:50:LEU:N      | 2.34                     | 0.42              |
| 2:C:12:ARG:HA     | 2:C:1195:PRO:O    | 2.19                     | 0.42              |
| 2:C:192:PHE:CE2   | 2:C:202:VAL:HG22  | 2.55                     | 0.42              |
| 2:C:227:LEU:HD11  | 2:C:359:LEU:HD12  | 2.01                     | 0.42              |
| 2:C:432:ASP:O     | 2:C:436:VAL:HG23  | 2.20                     | 0.42              |
| 2:C:528:PRO:HG2   | 2:C:800:LEU:CD1   | 2.46                     | 0.42              |
| 2:C:1105:PHE:O    | 2:C:1226:LEU:HD12 | 2.19                     | 0.42              |
| 2:C:1199:PRO:HD2  | 2:C:1203:GLY:CA   | 2.37                     | 0.42              |
| 3:D:127:MET:SD    | 3:D:225:ILE:HG13  | 2.59                     | 0.42              |
| 3:D:194:ILE:HD11  | 3:D:199:GLU:HG2   | 2.00                     | 0.42              |
| 3:D:571:THR:O     | 3:D:575:MET:HG3   | 2.19                     | 0.42              |
| 3:D:764:THR:HG22  | 3:D:767:GLU:CD    | 2.40                     | 0.42              |
| 3:D:819:ARG:CZ    | 3:D:874:GLN:HB3   | 2.50                     | 0.42              |
| 3:D:895:TYR:CZ    | 3:D:911:VAL:HG13  | 2.55                     | 0.42              |
| 2:C:38:PHE:HD2    | 2:C:39:LEU:HG     | 1.84                     | 0.42              |
| 2:C:529:LEU:HD12  | 2:C:674:LEU:HD12  | 2.02                     | 0.42              |
| 2:C:558:VAL:HG21  | 2:C:568:PRO:HB3   | 2.01                     | 0.42              |
| 2:C:711:MET:O     | 2:C:715:VAL:HG12  | 2.20                     | 0.42              |
| 2:C:764:ARG:HG2   | 2:C:765:SER:O     | 2.19                     | 0.42              |
| 2:C:824:ILE:CD1   | 2:C:1078:LEU:HD13 | 2.49                     | 0.42              |
| 2:C:1125:MET:HB3  | 3:D:759:PHE:CD2   | 2.55                     | 0.42              |
| 2:C:1154:GLN:OE1  | 2:C:1154:GLN:N    | 2.53                     | 0.42              |
| 3:D:57:LEU:CD2    | 3:D:271:TYR:HB3   | 2.49                     | 0.42              |
| 3:D:121:LEU:HB2   | 3:D:122:PRO:CD    | 2.48                     | 0.42              |
| 3:D:293:ILE:HD11  | 5:F:424:LEU:HD21  | 2.02                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:424:LEU:HD23  | 3:D:436:ILE:CG2   | 2.50                     | 0.42              |
| 3:D:842:GLU:H     | 3:D:877:LYS:HB3   | 1.85                     | 0.42              |
| 5:F:156:ALA:HB2   | 5:F:401:ILE:CD1   | 2.50                     | 0.42              |
| 5:F:169:LEU:HA    | 5:F:173:ARG:CB    | 2.50                     | 0.42              |
| 7:I:22:DT:C6      | 7:I:23:DT:H73     | 2.55                     | 0.42              |
| 1:B:12:PRO:CB     | 1:B:33:PRO:HD2    | 2.45                     | 0.42              |
| 2:C:643:GLY:O     | 2:C:650:THR:N     | 2.36                     | 0.42              |
| 2:C:674:LEU:HD21  | 2:C:711:MET:HG3   | 2.02                     | 0.42              |
| 3:D:432:HIS:HA    | 3:D:917:GLN:CB    | 2.31                     | 0.42              |
| 3:D:489:THR:CG2   | 3:D:618:VAL:HG21  | 2.40                     | 0.42              |
| 3:D:627:LEU:O     | 3:D:631:GLU:HG2   | 2.19                     | 0.42              |
| 3:D:756:VAL:O     | 3:D:756:VAL:HG13  | 2.20                     | 0.42              |
| 5:F:140:ARG:HG2   | 5:F:415:ALA:HB2   | 2.01                     | 0.42              |
| 5:F:510:MET:SD    | 5:F:518:PRO:HG3   | 2.60                     | 0.42              |
| 1:A:49:VAL:HG11   | 1:A:224:LEU:HD11  | 2.00                     | 0.42              |
| 1:A:224:LEU:O     | 1:A:228:LEU:HG    | 2.19                     | 0.42              |
| 1:B:57:ALA:HB1    | 1:B:148:VAL:CG2   | 2.50                     | 0.42              |
| 2:C:111:THR:HG23  | 2:C:115:THR:HB    | 2.01                     | 0.42              |
| 2:C:502:ASN:OD1   | 2:C:503:ALA:N     | 2.52                     | 0.42              |
| 2:C:1303:GLU:CA   | 2:C:1307:VAL:HG12 | 2.50                     | 0.42              |
| 2:C:1333:ILE:HG13 | 3:D:18:PHE:CE1    | 2.54                     | 0.42              |
| 3:D:115:ILE:HD11  | 3:D:313:ARG:HB2   | 2.01                     | 0.42              |
| 3:D:512:LEU:HD21  | 3:D:624:VAL:CG2   | 2.50                     | 0.42              |
| 3:D:743:MET:HG3   | 3:D:770:ASN:C     | 2.39                     | 0.42              |
| 5:F:454:LYS:HE2   | 6:H:-14:DG:OP1    | 2.18                     | 0.42              |
| 5:F:522:GLU:O     | 5:F:525:GLU:HG3   | 2.20                     | 0.42              |
| 5:F:629:GLN:O     | 5:F:633:LYS:HG3   | 2.20                     | 0.42              |
| 1:A:48:ARG:HG3    | 2:C:1101:GLU:HB2  | 2.01                     | 0.42              |
| 1:A:62:ILE:HD11   | 1:A:88:ILE:CG2    | 2.50                     | 0.42              |
| 1:B:110:PRO:HA    | 1:B:136:LEU:O     | 2.20                     | 0.42              |
| 1:B:185:ARG:NE    | 1:B:201:ILE:HD11  | 2.34                     | 0.42              |
| 1:B:188:PRO:HA    | 1:B:197:TYR:O     | 2.20                     | 0.42              |
| 2:C:99:PRO:HB3    | 2:C:129:TYR:CZ    | 2.54                     | 0.42              |
| 2:C:527:ASN:ND2   | 2:C:529:LEU:HB3   | 2.34                     | 0.42              |
| 2:C:826:GLU:N     | 2:C:1098:LEU:O    | 2.52                     | 0.42              |
| 2:C:827:ARG:HD3   | 2:C:1113:ASP:OD1  | 2.19                     | 0.42              |
| 3:D:23:ILE:HD11   | 3:D:1331:ALA:HB3  | 2.02                     | 0.42              |
| 3:D:294:ILE:HG22  | 3:D:298:LYS:HE3   | 2.02                     | 0.42              |
| 3:D:319:THR:HB    | 3:D:326:LEU:CD2   | 2.46                     | 0.42              |
| 3:D:382:PHE:HB3   | 3:D:417:VAL:HG21  | 2.01                     | 0.42              |
| 3:D:489:THR:O     | 3:D:492:ILE:HG13  | 2.20                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:D:513:TYR:CD2  | 3:D:720:MET:HG3   | 2.55                     | 0.42              |
| 3:D:571:THR:OG1  | 3:D:574:ARG:HD3   | 2.19                     | 0.42              |
| 3:D:615:LYS:O    | 3:D:618:VAL:HG12  | 2.20                     | 0.42              |
| 3:D:646:ILE:HG22 | 3:D:758:ASN:ND2   | 2.31                     | 0.42              |
| 3:D:1126:THR:O   | 3:D:1131:ARG:HB2  | 2.20                     | 0.42              |
| 3:D:1163:LYS:HG2 | 3:D:1164:ARG:N    | 2.35                     | 0.42              |
| 3:D:1343:LEU:O   | 3:D:1347:VAL:HG23 | 2.20                     | 0.42              |
| 5:F:594:ARG:O    | 5:F:598:VAL:HG22  | 2.20                     | 0.42              |
| 7:I:20:DG:H2'    | 7:I:21:DT:C7      | 2.50                     | 0.42              |
| 2:C:155:MET:CG   | 2:C:538:LEU:HB3   | 2.50                     | 0.41              |
| 2:C:951:ALA:HA   | 2:C:954:ILE:CD1   | 2.48                     | 0.41              |
| 2:C:1031:SER:HA  | 2:C:1034:ARG:CZ   | 2.50                     | 0.41              |
| 2:C:1178:ASP:OD1 | 2:C:1178:ASP:N    | 2.53                     | 0.41              |
| 3:D:222:ARG:O    | 3:D:226:LEU:HG    | 2.20                     | 0.41              |
| 3:D:427:ARG:HE   | 3:D:461:ALA:HA    | 1.85                     | 0.41              |
| 3:D:654:VAL:CG2  | 3:D:739:MET:HE1   | 2.50                     | 0.41              |
| 3:D:841:ALA:CA   | 3:D:879:ARG:HG3   | 2.50                     | 0.41              |
| 4:E:9:CYS:SG     | 4:E:19:LEU:HD21   | 2.60                     | 0.41              |
| 6:H:-45:DC:H2''  | 6:H:-44:DC:C6     | 2.55                     | 0.41              |
| 6:H:-16:DG:H2''  | 6:H:-15:DT:OP1    | 2.20                     | 0.41              |
| 1:B:84:ILE:O     | 1:B:88:ILE:HG12   | 2.19                     | 0.41              |
| 1:B:103:MET:HG2  | 1:B:124:ILE:HD11  | 2.02                     | 0.41              |
| 2:C:215:PHE:HE1  | 2:C:433:VAL:HG21  | 1.85                     | 0.41              |
| 2:C:553:PHE:CE2  | 3:D:777:LYS:HG3   | 2.55                     | 0.41              |
| 2:C:674:LEU:HD22 | 2:C:712:GLU:CG    | 2.50                     | 0.41              |
| 2:C:776:LEU:HD13 | 2:C:797:LEU:CA    | 2.49                     | 0.41              |
| 2:C:1084:MET:HE3 | 2:C:1094:ILE:HD13 | 2.02                     | 0.41              |
| 3:D:27:SER:O     | 3:D:31:ILE:HG12   | 2.20                     | 0.41              |
| 3:D:357:ILE:HG13 | 3:D:463:PHE:CD1   | 2.55                     | 0.41              |
| 3:D:881:VAL:HG11 | 3:D:1251:THR:HG22 | 2.02                     | 0.41              |
| 3:D:895:TYR:CE1  | 3:D:1247:LYS:HD3  | 2.55                     | 0.41              |
| 3:D:1155:GLU:HG3 | 3:D:1167:LYS:HB3  | 2.02                     | 0.41              |
| 5:F:422:ALA:C    | 5:F:423:ASN:ND2   | 2.73                     | 0.41              |
| 5:F:426:LEU:HD13 | 5:F:471:ALA:HB1   | 2.01                     | 0.41              |
| 5:F:437:ARG:NH2  | 7:I:10:DT:H1'     | 2.35                     | 0.41              |
| 5:F:598:VAL:O    | 5:F:616:VAL:HG21  | 2.19                     | 0.41              |
| 5:F:647:LEU:HA   | 5:F:650:PHE:HB2   | 2.03                     | 0.41              |
| 1:A:32:GLU:HA    | 1:A:200:LYS:HG3   | 2.02                     | 0.41              |
| 1:A:77:VAL:CG1   | 1:A:134:CYS:HB2   | 2.49                     | 0.41              |
| 1:A:218:ALA:HB1  | 1:B:233:PHE:CE2   | 2.47                     | 0.41              |
| 1:A:230:ILE:HD13 | 1:B:11:ARG:HG2    | 2.02                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:111:GLY:HA2  | 1:B:112:PRO:HD3   | 1.94                     | 0.41              |
| 2:C:824:ILE:HD11 | 2:C:1078:LEU:HD13 | 2.02                     | 0.41              |
| 2:C:894:THR:C    | 2:C:919:VAL:HG23  | 2.41                     | 0.41              |
| 2:C:1149:LEU:O   | 2:C:1149:LEU:HD23 | 2.20                     | 0.41              |
| 2:C:1336:SER:CB  | 3:D:347:LYS:HE3   | 2.51                     | 0.41              |
| 2:C:1342:LYS:HE2 | 2:C:1345:ARG:HD2  | 2.02                     | 0.41              |
| 3:D:103:MET:SD   | 3:D:248:PRO:HD3   | 2.60                     | 0.41              |
| 3:D:520:ASP:N    | 3:D:520:ASP:OD1   | 2.53                     | 0.41              |
| 3:D:557:MET:HA   | 3:D:563:LEU:HB3   | 2.01                     | 0.41              |
| 3:D:581:LEU:HD21 | 3:D:604:LEU:HD21  | 2.02                     | 0.41              |
| 3:D:1158:LYS:HG2 | 3:D:1161:LYS:HZ3  | 1.86                     | 0.41              |
| 3:D:1191:HIS:O   | 3:D:1192:ILE:HD13 | 2.20                     | 0.41              |
| 3:D:1217:LEU:CD1 | 3:D:1222:VAL:HA   | 2.50                     | 0.41              |
| 3:D:1309:SER:HB2 | 3:D:1318:ALA:HB1  | 2.02                     | 0.41              |
| 1:A:212:THR:HG23 | 1:A:215:ASP:HB2   | 2.02                     | 0.41              |
| 1:B:49:VAL:HA    | 1:B:52:SER:OG     | 2.20                     | 0.41              |
| 1:B:107:ALA:H    | 1:B:142:VAL:HG21  | 1.86                     | 0.41              |
| 1:B:183:ALA:O    | 1:B:203:GLU:N     | 2.42                     | 0.41              |
| 2:C:138:ASP:OD1  | 2:C:138:ASP:N     | 2.52                     | 0.41              |
| 2:C:513:PHE:O    | 2:C:517:SER:HB3   | 2.20                     | 0.41              |
| 2:C:567:CYS:HB3  | 2:C:669:SER:HB3   | 2.01                     | 0.41              |
| 2:C:692:MET:CB   | 2:C:1249:LEU:HD21 | 2.47                     | 0.41              |
| 2:C:1209:ILE:O   | 2:C:1213:LEU:HG   | 2.21                     | 0.41              |
| 2:C:1228:ASP:HB2 | 2:C:1235:PHE:CE1  | 2.55                     | 0.41              |
| 3:D:119:LYS:O    | 3:D:313:ARG:HG2   | 2.20                     | 0.41              |
| 3:D:496:ALA:HA   | 3:D:918:SER:OG    | 2.19                     | 0.41              |
| 3:D:548:ALA:HA   | 3:D:572:PRO:CD    | 2.35                     | 0.41              |
| 3:D:598:LYS:O    | 3:D:601:ILE:HG22  | 2.19                     | 0.41              |
| 3:D:655:GLU:HA   | 3:D:658:ARG:CD    | 2.51                     | 0.41              |
| 3:D:729:SER:O    | 3:D:733:MET:HG2   | 2.19                     | 0.41              |
| 3:D:795:ARG:HD2  | 3:D:1306:THR:CG2  | 2.50                     | 0.41              |
| 3:D:1316:ILE:HB  | 3:D:1338:ASP:OD2  | 2.20                     | 0.41              |
| 3:D:1346:ASN:ND2 | 3:D:1354:PRO:HD3  | 2.36                     | 0.41              |
| 1:A:183:ALA:HA   | 2:C:1109:GLY:HA3  | 2.03                     | 0.41              |
| 1:A:221:ALA:HA   | 1:B:227:LEU:HD21  | 2.01                     | 0.41              |
| 2:C:151:ILE:HG21 | 2:C:513:PHE:CZ    | 2.56                     | 0.41              |
| 2:C:263:ASP:H    | 2:C:268:GLU:N     | 2.19                     | 0.41              |
| 2:C:395:SER:HA   | 2:C:399:ASP:CB    | 2.48                     | 0.41              |
| 2:C:1344:MET:HE1 | 3:D:1328:LEU:HD21 | 2.03                     | 0.41              |
| 3:D:300:MET:SD   | 5:F:442:LEU:HD23  | 2.61                     | 0.41              |
| 3:D:529:PHE:H    | 3:D:552:ALA:HA    | 1.85                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:733:MET:HB3   | 3:D:733:MET:HE2   | 1.95                     | 0.41              |
| 3:D:837:GLY:HA2   | 3:D:897:ARG:HB3   | 2.01                     | 0.41              |
| 3:D:895:TYR:CD2   | 3:D:905:VAL:HG21  | 2.54                     | 0.41              |
| 3:D:1193:ALA:HB3  | 3:D:1206:ILE:HG13 | 2.03                     | 0.41              |
| 3:D:1353:ILE:O    | 3:D:1358:GLY:HA3  | 2.20                     | 0.41              |
| 3:D:1367:VAL:HG13 | 4:E:65:GLU:OE2    | 2.21                     | 0.41              |
| 1:B:17:ILE:O      | 1:B:30:VAL:HG23   | 2.21                     | 0.41              |
| 1:B:25:ARG:O      | 1:B:205:GLU:HA    | 2.20                     | 0.41              |
| 2:C:32:ARG:O      | 2:C:36:GLU:HG3    | 2.19                     | 0.41              |
| 2:C:263:ASP:H     | 2:C:267:GLY:HA2   | 1.86                     | 0.41              |
| 2:C:487:MET:HG3   | 2:C:500:LEU:HD13  | 2.02                     | 0.41              |
| 2:C:527:ASN:HD22  | 2:C:529:LEU:H     | 1.69                     | 0.41              |
| 2:C:532:ILE:HD12  | 2:C:715:VAL:CG2   | 2.51                     | 0.41              |
| 2:C:676:PRO:O     | 2:C:1088:HIS:NE2  | 2.53                     | 0.41              |
| 2:C:858:ARG:HE    | 2:C:868:LEU:HD21  | 1.85                     | 0.41              |
| 2:C:1074:VAL:CG1  | 2:C:1076:ARG:HG3  | 2.50                     | 0.41              |
| 3:D:556:GLU:OE1   | 3:D:558:THR:HB    | 2.19                     | 0.41              |
| 3:D:745:LYS:CE    | 3:D:746:PRO:HD2   | 2.42                     | 0.41              |
| 3:D:922:PRO:HB3   | 3:D:1242:VAL:HB   | 2.02                     | 0.41              |
| 3:D:1256:MET:HE2  | 3:D:1256:MET:HB2  | 1.91                     | 0.41              |
| 3:D:1264:GLU:OE2  | 3:D:1296:ALA:HB2  | 2.21                     | 0.41              |
| 6:H:-43:DT:H2'    | 6:H:-42:DT:H72    | 2.01                     | 0.41              |
| 1:A:64:ILE:HB     | 1:A:67:VAL:CG1    | 2.43                     | 0.41              |
| 2:C:410:ARG:HG2   | 2:C:422:SER:O     | 2.20                     | 0.41              |
| 2:C:479:MET:HE3   | 2:C:506:ALA:HB2   | 2.02                     | 0.41              |
| 2:C:702:SER:OG    | 2:C:794:SER:HA    | 2.21                     | 0.41              |
| 2:C:860:ILE:HG12  | 2:C:921:ASP:HA    | 2.02                     | 0.41              |
| 2:C:933:THR:O     | 2:C:1072:VAL:HG23 | 2.21                     | 0.41              |
| 2:C:982:LYS:O     | 2:C:986:ILE:HG23  | 2.19                     | 0.41              |
| 2:C:1036:PHE:O    | 2:C:1040:ARG:HG3  | 2.20                     | 0.41              |
| 2:C:1143:GLY:O    | 2:C:1147:THR:HG22 | 2.21                     | 0.41              |
| 3:D:314:ARG:HD3   | 3:D:314:ARG:HA    | 1.88                     | 0.41              |
| 3:D:322:ASN:ND2   | 3:D:324:ARG:HD3   | 2.35                     | 0.41              |
| 3:D:734:LYS:HE2   | 3:D:734:LYS:HB3   | 1.93                     | 0.41              |
| 3:D:1309:SER:HB2  | 3:D:1318:ALA:CA   | 2.51                     | 0.41              |
| 6:H:-9:DC:H2''    | 6:H:-8:DC:H5''    | 2.02                     | 0.41              |
| 7:I:18:DA:H1'     | 7:I:19:DT:H5'     | 2.02                     | 0.41              |
| 1:A:41:THR:HG22   | 1:B:48:ARG:CD     | 2.49                     | 0.41              |
| 1:B:10:ILE:HG13   | 1:B:197:TYR:CZ    | 2.55                     | 0.41              |
| 2:C:565:ARG:HB3   | 2:C:595:ILE:HG21  | 2.01                     | 0.41              |
| 2:C:771:ILE:CD1   | 2:C:793:PRO:HG3   | 2.48                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:811:MET:SD    | 2:C:1226:LEU:HD23 | 2.61                     | 0.41              |
| 2:C:977:ILE:HG12  | 2:C:1036:PHE:CD2  | 2.56                     | 0.41              |
| 2:C:978:SER:O     | 2:C:982:LYS:HD3   | 2.21                     | 0.41              |
| 2:C:1199:PRO:HB2  | 2:C:1202:ASP:H    | 1.86                     | 0.41              |
| 3:D:26:ALA:HA     | 3:D:30:LYS:HZ1    | 1.86                     | 0.41              |
| 3:D:109:ALA:HB3   | 3:D:281:LEU:CG    | 2.49                     | 0.41              |
| 3:D:832:GLY:O     | 3:D:836:LEU:HB2   | 2.21                     | 0.41              |
| 3:D:1205:TYR:CE2  | 3:D:1211:PRO:HB3  | 2.56                     | 0.41              |
| 3:D:1260:VAL:CG2  | 3:D:1279:PRO:HG2  | 2.50                     | 0.41              |
| 5:F:402:VAL:HA    | 5:F:405:VAL:CG1   | 2.50                     | 0.41              |
| 6:H:7:DG:H2'      | 6:H:8:DC:H6       | 1.85                     | 0.41              |
| 7:I:-11:DT:C2'    | 7:I:-10:DC:H5''   | 2.35                     | 0.41              |
| 1:A:62:ILE:HG22   | 1:A:64:ILE:HG13   | 2.02                     | 0.41              |
| 2:C:364:ASN:CB    | 2:C:369:ASP:HB3   | 2.51                     | 0.41              |
| 2:C:381:GLY:HA3   | 5:F:117:ARG:HB3   | 2.02                     | 0.41              |
| 2:C:559:HIS:O     | 2:C:562:HIS:HB2   | 2.21                     | 0.41              |
| 2:C:703:ASP:H     | 2:C:804:ARG:HD2   | 1.85                     | 0.41              |
| 2:C:834:PHE:CD2   | 2:C:1078:LEU:HD11 | 2.56                     | 0.41              |
| 2:C:835:THR:CG2   | 2:C:1077:LYS:HD3  | 2.48                     | 0.41              |
| 2:C:1053:LYS:HG3  | 2:C:1056:ARG:HH11 | 1.85                     | 0.41              |
| 2:C:1150:LEU:HD13 | 2:C:1187:ALA:CB   | 2.47                     | 0.41              |
| 2:C:1207:ASP:OD1  | 2:C:1208:ASP:N    | 2.53                     | 0.41              |
| 2:C:1226:LEU:HD22 | 2:C:1241:VAL:CG2  | 2.50                     | 0.41              |
| 2:C:1287:MET:CE   | 3:D:793:THR:HG21  | 2.51                     | 0.41              |
| 2:C:1345:ARG:HG2  | 3:D:34:TRP:CH2    | 2.56                     | 0.41              |
| 3:D:24:SER:HB2    | 3:D:234:ASN:ND2   | 2.36                     | 0.41              |
| 3:D:37:GLY:HA3    | 3:D:62:ILE:HG23   | 2.02                     | 0.41              |
| 3:D:39:ILE:HD11   | 3:D:106:ILE:HG12  | 2.02                     | 0.41              |
| 3:D:57:LEU:HD11   | 3:D:272:ARG:CA    | 2.51                     | 0.41              |
| 3:D:104:GLY:O     | 3:D:245:PRO:HA    | 2.21                     | 0.41              |
| 3:D:123:SER:OG    | 3:D:133:LEU:HD13  | 2.20                     | 0.41              |
| 3:D:290:PRO:HG2   | 5:F:420:VAL:HG11  | 2.01                     | 0.41              |
| 3:D:684:ASP:HA    | 3:D:688:LYS:CG    | 2.51                     | 0.41              |
| 3:D:746:PRO:HD3   | 3:D:773:HIS:NE2   | 2.36                     | 0.41              |
| 3:D:805:ILE:HG23  | 3:D:908:GLY:N     | 2.35                     | 0.41              |
| 3:D:835:VAL:HG21  | 3:D:876:VAL:HG11  | 2.03                     | 0.41              |
| 3:D:1259:LYS:HA   | 3:D:1274:ASP:O    | 2.20                     | 0.41              |
| 5:F:416:LYS:O     | 5:F:420:VAL:HG23  | 2.20                     | 0.41              |
| 5:F:425:ARG:HB2   | 5:F:425:ARG:CZ    | 2.50                     | 0.41              |
| 5:F:444:LEU:HD21  | 5:F:483:ILE:CD1   | 2.40                     | 0.41              |
| 7:I:43:DA:H2''    | 7:I:44:DG:C8      | 2.56                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:62:ILE:CG2   | 1:B:170:ILE:HB    | 2.50                     | 0.41              |
| 2:C:95:THR:HA    | 2:C:144:VAL:O     | 2.21                     | 0.41              |
| 2:C:210:LEU:HD23 | 2:C:210:LEU:H     | 1.86                     | 0.41              |
| 2:C:354:TYR:CZ   | 2:C:444:ARG:HD2   | 2.56                     | 0.41              |
| 2:C:759:MET:CG   | 2:C:773:GLN:HB2   | 2.51                     | 0.41              |
| 3:D:252:ARG:H    | 3:D:252:ARG:HG3   | 1.60                     | 0.41              |
| 3:D:373:LYS:HG3  | 3:D:447:LYS:HE3   | 2.01                     | 0.41              |
| 3:D:821:VAL:HG21 | 3:D:1238:ARG:CZ   | 2.50                     | 0.41              |
| 3:D:899:LEU:HD21 | 3:D:1245:ASN:ND2  | 2.29                     | 0.41              |
| 3:D:1139:ARG:CZ  | 3:D:1139:ARG:HB3  | 2.51                     | 0.41              |
| 3:D:1277:ASP:HA  | 3:D:1280:GLU:CD   | 2.41                     | 0.41              |
| 8:G:120:TRP:CE3  | 8:G:122:ILE:HG13  | 2.55                     | 0.41              |
| 1:A:4:ARG:HA     | 1:B:55:GLN:OE1    | 2.21                     | 0.40              |
| 1:A:203:LEU:HD22 | 1:A:217:VAL:HG21  | 2.02                     | 0.40              |
| 1:A:225:GLN:O    | 1:A:229:GLN:HG3   | 2.21                     | 0.40              |
| 1:B:10:ILE:HG13  | 1:B:197:TYR:CE2   | 2.56                     | 0.40              |
| 1:B:86:LEU:HD22  | 3:D:529:PHE:C     | 2.41                     | 0.40              |
| 2:C:263:ASP:N    | 2:C:267:GLY:HA2   | 2.36                     | 0.40              |
| 2:C:362:ASP:OD1  | 2:C:364:ASN:N     | 2.42                     | 0.40              |
| 2:C:604:ASP:N    | 2:C:604:ASP:OD1   | 2.53                     | 0.40              |
| 2:C:624:ILE:HG13 | 2:C:659:LEU:HB2   | 2.03                     | 0.40              |
| 2:C:748:ASP:HB2  | 2:C:751:ARG:CB    | 2.47                     | 0.40              |
| 2:C:828:ILE:HG13 | 2:C:833:VAL:CG1   | 2.51                     | 0.40              |
| 3:D:140:LEU:CD2  | 3:D:184:ALA:HA    | 2.51                     | 0.40              |
| 3:D:378:LEU:HD11 | 3:D:470:VAL:HG13  | 2.04                     | 0.40              |
| 3:D:557:MET:O    | 3:D:585:PRO:HA    | 2.21                     | 0.40              |
| 3:D:650:LYS:O    | 3:D:654:VAL:HG23  | 2.21                     | 0.40              |
| 3:D:819:ARG:CG   | 3:D:875:SER:HB3   | 2.51                     | 0.40              |
| 3:D:881:VAL:HG12 | 3:D:890:VAL:HG21  | 2.03                     | 0.40              |
| 3:D:1128:GLY:O   | 3:D:1132:VAL:HG23 | 2.21                     | 0.40              |
| 5:F:123:MET:HG3  | 5:F:428:ILE:HD11  | 2.03                     | 0.40              |
| 5:F:636:ARG:HA   | 5:F:639:LYS:HD2   | 2.02                     | 0.40              |
| 7:I:-4:DC:H6     | 7:I:-4:DC:H5''    | 1.84                     | 0.40              |
| 7:I:28:DC:H6     | 7:I:28:DC:H2'     | 1.67                     | 0.40              |
| 1:A:101:LYS:HG3  | 1:A:124:ILE:CG1   | 2.51                     | 0.40              |
| 1:B:58:ALA:CB    | 1:B:174:ALA:HB3   | 2.46                     | 0.40              |
| 2:C:641:VAL:O    | 2:C:652:LEU:HD23  | 2.20                     | 0.40              |
| 2:C:712:GLU:HA   | 2:C:715:VAL:CG1   | 2.50                     | 0.40              |
| 2:C:1247:LEU:HB3 | 2:C:1249:LEU:HD12 | 2.03                     | 0.40              |
| 3:D:383:ILE:O    | 3:D:387:LEU:HG    | 2.22                     | 0.40              |
| 3:D:538:ALA:O    | 3:D:543:VAL:HG12  | 2.21                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:816:ILE:HG22  | 3:D:880:SER:HB2   | 2.02                     | 0.40              |
| 3:D:1125:ILE:HG13 | 3:D:1130:PRO:HG2  | 2.04                     | 0.40              |
| 3:D:1149:GLU:HB2  | 3:D:1219:ILE:HD12 | 2.03                     | 0.40              |
| 5:F:580:LEU:HB2   | 5:F:650:PHE:CZ    | 2.55                     | 0.40              |
| 6:H:-44:DC:H2'    | 6:H:-43:DT:H72    | 2.03                     | 0.40              |
| 7:I:24:DC:H1'     | 7:I:25:DC:O5'     | 2.20                     | 0.40              |
| 7:I:31:DG:C2'     | 7:I:32:DT:H71     | 2.51                     | 0.40              |
| 1:A:46:LEU:HD13   | 1:B:227:LEU:HD11  | 2.02                     | 0.40              |
| 1:A:89:LYS:HE3    | 1:A:89:LYS:HB2    | 1.87                     | 0.40              |
| 1:A:229:GLN:HG3   | 1:B:224:GLN:NE2   | 2.37                     | 0.40              |
| 1:B:63:GLN:HG3    | 1:B:142:VAL:O     | 2.21                     | 0.40              |
| 1:B:104:THR:N     | 1:B:119:GLU:O     | 2.54                     | 0.40              |
| 2:C:416:ARG:HD3   | 2:C:451:ASP:OD2   | 2.22                     | 0.40              |
| 2:C:707:VAL:HG22  | 2:C:707:VAL:O     | 2.20                     | 0.40              |
| 2:C:710:GLY:CA    | 2:C:1197:ALA:HB1  | 2.52                     | 0.40              |
| 2:C:800:LEU:HD12  | 2:C:801:ALA:N     | 2.36                     | 0.40              |
| 2:C:823:LEU:HD21  | 2:C:1098:LEU:CD1  | 2.42                     | 0.40              |
| 2:C:1196:ILE:HD11 | 2:C:1212:HIS:HE1  | 1.83                     | 0.40              |
| 2:C:1223:GLN:HB2  | 2:C:1238:PRO:HB2  | 2.02                     | 0.40              |
| 2:C:1288:GLU:HG2  | 3:D:430:THR:CG2   | 2.52                     | 0.40              |
| 3:D:61:ARG:HA     | 3:D:91:VAL:HA     | 2.04                     | 0.40              |
| 3:D:292:ILE:HD13  | 5:F:421:GLU:OE1   | 2.21                     | 0.40              |
| 3:D:480:LEU:HD11  | 4:E:50:LEU:HG     | 2.02                     | 0.40              |
| 3:D:1222:VAL:CG2  | 3:D:1257:LEU:HD13 | 2.52                     | 0.40              |
| 3:D:1373:GLU:O    | 3:D:1377:GLN:HG3  | 2.21                     | 0.40              |
| 4:E:64:LYS:O      | 4:E:68:ILE:HG12   | 2.21                     | 0.40              |
| 1:A:82:VAL:O      | 1:A:86:LEU:HD23   | 2.21                     | 0.40              |
| 2:C:108:VAL:HG23  | 2:C:492:ILE:HD11  | 2.03                     | 0.40              |
| 2:C:487:MET:HE2   | 2:C:487:MET:HB2   | 1.91                     | 0.40              |
| 2:C:558:VAL:HG11  | 3:D:773:HIS:HA    | 2.03                     | 0.40              |
| 2:C:738:ARG:HD2   | 2:C:756:ILE:CD1   | 2.37                     | 0.40              |
| 2:C:1251:HIS:HA   | 2:C:1256:LYS:NZ   | 2.37                     | 0.40              |
| 2:C:1344:MET:CB   | 2:C:1351:VAL:HG21 | 2.51                     | 0.40              |
| 3:D:683:VAL:CA    | 3:D:687:ALA:HB3   | 2.42                     | 0.40              |
| 3:D:927:THR:HG22  | 3:D:1127:GLY:O    | 2.20                     | 0.40              |
| 3:D:1193:ALA:H    | 3:D:1206:ILE:HG12 | 1.85                     | 0.40              |
| 3:D:1328:LEU:HD23 | 3:D:1328:LEU:HA   | 1.90                     | 0.40              |
| 6:H:-9:DC:C2'     | 6:H:-8:DC:H5''    | 2.52                     | 0.40              |
| 2:C:38:PHE:HE1    | 2:C:469:GLU:HA    | 1.86                     | 0.40              |
| 2:C:583:LEU:HD11  | 2:C:595:ILE:CG2   | 2.52                     | 0.40              |
| 2:C:761:LYS:HG3   | 2:C:762:PHE:H     | 1.87                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:826:GLU:HA   | 2:C:829:VAL:HG12 | 2.04                     | 0.40              |
| 3:D:434:LEU:HD22 | 3:D:491:ASN:CB   | 2.43                     | 0.40              |
| 3:D:681:LYS:C    | 3:D:685:ALA:HB3  | 2.42                     | 0.40              |
| 3:D:881:VAL:CG1  | 3:D:890:VAL:HG21 | 2.51                     | 0.40              |
| 3:D:1152:GLY:N   | 3:D:1200:ILE:O   | 2.55                     | 0.40              |
| 6:H:-27:DC:H2''  | 6:H:-26:DG:O5'   | 2.21                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | A     | 300/338 (89%)   | 280 (93%)  | 19 (6%)  | 1 (0%)   | 41          | 74  |
| 1   | B     | 214/338 (63%)   | 202 (94%)  | 12 (6%)  | 0        | 100         | 100 |
| 2   | C     | 1291/1356 (95%) | 1207 (94%) | 84 (6%)  | 0        | 100         | 100 |
| 3   | D     | 1128/1396 (81%) | 1072 (95%) | 56 (5%)  | 0        | 100         | 100 |
| 4   | E     | 67/119 (56%)    | 64 (96%)   | 3 (4%)   | 0        | 100         | 100 |
| 5   | F     | 493/652 (76%)   | 477 (97%)  | 16 (3%)  | 0        | 100         | 100 |
| 8   | G     | 51/173 (30%)    | 49 (96%)   | 2 (4%)   | 0        | 100         | 100 |
| All | All   | 3544/4372 (81%) | 3351 (95%) | 192 (5%) | 1 (0%)   | 100         | 100 |

All (1) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 54  | LEU  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 1   | A     | 176/285 (62%)   | 175 (99%)   | 1 (1%)   | 86          | 92  |
| 1   | B     | 173/285 (61%)   | 173 (100%)  | 0        | 100         | 100 |
| 2   | C     | 975/1137 (86%)  | 971 (100%)  | 4 (0%)   | 91          | 95  |
| 3   | D     | 941/1157 (81%)  | 937 (100%)  | 4 (0%)   | 91          | 95  |
| 4   | E     | 56/100 (56%)    | 56 (100%)   | 0        | 100         | 100 |
| 5   | F     | 247/542 (46%)   | 244 (99%)   | 3 (1%)   | 71          | 84  |
| 8   | G     | 37/134 (28%)    | 37 (100%)   | 0        | 100         | 100 |
| All | All   | 2605/3640 (72%) | 2593 (100%) | 12 (0%)  | 89          | 94  |

All (12) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 102 | ARG  |
| 2   | C     | 35  | TYR  |
| 2   | C     | 149 | ARG  |
| 2   | C     | 231 | TYR  |
| 2   | C     | 550 | ARG  |
| 3   | D     | 252 | ARG  |
| 3   | D     | 727 | ARG  |
| 3   | D     | 776 | ARG  |
| 3   | D     | 901 | ARG  |
| 5   | F     | 491 | ARG  |
| 5   | F     | 581 | ARG  |
| 5   | F     | 602 | ARG  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 44  | ASN  |
| 1   | A     | 63  | GLN  |
| 1   | B     | 44  | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 224  | GLN  |
| 2   | C     | 154  | GLN  |
| 2   | C     | 357  | ASN  |
| 2   | C     | 419  | GLN  |
| 2   | C     | 458  | ASN  |
| 2   | C     | 527  | ASN  |
| 2   | C     | 590  | ASN  |
| 2   | C     | 628  | ASN  |
| 2   | C     | 666  | GLN  |
| 2   | C     | 693  | GLN  |
| 2   | C     | 695  | GLN  |
| 2   | C     | 767  | GLN  |
| 2   | C     | 773  | GLN  |
| 2   | C     | 870  | ASN  |
| 2   | C     | 941  | ASN  |
| 2   | C     | 974  | ASN  |
| 2   | C     | 976  | ASN  |
| 2   | C     | 1079 | GLN  |
| 2   | C     | 1129 | GLN  |
| 2   | C     | 1141 | ASN  |
| 2   | C     | 1155 | GLN  |
| 2   | C     | 1189 | ASN  |
| 2   | C     | 1258 | HIS  |
| 2   | C     | 1270 | GLN  |
| 3   | D     | 114  | HIS  |
| 3   | D     | 158  | HIS  |
| 3   | D     | 276  | ASN  |
| 3   | D     | 278  | ASN  |
| 3   | D     | 460  | ASN  |
| 3   | D     | 491  | ASN  |
| 3   | D     | 702  | GLN  |
| 3   | D     | 770  | ASN  |
| 3   | D     | 801  | GLN  |
| 3   | D     | 874  | GLN  |
| 3   | D     | 1227 | ASN  |
| 3   | D     | 1234 | GLN  |
| 3   | D     | 1245 | ASN  |
| 3   | D     | 1275 | HIS  |
| 3   | D     | 1285 | GLN  |
| 3   | D     | 1374 | GLN  |
| 4   | E     | 42   | ASN  |
| 5   | F     | 423  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | F     | 579 | ASN  |
| 5   | F     | 629 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 6   | 6MA  | H     | 11  | 7,6  | 18,24,25     | 3.10 | 10 (55%) | 15,34,37    | 2.02 | 3 (20%)  |
| 7   | 6MA  | I     | -13 | 7,6  | 18,24,25     | 3.12 | 10 (55%) | 15,34,37    | 2.03 | 3 (20%)  |
| 6   | 6MA  | H     | 3   | 6    | 18,24,25     | 3.09 | 10 (55%) | 15,34,37    | 2.20 | 4 (26%)  |
| 7   | 6MA  | I     | -5  | 7    | 18,24,25     | 3.13 | 10 (55%) | 15,34,37    | 2.09 | 3 (20%)  |

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   | 6MA  | H     | 11  | 7,6  | -       | 5/5/23/24 | 0/3/3/3 |
| 7   | 6MA  | I     | -13 | 7,6  | -       | 4/5/23/24 | 0/3/3/3 |
| 6   | 6MA  | H     | 3   | 6    | -       | 2/5/23/24 | 0/3/3/3 |
| 7   | 6MA  | I     | -5  | 7    | -       | 4/5/23/24 | 0/3/3/3 |

All (40) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 7   | I     | -5  | 6MA  | O4'-C4' | 8.03  | 1.63        | 1.45     |
| 7   | I     | -13 | 6MA  | C3'-C4' | -7.89 | 1.31        | 1.53     |
| 7   | I     | -13 | 6MA  | O4'-C4' | 7.89  | 1.62        | 1.45     |
| 6   | H     | 11  | 6MA  | O4'-C4' | 7.85  | 1.62        | 1.45     |
| 6   | H     | 11  | 6MA  | C3'-C4' | -7.82 | 1.31        | 1.53     |
| 7   | I     | -5  | 6MA  | C3'-C4' | -7.74 | 1.31        | 1.53     |
| 6   | H     | 3   | 6MA  | O4'-C4' | 7.70  | 1.62        | 1.45     |
| 6   | H     | 3   | 6MA  | C3'-C4' | -7.64 | 1.32        | 1.53     |
| 6   | H     | 3   | 6MA  | O4'-C1' | -3.08 | 1.35        | 1.42     |
| 6   | H     | 11  | 6MA  | C5-C4   | -2.81 | 1.33        | 1.40     |
| 7   | I     | -13 | 6MA  | C5-C4   | -2.79 | 1.33        | 1.40     |
| 7   | I     | -5  | 6MA  | O4'-C1' | -2.78 | 1.36        | 1.42     |
| 7   | I     | -5  | 6MA  | C5-C4   | -2.78 | 1.33        | 1.40     |
| 6   | H     | 3   | 6MA  | C5-C4   | -2.78 | 1.33        | 1.40     |
| 7   | I     | -13 | 6MA  | O4'-C1' | -2.74 | 1.36        | 1.42     |
| 6   | H     | 11  | 6MA  | O4'-C1' | -2.72 | 1.36        | 1.42     |
| 7   | I     | -5  | 6MA  | C1-N6   | 2.66  | 1.49        | 1.45     |
| 7   | I     | -13 | 6MA  | C1-N6   | 2.66  | 1.49        | 1.45     |
| 6   | H     | 3   | 6MA  | C1-N6   | 2.64  | 1.49        | 1.45     |
| 6   | H     | 11  | 6MA  | C1-N6   | 2.59  | 1.49        | 1.45     |
| 7   | I     | -5  | 6MA  | O3'-C3' | 2.40  | 1.48        | 1.43     |
| 6   | H     | 11  | 6MA  | O5'-C5' | -2.38 | 1.38        | 1.44     |
| 7   | I     | -13 | 6MA  | C2-N3   | 2.37  | 1.35        | 1.32     |
| 7   | I     | -5  | 6MA  | C2-N3   | 2.36  | 1.35        | 1.32     |
| 6   | H     | 11  | 6MA  | C2-N3   | 2.32  | 1.35        | 1.32     |
| 6   | H     | 3   | 6MA  | O5'-C5' | -2.31 | 1.39        | 1.44     |
| 6   | H     | 3   | 6MA  | O3'-C3' | 2.29  | 1.48        | 1.43     |
| 6   | H     | 3   | 6MA  | C2'-C3' | 2.28  | 1.58        | 1.52     |
| 7   | I     | -13 | 6MA  | O5'-C5' | -2.27 | 1.39        | 1.44     |
| 6   | H     | 3   | 6MA  | C2-N3   | 2.27  | 1.35        | 1.32     |
| 7   | I     | -5  | 6MA  | O5'-C5' | -2.27 | 1.39        | 1.44     |
| 7   | I     | -13 | 6MA  | O3'-C3' | 2.26  | 1.48        | 1.43     |
| 6   | H     | 11  | 6MA  | O3'-C3' | 2.23  | 1.48        | 1.43     |
| 6   | H     | 11  | 6MA  | C5-N7   | -2.14 | 1.32        | 1.39     |
| 6   | H     | 3   | 6MA  | C5-N7   | -2.13 | 1.32        | 1.39     |
| 7   | I     | -5  | 6MA  | C5-N7   | -2.13 | 1.32        | 1.39     |
| 7   | I     | -13 | 6MA  | C5-N7   | -2.11 | 1.32        | 1.39     |
| 6   | H     | 11  | 6MA  | C2'-C3' | 2.07  | 1.58        | 1.52     |
| 7   | I     | -5  | 6MA  | C2'-C3' | 2.04  | 1.58        | 1.52     |
| 7   | I     | -13 | 6MA  | C2'-C3' | 2.02  | 1.58        | 1.52     |

All (13) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 7   | I     | -13 | 6MA  | N3-C2-N1   | -5.62 | 119.89      | 128.68   |
| 6   | H     | 11  | 6MA  | N3-C2-N1   | -5.62 | 119.90      | 128.68   |
| 7   | I     | -5  | 6MA  | N3-C2-N1   | -5.53 | 120.03      | 128.68   |
| 6   | H     | 3   | 6MA  | N3-C2-N1   | -5.50 | 120.09      | 128.68   |
| 6   | H     | 3   | 6MA  | C1-N6-C6   | -3.76 | 119.64      | 122.87   |
| 7   | I     | -13 | 6MA  | C2-N1-C6   | 3.60  | 119.67      | 116.59   |
| 6   | H     | 3   | 6MA  | C2-N1-C6   | 3.59  | 119.67      | 116.59   |
| 6   | H     | 11  | 6MA  | C2-N1-C6   | 3.55  | 119.63      | 116.59   |
| 7   | I     | -13 | 6MA  | C1-N6-C6   | -3.52 | 119.84      | 122.87   |
| 7   | I     | -5  | 6MA  | C2-N1-C6   | 3.50  | 119.59      | 116.59   |
| 7   | I     | -5  | 6MA  | C1-N6-C6   | -3.48 | 119.87      | 122.87   |
| 6   | H     | 11  | 6MA  | C1-N6-C6   | -3.45 | 119.90      | 122.87   |
| 6   | H     | 3   | 6MA  | C2'-C1'-N9 | -2.02 | 109.62      | 114.27   |

There are no chirality outliers.

All (15) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 6   | H     | 3   | 6MA  | C5-C6-N6-C1     |
| 6   | H     | 3   | 6MA  | N1-C6-N6-C1     |
| 6   | H     | 11  | 6MA  | C5-C6-N6-C1     |
| 6   | H     | 11  | 6MA  | N1-C6-N6-C1     |
| 7   | I     | -13 | 6MA  | C3'-C4'-C5'-O5' |
| 7   | I     | -13 | 6MA  | C5-C6-N6-C1     |
| 7   | I     | -13 | 6MA  | N1-C6-N6-C1     |
| 7   | I     | -5  | 6MA  | O4'-C4'-C5'-O5' |
| 7   | I     | -5  | 6MA  | C3'-C4'-C5'-O5' |
| 7   | I     | -5  | 6MA  | C5-C6-N6-C1     |
| 7   | I     | -5  | 6MA  | N1-C6-N6-C1     |
| 7   | I     | -13 | 6MA  | O4'-C4'-C5'-O5' |
| 6   | H     | 11  | 6MA  | C3'-C4'-C5'-O5' |
| 6   | H     | 11  | 6MA  | O4'-C4'-C5'-O5' |
| 6   | H     | 11  | 6MA  | C4'-C5'-O5'-P   |

There are no ring outliers.

3 monomers are involved in 8 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 7   | I     | -13 | 6MA  | 3       | 0            |
| 6   | H     | 3   | 6MA  | 2       | 0            |
| 7   | I     | -5  | 6MA  | 3       | 0            |

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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.

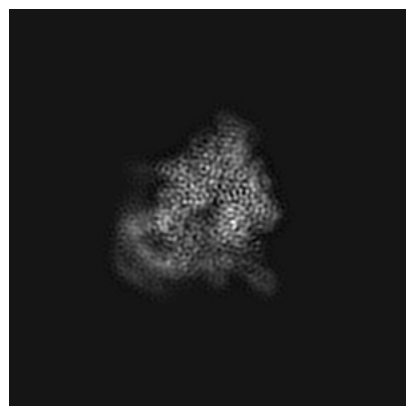
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33762. These allow visual inspection of the internal detail of the map and identification of artifacts.

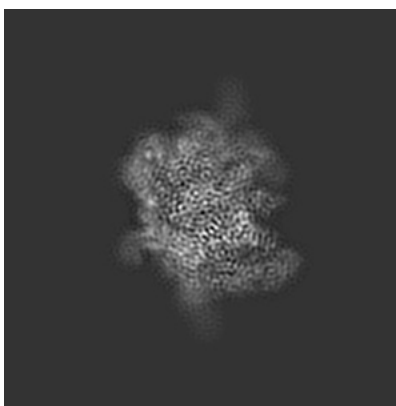
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

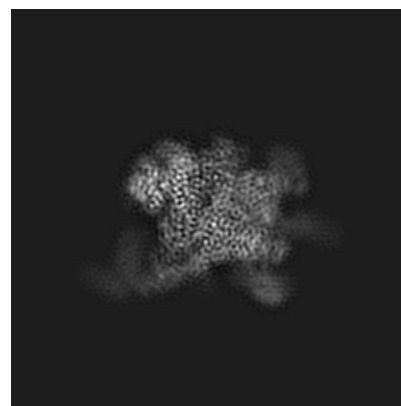
#### 6.1.1 Primary map



X

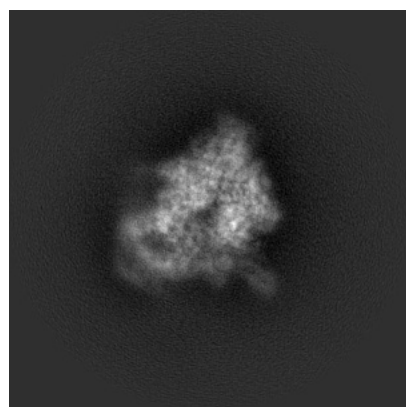


Y

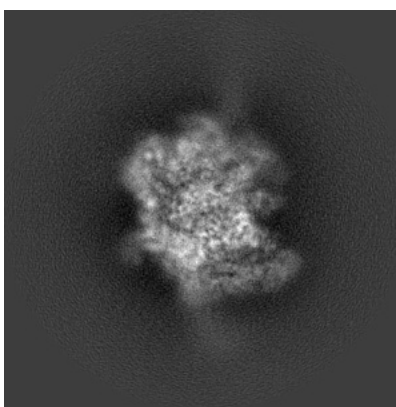


Z

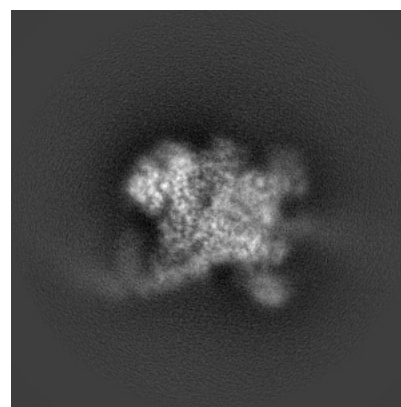
#### 6.1.2 Raw map



X



Y

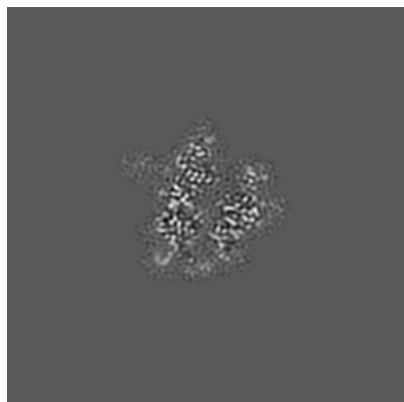


Z

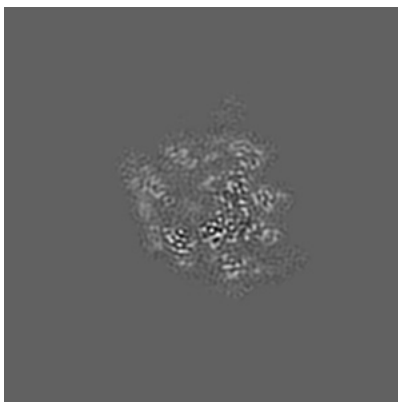
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

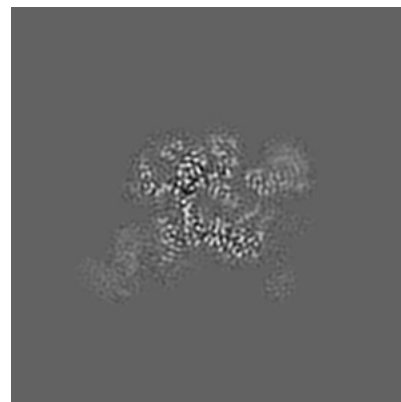
### 6.2.1 Primary map



X Index: 150

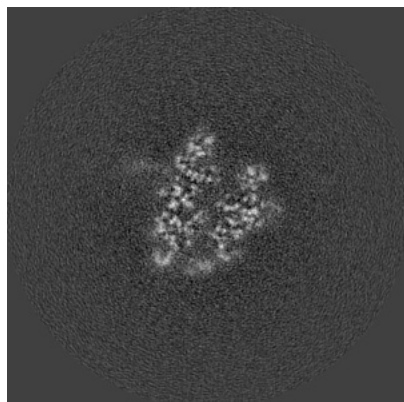


Y Index: 150

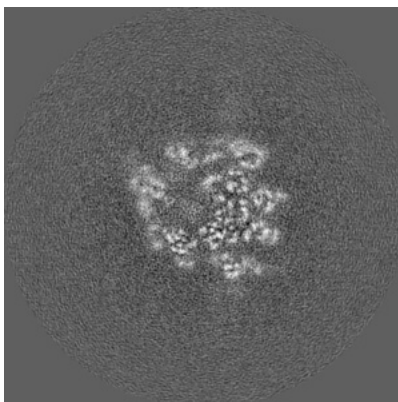


Z Index: 150

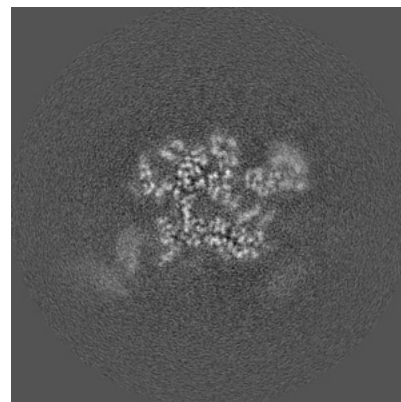
### 6.2.2 Raw map



X Index: 150



Y Index: 150

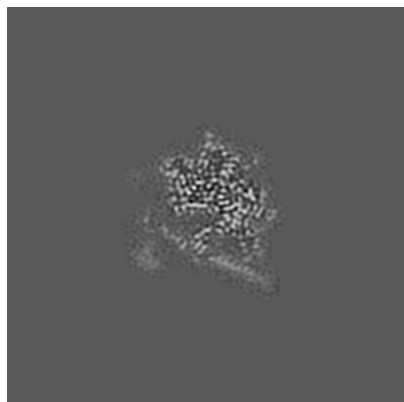


Z Index: 150

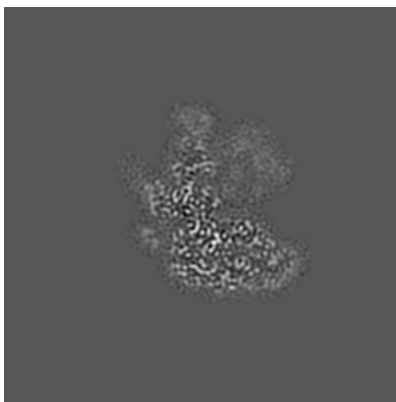
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

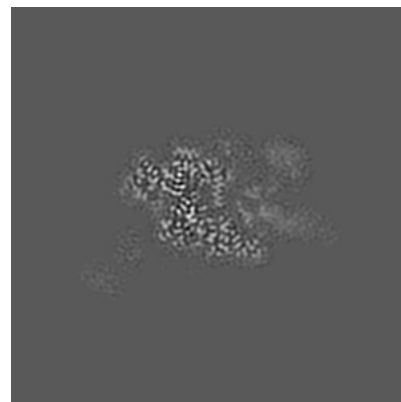
### 6.3.1 Primary map



X Index: 131

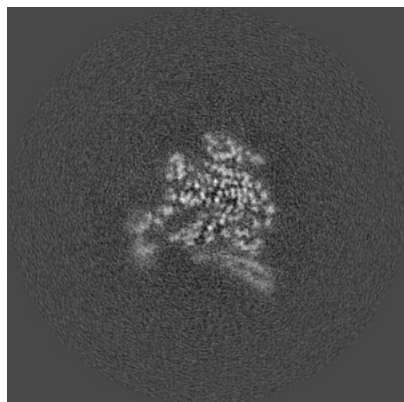


Y Index: 165

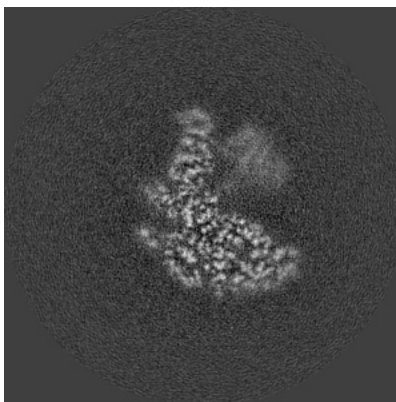


Z Index: 159

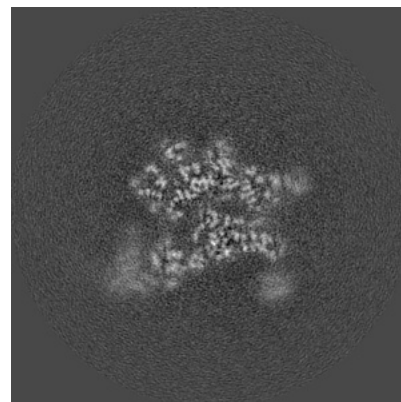
### 6.3.2 Raw map



X Index: 125



Y Index: 168



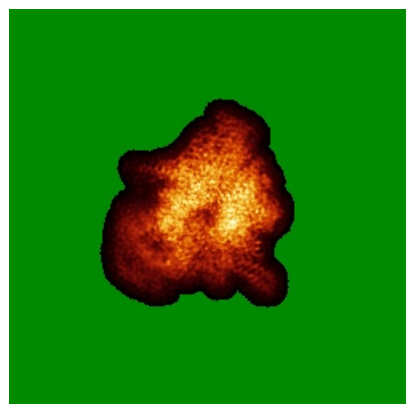
Z Index: 138

The images above show the largest variance slices of the map in three orthogonal directions.

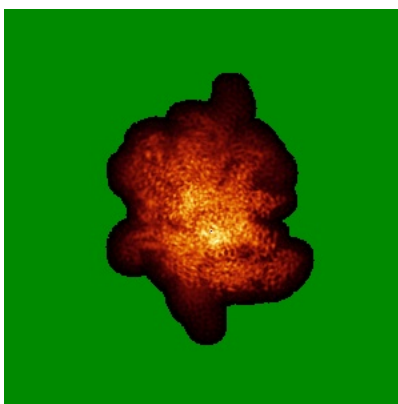


## 6.4 Orthogonal standard-deviation projections (False-color) ⓘ

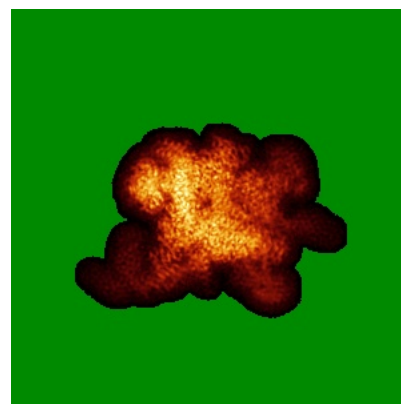
### 6.4.1 Primary map



X

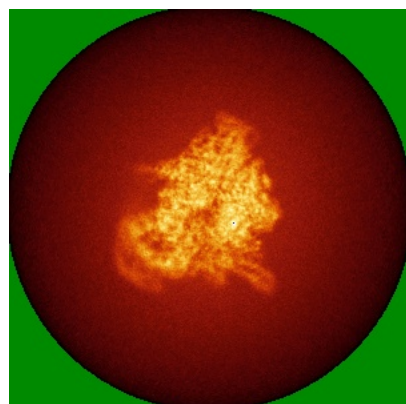


Y

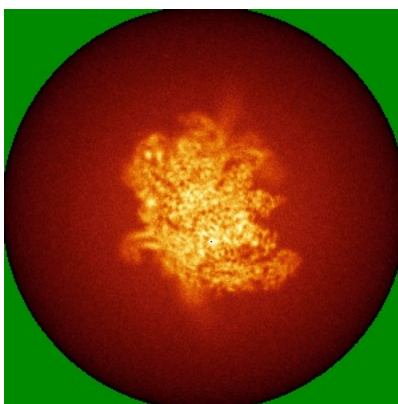


Z

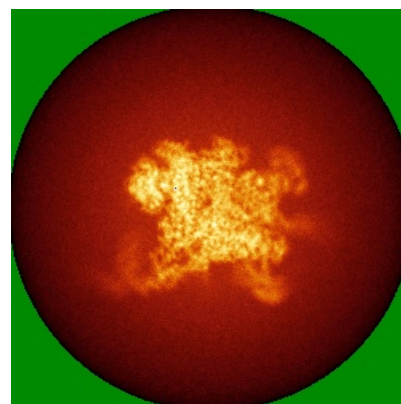
### 6.4.2 Raw map



X



Y

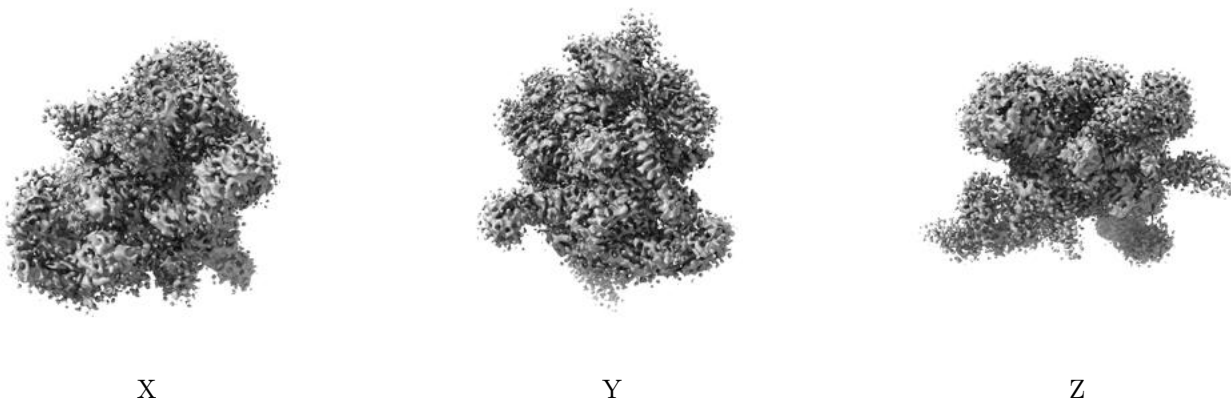


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

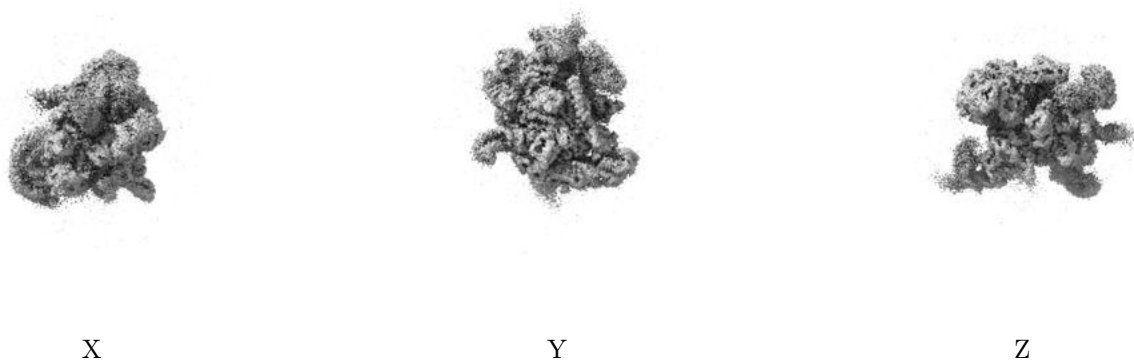
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

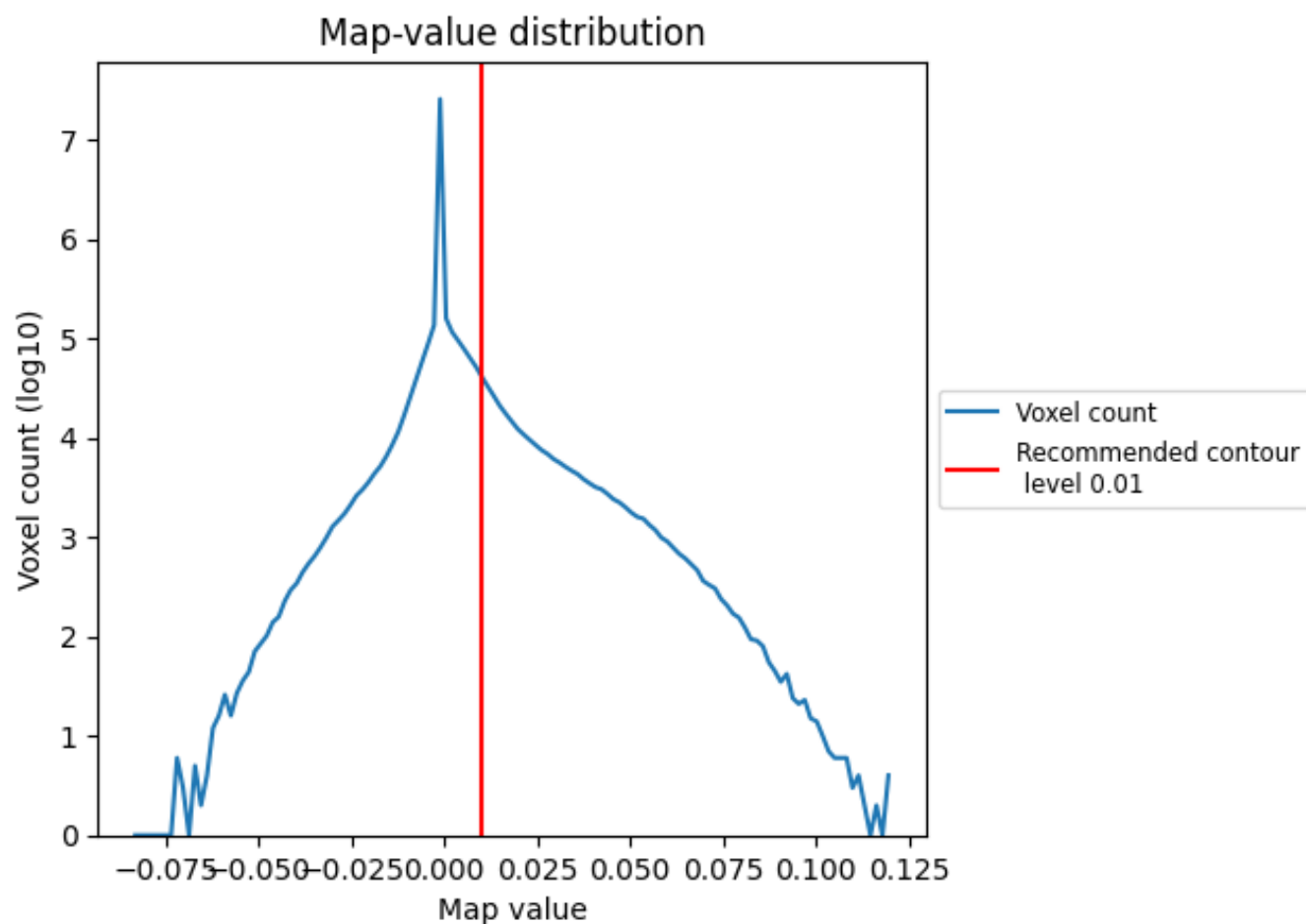
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

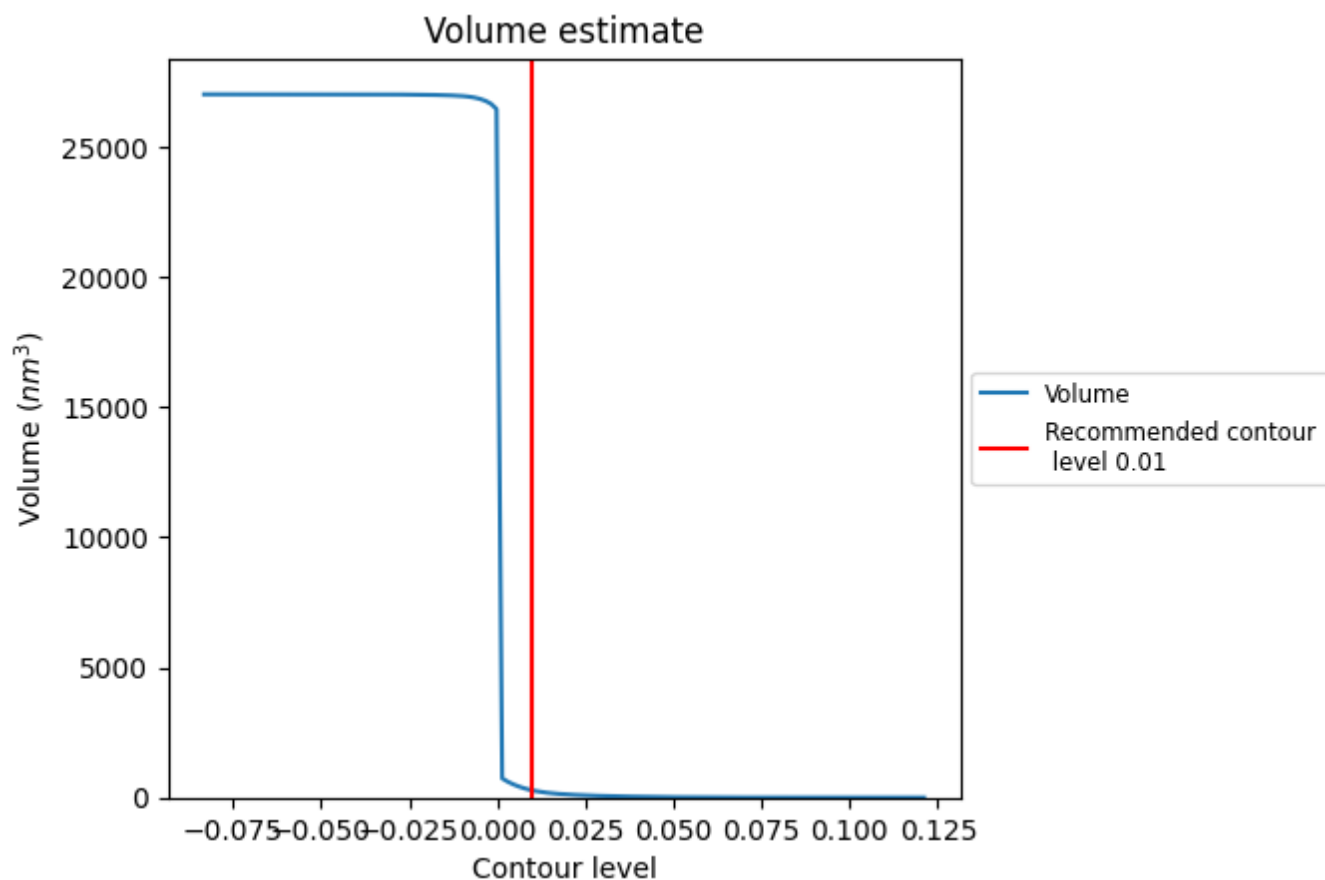
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

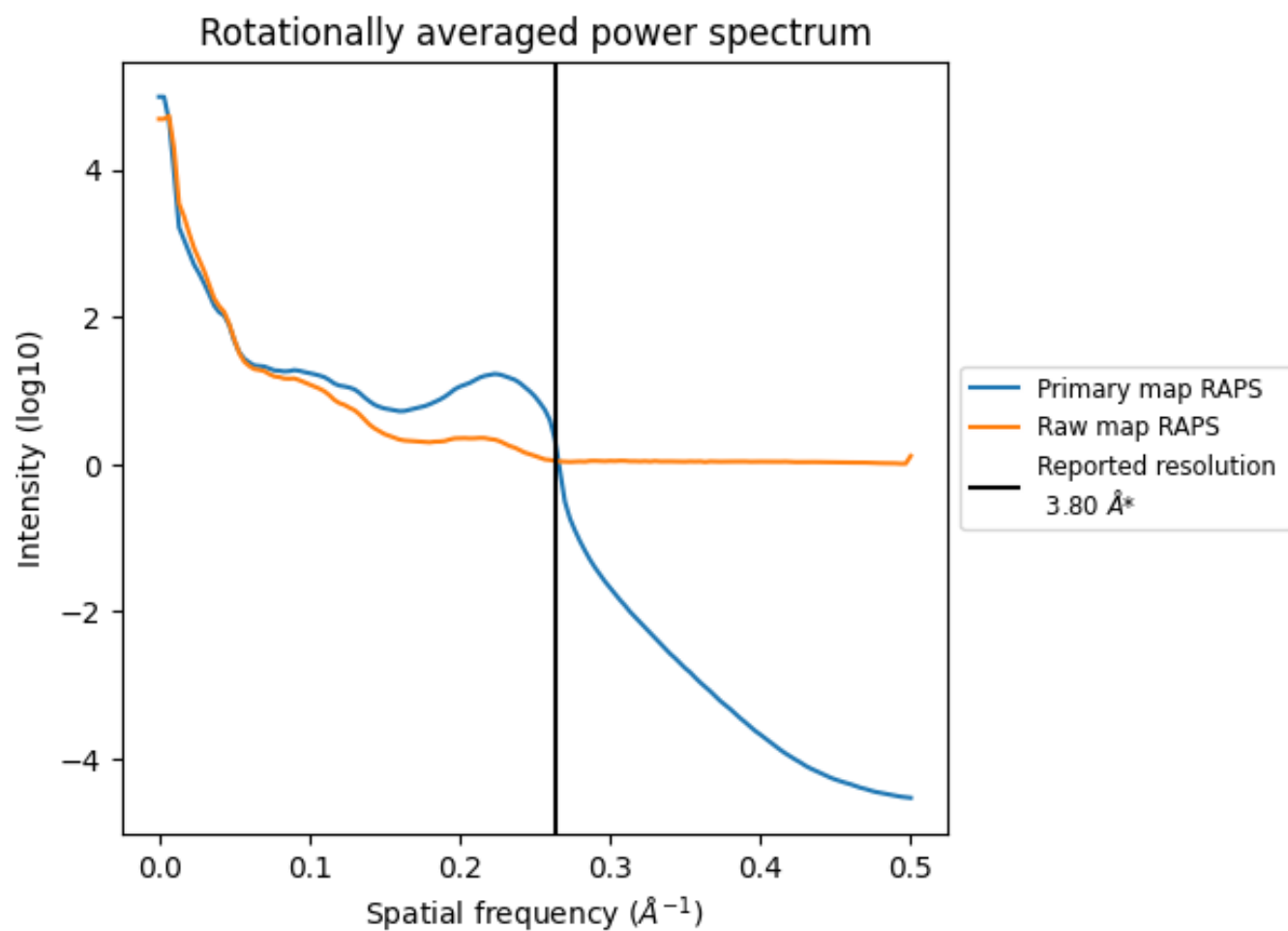
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 277 nm<sup>3</sup>; this corresponds to an approximate mass of 250 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

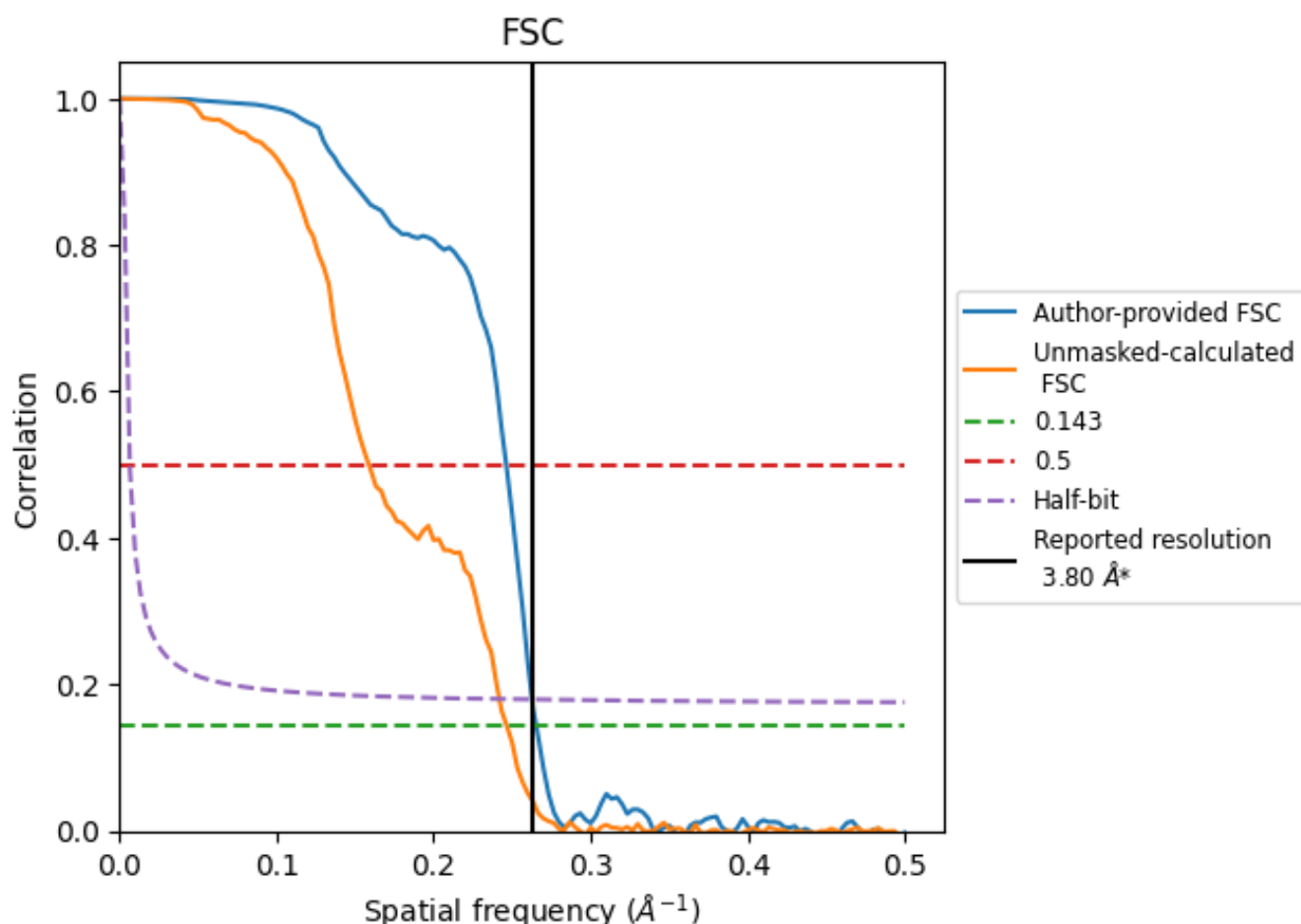


\*Reported resolution corresponds to spatial frequency of  $0.263 \text{ \AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.263 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.80                               | -    | -        |
| Author-provided FSC curve | 3.77                               | 4.06 | 3.81     |
| Unmasked-calculated*      | 4.06                               | 6.30 | 4.13     |

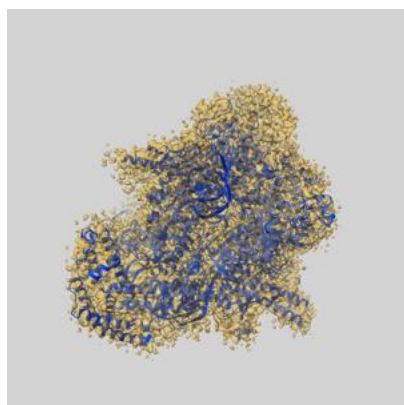
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.



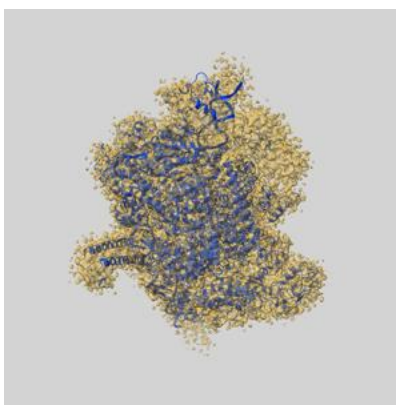
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-33762 and PDB model 7YE2. Per-residue inclusion information can be found in section [3](#) on page [6](#).

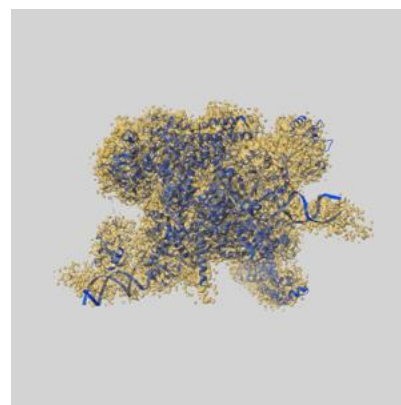
### 9.1 Map-model overlay [i](#)



X



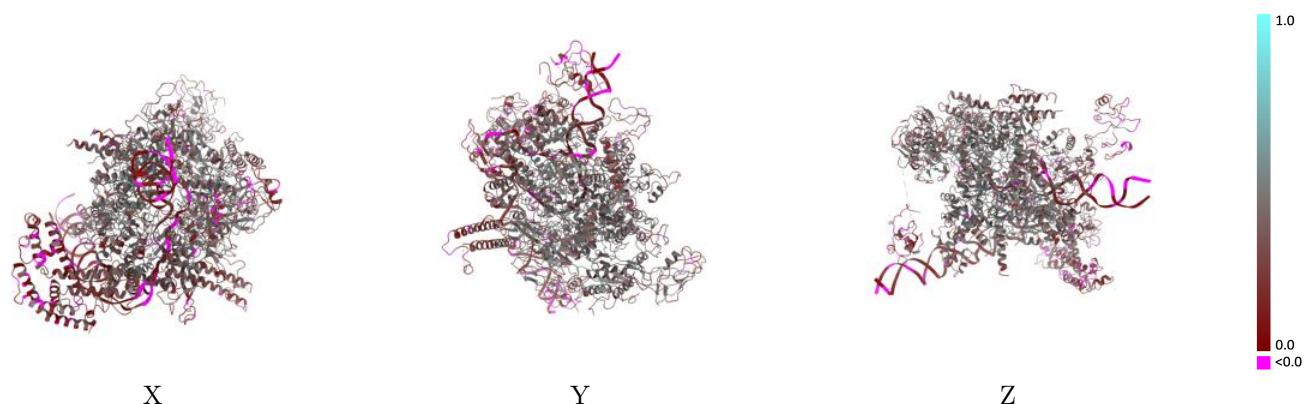
Y



Z

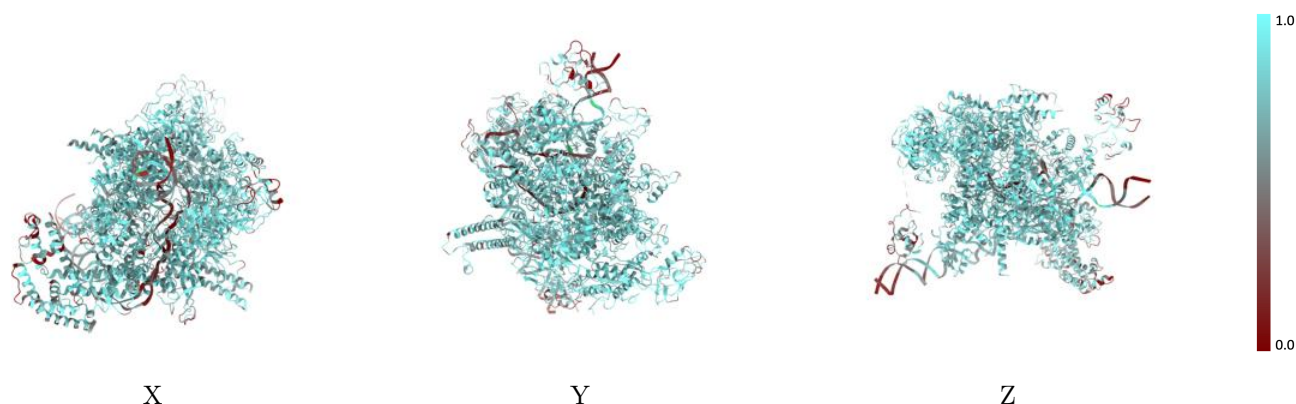
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



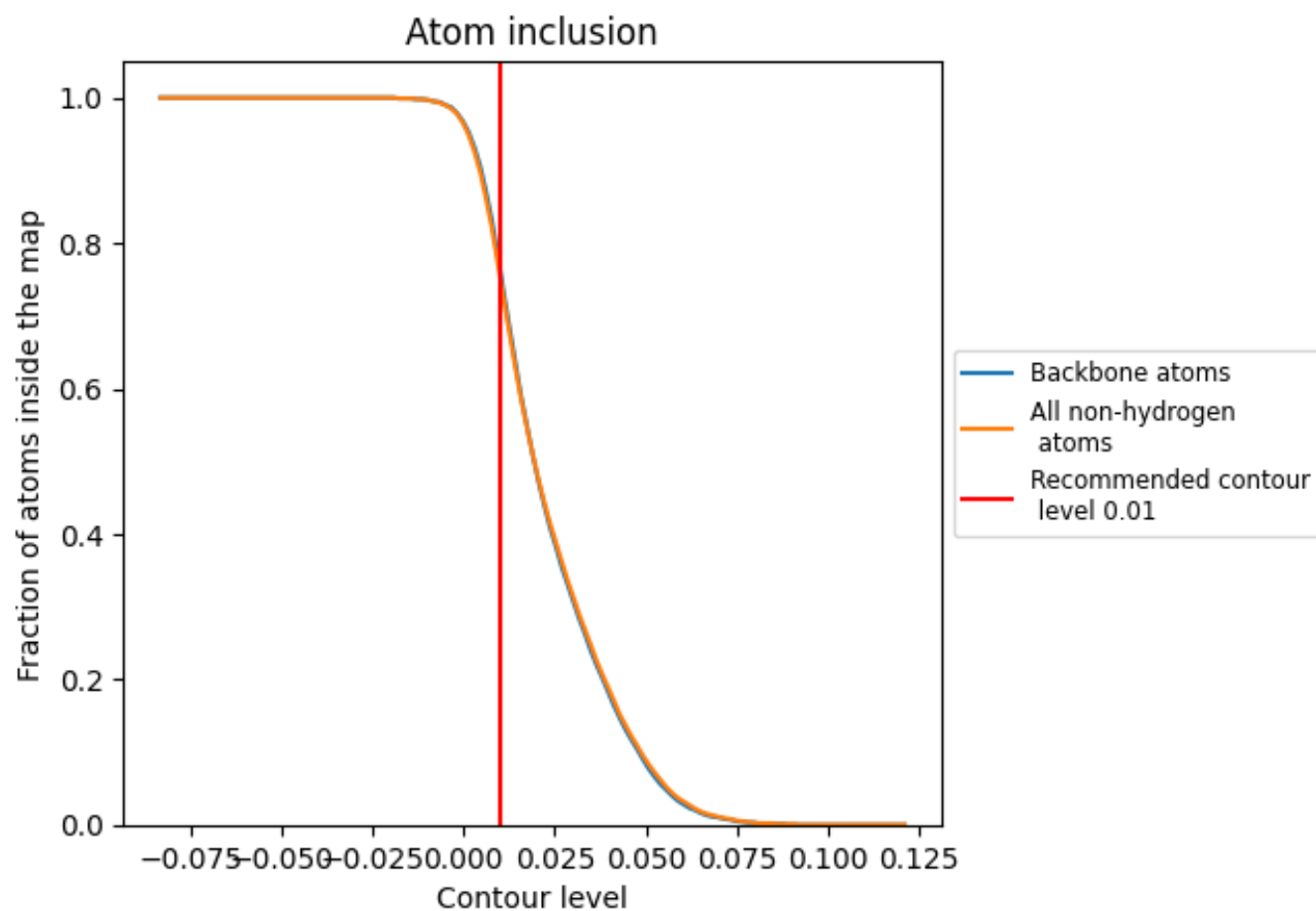
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                | Q-score                       |
|-------|-------------------------------|-------------------------------|
| All   | <div><div></div></div> 0.7550 | <div><div></div></div> 0.3540 |
| A     | <div><div></div></div> 0.7690 | <div><div></div></div> 0.3850 |
| B     | <div><div></div></div> 0.8060 | <div><div></div></div> 0.3890 |
| C     | <div><div></div></div> 0.7850 | <div><div></div></div> 0.3840 |
| D     | <div><div></div></div> 0.8030 | <div><div></div></div> 0.4060 |
| E     | <div><div></div></div> 0.8140 | <div><div></div></div> 0.4120 |
| F     | <div><div></div></div> 0.7330 | <div><div></div></div> 0.3080 |
| G     | <div><div></div></div> 0.6820 | <div><div></div></div> 0.2680 |
| H     | <div><div></div></div> 0.4960 | <div><div></div></div> 0.0990 |
| I     | <div><div></div></div> 0.4880 | <div><div></div></div> 0.0920 |

1.0

0.0

<0.0