



## Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:18 PM UTC

PDB ID : 6BZO / pdb\_00006bzo  
EMDB ID : EMD-7319  
Title : Mtb RNAP Holo/RbpA/Fidaxomicin/upstream fork DNA  
Authors : Darst, S.A.; Campbell, E.A.; Boyaci Selcuk, H.; Chen, J.  
Deposited on : 2017-12-25  
Resolution : 3.38 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:

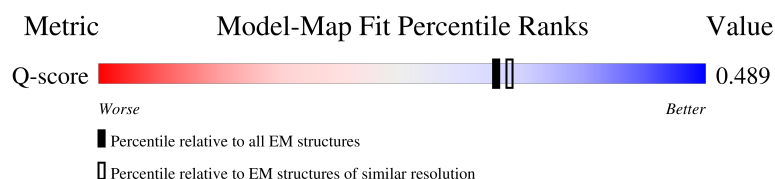
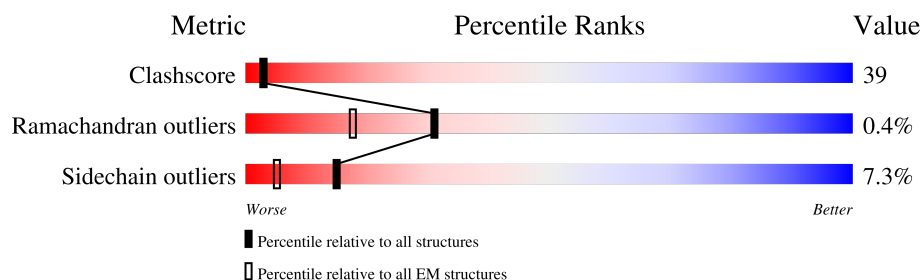
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 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 3.38 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) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 14261 ( 2.88 - 3.88 )                                    |

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     | 347    |                  |
| 1   | B     | 347    |                  |
| 2   | C     | 1181   |                  |
| 3   | D     | 1324   |                  |

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| Mol | Chain | Length | Quality of chain                                                            |
|-----|-------|--------|-----------------------------------------------------------------------------|
| 4   | E     | 110    | <div><div></div><div>27%</div><div>47%</div><div></div><div>25%</div></div> |
| 5   | F     | 531    | <div><div></div><div>28%</div><div>30%</div><div></div><div>39%</div></div> |
| 6   | J     | 111    | <div><div></div><div>48%</div><div>38%</div><div>11%</div><div></div></div> |
| 7   | O     | 31     | <div><div></div><div>26%</div><div>74%</div><div></div></div>               |
| 8   | P     | 26     | <div><div></div><div>38%</div><div>62%</div><div></div></div>               |

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 27336 atoms, of which 74 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     | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1724  | 1085 | 297 | 339 | 3 |         |       |
| 1   | B     | 237      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1775  | 1120 | 304 | 348 | 3 |         |       |

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

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 2   | C     | 1111     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 8556  | 5361 | 1504 | 1652 | 39 |         |       |

There are 9 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| C     | 1179    | LEU      | -      | expression tag | UNP V9Z879 |
| C     | 1180    | ALA      | -      | expression tag | UNP V9Z879 |
| C     | 1181    | ARG      | -      | expression tag | UNP V9Z879 |
| C     | 1182    | HIS      | -      | expression tag | UNP V9Z879 |
| C     | 1183    | GLY      | -      | expression tag | UNP V9Z879 |
| C     | 1184    | GLY      | -      | expression tag | UNP V9Z879 |
| C     | 1185    | SER      | -      | expression tag | UNP V9Z879 |
| C     | 1186    | GLY      | -      | expression tag | UNP V9Z879 |
| C     | 1187    | ALA      | -      | expression tag | UNP V9Z879 |

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

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 3   | D     | 1263     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 9857  | 6175 | 1791 | 1850 | 41 |         |       |

There are 8 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference      |
|-------|---------|----------|--------|----------------|----------------|
| D     | 1317    | HIS      | -      | expression tag | UNP A0A045J9E2 |
| D     | 1318    | HIS      | -      | expression tag | UNP A0A045J9E2 |
| D     | 1319    | HIS      | -      | expression tag | UNP A0A045J9E2 |
| D     | 1320    | HIS      | -      | expression tag | UNP A0A045J9E2 |
| D     | 1321    | HIS      | -      | expression tag | UNP A0A045J9E2 |
| D     | 1322    | HIS      | -      | expression tag | UNP A0A045J9E2 |
| D     | 1323    | HIS      | -      | expression tag | UNP A0A045J9E2 |
| D     | 1324    | HIS      | -      | expression tag | UNP A0A045J9E2 |

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

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 4   | E     | 83       | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 649   | 414 | 108 | 127 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference      |
|-------|---------|----------|--------|----------------|----------------|
| E     | 1       | GLY      | -      | expression tag | UNP A0A0T9N9K3 |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 5   | F     | 326      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2588  | 1617 | 467 | 495 | 9 |         |       |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference      |
|-------|---------|----------|--------|----------------|----------------|
| F     | -2      | GLY      | -      | expression tag | UNP A0A045HD00 |
| F     | -1      | PRO      | -      | expression tag | UNP A0A045HD00 |
| F     | 0       | HIS      | -      | expression tag | UNP A0A045HD00 |

- Molecule 6 is a protein called RNA polymerase-binding protein RbpA.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | J     | 107      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 872   | 539 | 162 | 168 | 3 |         |       |

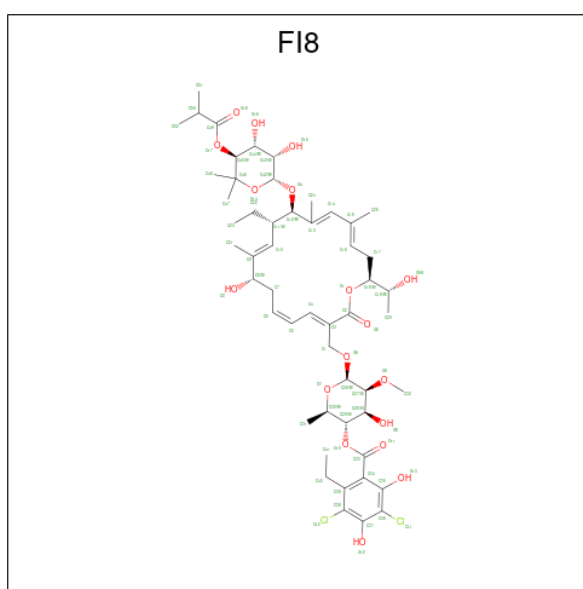
- Molecule 7 is a DNA chain called DNA (32-MER).

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 7   | O     | 31       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 634   | 305 | 114 | 185 | 30 |         |       |

- Molecule 8 is a DNA chain called DNA (26-MER).

| Mol | Chain | Residues | Atoms |     |    |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|-------|
| 8   | P     | 26       | Total | C   | N  | O   | P  | 0       | 0     |
|     |       |          | 526   | 254 | 94 | 153 | 25 |         |       |

- Molecule 9 is Fidaxomicin (CCD ID: FI8) (formula:  $C_{52}H_{74}Cl_2O_{18}$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |    |    |    | AltConf |
|-----|-------|----------|-------|----|----|----|----|---------|
| 9   | C     | 1        | Total | C  | Cl | H  | O  | 0       |
|     |       |          | 146   | 52 | 2  | 74 | 18 |         |

- Molecule 10 is ZINC ION (CCD ID: ZN) (formula:  $Zn$ ).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 10  | D     | 2        | Total | Zn | 0       |
|     |       |          | 2     | 2  |         |

- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula:  $Mg$ ).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 11  | D     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 12 is water.

| Mol | Chain | Residues | Atoms      |        | AltConf |
|-----|-------|----------|------------|--------|---------|
| 12  | C     | 2        | Total<br>2 | O<br>2 | 0       |
| 12  | D     | 4        | Total<br>4 | O<br>4 | 0       |

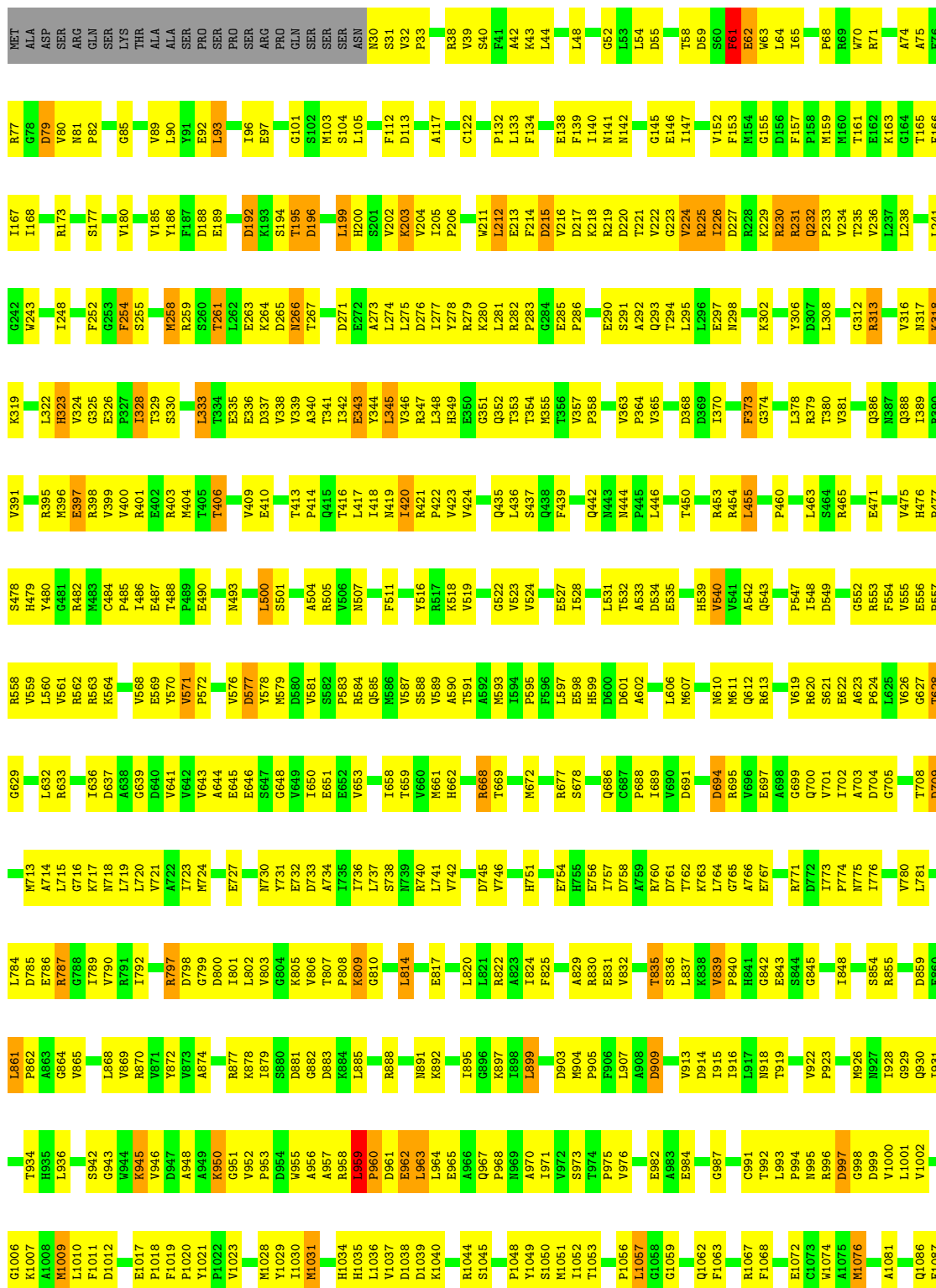




ALA  
TYR  
GLU  
GLN  
ASP  
TYR  
ALA  
GLU  
THR  
GLU  
GLN  
LEU

● Molecule 2: DNA-directed RNA polymerase subunit beta

Chain C: 42% 46% 5% 6%



|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| L1088 | L1091 | L1092 | S1093 | R1099 | V1102 | Y1103 | E1104 | Y1107 | E1110 | N1111 | I1112 | T1117 | F1118 | E1119 | V1123 | L1124 | L1125 | K1126 | E1127 | Q1129 | V1135 | S1140 | ASP | GLY | ALA | ALA | TLE | GLU | LEU | ARG | GLU | GLY | GLY | ASP | GLU | ASP | LEU | GLU | ARG | ALA | ALA | ASN | ASN | GLY | TLE | ASN | LEU | SER |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| ARG | ASN | GLU | SER | ALA | SER | VAL | GLU | ASP | LEU | ALA | LEU | ALA | ARG | HIS | GLY | GLY | SER | GLY | ALA |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

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



|     |     |     |    |    |    |     |     |     |     |      |      |      |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|----|----|----|-----|-----|-----|-----|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| RET | LEU | ASP | V4 | N5 | E9 | L10 | R11 | I12 | D19 | H104 | H103 | H105 | T20 | R21 | Q22 | Y25 | P31 | N35 | V36 | R37 | T38 | L39 | E49 | R50 | L51 | F52 | G53 | P54 | T55 | R56 | D57 | W58 | E59 | C60 | Y61 | G62 | G63 | K64 | Y65 | K66 | R67 | I73 | E76 | R77 | C78 | G79 | V80 | E81 | H82 | A83 | T84 | E85 | R86 | V87 |
|-----|-----|-----|----|----|----|-----|-----|-----|-----|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

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|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|------|------|-----|-----|------|------|------|------|
| R88 | R89 | E90 | R91 | N92 | E96 | V101 | T102 | H103 | H104 | H105 | H106 | F107 | P111 | S112 | R113 | Y116 | L117 | L118 | D119 | D120 | A121 | P122 | R123 | D124 | L125 | F126 | G127 | L128 | I129 | Y130 | Y134 | Y135 | I136 | T137 | S138 | V139 | D140 | E141 | E142 | M143 | R144 | H145 | N146 | E147 | L148 | S149 | T150 | L151 | E81 | A152 | R153 | T83 | R84 | E154 | M155 | A156 | V157 |
|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|------|------|-----|-----|------|------|------|------|

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| E158 | R159 | L160 | A161 | V162 | E163 | D164 | Q165 | R166 | E169 | L170 | H171 | A172 | R173 | A174 | Q175 | K176 | L177 | E178 | A179 | E185 | A186 | E187 | G188 | L189 | K190 | A191 | D192 | A193 | K196 | V197 | R198 | D199 | G200 | G201 | E202 | R203 | E204 | R205 | R206 | Q207 | T208 | R211 | A212 | Q213 | R214 | E215 | L216 | D217 | R218 | L219 | E220 | D221 | I222 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|

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|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| K223 | S224 | T225 | F226 | T227 | K228 | L229 | A230 | P231 | K232 | L234 | L235 | V236 | D237 | E238 | N239 | L240 | Y241 | R242 | E243 | L244 | V245 | D246 | R247 | Y248 | G249 | E250 | F251 | F252 | T253 | M256 | L261 | Q262 | K263 | F268 | D269 | L270 | E273 | A274 | E275 | L277 | R278 | D279 | V280 | Q287 | L290 | L293 | K294 | R295 | L296 | K297 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|

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| V298 | V299 | M310 | V313 | L314 | D315 | V317 | V318 | V319 | L320 | P321 | P322 | E323 | L324 | K327 | V328 | L330 | D331 | G332 | G333 | R334 | F335 | A336 | T337 | S338 | D339 | L340 | N341 | Y344 | R345 | L348 | N349 | L354 | L357 | L360 | G361 | A362 | P363 | E364 | L365 | L366 | V367 | N368 | N369 | E370 | K371 | R372 | K373 | L374 | Q375 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|

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| F382 | N383 | N384 | G385 | R386 | R387 | T392 | R397 | P398 | L399 | K400 | S401 | L402 | L405 | L406 | K407 | G408 | K409 | Q410 | G411 | R412 | F413 | R414 | K420 | R421 | Y429 | T430 | V431 | V432 | Q433 | P434 | Q435 | L436 | G442 | L443 | P444 | M447 | A448 | L449 | Q450 | L451 | F452 | K453 | P454 | F455 | V456 | R459 | L460 | L463 | M464 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|

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| H465 | A466 | Q467 | N468 | L469 | K470 | S471 | A472 | N475 | V476 | R477 | E478 | Q479 | L485 | V486 | L487 | E488 | E489 | V490 | L491 | H494 | P495 | N499 | R500 | T503 | L504 | H505 | R506 | P512 | E513 | P514 | N515 | L516 | V517 | K520 | A521 | L522 | Q523 | L524 | H525 | P526 | L527 | A534 | D535 | D539 | Q540 | L545 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|

|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| P546 | L547 | E554 | L557 | L558 | H559 | S561 | S567 | R572 | P573 | L574 | A575 | N576 | P577 | R578 | L579 | N580 | E581 | V582 | F587 | L588 | T589 | T590 | D595 | T596 | G597 | E598 | Y599 | Q600 | P601 | H606 | P607 | E608 | T609 | G610 | V611 | S614 | P615 | A616 | E617 | M620 | A621 | A622 | D623 | R624 | G625 | V626 | L627 | R628 | V629 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|

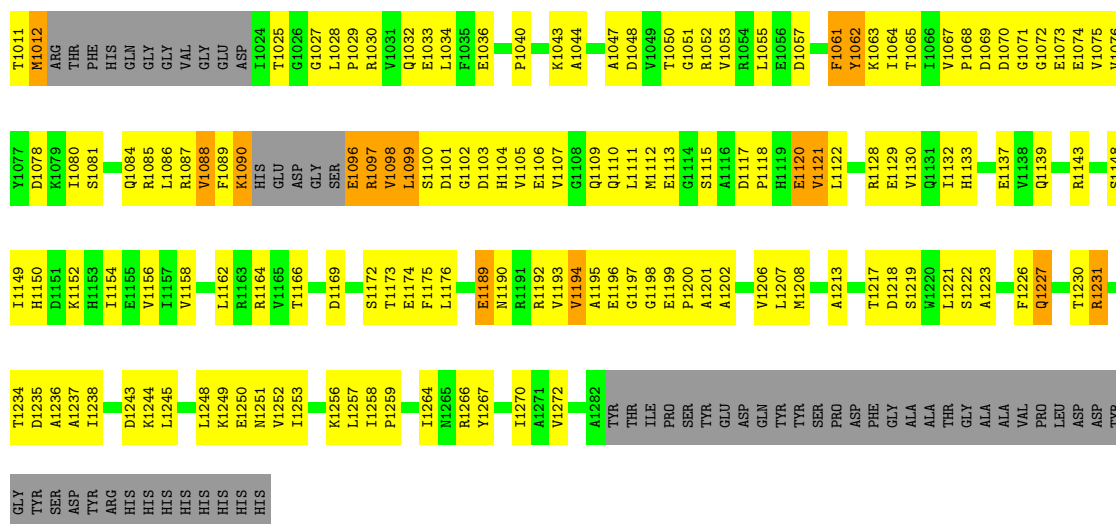
|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| R630 | A631 | K632 | L633 | K634 | V635 | R636 | L637 | T638 | Q639 | L640 | R641 | P642 | T646 | E647 | A648 | E649 | L650 | H653 | S654 | Q657 | D660 | A661 | M662 | N663 | A664 | E665 | T666 | K673 | L676 | L677 | P678 | L679 | V684 | N685 | K686 | Q687 | N688 | L697 | N698 | L699 | D699 | G699 | R703 | Y704 | P705 | M706 | I707 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|

|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| V708 | V709 | A710 | Q711 | V712 | V713 | L716 | K717 | D718 | F721 | P722 | W723 | A724 | T725 | R726 | T730 | V731 | S732 | M733 | A734 | D735 | V736 | L737 | V738 | P739 | R740 | R741 | A742 | K743 | E744 | L745 | L746 | Y749 | E750 | A753 | L756 | L757 | P758 | L759 | V765 | N766 | H767 | R770 | N771 | L774 | V775 | D776 | G777 | E778 | R779 | W780 | A781 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|

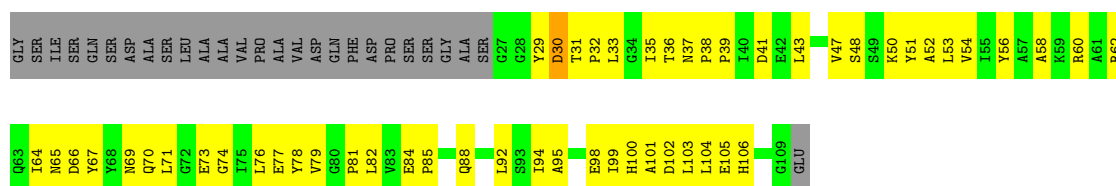
|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| T782 | D783 | A784 | V785 | R790 | E791 | L792 | H793 | N797 | L798 | T799 | T800 | A807 | T808 | F811 | L817 | N820 | K821 | G822 | V823 | L823 | V824 | E827 | R828 | P827 | E830 | F831 | T832 | P833 | R834 | P835 | V836 | K837 | F840 | R841 | L844 | T845 | V846 | L847 | E848 | Y849 | F850 | L851 | N852 | T853 | H854 | G855 | E856 | R857 | L860 | A861 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|

|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| D862 | T863 | A864 | L865 | R866 | T867 | L873 | T874 | R875 | R876 | L877 | S880 | S881 | Q882 | D883 | V884 | L885 | V886 | R887 | E888 | H889 | D890 | C891 | Q892 | T893 | E894 | N895 | R896 | L897 | V898 | V899 | E900 | T901 | A902 | E903 | R904 | A905 | G908 | T909 | L910 | R911 | R912 | D913 | P914 | Y915 | Y916 | E917 | Y921 | A922 | R923 | T924 | L925 | G926 | T927 | T928 | A929 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|

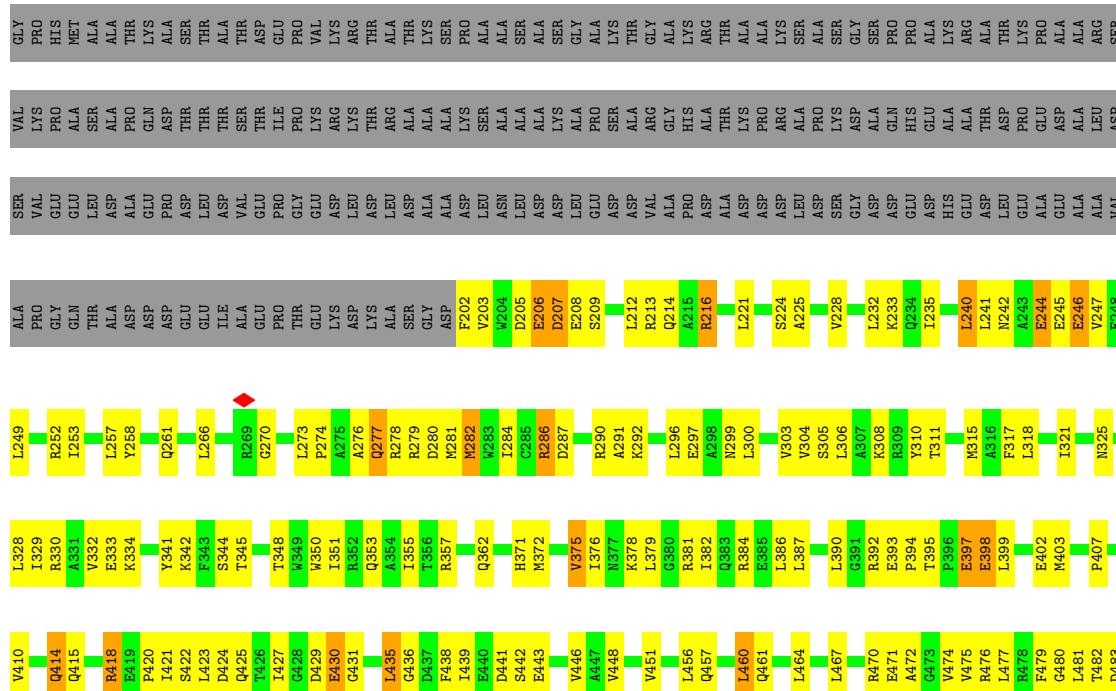
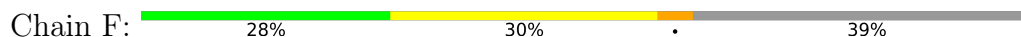
|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |       |       |       |       |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-------|-------|-------|-------|
| V930 | D931 | E932 | A933 | R934 | G935 | V936 | I937 | V938 | E939 | R940 | G941 | D942 | D943 | G945 | D946 | P947 | E948 | L952 | A955 | G956 | I957 | V960 | R961 | V962 | R963 | G964 | V965 | L966 | T967 | C968 | A969 | T970 | G973 | V974 | C975 | A976 | T977 | C978 | Y979 | G980 | R981 | S982 | V989 | D990 | I991 | G992 | E993 | E1005 | T1008 | Q1009 | L1010 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-------|-------|-------|-------|



• Molecule 4: DNA-directed RNA polymerase subunit omega

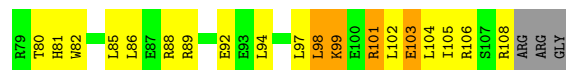
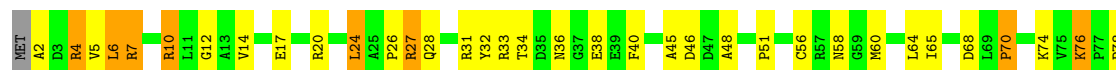


• Molecule 5: RNA polymerase sigma factor SigA

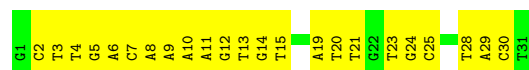




• Molecule 6: RNA polymerase-binding protein RbpA



• Molecule 7: DNA (32-MER)



• Molecule 8: DNA (26-MER)



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 173509                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 6.7                                     | Depositor |
| Minimum defocus (nm)                 | 800                                     | Depositor |
| Maximum defocus (nm)                 | 1800                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 3.278                                   | Depositor |
| Minimum map value                    | -1.545                                  | Depositor |
| Average map value                    | 0.011                                   | Depositor |
| Map value standard deviation         | 0.105                                   | Depositor |
| Recommended contour level            | 0.347                                   | Depositor |
| Map size ( $\text{\AA}$ )            | 330.0, 330.0, 330.0                     | wwPDB     |
| Map dimensions                       | 300, 300, 300                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.1, 1.1, 1.1                           | 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: ZN, FI8, 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     | 0.10         | 0/1750         | 0.30        | 0/2380         |
| 1   | B     | 0.10         | 0/1802         | 0.31        | 0/2454         |
| 2   | C     | 0.10         | 0/8714         | 0.33        | 2/11824 (0.0%) |
| 3   | D     | 0.15         | 0/10021        | 0.33        | 0/13549        |
| 4   | E     | 0.10         | 0/662          | 0.29        | 0/901          |
| 5   | F     | 0.10         | 0/2622         | 0.29        | 0/3538         |
| 6   | J     | 0.41         | 2/888 (0.2%)   | 0.42        | 0/1199         |
| 7   | O     | 0.18         | 0/710          | 0.37        | 0/1095         |
| 8   | P     | 0.20         | 0/589          | 0.39        | 0/906          |
| All | All   | 0.14         | 2/27758 (0.0%) | 0.33        | 2/37846 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2   | C     | 0                   | 3                   |
| 3   | D     | 0                   | 2                   |
| All | All   | 0                   | 5                   |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 6   | J     | 10  | ARG  | C-O   | -6.83 | 1.16        | 1.23     |
| 6   | J     | 10  | ARG  | CA-C  | -6.33 | 1.44        | 1.53     |

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 2   | C     | 254 | PHE  | CA-C-N | 5.37 | 131.37      | 121.70   |
| 2   | C     | 254 | PHE  | C-N-CA | 5.37 | 131.37      | 121.70   |

There are no chirality outliers.

All (5) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group   |
|-----|-------|------|------|---------|
| 2   | C     | 61   | PHE  | Peptide |
| 2   | C     | 958  | ARG  | Peptide |
| 2   | C     | 960  | PRO  | Peptide |
| 3   | D     | 1194 | VAL  | Peptide |
| 3   | D     | 600  | GLN  | Peptide |

## 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     | 1724  | 0        | 1768     | 130     | 0            |
| 1   | B     | 1775  | 0        | 1809     | 178     | 0            |
| 2   | C     | 8556  | 0        | 8459     | 769     | 0            |
| 3   | D     | 9857  | 0        | 9920     | 807     | 0            |
| 4   | E     | 649   | 0        | 645      | 57      | 0            |
| 5   | F     | 2588  | 0        | 2602     | 230     | 0            |
| 6   | J     | 872   | 0        | 852      | 61      | 0            |
| 7   | O     | 634   | 0        | 350      | 39      | 0            |
| 8   | P     | 526   | 0        | 296      | 38      | 0            |
| 9   | C     | 72    | 74       | 0        | 3       | 0            |
| 10  | D     | 2     | 0        | 0        | 0       | 0            |
| 11  | D     | 1     | 0        | 0        | 0       | 0            |
| 12  | C     | 2     | 0        | 0        | 0       | 0            |
| 12  | D     | 4     | 0        | 0        | 3       | 0            |
| All | All   | 27262 | 74       | 26701    | 2122    | 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 39.

All (2122) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:948:ALA:HB2   | 2:C:953:PRO:HD3   | 1.27                     | 1.16              |
| 2:C:658:ILE:HD11  | 2:C:688:PRO:HB3   | 1.33                     | 1.08              |
| 2:C:633:ARG:NH1   | 2:C:637:ASP:OD2   | 1.87                     | 1.07              |
| 2:C:225:ARG:HB2   | 2:C:231:ARG:HA    | 1.34                     | 1.06              |
| 2:C:960:PRO:HG2   | 2:C:963:LEU:HD12  | 1.35                     | 1.04              |
| 2:C:611:MET:HE1   | 2:C:892:LYS:HB3   | 1.39                     | 1.04              |
| 2:C:959:LEU:HB2   | 2:C:960:PRO:HD3   | 1.39                     | 1.04              |
| 7:O:19:DA:H2'     | 7:O:20:DT:H71     | 1.38                     | 1.04              |
| 2:C:571:VAL:HG22  | 2:C:572:PRO:HD2   | 1.40                     | 1.01              |
| 3:D:1025:THR:HG21 | 3:D:1029:PRO:HB2  | 1.42                     | 1.00              |
| 3:D:162:VAL:HG13  | 3:D:216:LEU:HD22  | 1.41                     | 1.00              |
| 2:C:163:LYS:NZ    | 2:C:639:GLY:O     | 1.97                     | 0.98              |
| 2:C:719:LEU:HD22  | 2:C:1030:ILE:HD11 | 1.41                     | 0.98              |
| 3:D:750:GLU:OE2   | 3:D:837:LYS:NZ    | 1.96                     | 0.97              |
| 1:B:183:VAL:HA    | 1:B:188:ASP:H     | 1.28                     | 0.97              |
| 1:B:104:GLU:HG2   | 1:B:127:THR:HG22  | 1.46                     | 0.97              |
| 3:D:1063:LYS:HZ1  | 3:D:1078:ASP:HA   | 1.27                     | 0.97              |
| 2:C:221:THR:HB    | 2:C:261:THR:HG22  | 1.46                     | 0.96              |
| 3:D:676:LEU:HD23  | 3:D:716:LEU:HD23  | 1.47                     | 0.96              |
| 2:C:152:VAL:HG21  | 2:C:418:ILE:HD12  | 1.46                     | 0.96              |
| 2:C:233:PRO:HB3   | 5:F:203:VAL:HG11  | 1.43                     | 0.96              |
| 3:D:823:LEU:HD23  | 3:D:835:PRO:HB3   | 1.48                     | 0.95              |
| 2:C:61:PHE:O      | 2:C:63:TRP:N      | 1.98                     | 0.95              |
| 2:C:222:VAL:O     | 2:C:231:ARG:NH1   | 1.99                     | 0.95              |
| 2:C:1135:VAL:HG12 | 3:D:12:ILE:HG12   | 1.49                     | 0.94              |
| 2:C:220:ASP:HB3   | 2:C:221:THR:HG22  | 1.48                     | 0.94              |
| 3:D:1089:PHE:CE2  | 3:D:1103:ASP:OD2  | 2.20                     | 0.94              |
| 1:A:186:ARG:HD2   | 1:B:147:VAL:HG23  | 1.49                     | 0.94              |
| 2:C:258:MET:HA    | 2:C:261:THR:HG23  | 1.49                     | 0.94              |
| 2:C:767:GLU:OE1   | 2:C:805:LYS:NZ    | 1.99                     | 0.94              |
| 3:D:89:ARG:NH1    | 12:D:1502:HOH:O   | 1.99                     | 0.94              |
| 2:C:825:PHE:HD2   | 5:F:527:LEU:HD12  | 1.33                     | 0.93              |
| 2:C:1038:ASP:OD1  | 3:D:520:LYS:NZ    | 2.01                     | 0.93              |
| 2:C:659:THR:HG22  | 2:C:669:THR:HG22  | 1.51                     | 0.93              |
| 1:B:106:THR:N     | 1:B:109:ASP:OD2   | 2.01                     | 0.92              |
| 2:C:736:ILE:HD11  | 2:C:916:ILE:HD12  | 1.51                     | 0.92              |
| 3:D:902:ALA:HB2   | 3:D:912:ARG:HA    | 1.50                     | 0.92              |
| 2:C:741:LEU:HD22  | 2:C:746:VAL:HG11  | 1.51                     | 0.91              |
| 1:A:34:LEU:HD11   | 1:B:218:LEU:HD21  | 1.50                     | 0.91              |
| 2:C:215:ASP:HB2   | 2:C:223:GLY:HA3   | 1.53                     | 0.91              |
| 2:C:648:GLY:O     | 2:C:695:ARG:NH1   | 2.02                     | 0.91              |
| 2:C:413:THR:HG22  | 2:C:416:THR:HG23  | 1.51                     | 0.91              |

Continued on next page...



*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:F:502:ARG:NH2   | 7:O:2:DC:OP2      | 2.04                     | 0.90              |
| 2:C:994:PRO:HB3   | 2:C:999:ASP:H     | 1.35                     | 0.90              |
| 3:D:1087:ARG:NH1  | 3:D:1110:GLN:OE1  | 2.04                     | 0.90              |
| 3:D:1067:VAL:HA   | 3:D:1074:GLU:HG2  | 1.50                     | 0.90              |
| 6:J:27:ARG:HB3    | 6:J:27:ARG:HH11   | 1.34                     | 0.90              |
| 3:D:1122:LEU:HB2  | 3:D:1130:VAL:HG21 | 1.54                     | 0.89              |
| 7:O:19:DA:H1'     | 7:O:20:DT:H5'     | 1.53                     | 0.89              |
| 2:C:1127:GLU:OE2  | 3:D:412:ARG:NH1   | 2.05                     | 0.89              |
| 1:A:40:ARG:HH12   | 2:C:903:ASP:HB3   | 1.39                     | 0.88              |
| 2:C:400:VAL:HG13  | 2:C:417:LEU:HB3   | 1.56                     | 0.88              |
| 2:C:230:ARG:NH1   | 2:C:230:ARG:HA    | 1.88                     | 0.88              |
| 1:B:94:THR:HG22   | 1:B:139:VAL:HG22  | 1.53                     | 0.88              |
| 2:C:581:VAL:HG22  | 2:C:585:GLN:HE21  | 1.38                     | 0.87              |
| 3:D:432:VAL:HG22  | 3:D:434:PRO:HD3   | 1.56                     | 0.87              |
| 2:C:267:THR:HG21  | 2:C:273:ALA:HB2   | 1.56                     | 0.87              |
| 3:D:1087:ARG:HG3  | 3:D:1088:VAL:H    | 1.40                     | 0.86              |
| 1:A:40:ARG:NH1    | 2:C:903:ASP:HB3   | 1.90                     | 0.86              |
| 2:C:1102:VAL:HG23 | 2:C:1112:ILE:HG23 | 1.54                     | 0.86              |
| 3:D:1128:ARG:HH22 | 3:D:1132:ILE:HD11 | 1.41                     | 0.86              |
| 5:F:206:GLU:OE1   | 5:F:207:ASP:N     | 2.08                     | 0.86              |
| 3:D:1128:ARG:HH12 | 3:D:1132:ILE:HG12 | 1.39                     | 0.86              |
| 2:C:764:LEU:HD22  | 2:C:810:GLY:HA2   | 1.56                     | 0.86              |
| 2:C:221:THR:CB    | 2:C:261:THR:HG22  | 2.05                     | 0.85              |
| 5:F:386:LEU:HD22  | 5:F:394:PRO:HG3   | 1.55                     | 0.85              |
| 2:C:229:LYS:HD3   | 2:C:281:LEU:HA    | 1.59                     | 0.85              |
| 3:D:1097:ARG:HH12 | 3:D:1100:SER:CB   | 1.89                     | 0.85              |
| 3:D:1080:ILE:HG21 | 3:D:1112:MET:HE3  | 1.59                     | 0.85              |
| 2:C:548:ILE:HD11  | 2:C:579:MET:HE1   | 1.57                     | 0.85              |
| 8:P:11:DA:H2''    | 8:P:12:DA:H5'     | 1.58                     | 0.85              |
| 3:D:323:GLU:OE2   | 12:D:1501:HOH:O   | 1.93                     | 0.84              |
| 1:B:202:ILE:HD13  | 1:B:207:ALA:HB2   | 1.59                     | 0.84              |
| 2:C:319:LYS:NZ    | 2:C:368:ASP:OD1   | 2.09                     | 0.84              |
| 2:C:877:ARG:HH11  | 2:C:1036:LEU:HD12 | 1.41                     | 0.84              |
| 5:F:502:ARG:NH1   | 5:F:505:GLN:OE1   | 2.10                     | 0.84              |
| 2:C:285:GLU:HG3   | 2:C:286:PRO:HD2   | 1.59                     | 0.84              |
| 2:C:233:PRO:HG3   | 5:F:203:VAL:HG21  | 1.57                     | 0.84              |
| 2:C:959:LEU:HD13  | 2:C:960:PRO:HD2   | 1.60                     | 0.84              |
| 5:F:240:LEU:HD23  | 5:F:241:LEU:H     | 1.43                     | 0.83              |
| 3:D:737:LEU:HB2   | 3:D:793:TYR:HE1   | 1.43                     | 0.83              |
| 2:C:396:MET:HE3   | 2:C:418:ILE:HG23  | 1.59                     | 0.83              |
| 2:C:43:LYS:HE3    | 2:C:959:LEU:HA    | 1.61                     | 0.83              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:231:ARG:HD2   | 5:F:205:ASP:HB3   | 1.60                     | 0.83              |
| 5:F:306:LEU:HD11  | 5:F:348:THR:HG23  | 1.58                     | 0.83              |
| 2:C:339:VAL:HA    | 2:C:342:ILE:HD12  | 1.58                     | 0.82              |
| 5:F:303:VAL:HG22  | 5:F:351:ILE:HD13  | 1.62                     | 0.82              |
| 2:C:1111:ASN:ND2  | 4:E:66:ASP:OD1    | 2.12                     | 0.82              |
| 3:D:909:THR:C     | 3:D:910:LEU:HG    | 2.03                     | 0.82              |
| 3:D:173:ARG:NH1   | 3:D:173:ARG:HB2   | 1.94                     | 0.81              |
| 3:D:970:THR:OG1   | 3:D:973:GLY:O     | 1.97                     | 0.81              |
| 3:D:337:THR:OG1   | 3:D:341:ASN:ND2   | 2.14                     | 0.81              |
| 3:D:1063:LYS:NZ   | 3:D:1078:ASP:HA   | 1.95                     | 0.81              |
| 2:C:490:GLU:OE2   | 2:C:607:MET:HG2   | 1.81                     | 0.81              |
| 3:D:162:VAL:CG1   | 3:D:216:LEU:HD22  | 2.11                     | 0.81              |
| 3:D:1099:LEU:O    | 3:D:1099:LEU:HD23 | 1.79                     | 0.81              |
| 3:D:1250:GLU:OE1  | 3:D:1250:GLU:N    | 2.14                     | 0.81              |
| 2:C:336:GLU:O     | 2:C:339:VAL:HG22  | 1.79                     | 0.80              |
| 3:D:579:LEU:HD22  | 3:D:808:THR:HB    | 1.63                     | 0.80              |
| 3:D:1052:ARG:HG2  | 3:D:1067:VAL:HB   | 1.63                     | 0.80              |
| 5:F:282:MET:O     | 5:F:286:ARG:HG2   | 1.80                     | 0.80              |
| 3:D:1128:ARG:NH1  | 3:D:1132:ILE:HG12 | 1.96                     | 0.80              |
| 2:C:487:GLU:OE2   | 2:C:613:ARG:NH2   | 2.15                     | 0.80              |
| 2:C:909:ASP:OD2   | 2:C:1001:LEU:HD11 | 1.81                     | 0.80              |
| 2:C:254:PHE:H     | 2:C:255:SER:HB2   | 1.44                     | 0.80              |
| 3:D:908:GLY:O     | 3:D:910:LEU:N     | 2.14                     | 0.80              |
| 2:C:213:GLU:OE1   | 2:C:213:GLU:N     | 2.15                     | 0.80              |
| 1:A:177:LYS:HE2   | 1:A:193:ILE:HD11  | 1.64                     | 0.80              |
| 1:B:154:ALA:HB3   | 1:B:158:GLU:HG2   | 1.62                     | 0.80              |
| 3:D:993:GLU:OE2   | 4:E:51:TYR:OH     | 2.00                     | 0.80              |
| 3:D:952:LEU:HB3   | 3:D:957:ILE:HD11  | 1.64                     | 0.79              |
| 3:D:742:LYS:HE2   | 3:D:746:LEU:HD11  | 1.65                     | 0.79              |
| 3:D:177:LEU:CD1   | 3:D:201:GLY:HA3   | 2.12                     | 0.79              |
| 5:F:286:ARG:HB2   | 5:F:290:ARG:HH12  | 1.45                     | 0.79              |
| 5:F:299:ASN:HB2   | 5:F:328:LEU:HD11  | 1.63                     | 0.79              |
| 2:C:758:ASP:HB3   | 2:C:868:LEU:HD23  | 1.64                     | 0.79              |
| 2:C:945:LYS:N     | 2:C:991:CYS:SG    | 2.53                     | 0.79              |
| 2:C:347:ARG:NH2   | 2:C:352:GLN:OE1   | 2.16                     | 0.79              |
| 1:B:182:ARG:NH2   | 3:D:488:GLU:OE2   | 2.15                     | 0.79              |
| 1:A:144:ARG:HG2   | 1:B:1:MET:HE2     | 1.62                     | 0.79              |
| 3:D:1128:ARG:HH12 | 3:D:1132:ILE:CG1  | 1.95                     | 0.79              |
| 2:C:258:MET:HA    | 2:C:261:THR:CG2   | 2.12                     | 0.79              |
| 2:C:767:GLU:HG2   | 2:C:807:THR:HG22  | 1.64                     | 0.79              |
| 3:D:144:ARG:NH1   | 3:D:227:THR:O     | 2.15                     | 0.79              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:911:ILE:H     | 3:D:911:ILE:HD13  | 1.48                     | 0.79              |
| 2:C:831:GLU:OE1   | 2:C:831:GLU:N     | 2.16                     | 0.78              |
| 2:C:233:PRO:HG2   | 2:C:236:VAL:HG23  | 1.63                     | 0.78              |
| 2:C:1045:SER:OG   | 3:D:453:LYS:NZ    | 2.16                     | 0.78              |
| 3:D:1061:PHE:HB3  | 3:D:1081:SER:HA   | 1.65                     | 0.78              |
| 2:C:453:ARG:NH2   | 2:C:501:SER:O     | 2.15                     | 0.78              |
| 3:D:159:ARG:NH2   | 3:D:220:GLU:OE1   | 2.15                     | 0.78              |
| 2:C:961:ASP:OD1   | 2:C:962:GLU:N     | 2.16                     | 0.78              |
| 2:C:817:GLU:OE1   | 2:C:817:GLU:N     | 2.14                     | 0.78              |
| 3:D:190:LYS:NZ    | 3:D:192:ASP:HB3   | 1.99                     | 0.78              |
| 2:C:435:GLN:HG3   | 2:C:460:PRO:HD3   | 1.66                     | 0.78              |
| 2:C:543:GLN:HE22  | 3:D:847:LEU:HD13  | 1.47                     | 0.78              |
| 2:C:222:VAL:HG21  | 2:C:234:VAL:H     | 1.48                     | 0.78              |
| 3:D:64:LYS:NZ     | 3:D:76:GLU:OE2    | 2.14                     | 0.78              |
| 6:J:106:ARG:O     | 6:J:108:ARG:NH2   | 2.17                     | 0.78              |
| 3:D:908:GLY:C     | 3:D:910:LEU:H     | 1.91                     | 0.77              |
| 3:D:657:GLN:NE2   | 3:D:660:ASP:O     | 2.16                     | 0.77              |
| 3:D:684:VAL:HG11  | 3:D:688:MET:HE1   | 1.66                     | 0.77              |
| 2:C:809:LYS:HB2   | 2:C:809:LYS:HZ2   | 1.48                     | 0.77              |
| 5:F:439:ILE:HD13  | 6:J:6:LEU:HD13    | 1.65                     | 0.77              |
| 2:C:797:ARG:O     | 2:C:839:VAL:HG11  | 1.85                     | 0.77              |
| 2:C:598:GLU:OE1   | 2:C:598:GLU:N     | 2.14                     | 0.77              |
| 2:C:967:GLN:HG3   | 2:C:968:PRO:HD2   | 1.66                     | 0.77              |
| 5:F:303:VAL:HG23  | 5:F:328:LEU:HD12  | 1.67                     | 0.77              |
| 4:E:70:GLN:NE2    | 4:E:73:GLU:OE2    | 2.19                     | 0.76              |
| 3:D:486:VAL:O     | 3:D:490:VAL:HG13  | 1.86                     | 0.76              |
| 6:J:27:ARG:HB3    | 6:J:27:ARG:NH1    | 1.99                     | 0.76              |
| 2:C:254:PHE:CG    | 2:C:255:SER:HB2   | 2.20                     | 0.76              |
| 3:D:362:ALA:HB1   | 3:D:363:PRO:HD2   | 1.66                     | 0.76              |
| 3:D:198:ARG:O     | 3:D:202:GLU:HG2   | 1.86                     | 0.76              |
| 4:E:56:TYR:OH     | 4:E:104:LEU:HG    | 1.85                     | 0.76              |
| 3:D:641:ARG:HA    | 3:D:657:GLN:HG2   | 1.67                     | 0.76              |
| 1:A:95:MET:HE3    | 1:A:112:PRO:HB3   | 1.66                     | 0.76              |
| 5:F:498:VAL:HB    | 5:F:502:ARG:HB3   | 1.67                     | 0.75              |
| 7:O:12:DG:H2'     | 7:O:13:DT:H71     | 1.68                     | 0.75              |
| 3:D:928:ASP:OD1   | 3:D:940:ARG:N     | 2.17                     | 0.75              |
| 3:D:1064:ILE:HD11 | 3:D:1112:MET:HE2  | 1.68                     | 0.75              |
| 8:P:18:DT:H2'     | 8:P:19:DT:H71     | 1.67                     | 0.75              |
| 2:C:275:LEU:O     | 2:C:279:ARG:HG3   | 1.87                     | 0.75              |
| 3:D:1231:ARG:HA   | 3:D:1234:THR:HG22 | 1.69                     | 0.75              |
| 2:C:809:LYS:HB2   | 2:C:809:LYS:NZ    | 2.00                     | 0.75              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:736:VAL:HG22  | 3:D:799:ILE:CD1  | 2.17                     | 0.75              |
| 2:C:252:PHE:HB3   | 2:C:258:MET:SD   | 2.27                     | 0.75              |
| 3:D:187:GLU:OE1   | 3:D:187:GLU:N    | 2.20                     | 0.75              |
| 3:D:365:ILE:H     | 3:D:365:ILE:HD12 | 1.52                     | 0.75              |
| 2:C:233:PRO:HG2   | 2:C:236:VAL:CG2  | 2.17                     | 0.75              |
| 8:P:11:DA:H4'     | 8:P:12:DA:OP1    | 1.85                     | 0.74              |
| 1:A:56:ILE:HB     | 1:A:59:VAL:HG22  | 1.69                     | 0.74              |
| 2:C:231:ARG:CD    | 5:F:205:ASP:HB3  | 2.17                     | 0.74              |
| 2:C:540:VAL:HG13  | 2:C:561:VAL:CG2  | 2.17                     | 0.74              |
| 3:D:1128:ARG:HH12 | 3:D:1132:ILE:CD1 | 1.99                     | 0.74              |
| 3:D:500:ARG:HD2   | 3:D:534:ALA:HB2  | 1.69                     | 0.74              |
| 6:J:4:ARG:HD3     | 6:J:5:VAL:H      | 1.51                     | 0.74              |
| 1:B:84:VAL:HB     | 1:B:199:LYS:HD3  | 1.70                     | 0.74              |
| 2:C:206:PRO:HG3   | 2:C:306:TYR:CE1  | 2.23                     | 0.74              |
| 1:B:107:ALA:HB3   | 1:B:121:PRO:HA   | 1.69                     | 0.74              |
| 2:C:202:VAL:HG12  | 2:C:214:PHE:HB2  | 1.68                     | 0.74              |
| 3:D:263:LYS:HB2   | 3:D:263:LYS:NZ   | 2.03                     | 0.74              |
| 3:D:31:PRO:HG3    | 3:D:349:ASN:OD1  | 1.88                     | 0.73              |
| 2:C:803:VAL:O     | 2:C:836:SER:OG   | 2.05                     | 0.73              |
| 2:C:861:LEU:HB2   | 2:C:862:PRO:HD2  | 1.68                     | 0.73              |
| 2:C:948:ALA:HB2   | 2:C:953:PRO:CD   | 2.15                     | 0.73              |
| 3:D:895:ARG:NH1   | 3:D:967:THR:HB   | 2.03                     | 0.73              |
| 3:D:397:ARG:NH2   | 5:F:422:SER:OG   | 2.21                     | 0.73              |
| 5:F:216:ARG:HB2   | 5:F:216:ARG:HH11 | 1.53                     | 0.73              |
| 2:C:259:ARG:O     | 2:C:263:GLU:HG2  | 1.88                     | 0.73              |
| 3:D:190:LYS:HZ2   | 3:D:192:ASP:HB3  | 1.53                     | 0.73              |
| 3:D:614:SER:HB2   | 3:D:615:PRO:HD2  | 1.69                     | 0.73              |
| 1:A:223:ARG:HD2   | 1:A:224:GLU:H    | 1.53                     | 0.73              |
| 3:D:673:PHE:CE2   | 3:D:688:MET:HE3  | 2.23                     | 0.73              |
| 3:D:939:GLU:OE1   | 3:D:939:GLU:N    | 2.20                     | 0.73              |
| 3:D:820:MET:HE2   | 3:D:822:GLY:HA2  | 1.70                     | 0.73              |
| 1:B:182:ARG:HA    | 1:B:182:ARG:HE   | 1.54                     | 0.73              |
| 2:C:277:ILE:O     | 2:C:281:LEU:HD13 | 1.88                     | 0.73              |
| 3:D:670:ARG:NH1   | 3:D:685:ASN:OD1  | 2.20                     | 0.73              |
| 3:D:913:ASP:OD1   | 3:D:914:PRO:HD2  | 1.89                     | 0.73              |
| 3:D:92:MET:HG2    | 3:D:321:PRO:HD3  | 1.70                     | 0.72              |
| 6:J:89:ARG:HG2    | 6:J:94:LEU:HD21  | 1.71                     | 0.72              |
| 2:C:177:SER:HB2   | 2:C:378:LEU:HD11 | 1.71                     | 0.72              |
| 2:C:577:ASP:N     | 2:C:577:ASP:OD1  | 2.19                     | 0.72              |
| 6:J:51:PRO:O      | 6:J:64:LEU:HD11  | 1.88                     | 0.72              |
| 2:C:52:GLY:O      | 2:C:55:ASP:N     | 2.21                     | 0.72              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:540:VAL:HG13  | 2:C:561:VAL:HG21 | 1.71                     | 0.72              |
| 1:B:128:LEU:HD23  | 1:B:132:GLY:O    | 1.88                     | 0.72              |
| 2:C:103:MET:HG3   | 2:C:404:MET:HE2  | 1.71                     | 0.72              |
| 2:C:563:ARG:HB2   | 2:C:563:ARG:HH11 | 1.54                     | 0.72              |
| 3:D:293:LEU:HD22  | 3:D:1176:LEU:HG  | 1.70                     | 0.72              |
| 3:D:606:HIS:HB2   | 3:D:607:PRO:HD2  | 1.71                     | 0.72              |
| 2:C:340:ALA:O     | 2:C:343:GLU:HG3  | 1.89                     | 0.72              |
| 3:D:1193:VAL:HG23 | 3:D:1199:GLU:HG2 | 1.70                     | 0.72              |
| 5:F:397:GLU:OE1   | 5:F:398:GLU:N    | 2.22                     | 0.72              |
| 2:C:230:ARG:HA    | 2:C:230:ARG:HH11 | 1.51                     | 0.72              |
| 2:C:231:ARG:O     | 2:C:232:GLN:NE2  | 2.22                     | 0.72              |
| 2:C:435:GLN:HE21  | 2:C:460:PRO:HG3  | 1.54                     | 0.72              |
| 2:C:325:GLY:O     | 2:C:326:GLU:HG2  | 1.89                     | 0.72              |
| 3:D:1097:ARG:HH12 | 3:D:1100:SER:HB2 | 1.54                     | 0.72              |
| 2:C:727:GLU:HG2   | 3:D:725:THR:HG21 | 1.72                     | 0.72              |
| 1:A:9:LEU:HD12    | 1:A:23:ILE:HD11  | 1.72                     | 0.71              |
| 2:C:223:GLY:HA2   | 2:C:231:ARG:NH1  | 2.04                     | 0.71              |
| 2:C:1039:ASP:HB2  | 2:C:1040:LYS:HE3 | 1.72                     | 0.71              |
| 5:F:299:ASN:CB    | 5:F:328:LEU:HD11 | 2.20                     | 0.71              |
| 5:F:489:LEU:CD1   | 8:P:20:DG:H2'    | 2.19                     | 0.71              |
| 2:C:959:LEU:HB2   | 2:C:960:PRO:CD   | 2.17                     | 0.71              |
| 5:F:425:GLN:OE1   | 5:F:425:GLN:N    | 2.24                     | 0.71              |
| 1:A:186:ARG:HG3   | 1:B:150:VAL:HB   | 1.72                     | 0.71              |
| 1:B:24:GLU:HG2    | 1:B:191:LYS:HG3  | 1.71                     | 0.71              |
| 2:C:264:LYS:O     | 5:F:202:PHE:N    | 2.24                     | 0.71              |
| 2:C:563:ARG:NH1   | 2:C:569:GLU:OE1  | 2.23                     | 0.71              |
| 5:F:390:LEU:HG    | 5:F:392:ARG:HG3  | 1.72                     | 0.71              |
| 3:D:54:PRO:HG3    | 3:D:81:GLU:O     | 1.90                     | 0.71              |
| 3:D:471:SER:HB3   | 5:F:525:ASP:OD2  | 1.89                     | 0.71              |
| 5:F:446:VAL:HG12  | 5:F:448:VAL:HG12 | 1.73                     | 0.71              |
| 2:C:787:ARG:HD3   | 2:C:787:ARG:O    | 1.91                     | 0.71              |
| 3:D:1190:ASN:HD21 | 3:D:1201:ALA:HB3 | 1.55                     | 0.71              |
| 7:O:19:DA:H4'     | 7:O:20:DT:OP1    | 1.89                     | 0.71              |
| 1:B:28:PRO:HD3    | 1:B:189:PHE:HD1  | 1.55                     | 0.71              |
| 1:B:183:VAL:HA    | 1:B:188:ASP:N    | 2.05                     | 0.71              |
| 5:F:427:ILE:HD11  | 6:J:2:ALA:N      | 2.06                     | 0.71              |
| 2:C:959:LEU:HD23  | 2:C:984:GLU:OE1  | 1.90                     | 0.70              |
| 3:D:1198:GLY:O    | 3:D:1200:PRO:HD3 | 1.91                     | 0.70              |
| 1:B:64:THR:O      | 1:B:65:THR:OG1   | 2.07                     | 0.70              |
| 1:B:154:ALA:CB    | 1:B:158:GLU:HG2  | 2.20                     | 0.70              |
| 3:D:152:GLU:OE2   | 3:D:153:ALA:N    | 2.23                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:386:ARG:NH2   | 3:D:1230:THR:HG21 | 2.07                     | 0.70              |
| 3:D:699:ASP:OD1   | 3:D:703:ARG:HD3   | 1.90                     | 0.70              |
| 3:D:67:ARG:HA     | 3:D:67:ARG:NE     | 2.05                     | 0.70              |
| 5:F:507:GLU:O     | 5:F:511:MET:HG2   | 1.90                     | 0.70              |
| 2:C:63:TRP:O      | 2:C:85:GLY:N      | 2.22                     | 0.70              |
| 3:D:125:LEU:HD11  | 3:D:261:ILE:HD11  | 1.74                     | 0.70              |
| 5:F:278:ARG:NH2   | 5:F:282:MET:SD    | 2.65                     | 0.70              |
| 3:D:460:LEU:HD11  | 3:D:472:ALA:HB1   | 1.72                     | 0.70              |
| 3:D:1096:GLU:HA   | 3:D:1096:GLU:OE1  | 1.91                     | 0.70              |
| 5:F:489:LEU:N     | 8:P:20:DG:OP2     | 2.15                     | 0.70              |
| 2:C:254:PHE:N     | 2:C:255:SER:HB2   | 2.06                     | 0.70              |
| 3:D:826:ASN:OD1   | 3:D:832:ILE:HD11  | 1.92                     | 0.70              |
| 3:D:847:LEU:O     | 3:D:851:ILE:HG12  | 1.91                     | 0.70              |
| 5:F:357:ARG:NH1   | 7:O:23:DT:H72     | 2.07                     | 0.70              |
| 3:D:269:ASP:O     | 3:D:273:GLU:HG2   | 1.92                     | 0.69              |
| 2:C:215:ASP:CB    | 2:C:223:GLY:HA3   | 2.22                     | 0.69              |
| 3:D:237:ASP:OD2   | 3:D:240:LEU:HB2   | 1.92                     | 0.69              |
| 1:B:40:ARG:HH12   | 3:D:623:ASP:HB3   | 1.58                     | 0.69              |
| 3:D:642:PRO:HG2   | 3:D:647:GLU:HB3   | 1.74                     | 0.69              |
| 3:D:1162:LEU:HD21 | 3:D:1207:LEU:HD23 | 1.74                     | 0.69              |
| 1:A:177:LYS:CE    | 1:A:193:ILE:HD11  | 2.23                     | 0.69              |
| 3:D:1010:LEU:HD23 | 3:D:1028:LEU:HA   | 1.74                     | 0.69              |
| 7:O:5:DG:H2'      | 7:O:6:DA:C8       | 2.26                     | 0.69              |
| 1:B:15:THR:HG23   | 1:B:18:ARG:HB2    | 1.74                     | 0.69              |
| 2:C:621:SER:O     | 2:C:709:ASP:HB2   | 1.93                     | 0.69              |
| 3:D:407:LYS:HG2   | 3:D:408:GLY:H     | 1.58                     | 0.69              |
| 3:D:1084:GLN:HE21 | 3:D:1112:MET:HB2  | 1.57                     | 0.69              |
| 5:F:252:ARG:NH2   | 5:F:287:ASP:OD1   | 2.22                     | 0.69              |
| 1:B:60:LEU:HD22   | 1:B:60:LEU:H      | 1.58                     | 0.69              |
| 3:D:155:MET:HE1   | 3:D:219:LEU:HD12  | 1.74                     | 0.69              |
| 3:D:834:ARG:HA    | 3:D:834:ARG:HE    | 1.56                     | 0.69              |
| 8:P:1:DA:H5''     | 8:P:1:DA:H8       | 1.56                     | 0.69              |
| 2:C:39:VAL:HG11   | 2:C:963:LEU:HG    | 1.73                     | 0.69              |
| 2:C:225:ARG:HB2   | 2:C:231:ARG:CA    | 2.19                     | 0.69              |
| 8:P:11:DA:H2''    | 8:P:12:DA:C5'     | 2.22                     | 0.69              |
| 2:C:1044:ARG:HB2  | 2:C:1063:PHE:HB3  | 1.74                     | 0.69              |
| 2:C:1067:ARG:HA   | 3:D:421:ARG:HA    | 1.75                     | 0.69              |
| 2:C:738:SER:OG    | 2:C:904:MET:HE3   | 1.92                     | 0.68              |
| 2:C:229:LYS:CD    | 2:C:281:LEU:HA    | 2.23                     | 0.68              |
| 3:D:295:ARG:O     | 3:D:299:VAL:HG23  | 1.93                     | 0.68              |
| 3:D:909:THR:HG22  | 3:D:910:LEU:HG    | 1.74                     | 0.68              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:149:ALA:N     | 1:B:165:ASP:OD1  | 2.27                     | 0.68              |
| 2:C:959:LEU:HD13  | 2:C:960:PRO:CD   | 2.22                     | 0.68              |
| 3:D:1012:MET:C    | 3:D:1027:GLY:N   | 2.52                     | 0.68              |
| 1:A:6:ARG:NH1     | 1:A:6:ARG:HB3    | 2.08                     | 0.68              |
| 2:C:220:ASP:HB3   | 2:C:221:THR:CG2  | 2.21                     | 0.68              |
| 3:D:435:GLN:OE1   | 3:D:435:GLN:N    | 2.25                     | 0.68              |
| 2:C:233:PRO:HB3   | 5:F:203:VAL:CG1  | 2.23                     | 0.68              |
| 2:C:719:LEU:HD22  | 2:C:1030:ILE:CD1 | 2.22                     | 0.68              |
| 3:D:926:GLY:O     | 3:D:940:ARG:NH2  | 2.27                     | 0.68              |
| 2:C:771:ARG:HG2   | 2:C:781:LEU:HD11 | 1.75                     | 0.68              |
| 3:D:705:PRO:HB2   | 4:E:41:ASP:OD2   | 1.93                     | 0.68              |
| 3:D:1164:ARG:HD2  | 3:D:1208:MET:HE1 | 1.74                     | 0.68              |
| 2:C:563:ARG:HB2   | 2:C:563:ARG:NH1  | 2.07                     | 0.68              |
| 2:C:961:ASP:O     | 2:C:962:GLU:HG3  | 1.94                     | 0.68              |
| 3:D:1070:ASP:N    | 3:D:1071:GLY:HA2 | 2.09                     | 0.68              |
| 2:C:326:GLU:HB3   | 2:C:328:ILE:HG23 | 1.76                     | 0.68              |
| 2:C:948:ALA:CB    | 2:C:953:PRO:HD3  | 2.16                     | 0.68              |
| 3:D:121:ALA:HB3   | 3:D:124:ASP:OD2  | 1.94                     | 0.68              |
| 3:D:277:LEU:HD11  | 3:D:295:ARG:NH1  | 2.09                     | 0.68              |
| 3:D:823:LEU:HD23  | 3:D:835:PRO:CB   | 2.22                     | 0.68              |
| 1:A:142:ARG:NH2   | 1:B:230:GLU:OE1  | 2.27                     | 0.68              |
| 1:B:81:LYS:NZ     | 3:D:617:GLU:OE2  | 2.23                     | 0.68              |
| 2:C:338:VAL:O     | 2:C:342:ILE:HG13 | 1.94                     | 0.68              |
| 2:C:825:PHE:CE2   | 5:F:524:ARG:HA   | 2.29                     | 0.68              |
| 3:D:749:TYR:CD1   | 3:D:781:ALA:HB2  | 2.29                     | 0.68              |
| 2:C:230:ARG:O     | 2:C:231:ARG:HB2  | 1.94                     | 0.67              |
| 2:C:542:ALA:HB2   | 2:C:576:VAL:CG1  | 2.24                     | 0.67              |
| 2:C:741:LEU:CD2   | 2:C:746:VAL:HG11 | 2.24                     | 0.67              |
| 3:D:320:ILE:HG13  | 3:D:321:PRO:HD2  | 1.76                     | 0.67              |
| 3:D:1080:ILE:HG21 | 3:D:1112:MET:HG3 | 1.75                     | 0.67              |
| 2:C:254:PHE:CD2   | 2:C:255:SER:HB2  | 2.29                     | 0.67              |
| 3:D:1139:GLN:O    | 3:D:1143:ARG:HG3 | 1.94                     | 0.67              |
| 5:F:286:ARG:HB2   | 5:F:290:ARG:NH1  | 2.09                     | 0.67              |
| 2:C:96:ILE:HB     | 2:C:105:LEU:HB3  | 1.77                     | 0.67              |
| 2:C:343:GLU:O     | 2:C:346:VAL:HG12 | 1.94                     | 0.67              |
| 1:B:104:GLU:HG2   | 1:B:127:THR:CG2  | 2.24                     | 0.67              |
| 2:C:584:ARG:HH21  | 2:C:975:PRO:HB3  | 1.60                     | 0.67              |
| 3:D:163:GLU:OE1   | 3:D:166:ARG:NH2  | 2.22                     | 0.67              |
| 3:D:737:LEU:HB2   | 3:D:793:TYR:CE1  | 2.29                     | 0.67              |
| 4:E:43:LEU:HD21   | 4:E:100:HIS:HB2  | 1.76                     | 0.67              |
| 5:F:441:ASP:OD1   | 5:F:443:GLU:N    | 2.24                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:737:LEU:HD11  | 2:C:895:ILE:HD13  | 1.76                     | 0.67              |
| 2:C:745:ASP:OD1   | 2:C:878:LYS:HE2   | 1.95                     | 0.67              |
| 5:F:246:GLU:OE1   | 5:F:247:VAL:N     | 2.28                     | 0.67              |
| 7:O:14:DG:H2'     | 7:O:15:DT:H71     | 1.75                     | 0.67              |
| 2:C:581:VAL:HG22  | 2:C:585:GLN:NE2   | 2.08                     | 0.67              |
| 2:C:919:THR:HG23  | 3:D:731:VAL:HG23  | 1.76                     | 0.67              |
| 1:A:3:ILE:HD12    | 1:A:3:ILE:O       | 1.94                     | 0.67              |
| 2:C:785:ASP:OD2   | 2:C:787:ARG:HD2   | 1.95                     | 0.67              |
| 2:C:967:GLN:CG    | 2:C:968:PRO:HD2   | 2.24                     | 0.67              |
| 3:D:849:TYR:O     | 3:D:853:THR:HG23  | 1.94                     | 0.67              |
| 8:P:24:DA:H2'     | 8:P:25:DG:H8      | 1.60                     | 0.67              |
| 1:A:56:ILE:HB     | 1:A:59:VAL:CG2    | 2.24                     | 0.67              |
| 1:B:175:THR:HG23  | 1:B:195:ASP:HB3   | 1.76                     | 0.67              |
| 2:C:233:PRO:CG    | 5:F:203:VAL:HG21  | 2.25                     | 0.67              |
| 3:D:736:VAL:HG11  | 3:D:817:LEU:HD22  | 1.75                     | 0.67              |
| 5:F:395:THR:OG1   | 5:F:398:GLU:HB2   | 1.94                     | 0.67              |
| 3:D:228:LYS:O     | 3:D:233:GLN:NE2   | 2.24                     | 0.66              |
| 3:D:386:ARG:HH22  | 3:D:1230:THR:HG21 | 1.60                     | 0.66              |
| 5:F:315:MET:HE3   | 5:F:362:GLN:HB2   | 1.77                     | 0.66              |
| 1:A:219:PHE:HE1   | 1:B:38:LEU:HD22   | 1.61                     | 0.66              |
| 1:B:102:PRO:HB3   | 1:B:130:ASP:HA    | 1.76                     | 0.66              |
| 2:C:290:GLU:HA    | 2:C:294:THR:HG23  | 1.76                     | 0.66              |
| 3:D:212:ALA:O     | 3:D:216:LEU:HG    | 1.95                     | 0.66              |
| 5:F:253:ILE:O     | 5:F:257:LEU:HD13  | 1.96                     | 0.66              |
| 5:F:281:MET:O     | 5:F:284:ILE:HG22  | 1.94                     | 0.66              |
| 1:A:176:TYR:HB3   | 1:A:194:LEU:HD23  | 1.78                     | 0.66              |
| 2:C:950:LYS:HD3   | 2:C:951:GLY:H     | 1.59                     | 0.66              |
| 2:C:997:ASP:N     | 2:C:997:ASP:OD1   | 2.26                     | 0.66              |
| 3:D:465:HIS:O     | 3:D:475:MET:HE1   | 1.96                     | 0.66              |
| 3:D:1173:THR:HG21 | 3:D:1189:GLU:OE2  | 1.95                     | 0.66              |
| 1:A:120:ASN:HD21  | 1:A:123:MET:HE3   | 1.61                     | 0.66              |
| 5:F:303:VAL:CG2   | 5:F:328:LEU:HD12  | 2.25                     | 0.66              |
| 5:F:489:LEU:HD11  | 8:P:20:DG:H2'     | 1.75                     | 0.66              |
| 8:P:14:DA:H5'     | 8:P:14:DA:C8      | 2.31                     | 0.66              |
| 2:C:413:THR:O     | 2:C:416:THR:OG1   | 2.13                     | 0.66              |
| 3:D:364:GLU:HG3   | 3:D:368:ASN:OD1   | 1.95                     | 0.66              |
| 5:F:488:THR:OG1   | 5:F:491:GLU:HB2   | 1.96                     | 0.66              |
| 2:C:192:ASP:OD2   | 2:C:195:THR:HG23  | 1.94                     | 0.66              |
| 3:D:1043:LYS:HD3  | 3:D:1044:ALA:N    | 2.11                     | 0.66              |
| 5:F:386:LEU:HD22  | 5:F:394:PRO:CG    | 2.23                     | 0.66              |
| 2:C:413:THR:HG22  | 2:C:416:THR:CG2   | 2.26                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:558:ARG:HH21  | 2:C:572:PRO:HD3   | 1.59                     | 0.66              |
| 2:C:994:PRO:CB    | 2:C:998:GLY:HA2   | 2.26                     | 0.66              |
| 3:D:909:THR:O     | 3:D:910:LEU:HG    | 1.95                     | 0.66              |
| 5:F:446:VAL:CG1   | 5:F:448:VAL:HG12  | 2.25                     | 0.66              |
| 2:C:825:PHE:CD2   | 5:F:527:LEU:HD12  | 2.25                     | 0.66              |
| 3:D:155:MET:O     | 3:D:159:ARG:HG2   | 1.95                     | 0.66              |
| 3:D:201:GLY:O     | 3:D:205:MET:HG3   | 1.95                     | 0.66              |
| 3:D:447:MET:O     | 3:D:451:LEU:HD23  | 1.96                     | 0.66              |
| 4:E:105:GLU:OE1   | 4:E:105:GLU:N     | 2.25                     | 0.66              |
| 2:C:153:PHE:CE2   | 2:C:155:GLY:HA2   | 2.31                     | 0.66              |
| 2:C:602:ALA:HB3   | 3:D:856:ALA:CB    | 2.26                     | 0.66              |
| 5:F:228:VAL:O     | 5:F:232:LEU:HG    | 1.96                     | 0.66              |
| 5:F:257:LEU:HD21  | 6:J:81:HIS:ND1    | 2.11                     | 0.66              |
| 1:A:21:PHE:CD2    | 1:A:208:LEU:HD22  | 2.30                     | 0.66              |
| 2:C:180:VAL:HG21  | 2:C:379:ARG:NH1   | 2.10                     | 0.66              |
| 2:C:757:ILE:HB    | 2:C:837:LEU:HD22  | 1.77                     | 0.66              |
| 2:C:952:VAL:HG11  | 2:C:957:ALA:HA    | 1.78                     | 0.66              |
| 3:D:776:GLU:O     | 3:D:780:GLU:HG2   | 1.95                     | 0.66              |
| 3:D:826:ASN:HB2   | 3:D:830:GLU:O     | 1.95                     | 0.66              |
| 3:D:946:ASP:HB2   | 3:D:947:PRO:HD3   | 1.77                     | 0.66              |
| 3:D:1067:VAL:HG22 | 3:D:1074:GLU:CD   | 2.21                     | 0.66              |
| 2:C:861:LEU:HD22  | 2:C:865:VAL:HG12  | 1.78                     | 0.65              |
| 2:C:186:TYR:CE2   | 2:C:205:ILE:HD11  | 2.31                     | 0.65              |
| 5:F:261:GLN:HG2   | 6:J:82:TRP:CZ2    | 2.32                     | 0.65              |
| 1:A:221:LEU:HD13  | 1:B:7:PRO:HG2     | 1.78                     | 0.65              |
| 1:B:38:LEU:O      | 1:B:42:LEU:HD13   | 1.96                     | 0.65              |
| 2:C:220:ASP:HB3   | 2:C:221:THR:HA    | 1.77                     | 0.65              |
| 2:C:960:PRO:HG2   | 2:C:963:LEU:CD1   | 2.21                     | 0.65              |
| 3:D:749:TYR:HE1   | 3:D:780:GLU:HB2   | 1.61                     | 0.65              |
| 5:F:317:PHE:CE2   | 5:F:321:ILE:HD11  | 2.31                     | 0.65              |
| 2:C:771:ARG:HH11  | 2:C:786:GLU:HA    | 1.61                     | 0.65              |
| 2:C:918:ASN:OD1   | 2:C:919:THR:N     | 2.29                     | 0.65              |
| 3:D:173:ARG:HB2   | 3:D:173:ARG:HH11  | 1.59                     | 0.65              |
| 3:D:344:TYR:O     | 3:D:348:ILE:HG22  | 1.97                     | 0.65              |
| 5:F:516:HIS:ND1   | 5:F:517:PRO:HD2   | 2.11                     | 0.65              |
| 8:P:24:DA:H2'     | 8:P:25:DG:C8      | 2.32                     | 0.65              |
| 2:C:524:VAL:HG21  | 2:C:548:ILE:HD11  | 1.79                     | 0.65              |
| 3:D:1150:HIS:CE1  | 3:D:1152:LYS:HE3  | 2.32                     | 0.65              |
| 3:D:790:ARG:HB2   | 3:D:811:PHE:CZ    | 2.31                     | 0.65              |
| 3:D:917:GLU:HA    | 3:D:921:TYR:CD2   | 2.31                     | 0.65              |
| 3:D:1065:THR:HG23 | 3:D:1076:VAL:HG22 | 1.77                     | 0.65              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:E:56:TYR:OH    | 4:E:104:LEU:O     | 2.14                     | 0.65              |
| 7:O:8:DA:H2''    | 7:O:9:DA:C8       | 2.32                     | 0.65              |
| 2:C:85:GLY:O     | 2:C:386:GLN:NE2   | 2.28                     | 0.65              |
| 2:C:152:VAL:HG21 | 2:C:418:ILE:CD1   | 2.25                     | 0.65              |
| 2:C:357:VAL:CG2  | 2:C:358:PRO:HD2   | 2.27                     | 0.65              |
| 2:C:610:ASN:OD1  | 2:C:613:ARG:NH1   | 2.23                     | 0.65              |
| 3:D:595:ASP:OD1  | 3:D:596:THR:N     | 2.25                     | 0.65              |
| 3:D:885:ILE:HD11 | 3:D:887:ARG:NH1   | 2.11                     | 0.65              |
| 2:C:790:VAL:HG13 | 2:C:802:LEU:O     | 1.97                     | 0.65              |
| 3:D:494:HIS:CE1  | 3:D:545:LEU:HD11  | 2.31                     | 0.65              |
| 3:D:1267:TYR:O   | 3:D:1270:ILE:HG13 | 1.96                     | 0.65              |
| 6:J:34:THR:OG1   | 6:J:38:GLU:HB2    | 1.97                     | 0.65              |
| 2:C:232:GLN:HG2  | 2:C:277:ILE:CD1   | 2.27                     | 0.65              |
| 2:C:442:GLN:O    | 2:C:678:SER:OG    | 2.13                     | 0.65              |
| 1:A:120:ASN:ND2  | 1:A:123:MET:HE3   | 2.12                     | 0.64              |
| 2:C:224:VAL:HG21 | 2:C:234:VAL:N     | 2.12                     | 0.64              |
| 2:C:229:LYS:HZ2  | 2:C:281:LEU:HG    | 1.62                     | 0.64              |
| 3:D:84:ARG:HG3   | 3:D:84:ARG:HH11   | 1.62                     | 0.64              |
| 3:D:314:LEU:HD21 | 3:D:382:PHE:HE2   | 1.62                     | 0.64              |
| 3:D:923:ARG:HB3  | 3:D:962:VAL:CG1   | 2.28                     | 0.64              |
| 5:F:306:LEU:CD1  | 5:F:348:THR:HG23  | 2.27                     | 0.64              |
| 7:O:5:DG:H2''    | 7:O:6:DA:C5'      | 2.27                     | 0.64              |
| 1:B:28:PRO:HD3   | 1:B:189:PHE:CD1   | 2.31                     | 0.64              |
| 2:C:482:ARG:HH11 | 2:C:532:THR:C     | 2.06                     | 0.64              |
| 3:D:662:TRP:CZ3  | 3:D:664:ALA:HB2   | 2.33                     | 0.64              |
| 1:A:78:LEU:HD13  | 2:C:620:ARG:HD3   | 1.78                     | 0.64              |
| 1:B:102:PRO:HD3  | 1:B:131:LYS:H     | 1.63                     | 0.64              |
| 2:C:285:GLU:CG   | 2:C:286:PRO:HD2   | 2.28                     | 0.64              |
| 2:C:786:GLU:OE1  | 2:C:786:GLU:N     | 2.30                     | 0.64              |
| 3:D:177:LEU:HD12 | 3:D:201:GLY:HA3   | 1.80                     | 0.64              |
| 3:D:1050:THR:O   | 3:D:1069:ASP:N    | 2.23                     | 0.64              |
| 1:A:40:ARG:HH12  | 2:C:903:ASP:CB    | 2.09                     | 0.64              |
| 1:A:152:ASN:OD1  | 1:A:157:ALA:HB3   | 1.98                     | 0.64              |
| 1:B:2:LEU:HD23   | 1:B:3:ILE:N       | 2.13                     | 0.64              |
| 2:C:760:ARG:HG2  | 2:C:865:VAL:HG22  | 1.78                     | 0.64              |
| 2:C:774:PRO:HG3  | 2:C:832:VAL:HG23  | 1.80                     | 0.64              |
| 5:F:249:LEU:O    | 5:F:253:ILE:HG13  | 1.97                     | 0.64              |
| 8:P:24:DA:H2''   | 8:P:25:DG:C5'     | 2.28                     | 0.64              |
| 1:B:4:SER:O      | 1:B:5:GLN:HG2     | 1.97                     | 0.64              |
| 2:C:757:ILE:O    | 2:C:868:LEU:HD22  | 1.96                     | 0.64              |
| 4:E:73:GLU:OE1   | 4:E:74:GLY:N      | 2.31                     | 0.64              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:F:342:LYS:HG2   | 7:O:30:DC:OP2    | 1.97                     | 0.64              |
| 2:C:622:GLU:O     | 2:C:714:ALA:HB1  | 1.96                     | 0.64              |
| 3:D:760:PHE:CD1   | 3:D:770:ARG:HG2  | 2.33                     | 0.64              |
| 3:D:902:ALA:CB    | 3:D:912:ARG:HA   | 2.27                     | 0.64              |
| 2:C:214:PHE:HE2   | 2:C:342:ILE:HG12 | 1.63                     | 0.64              |
| 3:D:134:TYR:HE2   | 3:D:238:GLU:HG3  | 1.61                     | 0.64              |
| 3:D:436:LEU:HD22  | 3:D:515:MET:HE2  | 1.80                     | 0.64              |
| 3:D:599:TYR:OH    | 3:D:608:GLU:OE1  | 2.09                     | 0.64              |
| 5:F:378:LYS:HG2   | 5:F:403:MET:HE3  | 1.80                     | 0.64              |
| 5:F:399:LEU:O     | 5:F:403:MET:N    | 2.27                     | 0.64              |
| 6:J:26:PRO:O      | 6:J:46:ASP:HB2   | 1.98                     | 0.64              |
| 1:A:183:VAL:HG22  | 1:A:185:GLN:OE1  | 1.97                     | 0.64              |
| 2:C:202:VAL:CG1   | 2:C:214:PHE:HB2  | 2.27                     | 0.64              |
| 2:C:357:VAL:HG22  | 2:C:358:PRO:HD2  | 1.80                     | 0.64              |
| 3:D:940:ARG:NH1   | 3:D:963:ARG:HH22 | 1.96                     | 0.64              |
| 6:J:24:LEU:HD23   | 6:J:24:LEU:H     | 1.63                     | 0.64              |
| 3:D:638:THR:O     | 3:D:639:GLN:NE2  | 2.31                     | 0.63              |
| 1:B:210:SER:O     | 1:B:214:THR:HG23 | 1.98                     | 0.63              |
| 2:C:399:VAL:O     | 2:C:403:ARG:HG2  | 1.98                     | 0.63              |
| 2:C:542:ALA:HB2   | 2:C:576:VAL:HG13 | 1.80                     | 0.63              |
| 2:C:767:GLU:CG    | 2:C:807:THR:HG22 | 2.28                     | 0.63              |
| 3:D:153:ALA:O     | 3:D:157:VAL:HG23 | 1.97                     | 0.63              |
| 2:C:737:LEU:CD2   | 2:C:915:ILE:HG22 | 2.28                     | 0.63              |
| 3:D:721:PHE:O     | 3:D:725:THR:HG23 | 1.98                     | 0.63              |
| 1:A:6:ARG:HB3     | 1:A:6:ARG:HH11   | 1.63                     | 0.63              |
| 2:C:891:ASN:HD21  | 2:C:1028:MET:HE1 | 1.63                     | 0.63              |
| 2:C:363:VAL:CG1   | 2:C:364:PRO:HD2  | 2.29                     | 0.63              |
| 2:C:396:MET:CE    | 2:C:418:ILE:HG23 | 2.29                     | 0.63              |
| 2:C:413:THR:CG2   | 2:C:416:THR:HG23 | 2.28                     | 0.63              |
| 3:D:166:ARG:HD3   | 3:D:216:LEU:HD11 | 1.81                     | 0.63              |
| 1:A:110:ILE:O     | 1:A:112:PRO:HD3  | 1.97                     | 0.63              |
| 2:C:806:VAL:HG22  | 2:C:832:VAL:HB   | 1.80                     | 0.63              |
| 3:D:1192:ARG:HG2  | 3:D:1192:ARG:O   | 1.98                     | 0.63              |
| 3:D:1217:THR:HG22 | 3:D:1223:ALA:HB2 | 1.80                     | 0.63              |
| 5:F:467:LEU:HD21  | 5:F:519:ARG:NH1  | 2.13                     | 0.63              |
| 2:C:583:PRO:O     | 2:C:584:ARG:HG2  | 1.99                     | 0.63              |
| 3:D:1089:PHE:CZ   | 3:D:1103:ASP:OD2 | 2.51                     | 0.63              |
| 5:F:311:THR:HG21  | 5:F:317:PHE:HD1  | 1.64                     | 0.63              |
| 5:F:399:LEU:HA    | 5:F:402:GLU:HB3  | 1.79                     | 0.63              |
| 2:C:950:LYS:HD3   | 2:C:951:GLY:N    | 2.13                     | 0.63              |
| 5:F:315:MET:CE    | 5:F:362:GLN:HB2  | 2.29                     | 0.63              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:E:82:LEU:N      | 4:E:98:GLU:OE2   | 2.30                     | 0.62              |
| 2:C:697:GLU:OE1   | 2:C:697:GLU:N    | 2.32                     | 0.62              |
| 3:D:58:TRP:HA     | 3:D:82:VAL:HG23  | 1.82                     | 0.62              |
| 3:D:219:LEU:O     | 3:D:222:ILE:HG23 | 1.99                     | 0.62              |
| 5:F:325:ASN:O     | 5:F:329:ILE:HG13 | 1.99                     | 0.62              |
| 2:C:488:THR:O     | 2:C:610:ASN:ND2  | 2.28                     | 0.62              |
| 3:D:52:PHE:O      | 3:D:91:ARG:HD2   | 1.98                     | 0.62              |
| 3:D:73:ILE:HG22   | 6:J:27:ARG:NH1   | 2.15                     | 0.62              |
| 5:F:386:LEU:HD11  | 5:F:398:GLU:CD   | 2.25                     | 0.62              |
| 1:B:152:ASN:ND2   | 1:B:158:GLU:HG3  | 2.14                     | 0.62              |
| 3:D:642:PRO:HB3   | 3:D:662:TRP:CD2  | 2.34                     | 0.62              |
| 5:F:317:PHE:HE2   | 5:F:321:ILE:HD11 | 1.64                     | 0.62              |
| 3:D:888:GLU:OE2   | 3:D:891:CYS:HA   | 1.99                     | 0.62              |
| 5:F:381:ARG:HD2   | 5:F:382:ILE:HD12 | 1.80                     | 0.62              |
| 8:P:24:DA:H2''    | 8:P:25:DG:H5'    | 1.81                     | 0.62              |
| 1:B:41:THR:O      | 1:B:45:SER:HB3   | 2.00                     | 0.62              |
| 1:B:85:VAL:HG23   | 1:B:117:THR:O    | 1.99                     | 0.62              |
| 2:C:274:LEU:CD2   | 2:C:292:ALA:HB1  | 2.29                     | 0.62              |
| 2:C:400:VAL:HG22  | 2:C:417:LEU:O    | 2.00                     | 0.62              |
| 2:C:101:GLY:O     | 2:C:142:ASN:ND2  | 2.28                     | 0.62              |
| 2:C:214:PHE:CE2   | 2:C:342:ILE:HG12 | 2.34                     | 0.62              |
| 2:C:274:LEU:HD11  | 2:C:292:ALA:O    | 2.00                     | 0.62              |
| 2:C:486:ILE:HD11  | 3:D:849:TYR:HE2  | 1.64                     | 0.62              |
| 2:C:789:ILE:HD12  | 2:C:789:ILE:O    | 1.99                     | 0.62              |
| 2:C:959:LEU:CB    | 2:C:960:PRO:HD3  | 2.25                     | 0.62              |
| 5:F:471:GLU:O     | 5:F:475:VAL:HG23 | 2.00                     | 0.62              |
| 2:C:623:ALA:HA    | 2:C:714:ALA:HB2  | 1.81                     | 0.62              |
| 2:C:1128:LEU:HD23 | 3:D:406:LEU:HD21 | 1.81                     | 0.62              |
| 3:D:599:TYR:CZ    | 3:D:601:PRO:HG3  | 2.35                     | 0.62              |
| 3:D:882:GLN:HE22  | 3:D:1249:LYS:HE2 | 1.64                     | 0.62              |
| 3:D:1231:ARG:HA   | 3:D:1234:THR:CG2 | 2.29                     | 0.62              |
| 2:C:507:ASN:HB2   | 2:C:511:PHE:O    | 1.99                     | 0.61              |
| 3:D:1033:GLU:OE2  | 3:D:1040:PRO:HB3 | 1.99                     | 0.61              |
| 2:C:220:ASP:CB    | 2:C:221:THR:HG22 | 2.27                     | 0.61              |
| 3:D:453:LYS:NZ    | 3:D:453:LYS:HB3  | 2.15                     | 0.61              |
| 3:D:143:MET:HA    | 3:D:146:ASN:OD1  | 2.00                     | 0.61              |
| 3:D:741:ARG:HB2   | 3:D:744:GLU:OE2  | 1.98                     | 0.61              |
| 3:D:913:ASP:O     | 3:D:916:ILE:HG13 | 2.01                     | 0.61              |
| 3:D:1219:SER:HB2  | 3:D:1243:ASP:OD2 | 1.99                     | 0.61              |
| 5:F:486:PRO:O     | 5:F:487:ARG:HD3  | 1.99                     | 0.61              |
| 2:C:220:ASP:CB    | 2:C:221:THR:HA   | 2.30                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:222:VAL:HG21 | 2:C:234:VAL:N    | 2.14                     | 0.61              |
| 2:C:278:TYR:CD1  | 2:C:291:SER:HB2  | 2.35                     | 0.61              |
| 1:A:153:ARG:CZ   | 2:C:797:ARG:HG2  | 2.30                     | 0.61              |
| 2:C:922:VAL:HB   | 2:C:923:PRO:HD3  | 1.82                     | 0.61              |
| 3:D:873:LEU:O    | 3:D:877:LEU:HD23 | 2.00                     | 0.61              |
| 7:O:5:DG:H2''    | 7:O:6:DA:H5'     | 1.82                     | 0.61              |
| 1:B:96:TYR:CD1   | 1:B:137:GLU:HG2  | 2.35                     | 0.61              |
| 2:C:140:ILE:HG12 | 2:C:146:GLU:O    | 2.00                     | 0.61              |
| 3:D:709:VAL:O    | 3:D:713:VAL:HG23 | 2.00                     | 0.61              |
| 2:C:103:MET:HB2  | 2:C:139:PHE:CE1  | 2.36                     | 0.61              |
| 2:C:646:GLU:HB3  | 2:C:662:HIS:CE1  | 2.36                     | 0.61              |
| 2:C:855:ARG:HH11 | 2:C:861:LEU:HD12 | 1.66                     | 0.61              |
| 2:C:1040:LYS:HD3 | 3:D:540:GLN:HE22 | 1.65                     | 0.61              |
| 3:D:460:LEU:HD11 | 3:D:472:ALA:CB   | 2.30                     | 0.61              |
| 2:C:58:THR:O     | 2:C:62:GLU:HB2   | 2.00                     | 0.61              |
| 2:C:599:HIS:HB3  | 2:C:928:ILE:CD1  | 2.31                     | 0.61              |
| 2:C:1044:ARG:HB2 | 2:C:1063:PHE:CB  | 2.31                     | 0.61              |
| 3:D:467:GLN:HA   | 3:D:467:GLN:HE21 | 1.65                     | 0.61              |
| 3:D:963:ARG:HD3  | 3:D:978:CYS:SG   | 2.41                     | 0.61              |
| 4:E:85:PRO:HB3   | 4:E:94:ILE:CD1   | 2.31                     | 0.61              |
| 2:C:400:VAL:O    | 2:C:404:MET:HB2  | 2.00                     | 0.61              |
| 4:E:47:VAL:CG1   | 4:E:52:ALA:HB3   | 2.31                     | 0.61              |
| 2:C:290:GLU:HG2  | 2:C:294:THR:OG1  | 2.01                     | 0.60              |
| 3:D:767:HIS:O    | 3:D:770:ARG:HG3  | 2.00                     | 0.60              |
| 1:B:182:ARG:HA   | 1:B:182:ARG:NE   | 2.13                     | 0.60              |
| 2:C:225:ARG:HD3  | 2:C:230:ARG:CA   | 2.30                     | 0.60              |
| 9:C:1201:FI8:O8  | 9:C:1201:FI8:O11 | 2.19                     | 0.60              |
| 3:D:668:LEU:HD22 | 3:D:672:MET:HE2  | 1.82                     | 0.60              |
| 5:F:305:SER:O    | 5:F:308:LYS:HG2  | 2.01                     | 0.60              |
| 2:C:531:LEU:HD11 | 2:C:578:TYR:CE2  | 2.36                     | 0.60              |
| 2:C:993:LEU:HD22 | 2:C:993:LEU:H    | 1.64                     | 0.60              |
| 5:F:429:ASP:OD1  | 5:F:430:GLU:N    | 2.27                     | 0.60              |
| 1:A:18:ARG:NH1   | 1:A:195:ASP:OD2  | 2.33                     | 0.60              |
| 1:A:105:VAL:HG23 | 1:A:128:LEU:HD13 | 1.81                     | 0.60              |
| 2:C:205:ILE:HG22 | 2:C:211:TRP:CE2  | 2.36                     | 0.60              |
| 3:D:111:PRO:HB2  | 3:D:116:TYR:CE2  | 2.36                     | 0.60              |
| 3:D:155:MET:HE3  | 3:D:159:ARG:HD3  | 1.83                     | 0.60              |
| 3:D:929:ALA:O    | 3:D:937:ILE:HG22 | 2.01                     | 0.60              |
| 3:D:931:ASP:HB3  | 3:D:955:ALA:HB1  | 1.83                     | 0.60              |
| 3:D:1139:GLN:HG3 | 3:D:1143:ARG:HE  | 1.66                     | 0.60              |
| 6:J:7:ARG:HD2    | 6:J:7:ARG:O      | 2.01                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:O:3:DT:C6       | 7:O:4:DT:H72      | 2.36                     | 0.60              |
| 1:A:10:SER:OG     | 1:A:22:VAL:HG13   | 2.02                     | 0.60              |
| 1:A:82:SER:C      | 1:A:123:MET:HE1   | 2.27                     | 0.60              |
| 2:C:724:MET:HE1   | 2:C:1019:PHE:CE2  | 2.37                     | 0.60              |
| 2:C:1044:ARG:CZ   | 2:C:1056:PRO:HB3  | 2.30                     | 0.60              |
| 1:A:40:ARG:CD     | 1:B:33:THR:HG22   | 2.30                     | 0.60              |
| 1:B:95:MET:HG2    | 1:B:113:PRO:CD    | 2.32                     | 0.60              |
| 1:B:202:ILE:HD12  | 1:B:202:ILE:O     | 2.01                     | 0.60              |
| 2:C:103:MET:SD    | 2:C:404:MET:HG2   | 2.41                     | 0.60              |
| 2:C:721:VAL:HG23  | 2:C:915:ILE:HG13  | 1.83                     | 0.60              |
| 2:C:797:ARG:HG3   | 2:C:800:ASP:OD2   | 2.01                     | 0.60              |
| 3:D:1122:LEU:CB   | 3:D:1130:VAL:HG21 | 2.31                     | 0.60              |
| 3:D:1164:ARG:CD   | 3:D:1208:MET:HE1  | 2.32                     | 0.60              |
| 2:C:323:HIS:HB3   | 2:C:326:GLU:HG3   | 1.82                     | 0.60              |
| 3:D:215:GLU:HG2   | 3:D:218:ARG:HH21  | 1.64                     | 0.60              |
| 6:J:101:ARG:HA    | 6:J:101:ARG:HH11  | 1.65                     | 0.60              |
| 1:A:105:VAL:O     | 1:A:125:ILE:HB    | 2.02                     | 0.60              |
| 2:C:322:LEU:C     | 2:C:324:VAL:H     | 2.10                     | 0.60              |
| 2:C:905:PRO:O     | 2:C:913:VAL:HG13  | 2.02                     | 0.60              |
| 3:D:1087:ARG:CG   | 3:D:1088:VAL:H    | 2.11                     | 0.60              |
| 2:C:200:HIS:O     | 2:C:345:LEU:HD21  | 2.01                     | 0.60              |
| 2:C:290:GLU:OE1   | 2:C:291:SER:N     | 2.35                     | 0.60              |
| 3:D:1099:LEU:HD23 | 3:D:1099:LEU:C    | 2.27                     | 0.60              |
| 2:C:454:ARG:C     | 2:C:455:LEU:HD23  | 2.27                     | 0.59              |
| 2:C:1110:GLU:HG2  | 4:E:69:ASN:HD21   | 1.67                     | 0.59              |
| 3:D:219:LEU:HA    | 3:D:222:ILE:CG2   | 2.32                     | 0.59              |
| 3:D:1098:VAL:O    | 3:D:1098:VAL:HG22 | 2.01                     | 0.59              |
| 5:F:516:HIS:CG    | 5:F:517:PRO:HD2   | 2.37                     | 0.59              |
| 8:P:23:DA:H2''    | 8:P:24:DA:C5'     | 2.31                     | 0.59              |
| 2:C:602:ALA:HB3   | 3:D:856:ALA:HB1   | 1.84                     | 0.59              |
| 3:D:22:GLN:O      | 3:D:22:GLN:HG2    | 2.02                     | 0.59              |
| 3:D:1064:ILE:CD1  | 3:D:1112:MET:HE2  | 2.31                     | 0.59              |
| 1:A:186:ARG:HD2   | 1:B:147:VAL:CG2   | 2.27                     | 0.59              |
| 2:C:278:TYR:CG    | 2:C:291:SER:HB2   | 2.37                     | 0.59              |
| 2:C:946:VAL:HB    | 2:C:964:LEU:HB3   | 1.84                     | 0.59              |
| 5:F:492:ILE:O     | 5:F:495:VAL:HG12  | 2.02                     | 0.59              |
| 6:J:40:PHE:CD2    | 6:J:56:CYS:HB3    | 2.36                     | 0.59              |
| 6:J:102:LEU:O     | 6:J:105:ILE:HG22  | 2.01                     | 0.59              |
| 8:P:23:DA:H2''    | 8:P:24:DA:H5'     | 1.85                     | 0.59              |
| 1:A:144:ARG:NE    | 1:B:232:ILE:HD11  | 2.17                     | 0.59              |
| 2:C:241:LEU:HD21  | 2:C:335:GLU:CB    | 2.33                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:925:LEU:HD21  | 3:D:944:LEU:HD11  | 1.84                     | 0.59              |
| 3:D:711:GLN:OE1   | 4:E:30:ASP:HB2    | 2.02                     | 0.59              |
| 3:D:1051:GLY:HA2  | 3:D:1069:ASP:HB2  | 1.85                     | 0.59              |
| 1:A:218:LEU:O     | 1:A:221:LEU:HD22  | 2.02                     | 0.59              |
| 1:B:71:GLU:OE1    | 1:B:71:GLU:N      | 2.28                     | 0.59              |
| 2:C:220:ASP:HB3   | 2:C:221:THR:CA    | 2.33                     | 0.59              |
| 2:C:338:VAL:O     | 2:C:341:THR:HG22  | 2.02                     | 0.59              |
| 1:A:105:VAL:HG23  | 1:A:128:LEU:CD1   | 2.33                     | 0.59              |
| 1:B:55:ARG:NH1    | 1:B:55:ARG:HB2    | 2.18                     | 0.59              |
| 2:C:77:ARG:NH2    | 2:C:505:ARG:HH12  | 2.00                     | 0.59              |
| 2:C:446:LEU:O     | 2:C:446:LEU:HD23  | 2.02                     | 0.59              |
| 3:D:125:LEU:O     | 3:D:129:ILE:HG23  | 2.03                     | 0.59              |
| 3:D:725:THR:OG1   | 3:D:726:ARG:HD2   | 2.03                     | 0.59              |
| 2:C:231:ARG:HB2   | 5:F:205:ASP:HB3   | 1.84                     | 0.59              |
| 2:C:1050:SER:HB3  | 2:C:1053:THR:O    | 2.03                     | 0.59              |
| 3:D:638:THR:HG22  | 3:D:661:ALA:HB2   | 1.85                     | 0.59              |
| 3:D:1172:SER:HB3  | 3:D:1199:GLU:CB   | 2.33                     | 0.59              |
| 5:F:390:LEU:HG    | 5:F:392:ARG:CG    | 2.32                     | 0.59              |
| 1:B:124:HIS:CE1   | 1:B:127:THR:HG23  | 2.38                     | 0.59              |
| 2:C:267:THR:HG21  | 2:C:273:ALA:CB    | 2.31                     | 0.59              |
| 2:C:559:VAL:HG12  | 2:C:560:LEU:O     | 2.03                     | 0.59              |
| 2:C:737:LEU:CD1   | 2:C:895:ILE:HD13  | 2.33                     | 0.59              |
| 2:C:1059:GLY:H    | 2:C:1062:GLN:CB   | 2.16                     | 0.59              |
| 3:D:666:THR:HG22  | 3:D:685:ASN:ND2   | 2.18                     | 0.59              |
| 3:D:1221:LEU:HD23 | 3:D:1221:LEU:H    | 1.68                     | 0.59              |
| 5:F:490:ASP:HB2   | 5:F:500:ARG:HD3   | 1.85                     | 0.59              |
| 2:C:224:VAL:O     | 2:C:226:ILE:HG22  | 2.02                     | 0.58              |
| 2:C:1048:PRO:HG2  | 2:C:1057:LEU:O    | 2.01                     | 0.58              |
| 3:D:297:LYS:NZ    | 3:D:1176:LEU:HD11 | 2.18                     | 0.58              |
| 3:D:740:PRO:HD3   | 3:D:792:HIS:CD2   | 2.38                     | 0.58              |
| 3:D:1053:VAL:HG12 | 3:D:1103:ASP:O    | 2.04                     | 0.58              |
| 3:D:1067:VAL:HG22 | 3:D:1074:GLU:OE2  | 2.03                     | 0.58              |
| 3:D:1128:ARG:NH2  | 3:D:1132:ILE:HD11 | 2.14                     | 0.58              |
| 3:D:1166:THR:HB   | 3:D:1206:VAL:HG21 | 1.84                     | 0.58              |
| 5:F:334:LYS:HE3   | 7:O:25:DC:P       | 2.43                     | 0.58              |
| 5:F:418:ARG:HB2   | 5:F:418:ARG:NH2   | 2.18                     | 0.58              |
| 5:F:474:VAL:HG22  | 5:F:496:TYR:HE2   | 1.66                     | 0.58              |
| 1:B:84:VAL:HG22   | 1:B:119:HIS:HB2   | 1.85                     | 0.58              |
| 2:C:519:VAL:N     | 2:C:577:ASP:O     | 2.31                     | 0.58              |
| 2:C:789:ILE:HG21  | 2:C:869:VAL:HG21  | 1.85                     | 0.58              |
| 3:D:866:ARG:HD2   | 3:D:1010:LEU:O    | 2.03                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1150:HIS:ND1  | 3:D:1152:LYS:HG2  | 2.18                     | 0.58              |
| 2:C:318:LYS:HZ3   | 2:C:318:LYS:HB2   | 1.67                     | 0.58              |
| 3:D:902:ALA:H     | 3:D:913:ASP:HB2   | 1.68                     | 0.58              |
| 3:D:1162:LEU:CD2  | 3:D:1207:LEU:HD23 | 2.33                     | 0.58              |
| 1:B:136:VAL:HG12  | 1:B:138:LEU:HD12  | 1.85                     | 0.58              |
| 2:C:267:THR:CG2   | 2:C:273:ALA:HB2   | 2.29                     | 0.58              |
| 2:C:328:ILE:HD12  | 2:C:328:ILE:O     | 2.03                     | 0.58              |
| 2:C:539:HIS:HD1   | 2:C:578:TYR:HE2   | 1.49                     | 0.58              |
| 9:C:1201:FI8:O14  | 3:D:412:ARG:NH2   | 2.36                     | 0.58              |
| 3:D:245:VAL:O     | 3:D:249:GLY:HA3   | 2.04                     | 0.58              |
| 3:D:354:LEU:HB2   | 3:D:370:GLU:CG    | 2.33                     | 0.58              |
| 2:C:715:LEU:N     | 2:C:1029:TYR:OH   | 2.37                     | 0.58              |
| 2:C:1044:ARG:NH1  | 2:C:1056:PRO:HB3  | 2.18                     | 0.58              |
| 3:D:707:ILE:HD12  | 4:E:39:PRO:HB3    | 1.85                     | 0.58              |
| 3:D:766:ASN:HD22  | 3:D:766:ASN:H     | 1.51                     | 0.58              |
| 3:D:899:VAL:HG12  | 3:D:900:GLU:H     | 1.68                     | 0.58              |
| 2:C:217:ASP:OD1   | 2:C:231:ARG:NH2   | 2.37                     | 0.58              |
| 3:D:273:GLU:O     | 3:D:277:LEU:HD13  | 2.04                     | 0.58              |
| 3:D:1068:PRO:HG2  | 3:D:1072:GLY:N    | 2.19                     | 0.58              |
| 2:C:646:GLU:HB3   | 2:C:662:HIS:ND1   | 2.18                     | 0.58              |
| 3:D:119:ASP:C     | 3:D:120:LEU:HD12  | 2.29                     | 0.58              |
| 3:D:930:VAL:HG12  | 3:D:936:VAL:HA    | 1.86                     | 0.58              |
| 1:B:62:GLU:OE2    | 1:B:65:THR:HB     | 2.04                     | 0.58              |
| 2:C:103:MET:CG    | 2:C:404:MET:HE2   | 2.32                     | 0.58              |
| 2:C:222:VAL:CB    | 2:C:234:VAL:HG13  | 2.34                     | 0.58              |
| 2:C:1002:VAL:CG1  | 2:C:1006:GLY:HA2  | 2.34                     | 0.58              |
| 3:D:991:ILE:HG22  | 3:D:991:ILE:O     | 2.02                     | 0.58              |
| 2:C:1081:ALA:HB1  | 3:D:554:GLU:OE1   | 2.03                     | 0.58              |
| 1:A:40:ARG:HG2    | 1:B:33:THR:HG22   | 1.85                     | 0.57              |
| 3:D:31:PRO:HB3    | 3:D:348:ILE:CG2   | 2.34                     | 0.57              |
| 3:D:226:PHE:CE1   | 3:D:248:TYR:HB3   | 2.38                     | 0.57              |
| 3:D:369:ASN:O     | 3:D:373:MET:HG3   | 2.04                     | 0.57              |
| 5:F:296:LEU:O     | 5:F:300:LEU:HG    | 2.03                     | 0.57              |
| 1:A:182:ARG:HH11  | 3:D:624:ARG:NH1   | 2.02                     | 0.57              |
| 2:C:80:VAL:HG12   | 2:C:81:ASN:OD1    | 2.05                     | 0.57              |
| 2:C:584:ARG:NH2   | 2:C:975:PRO:HB3   | 2.19                     | 0.57              |
| 2:C:1087:GLU:OE2  | 3:D:547:LEU:HB2   | 2.03                     | 0.57              |
| 2:C:623:ALA:HA    | 2:C:714:ALA:CB    | 2.34                     | 0.57              |
| 3:D:736:VAL:HG22  | 3:D:799:ILE:HD11  | 1.87                     | 0.57              |
| 3:D:1010:LEU:HD23 | 3:D:1028:LEU:CA   | 2.35                     | 0.57              |
| 2:C:152:VAL:HG11  | 2:C:418:ILE:HG21  | 1.87                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:343:GLU:OE2   | 2:C:355:MET:HE2   | 2.03                     | 0.57              |
| 2:C:524:VAL:N     | 2:C:552:GLY:O     | 2.27                     | 0.57              |
| 5:F:379:LEU:HD11  | 5:F:410:VAL:HG23  | 1.87                     | 0.57              |
| 5:F:514:LEU:O     | 5:F:519:ARG:HB2   | 2.03                     | 0.57              |
| 2:C:231:ARG:CB    | 5:F:205:ASP:HB3   | 2.35                     | 0.57              |
| 2:C:313:ARG:HG3   | 2:C:330:SER:O     | 2.05                     | 0.57              |
| 2:C:982:GLU:OE1   | 3:D:841:ARG:NH2   | 2.37                     | 0.57              |
| 3:D:1084:GLN:HE21 | 3:D:1112:MET:CB   | 2.17                     | 0.57              |
| 7:O:6:DA:H1'      | 7:O:7:DC:H5'      | 1.87                     | 0.57              |
| 1:B:3:ILE:HD11    | 1:B:27:GLU:HG2    | 1.87                     | 0.57              |
| 2:C:718:ASN:C     | 2:C:719:LEU:HD12  | 2.29                     | 0.57              |
| 3:D:557:ILE:HD12  | 4:E:54:VAL:HG22   | 1.87                     | 0.57              |
| 3:D:668:LEU:HD23  | 3:D:668:LEU:O     | 2.05                     | 0.57              |
| 5:F:511:MET:HB3   | 5:F:515:ARG:HH12  | 1.70                     | 0.57              |
| 2:C:293:GLN:NE2   | 2:C:297:GLU:OE2   | 2.38                     | 0.57              |
| 2:C:531:LEU:HD11  | 2:C:578:TYR:CD2   | 2.40                     | 0.57              |
| 2:C:899:LEU:H     | 2:C:899:LEU:HD22  | 1.68                     | 0.57              |
| 3:D:125:LEU:HD11  | 3:D:261:ILE:CD1   | 2.35                     | 0.57              |
| 3:D:981:ARG:HG2   | 3:D:982:SER:O     | 2.05                     | 0.57              |
| 3:D:1050:THR:HG22 | 3:D:1106:GLU:HA   | 1.86                     | 0.57              |
| 4:E:58:ALA:O      | 4:E:62:ARG:HG3    | 2.05                     | 0.57              |
| 2:C:215:ASP:O     | 2:C:223:GLY:N     | 2.37                     | 0.57              |
| 3:D:136:ILE:HD11  | 3:D:235:ILE:CD1   | 2.35                     | 0.57              |
| 3:D:738:VAL:HG13  | 3:D:739:PRO:HD2   | 1.86                     | 0.57              |
| 3:D:1087:ARG:HG3  | 3:D:1088:VAL:N    | 2.17                     | 0.57              |
| 1:A:102:PRO:HG3   | 1:A:130:ASP:OD1   | 2.04                     | 0.57              |
| 6:J:101:ARG:NH1   | 6:J:101:ARG:HB3   | 2.19                     | 0.57              |
| 2:C:650:ILE:HG21  | 2:C:691:ASP:O     | 2.04                     | 0.56              |
| 2:C:727:GLU:CG    | 3:D:725:THR:HG21  | 2.35                     | 0.56              |
| 3:D:665:GLU:HG3   | 3:D:665:GLU:O     | 2.05                     | 0.56              |
| 3:D:910:LEU:HD12  | 3:D:910:LEU:O     | 2.05                     | 0.56              |
| 5:F:395:THR:HB    | 5:F:397:GLU:OE2   | 2.04                     | 0.56              |
| 1:B:153:ARG:HA    | 1:B:153:ARG:NE    | 2.20                     | 0.56              |
| 2:C:882:GLY:HA3   | 2:C:1037:VAL:HG11 | 1.87                     | 0.56              |
| 1:A:89:GLU:OE2    | 1:A:93:VAL:HG11   | 2.06                     | 0.56              |
| 1:A:221:LEU:CD1   | 1:B:7:PRO:HG2     | 2.35                     | 0.56              |
| 2:C:40:SER:HA     | 2:C:973:SER:OG    | 2.05                     | 0.56              |
| 2:C:388:GLN:O     | 2:C:391:VAL:HG12  | 2.04                     | 0.56              |
| 2:C:519:VAL:HG23  | 2:C:523:VAL:C     | 2.30                     | 0.56              |
| 2:C:742:VAL:HG22  | 2:C:879:ILE:HG22  | 1.87                     | 0.56              |
| 2:C:926:MET:HE1   | 3:D:817:LEU:CA    | 2.36                     | 0.56              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:D:162:VAL:HG13 | 3:D:216:LEU:CD2   | 2.27                     | 0.56              |
| 3:D:177:LEU:HD13 | 3:D:205:MET:HE3   | 1.86                     | 0.56              |
| 3:D:826:ASN:CG   | 3:D:827:PRO:HD2   | 2.30                     | 0.56              |
| 3:D:1061:PHE:HB3 | 3:D:1081:SER:CA   | 2.35                     | 0.56              |
| 3:D:1068:PRO:HD3 | 3:D:1074:GLU:HA   | 1.86                     | 0.56              |
| 3:D:1080:ILE:CG2 | 3:D:1112:MET:HE3  | 2.34                     | 0.56              |
| 3:D:1195:ALA:O   | 3:D:1197:GLY:N    | 2.38                     | 0.56              |
| 5:F:415:GLN:O    | 5:F:418:ARG:NH2   | 2.38                     | 0.56              |
| 5:F:498:VAL:HG23 | 5:F:503:ILE:HG12  | 1.87                     | 0.56              |
| 7:O:19:DA:H2''   | 7:O:20:DT:O5'     | 2.05                     | 0.56              |
| 1:B:96:TYR:O     | 1:B:110:ILE:HG13  | 2.04                     | 0.56              |
| 2:C:926:MET:HE1  | 3:D:817:LEU:HA    | 1.87                     | 0.56              |
| 3:D:101:VAL:HG13 | 3:D:375:GLN:OE1   | 2.05                     | 0.56              |
| 3:D:146:ASN:OD1  | 3:D:147:GLU:N     | 2.36                     | 0.56              |
| 3:D:797:ASN:O    | 3:D:800:ILE:HG22  | 2.06                     | 0.56              |
| 3:D:909:THR:O    | 3:D:910:LEU:CG    | 2.53                     | 0.56              |
| 5:F:328:LEU:O    | 5:F:328:LEU:HD23  | 2.05                     | 0.56              |
| 5:F:213:ARG:N    | 5:F:213:ARG:HD2   | 2.20                     | 0.56              |
| 1:A:95:MET:HE2   | 1:A:110:ILE:CG2   | 2.35                     | 0.56              |
| 5:F:213:ARG:O    | 5:F:216:ARG:HG3   | 2.06                     | 0.56              |
| 2:C:848:ILE:CD1  | 2:C:874:ALA:HB2   | 2.35                     | 0.56              |
| 2:C:885:LEU:HD23 | 2:C:1030:ILE:HD12 | 1.86                     | 0.56              |
| 3:D:276:SER:O    | 3:D:280:VAL:HG23  | 2.05                     | 0.56              |
| 3:D:1012:MET:C   | 3:D:1027:GLY:HA3  | 2.30                     | 0.56              |
| 3:D:1235:ASP:OD1 | 3:D:1236:ALA:N    | 2.38                     | 0.56              |
| 1:A:34:LEU:HD11  | 1:B:218:LEU:CD2   | 2.28                     | 0.56              |
| 3:D:35:ASN:OD1   | 3:D:38:THR:HG22   | 2.05                     | 0.56              |
| 3:D:480:ARG:O    | 3:D:483:VAL:HG13  | 2.06                     | 0.56              |
| 3:D:599:TYR:CE2  | 3:D:601:PRO:HG3   | 2.40                     | 0.56              |
| 3:D:736:VAL:HG11 | 3:D:817:LEU:CD2   | 2.35                     | 0.56              |
| 3:D:866:ARG:NH1  | 3:D:1011:THR:HA   | 2.21                     | 0.56              |
| 3:D:963:ARG:CD   | 3:D:978:CYS:HA    | 2.36                     | 0.56              |
| 3:D:1133:HIS:O   | 3:D:1137:GLU:HG2  | 2.06                     | 0.56              |
| 1:B:99:LYS:HD3   | 1:B:105:VAL:HG22  | 1.88                     | 0.56              |
| 3:D:330:LEU:HD11 | 5:F:439:ILE:HD12  | 1.87                     | 0.56              |
| 3:D:733:MET:O    | 3:D:733:MET:HG2   | 2.06                     | 0.56              |
| 5:F:414:GLN:HE21 | 5:F:414:GLN:HA    | 1.69                     | 0.56              |
| 2:C:173:ARG:NH2  | 2:C:437:SER:O     | 2.37                     | 0.56              |
| 2:C:203:LYS:HG2  | 2:C:205:ILE:HG23  | 1.87                     | 0.56              |
| 2:C:727:GLU:H    | 3:D:725:THR:HG22  | 1.71                     | 0.56              |
| 3:D:222:ILE:HD13 | 3:D:223:TRP:N     | 2.21                     | 0.56              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:F:334:LYS:HG2  | 5:F:334:LYS:O     | 2.06                     | 0.56              |
| 2:C:258:MET:CA   | 2:C:261:THR:HG23  | 2.31                     | 0.55              |
| 2:C:355:MET:HB2  | 2:C:365:VAL:CG2   | 2.36                     | 0.55              |
| 3:D:599:TYR:CD1  | 3:D:601:PRO:HD3   | 2.41                     | 0.55              |
| 3:D:632:LYS:NZ   | 3:D:665:GLU:OE1   | 2.29                     | 0.55              |
| 3:D:1173:THR:HA  | 3:D:1174:GLU:OE1  | 2.07                     | 0.55              |
| 4:E:37:ASN:OD1   | 4:E:38:PRO:HA     | 2.06                     | 0.55              |
| 8:P:1:DA:H5"     | 8:P:1:DA:C8       | 2.40                     | 0.55              |
| 3:D:1052:ARG:CG  | 3:D:1067:VAL:HB   | 2.36                     | 0.55              |
| 5:F:305:SER:HA   | 5:F:308:LYS:HD2   | 1.88                     | 0.55              |
| 5:F:489:LEU:HG   | 8:P:20:DG:P       | 2.46                     | 0.55              |
| 1:B:70:LYS:HE3   | 1:B:127:THR:OG1   | 2.06                     | 0.55              |
| 2:C:224:VAL:HG21 | 2:C:234:VAL:HA    | 1.88                     | 0.55              |
| 2:C:622:GLU:HB3  | 2:C:717:LYS:HD3   | 1.87                     | 0.55              |
| 2:C:773:ILE:HG23 | 2:C:774:PRO:HD2   | 1.87                     | 0.55              |
| 1:A:221:LEU:HD12 | 1:B:7:PRO:O       | 2.07                     | 0.55              |
| 1:B:182:ARG:HB3  | 1:B:186:ARG:CB    | 2.36                     | 0.55              |
| 2:C:222:VAL:HG11 | 2:C:234:VAL:CG2   | 2.36                     | 0.55              |
| 2:C:842:GLY:O    | 2:C:843:GLU:HG3   | 2.06                     | 0.55              |
| 3:D:218:ARG:O    | 3:D:222:ILE:HG22  | 2.05                     | 0.55              |
| 3:D:452:PHE:O    | 3:D:456:VAL:HG12  | 2.05                     | 0.55              |
| 3:D:608:GLU:O    | 3:D:609:THR:OG1   | 2.19                     | 0.55              |
| 3:D:760:PHE:CE1  | 3:D:767:HIS:HA    | 2.41                     | 0.55              |
| 3:D:913:ASP:HB3  | 3:D:916:ILE:CG1   | 2.36                     | 0.55              |
| 2:C:569:GLU:HG2  | 2:C:570:TYR:H     | 1.72                     | 0.55              |
| 2:C:595:PRO:HG3  | 2:C:888:ARG:NH2   | 2.21                     | 0.55              |
| 2:C:992:THR:HG23 | 2:C:1000:VAL:HG13 | 1.88                     | 0.55              |
| 3:D:320:ILE:CG1  | 3:D:321:PRO:HD2   | 2.36                     | 0.55              |
| 3:D:598:GLU:HG2  | 3:D:599:TYR:N     | 2.22                     | 0.55              |
| 3:D:765:LEU:HD23 | 3:D:765:LEU:H     | 1.72                     | 0.55              |
| 3:D:1190:ASN:ND2 | 3:D:1201:ALA:HB3  | 2.21                     | 0.55              |
| 3:D:1217:THR:CG2 | 3:D:1223:ALA:HB2  | 2.36                     | 0.55              |
| 6:J:40:PHE:CZ    | 6:J:58:ASN:HB2    | 2.42                     | 0.55              |
| 1:A:95:MET:HE2   | 1:A:110:ILE:HG21  | 1.88                     | 0.55              |
| 2:C:322:LEU:O    | 2:C:324:VAL:N     | 2.38                     | 0.55              |
| 2:C:522:GLY:O    | 2:C:553:ARG:HA    | 2.07                     | 0.55              |
| 2:C:919:THR:HG23 | 3:D:731:VAL:CG2   | 2.36                     | 0.55              |
| 2:C:982:GLU:HB2  | 3:D:841:ARG:HH22  | 1.72                     | 0.55              |
| 3:D:173:ARG:HE   | 3:D:205:MET:HG2   | 1.70                     | 0.55              |
| 1:A:94:THR:O     | 1:A:113:PRO:HG3   | 2.07                     | 0.55              |
| 1:B:97:LEU:HB2   | 1:B:110:ILE:HD12  | 1.87                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:222:VAL:HG21  | 2:C:234:VAL:HG13  | 1.87                     | 0.55              |
| 3:D:876:ARG:NH1   | 3:D:1036:GLU:OE1  | 2.40                     | 0.55              |
| 6:J:103:GLU:OE1   | 6:J:104:LEU:N     | 2.40                     | 0.55              |
| 1:B:24:GLU:CG     | 1:B:191:LYS:HG3   | 2.36                     | 0.55              |
| 2:C:42:ALA:HB2    | 2:C:975:PRO:HG2   | 1.87                     | 0.55              |
| 2:C:224:VAL:HG21  | 2:C:234:VAL:CA    | 2.37                     | 0.55              |
| 2:C:542:ALA:HB3   | 2:C:579:MET:HB2   | 1.89                     | 0.55              |
| 2:C:820:LEU:CD2   | 5:F:481:LEU:HD11  | 2.37                     | 0.55              |
| 3:D:35:ASN:CG     | 3:D:38:THR:HG22   | 2.32                     | 0.55              |
| 3:D:447:MET:HE1   | 3:D:522:ILE:HD11  | 1.88                     | 0.55              |
| 3:D:944:LEU:HA    | 3:D:948:GLU:HG3   | 1.88                     | 0.55              |
| 3:D:1064:ILE:HD12 | 3:D:1080:ILE:HD12 | 1.89                     | 0.55              |
| 3:D:1118:PRO:HA   | 3:D:1121:VAL:CG1  | 2.37                     | 0.55              |
| 5:F:266:LEU:O     | 5:F:266:LEU:HD13  | 2.06                     | 0.55              |
| 5:F:311:THR:HG21  | 5:F:317:PHE:CD1   | 2.41                     | 0.55              |
| 5:F:490:ASP:HB2   | 5:F:500:ARG:CD    | 2.36                     | 0.55              |
| 2:C:475:VAL:HG23  | 3:D:854:HIS:CE1   | 2.42                     | 0.55              |
| 2:C:764:LEU:HD23  | 2:C:808:PRO:CB    | 2.37                     | 0.55              |
| 2:C:959:LEU:HD12  | 2:C:959:LEU:N     | 2.22                     | 0.55              |
| 3:D:31:PRO:HB3    | 3:D:348:ILE:HG23  | 1.88                     | 0.55              |
| 2:C:281:LEU:HD23  | 2:C:295:LEU:HD21  | 1.88                     | 0.55              |
| 2:C:500:LEU:CD2   | 2:C:504:ALA:HB3   | 2.36                     | 0.55              |
| 2:C:1034:HIS:O    | 2:C:1035:HIS:ND1  | 2.40                     | 0.55              |
| 3:D:915:TYR:CZ    | 3:D:1143:ARG:HD3  | 2.42                     | 0.55              |
| 3:D:1080:ILE:HG21 | 3:D:1112:MET:CE   | 2.36                     | 0.55              |
| 5:F:372:MET:O     | 5:F:376:ILE:HG13  | 2.07                     | 0.55              |
| 2:C:133:LEU:HD23  | 2:C:134:PHE:N     | 2.22                     | 0.54              |
| 2:C:686:GLN:HG3   | 2:C:704:ASP:O     | 2.08                     | 0.54              |
| 2:C:1068:PHE:HZ   | 2:C:1076:MET:HG3  | 1.72                     | 0.54              |
| 3:D:193:ALA:O     | 3:D:197:VAL:HG23  | 2.07                     | 0.54              |
| 3:D:459:ARG:HH12  | 3:D:463:LEU:HD23  | 1.71                     | 0.54              |
| 3:D:706:MET:N     | 4:E:41:ASP:OD2    | 2.37                     | 0.54              |
| 1:B:38:LEU:HD12   | 1:B:42:LEU:CD1    | 2.37                     | 0.54              |
| 2:C:413:THR:OG1   | 2:C:414:PRO:HD2   | 2.07                     | 0.54              |
| 2:C:554:PHE:CD1   | 2:C:559:VAL:HG21  | 2.43                     | 0.54              |
| 3:D:107:PHE:CE2   | 3:D:129:ILE:HD11  | 2.42                     | 0.54              |
| 3:D:170:LEU:O     | 3:D:173:ARG:HG3   | 2.07                     | 0.54              |
| 3:D:778:TRP:CD1   | 3:D:835:PRO:HD3   | 2.42                     | 0.54              |
| 3:D:895:ARG:HH11  | 3:D:967:THR:HB    | 1.71                     | 0.54              |
| 1:A:25:PRO:O      | 1:A:26:LEU:HD23   | 2.08                     | 0.54              |
| 1:B:89:GLU:OE1    | 1:B:89:GLU:N      | 2.41                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:146:TYR:HB2   | 3:D:620:MET:HE2   | 1.88                     | 0.54              |
| 2:C:163:LYS:HG3   | 2:C:639:GLY:HA3   | 1.89                     | 0.54              |
| 2:C:549:ASP:HB2   | 2:C:555:VAL:CG2   | 2.38                     | 0.54              |
| 3:D:641:ARG:HA    | 3:D:657:GLN:CG    | 2.35                     | 0.54              |
| 3:D:923:ARG:HB3   | 3:D:962:VAL:HG11  | 1.88                     | 0.54              |
| 3:D:1025:THR:CG2  | 3:D:1029:PRO:HB2  | 2.26                     | 0.54              |
| 8:P:14:DA:H2''    | 8:P:15:DC:O5'     | 2.06                     | 0.54              |
| 2:C:32:VAL:HG21   | 2:C:632:LEU:HD11  | 1.88                     | 0.54              |
| 2:C:224:VAL:O     | 2:C:224:VAL:HG12  | 2.07                     | 0.54              |
| 2:C:587:VAL:HG13  | 2:C:591:THR:HB    | 1.88                     | 0.54              |
| 2:C:632:LEU:O     | 2:C:632:LEU:HD22  | 2.07                     | 0.54              |
| 2:C:959:LEU:CB    | 2:C:960:PRO:CD    | 2.84                     | 0.54              |
| 3:D:57:ASP:OD2    | 6:J:14:VAL:HA     | 2.06                     | 0.54              |
| 5:F:221:LEU:O     | 5:F:224:SER:OG    | 2.22                     | 0.54              |
| 5:F:371:HIS:NE2   | 7:O:21:DT:OP2     | 2.39                     | 0.54              |
| 6:J:85:LEU:HA     | 6:J:88:ARG:NH1    | 2.21                     | 0.54              |
| 1:B:107:ALA:HB3   | 1:B:121:PRO:CA    | 2.38                     | 0.54              |
| 2:C:134:PHE:HE1   | 2:C:153:PHE:HB2   | 1.72                     | 0.54              |
| 2:C:543:GLN:OE1   | 2:C:543:GLN:HA    | 2.08                     | 0.54              |
| 2:C:754:GLU:OE2   | 2:C:870:ARG:HD2   | 2.07                     | 0.54              |
| 2:C:799:GLY:H     | 2:C:839:VAL:HG13  | 1.73                     | 0.54              |
| 2:C:822:ARG:NH1   | 2:C:829:ALA:HB2   | 2.23                     | 0.54              |
| 2:C:1093:SER:CB   | 3:D:420:LYS:HD3   | 2.37                     | 0.54              |
| 3:D:113:ARG:NH2   | 3:D:1235:ASP:HB3  | 2.22                     | 0.54              |
| 3:D:297:LYS:HZ3   | 3:D:1176:LEU:HD11 | 1.71                     | 0.54              |
| 3:D:948:GLU:O     | 3:D:952:LEU:HG    | 2.08                     | 0.54              |
| 3:D:1064:ILE:HD11 | 3:D:1112:MET:CE   | 2.37                     | 0.54              |
| 6:J:28:GLN:NE2    | 6:J:46:ASP:O      | 2.41                     | 0.54              |
| 2:C:519:VAL:HG11  | 2:C:576:VAL:HG12  | 1.90                     | 0.54              |
| 3:D:190:LYS:HG2   | 3:D:192:ASP:H     | 1.72                     | 0.54              |
| 6:J:99:LYS:HZ3    | 6:J:99:LYS:HB2    | 1.73                     | 0.54              |
| 2:C:561:VAL:HG22  | 2:C:562:ARG:H     | 1.72                     | 0.54              |
| 3:D:373:MET:HE3   | 5:F:318:LEU:HB3   | 1.89                     | 0.54              |
| 3:D:873:LEU:HD22  | 3:D:1028:LEU:HD11 | 1.89                     | 0.54              |
| 3:D:925:LEU:HD22  | 3:D:960:VAL:HG12  | 1.89                     | 0.54              |
| 4:E:76:LEU:HG     | 4:E:77:GLU:H      | 1.71                     | 0.54              |
| 1:A:71:GLU:HB3    | 1:A:75:GLU:HB3    | 1.89                     | 0.54              |
| 2:C:485:PRO:O     | 3:D:857:ARG:NH2   | 2.41                     | 0.54              |
| 2:C:518:LYS:HA    | 2:C:578:TYR:HD1   | 1.73                     | 0.54              |
| 3:D:78:CYS:O      | 3:D:80:VAL:HG23   | 2.07                     | 0.54              |
| 3:D:199:ASP:O     | 3:D:203:ARG:HG2   | 2.08                     | 0.54              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:1244:LYS:HE2  | 3:D:1244:LYS:HA  | 1.89                     | 0.54              |
| 3:D:1264:ILE:CG2  | 3:D:1266:ARG:HG2 | 2.38                     | 0.54              |
| 4:E:85:PRO:HB3    | 4:E:94:ILE:HD13  | 1.90                     | 0.54              |
| 5:F:342:LYS:HG2   | 7:O:29:DA:H3'    | 1.90                     | 0.54              |
| 5:F:476:ARG:O     | 5:F:480:GLY:N    | 2.40                     | 0.54              |
| 8:P:14:DA:H1'     | 8:P:15:DC:H5'    | 1.89                     | 0.54              |
| 1:A:147:VAL:HG12  | 1:A:168:TYR:HE2  | 1.73                     | 0.54              |
| 1:A:221:LEU:HD23  | 1:A:222:ALA:N    | 2.22                     | 0.54              |
| 2:C:177:SER:HB2   | 2:C:378:LEU:CD1  | 2.37                     | 0.54              |
| 2:C:532:THR:CG2   | 2:C:535:GLU:HG2  | 2.38                     | 0.54              |
| 2:C:571:VAL:HG13  | 2:C:572:PRO:O    | 2.07                     | 0.54              |
| 2:C:805:LYS:HB3   | 2:C:836:SER:HA   | 1.90                     | 0.54              |
| 3:D:174:ALA:O     | 3:D:178:GLU:HG3  | 2.07                     | 0.54              |
| 3:D:410:GLN:HA    | 3:D:410:GLN:HE21 | 1.73                     | 0.54              |
| 3:D:504:LEU:HB3   | 3:D:1005:GLU:HG2 | 1.89                     | 0.54              |
| 4:E:32:PRO:HB2    | 4:E:36:THR:HG23  | 1.90                     | 0.54              |
| 2:C:705:GLY:N     | 2:C:708:THR:OG1  | 2.31                     | 0.54              |
| 2:C:885:LEU:HD13  | 2:C:895:ILE:HD11 | 1.89                     | 0.54              |
| 2:C:1044:ARG:HD2  | 2:C:1063:PHE:HB2 | 1.90                     | 0.54              |
| 3:D:314:LEU:HD21  | 3:D:382:PHE:CE2  | 2.43                     | 0.54              |
| 5:F:334:LYS:HD2   | 5:F:350:TRP:CZ2  | 2.42                     | 0.54              |
| 1:A:185:GLN:OE1   | 1:A:185:GLN:N    | 2.42                     | 0.53              |
| 2:C:192:ASP:O     | 2:C:196:ASP:HA   | 2.07                     | 0.53              |
| 2:C:225:ARG:HD3   | 2:C:230:ARG:N    | 2.23                     | 0.53              |
| 3:D:1063:LYS:HZ1  | 3:D:1078:ASP:CA  | 2.11                     | 0.53              |
| 3:D:1063:LYS:HD3  | 3:D:1064:ILE:N   | 2.23                     | 0.53              |
| 3:D:1105:VAL:HG13 | 3:D:1109:GLN:HB3 | 1.89                     | 0.53              |
| 3:D:1219:SER:OG   | 3:D:1222:SER:HB3 | 2.07                     | 0.53              |
| 5:F:328:LEU:HD23  | 5:F:328:LEU:C    | 2.33                     | 0.53              |
| 5:F:489:LEU:HD12  | 8:P:20:DG:H2'    | 1.90                     | 0.53              |
| 6:J:89:ARG:HG2    | 6:J:94:LEU:CD2   | 2.37                     | 0.53              |
| 2:C:771:ARG:CG    | 2:C:781:LEU:HD11 | 2.39                     | 0.53              |
| 3:D:1097:ARG:HH12 | 3:D:1100:SER:N   | 2.06                     | 0.53              |
| 3:D:1097:ARG:NH1  | 3:D:1100:SER:CB  | 2.66                     | 0.53              |
| 5:F:303:VAL:HG22  | 5:F:351:ILE:CD1  | 2.36                     | 0.53              |
| 6:J:68:ASP:OD2    | 6:J:70:PRO:HD3   | 2.09                     | 0.53              |
| 1:B:55:ARG:HD3    | 1:B:137:GLU:OE1  | 2.08                     | 0.53              |
| 2:C:271:ASP:HA    | 2:C:274:LEU:HB3  | 1.89                     | 0.53              |
| 2:C:789:ILE:HG22  | 2:C:803:VAL:HG22 | 1.91                     | 0.53              |
| 2:C:1007:LYS:NZ   | 3:D:735:ASP:OD2  | 2.38                     | 0.53              |
| 2:C:1110:GLU:HG2  | 4:E:69:ASN:ND2   | 2.23                     | 0.53              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:354:LEU:HB2   | 3:D:370:GLU:HG3  | 1.89                     | 0.53              |
| 3:D:1068:PRO:HG3  | 3:D:1073:GLU:O   | 2.09                     | 0.53              |
| 3:D:1070:ASP:HB2  | 3:D:1071:GLY:CA  | 2.39                     | 0.53              |
| 2:C:254:PHE:HE1   | 2:C:347:ARG:HH11 | 1.56                     | 0.53              |
| 2:C:1125:LEU:O    | 2:C:1129:GLN:HG3 | 2.08                     | 0.53              |
| 3:D:241:TYR:O     | 3:D:245:VAL:HG23 | 2.08                     | 0.53              |
| 3:D:262:GLN:HE21  | 3:D:310:MET:HE1  | 1.72                     | 0.53              |
| 2:C:446:LEU:HB2   | 2:C:713:MET:HE2  | 1.89                     | 0.53              |
| 2:C:547:PRO:O     | 2:C:555:VAL:HG23 | 2.08                     | 0.53              |
| 2:C:1117:ILE:CD1  | 3:D:5:ASN:HA     | 2.38                     | 0.53              |
| 3:D:1208:MET:HG3  | 3:D:1213:ALA:HB2 | 1.89                     | 0.53              |
| 5:F:498:VAL:CG2   | 5:F:503:ILE:HG12 | 2.38                     | 0.53              |
| 1:B:218:LEU:O     | 1:B:218:LEU:HD23 | 2.07                     | 0.53              |
| 3:D:383:ASP:OD2   | 3:D:386:ARG:HB2  | 2.08                     | 0.53              |
| 3:D:957:ILE:HD12  | 3:D:957:ILE:O    | 2.09                     | 0.53              |
| 3:D:1272:VAL:HG13 | 4:E:56:TYR:HE1   | 1.73                     | 0.53              |
| 5:F:407:PRO:HA    | 5:F:410:VAL:HG12 | 1.90                     | 0.53              |
| 2:C:222:VAL:HG23  | 2:C:224:VAL:HG23 | 1.90                     | 0.53              |
| 2:C:397:GLU:OE1   | 2:C:398:ARG:N    | 2.41                     | 0.53              |
| 2:C:756:GLU:OE1   | 2:C:870:ARG:HD3  | 2.08                     | 0.53              |
| 3:D:12:ILE:HG22   | 3:D:1237:ALA:HA  | 1.90                     | 0.53              |
| 3:D:73:ILE:HG22   | 6:J:27:ARG:HH11  | 1.72                     | 0.53              |
| 3:D:277:LEU:HD23  | 3:D:296:LEU:CA   | 2.38                     | 0.53              |
| 3:D:866:ARG:CD    | 3:D:1010:LEU:O   | 2.56                     | 0.53              |
| 5:F:276:ALA:HA    | 5:F:279:ARG:NH2  | 2.24                     | 0.53              |
| 1:A:40:ARG:CG     | 1:B:33:THR:HG22  | 2.38                     | 0.53              |
| 2:C:224:VAL:HG21  | 2:C:233:PRO:C    | 2.33                     | 0.53              |
| 2:C:486:ILE:HD11  | 3:D:849:TYR:CE2  | 2.43                     | 0.53              |
| 3:D:128:ILE:HD13  | 3:D:135:VAL:HG21 | 1.90                     | 0.53              |
| 4:E:101:ALA:HB3   | 4:E:103:LEU:HD13 | 1.89                     | 0.53              |
| 1:B:182:ARG:HG3   | 1:B:185:GLN:HB3  | 1.90                     | 0.53              |
| 2:C:216:VAL:HG11  | 2:C:349:HIS:HD2  | 1.74                     | 0.53              |
| 2:C:252:PHE:HB3   | 2:C:258:MET:CE   | 2.39                     | 0.53              |
| 2:C:338:VAL:HG12  | 2:C:342:ILE:HD11 | 1.91                     | 0.53              |
| 2:C:1117:ILE:HD13 | 3:D:5:ASN:HA     | 1.90                     | 0.53              |
| 3:D:263:LYS:HB2   | 3:D:263:LYS:HZ3  | 1.74                     | 0.53              |
| 3:D:657:GLN:NE2   | 3:D:660:ASP:OD1  | 2.41                     | 0.53              |
| 3:D:1012:MET:C    | 3:D:1027:GLY:H   | 2.16                     | 0.53              |
| 3:D:1190:ASN:O    | 3:D:1193:VAL:HB  | 2.08                     | 0.53              |
| 5:F:498:VAL:HB    | 5:F:502:ARG:CB   | 2.35                     | 0.53              |
| 2:C:518:LYS:HD3   | 2:C:527:GLU:OE1  | 2.09                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:1037:VAL:HG21 | 3:D:520:LYS:HB2   | 1.91                     | 0.53              |
| 3:D:782:THR:O     | 3:D:785:VAL:HG12  | 2.09                     | 0.53              |
| 3:D:1175:PHE:CE2  | 3:D:1189:GLU:HG2  | 2.43                     | 0.53              |
| 2:C:420:ILE:HD13  | 2:C:421:ARG:N     | 2.23                     | 0.52              |
| 2:C:727:GLU:H     | 3:D:725:THR:CG2   | 2.22                     | 0.52              |
| 3:D:965:VAL:HG13  | 3:D:979:TYR:HA    | 1.90                     | 0.52              |
| 3:D:1097:ARG:NH1  | 3:D:1100:SER:OG   | 2.42                     | 0.52              |
| 3:D:134:TYR:CE2   | 3:D:238:GLU:HG3   | 2.42                     | 0.52              |
| 3:D:525:HIS:CG    | 3:D:526:PRO:HD2   | 2.43                     | 0.52              |
| 1:B:147:VAL:HG13  | 1:B:166:SER:HB2   | 1.91                     | 0.52              |
| 2:C:275:LEU:CD1   | 2:C:279:ARG:HE    | 2.22                     | 0.52              |
| 2:C:1011:PHE:CD1  | 2:C:1018:PRO:HB3  | 2.44                     | 0.52              |
| 3:D:797:ASN:HB3   | 3:D:800:ILE:HG22  | 1.90                     | 0.52              |
| 6:J:40:PHE:CE2    | 6:J:58:ASN:HB2    | 2.44                     | 0.52              |
| 1:A:138:LEU:HD12  | 1:A:138:LEU:N     | 2.24                     | 0.52              |
| 1:B:66:VAL:HB     | 1:B:69:VAL:CG2    | 2.39                     | 0.52              |
| 3:D:155:MET:CE    | 3:D:219:LEU:HD12  | 2.40                     | 0.52              |
| 3:D:433:GLY:O     | 3:D:435:GLN:N     | 2.43                     | 0.52              |
| 2:C:223:GLY:C     | 2:C:225:ARG:H     | 2.18                     | 0.52              |
| 2:C:764:LEU:HD23  | 2:C:808:PRO:HB2   | 1.90                     | 0.52              |
| 3:D:136:ILE:HD11  | 3:D:235:ILE:HD12  | 1.92                     | 0.52              |
| 3:D:268:PHE:HE2   | 3:D:270:ILE:HG12  | 1.75                     | 0.52              |
| 3:D:387:ARG:CZ    | 5:F:225:ALA:HA    | 2.40                     | 0.52              |
| 3:D:876:ARG:O     | 3:D:880:VAL:HG12  | 2.09                     | 0.52              |
| 3:D:913:ASP:HB3   | 3:D:916:ILE:HG13  | 1.91                     | 0.52              |
| 3:D:1086:LEU:HD23 | 3:D:1112:MET:SD   | 2.49                     | 0.52              |
| 3:D:1176:LEU:H    | 3:D:1176:LEU:HD12 | 1.74                     | 0.52              |
| 2:C:203:LYS:HD2   | 2:C:211:TRP:CE3   | 2.45                     | 0.52              |
| 2:C:500:LEU:HD22  | 2:C:504:ALA:HB3   | 1.92                     | 0.52              |
| 2:C:926:MET:HE1   | 3:D:817:LEU:CB    | 2.40                     | 0.52              |
| 3:D:1064:ILE:HD12 | 3:D:1080:ILE:CD1  | 2.39                     | 0.52              |
| 2:C:476:HIS:CG    | 2:C:477:PRO:HD2   | 2.45                     | 0.52              |
| 3:D:39:LEU:HD22   | 3:D:335:PHE:HZ    | 1.75                     | 0.52              |
| 3:D:736:VAL:HG22  | 3:D:799:ILE:HD12  | 1.91                     | 0.52              |
| 3:D:750:GLU:HA    | 3:D:750:GLU:OE1   | 2.09                     | 0.52              |
| 1:A:60:LEU:H      | 1:A:60:LEU:HD12   | 1.75                     | 0.52              |
| 2:C:232:GLN:HG2   | 2:C:277:ILE:HD13  | 1.92                     | 0.52              |
| 2:C:1104:GLU:HB2  | 5:F:451:VAL:HG22  | 1.92                     | 0.52              |
| 3:D:924:THR:HA    | 3:D:942:GLN:O     | 2.10                     | 0.52              |
| 4:E:95:ALA:O      | 4:E:99:ILE:HG13   | 2.09                     | 0.52              |
| 6:J:74:LYS:O      | 6:J:74:LYS:HD3    | 2.09                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:138:SER:HB3   | 3:D:253:THR:OG1   | 2.10                     | 0.52              |
| 3:D:634:LYS:HE2   | 3:D:663:MET:CE    | 2.40                     | 0.52              |
| 3:D:913:ASP:H     | 3:D:916:ILE:HD11  | 1.74                     | 0.52              |
| 3:D:1044:ALA:HA   | 3:D:1084:GLN:HE22 | 1.73                     | 0.52              |
| 3:D:1174:GLU:OE1  | 3:D:1174:GLU:N    | 2.42                     | 0.52              |
| 1:A:193:ILE:HG13  | 1:A:193:ILE:O     | 2.10                     | 0.52              |
| 2:C:39:VAL:CG1    | 2:C:963:LEU:HG    | 2.38                     | 0.52              |
| 2:C:516:TYR:CD2   | 2:C:531:LEU:HD12  | 2.45                     | 0.52              |
| 2:C:928:ILE:HD11  | 3:D:840:PHE:O     | 2.09                     | 0.52              |
| 3:D:224:SER:O     | 3:D:227:THR:OG1   | 2.27                     | 0.52              |
| 3:D:891:CYS:HB2   | 3:D:969:ALA:HB3   | 1.92                     | 0.52              |
| 3:D:938:VAL:HG13  | 3:D:942:GLN:OE1   | 2.10                     | 0.52              |
| 3:D:1088:VAL:HG13 | 3:D:1098:VAL:HA   | 1.92                     | 0.52              |
| 1:B:11:GLU:OE1    | 1:B:12:ASP:N      | 2.42                     | 0.51              |
| 1:B:192:LEU:HD12  | 1:B:193:ILE:H     | 1.74                     | 0.51              |
| 2:C:43:LYS:HE3    | 2:C:959:LEU:CA    | 2.37                     | 0.51              |
| 2:C:89:VAL:O      | 2:C:92:GLU:HG2    | 2.09                     | 0.51              |
| 2:C:254:PHE:HE1   | 2:C:347:ARG:HG2   | 1.74                     | 0.51              |
| 2:C:282:ARG:HB2   | 2:C:283:PRO:HA    | 1.91                     | 0.51              |
| 2:C:689:ILE:O     | 2:C:689:ILE:HG13  | 2.08                     | 0.51              |
| 2:C:773:ILE:HG22  | 2:C:774:PRO:O     | 2.09                     | 0.51              |
| 2:C:855:ARG:HH11  | 2:C:861:LEU:CD1   | 2.22                     | 0.51              |
| 3:D:500:ARG:CD    | 3:D:534:ALA:HB2   | 2.39                     | 0.51              |
| 3:D:1062:TYR:HB2  | 3:D:1080:ILE:HB   | 1.93                     | 0.51              |
| 12:D:1501:HOH:O   | 6:J:10:ARG:NH1    | 2.43                     | 0.51              |
| 6:J:4:ARG:HA      | 6:J:4:ARG:NE      | 2.24                     | 0.51              |
| 1:A:60:LEU:HD12   | 1:A:60:LEU:N      | 2.25                     | 0.51              |
| 2:C:628:THR:OG1   | 2:C:629:GLY:N     | 2.43                     | 0.51              |
| 2:C:672:MET:SD    | 2:C:688:PRO:HD3   | 2.50                     | 0.51              |
| 2:C:955:TRP:NE1   | 2:C:987:GLY:HA3   | 2.24                     | 0.51              |
| 3:D:262:GLN:HG3   | 3:D:310:MET:HE1   | 1.91                     | 0.51              |
| 2:C:167:ILE:O     | 2:C:168:ILE:HD13  | 2.09                     | 0.51              |
| 2:C:716:GLY:N     | 2:C:1029:TYR:OH   | 2.35                     | 0.51              |
| 3:D:240:LEU:O     | 3:D:240:LEU:HD23  | 2.10                     | 0.51              |
| 3:D:600:GLN:HA    | 3:D:600:GLN:NE2   | 2.25                     | 0.51              |
| 5:F:273:LEU:HB3   | 5:F:274:PRO:HD2   | 1.92                     | 0.51              |
| 1:B:68:GLY:O      | 1:B:128:LEU:HA    | 2.09                     | 0.51              |
| 2:C:189:GLU:HB2   | 2:C:200:HIS:CD2   | 2.46                     | 0.51              |
| 2:C:1086:GLN:OE1  | 3:D:1257:LEU:HD13 | 2.11                     | 0.51              |
| 3:D:277:LEU:HD11  | 3:D:295:ARG:HH11  | 1.73                     | 0.51              |
| 3:D:923:ARG:HB3   | 3:D:962:VAL:HG13  | 1.93                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:153:PHE:CZ    | 2:C:155:GLY:HA2   | 2.46                     | 0.51              |
| 3:D:897:ILE:HB    | 3:D:1128:ARG:HH21 | 1.76                     | 0.51              |
| 3:D:1086:LEU:HD23 | 3:D:1112:MET:HE1  | 1.92                     | 0.51              |
| 6:J:24:LEU:HD23   | 6:J:24:LEU:N      | 2.26                     | 0.51              |
| 1:A:42:LEU:O      | 1:A:171:VAL:HG11  | 2.11                     | 0.51              |
| 2:C:549:ASP:HB2   | 2:C:555:VAL:HG22  | 1.91                     | 0.51              |
| 3:D:1169:ASP:HB2  | 3:D:1202:ALA:HB3  | 1.91                     | 0.51              |
| 1:A:95:MET:HE3    | 1:A:112:PRO:CB    | 2.39                     | 0.51              |
| 2:C:33:PRO:HG2    | 2:C:700:GLN:HA    | 1.92                     | 0.51              |
| 2:C:641:VAL:O     | 2:C:643:VAL:HG23  | 2.10                     | 0.51              |
| 5:F:244:GLU:HA    | 5:F:247:VAL:HG23  | 1.92                     | 0.51              |
| 2:C:64:LEU:HA     | 2:C:85:GLY:HA3    | 1.93                     | 0.51              |
| 2:C:177:SER:CB    | 2:C:378:LEU:HD11  | 2.40                     | 0.51              |
| 2:C:1099:ARG:O    | 2:C:1102:VAL:HG12 | 2.10                     | 0.51              |
| 3:D:103:HIS:CE1   | 3:D:105:TRP:HB2   | 2.46                     | 0.51              |
| 3:D:134:TYR:HA    | 3:D:256:MET:HG2   | 1.93                     | 0.51              |
| 3:D:736:VAL:CG1   | 3:D:817:LEU:HD22  | 2.41                     | 0.51              |
| 5:F:266:LEU:O     | 5:F:270:GLY:N     | 2.44                     | 0.51              |
| 5:F:415:GLN:HE22  | 5:F:418:ARG:HH12  | 1.59                     | 0.51              |
| 2:C:809:LYS:N     | 2:C:831:GLU:O     | 2.29                     | 0.51              |
| 2:C:948:ALA:CB    | 2:C:952:VAL:HA    | 2.41                     | 0.51              |
| 2:C:1023:VAL:HA   | 3:D:730:THR:HG21  | 1.92                     | 0.51              |
| 3:D:468:ASN:HD21  | 3:D:470:LYS:HB3   | 1.76                     | 0.51              |
| 3:D:1173:THR:O    | 3:D:1175:PHE:N    | 2.44                     | 0.51              |
| 5:F:467:LEU:HD11  | 5:F:514:LEU:HD21  | 1.92                     | 0.51              |
| 1:B:154:ALA:HB1   | 1:B:157:ALA:HB3   | 1.93                     | 0.51              |
| 2:C:200:HIS:CD2   | 2:C:348:LEU:HG    | 2.46                     | 0.51              |
| 2:C:225:ARG:O     | 2:C:225:ARG:HG2   | 2.10                     | 0.51              |
| 2:C:409:VAL:O     | 2:C:410:GLU:HB3   | 2.11                     | 0.51              |
| 3:D:9:GLU:OE2     | 3:D:1244:LYS:NZ   | 2.44                     | 0.51              |
| 3:D:61:TYR:HB2    | 3:D:80:VAL:HG21   | 1.93                     | 0.51              |
| 3:D:567:SER:OG    | 3:D:574:LEU:HD13  | 2.11                     | 0.51              |
| 3:D:749:TYR:CG    | 3:D:781:ALA:HB2   | 2.46                     | 0.51              |
| 5:F:387:LEU:HB2   | 5:F:394:PRO:HD3   | 1.93                     | 0.51              |
| 1:B:107:ALA:HB3   | 1:B:121:PRO:C     | 2.36                     | 0.50              |
| 1:B:134:LEU:HD21  | 1:B:136:VAL:HG23  | 1.93                     | 0.50              |
| 2:C:380:THR:OG1   | 2:C:381:VAL:N     | 2.44                     | 0.50              |
| 2:C:644:ALA:HB2   | 2:C:702:ILE:HD11  | 1.93                     | 0.50              |
| 3:D:1221:LEU:H    | 3:D:1221:LEU:CD2  | 2.23                     | 0.50              |
| 5:F:344:SER:OG    | 7:O:30:DC:OP2     | 2.28                     | 0.50              |
| 8:P:14:DA:H5'     | 8:P:14:DA:H8      | 1.74                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:157:PHE:CE1   | 2:C:389:ILE:HD11  | 2.45                     | 0.50              |
| 2:C:312:GLY:O     | 2:C:316:VAL:HG23  | 2.10                     | 0.50              |
| 2:C:593:MET:HA    | 2:C:628:THR:CG2   | 2.41                     | 0.50              |
| 2:C:907:LEU:HD23  | 2:C:1010:LEU:CD2  | 2.41                     | 0.50              |
| 3:D:129:ILE:HG13  | 3:D:130:TYR:CD2   | 2.46                     | 0.50              |
| 3:D:475:MET:HG3   | 3:D:480:ARG:CG    | 2.41                     | 0.50              |
| 3:D:607:PRO:O     | 3:D:609:THR:HG23  | 2.11                     | 0.50              |
| 4:E:33:LEU:O      | 4:E:36:THR:HG22   | 2.10                     | 0.50              |
| 5:F:208:GLU:O     | 5:F:212:LEU:HG    | 2.12                     | 0.50              |
| 5:F:249:LEU:HD22  | 5:F:291:ALA:HB1   | 1.93                     | 0.50              |
| 1:B:102:PRO:HB3   | 1:B:129:ASN:O     | 2.11                     | 0.50              |
| 2:C:281:LEU:HD23  | 2:C:295:LEU:CD2   | 2.41                     | 0.50              |
| 2:C:737:LEU:HD22  | 2:C:915:ILE:HG22  | 1.93                     | 0.50              |
| 2:C:801:ILE:N     | 2:C:801:ILE:HD12  | 2.26                     | 0.50              |
| 2:C:943:GLY:O     | 2:C:993:LEU:HD23  | 2.10                     | 0.50              |
| 2:C:1011:PHE:CE1  | 2:C:1018:PRO:HB3  | 2.46                     | 0.50              |
| 3:D:360:LEU:HD12  | 3:D:360:LEU:H     | 1.75                     | 0.50              |
| 3:D:407:LYS:HG2   | 3:D:408:GLY:N     | 2.26                     | 0.50              |
| 3:D:1055:LEU:H    | 3:D:1101:ASP:CG   | 2.20                     | 0.50              |
| 3:D:1128:ARG:HH12 | 3:D:1132:ILE:HD11 | 1.77                     | 0.50              |
| 4:E:84:GLU:H      | 4:E:84:GLU:CD     | 2.20                     | 0.50              |
| 5:F:206:GLU:O     | 5:F:208:GLU:N     | 2.44                     | 0.50              |
| 5:F:334:LYS:HD2   | 5:F:350:TRP:HZ2   | 1.76                     | 0.50              |
| 5:F:341:TYR:CE1   | 7:O:28:DT:H5''    | 2.47                     | 0.50              |
| 1:A:225:LEU:O     | 1:A:225:LEU:HD22  | 2.11                     | 0.50              |
| 1:B:201:SER:O     | 1:B:202:ILE:HG23  | 2.10                     | 0.50              |
| 2:C:370:ILE:HD12  | 2:C:370:ILE:N     | 2.26                     | 0.50              |
| 2:C:822:ARG:NE    | 5:F:527:LEU:HD21  | 2.27                     | 0.50              |
| 3:D:151:LEU:HD21  | 3:D:251:TYR:CE2   | 2.46                     | 0.50              |
| 3:D:405:LEU:C     | 3:D:406:LEU:HD12  | 2.36                     | 0.50              |
| 3:D:588:LEU:HD23  | 3:D:723:TRP:CE2   | 2.47                     | 0.50              |
| 8:P:20:DG:H2''    | 8:P:21:DT:O5'     | 2.12                     | 0.50              |
| 1:A:219:PHE:CE1   | 1:B:38:LEU:HD22   | 2.43                     | 0.50              |
| 1:B:3:ILE:CD1     | 1:B:27:GLU:HG2    | 2.42                     | 0.50              |
| 1:B:218:LEU:HD23  | 1:B:218:LEU:C     | 2.37                     | 0.50              |
| 2:C:363:VAL:HG12  | 2:C:364:PRO:HD2   | 1.94                     | 0.50              |
| 2:C:1117:ILE:HD12 | 2:C:1117:ILE:N    | 2.26                     | 0.50              |
| 3:D:113:ARG:HG2   | 3:D:1238:ILE:CD1  | 2.42                     | 0.50              |
| 3:D:611:VAL:HG12  | 3:D:634:LYS:HB2   | 1.93                     | 0.50              |
| 3:D:634:LYS:HG2   | 3:D:665:GLU:HB3   | 1.93                     | 0.50              |
| 3:D:639:GLN:O     | 3:D:640:LEU:HD23  | 2.11                     | 0.50              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:1226:PHE:O    | 3:D:1227:GLN:HG3 | 2.11                     | 0.50              |
| 5:F:209:SER:O     | 5:F:213:ARG:HG2  | 2.11                     | 0.50              |
| 2:C:147:ILE:O     | 2:C:147:ILE:HG22 | 2.12                     | 0.50              |
| 2:C:274:LEU:HG    | 2:C:292:ALA:HB1  | 1.93                     | 0.50              |
| 2:C:274:LEU:HD21  | 2:C:292:ALA:O    | 2.11                     | 0.50              |
| 2:C:363:VAL:HG13  | 2:C:364:PRO:HD2  | 1.93                     | 0.50              |
| 2:C:450:THR:HG21  | 2:C:590:ALA:HB2  | 1.93                     | 0.50              |
| 2:C:524:VAL:HG21  | 2:C:548:ILE:CD1  | 2.40                     | 0.50              |
| 2:C:691:ASP:HB2   | 2:C:694:ASP:OD1  | 2.12                     | 0.50              |
| 3:D:1012:MET:C    | 3:D:1027:GLY:CA  | 2.85                     | 0.50              |
| 5:F:216:ARG:HB2   | 5:F:216:ARG:NH1  | 2.24                     | 0.50              |
| 8:P:19:DT:H2''    | 8:P:20:DG:H8     | 1.77                     | 0.50              |
| 1:A:186:ARG:HG3   | 1:B:150:VAL:CB   | 2.41                     | 0.50              |
| 2:C:192:ASP:OD1   | 2:C:194:SER:OG   | 2.21                     | 0.50              |
| 2:C:290:GLU:HA    | 2:C:294:THR:CG2  | 2.41                     | 0.50              |
| 2:C:606:LEU:HD23  | 2:C:606:LEU:C    | 2.36                     | 0.50              |
| 3:D:468:ASN:HD22  | 3:D:470:LYS:H    | 1.59                     | 0.50              |
| 3:D:590:THR:HG23  | 3:D:630:ARG:HE   | 1.77                     | 0.50              |
| 1:B:15:THR:CG2    | 1:B:18:ARG:HB2   | 2.39                     | 0.50              |
| 2:C:653:VAL:HG12  | 2:C:658:ILE:HG23 | 1.94                     | 0.50              |
| 3:D:84:ARG:HG3    | 3:D:84:ARG:NH1   | 2.24                     | 0.50              |
| 3:D:1086:LEU:HA   | 3:D:1112:MET:SD  | 2.51                     | 0.50              |
| 3:D:1264:ILE:HG22 | 3:D:1266:ARG:HG2 | 1.93                     | 0.50              |
| 4:E:60:ARG:NH1    | 4:E:64:ILE:HG13  | 2.26                     | 0.50              |
| 5:F:244:GLU:HA    | 5:F:247:VAL:CG2  | 2.42                     | 0.50              |
| 7:O:19:DA:C1'     | 7:O:20:DT:H5'    | 2.32                     | 0.50              |
| 2:C:70:TRP:CH2    | 2:C:82:PRO:HB2   | 2.47                     | 0.50              |
| 2:C:736:ILE:HD11  | 2:C:916:ILE:CD1  | 2.33                     | 0.50              |
| 3:D:373:MET:HE3   | 5:F:318:LEU:CB   | 2.42                     | 0.50              |
| 3:D:1103:ASP:OD1  | 3:D:1104:HIS:N   | 2.45                     | 0.50              |
| 4:E:104:LEU:HD23  | 4:E:104:LEU:N    | 2.27                     | 0.50              |
| 1:A:11:GLU:CD     | 1:A:205:ARG:HE   | 2.20                     | 0.49              |
| 1:A:42:LEU:HD23   | 1:A:211:ALA:HB2  | 1.93                     | 0.49              |
| 1:B:2:LEU:CD2     | 1:B:4:SER:H      | 2.24                     | 0.49              |
| 2:C:180:VAL:HG21  | 2:C:379:ARG:HH11 | 1.77                     | 0.49              |
| 2:C:771:ARG:NH1   | 2:C:786:GLU:HA   | 2.27                     | 0.49              |
| 2:C:781:LEU:O     | 2:C:781:LEU:HD23 | 2.12                     | 0.49              |
| 3:D:832:ILE:HG22  | 3:D:834:ARG:H    | 1.77                     | 0.49              |
| 3:D:891:CYS:SG    | 3:D:893:THR:HG22 | 2.52                     | 0.49              |
| 1:B:124:HIS:HE1   | 1:B:127:THR:HG23 | 1.76                     | 0.49              |
| 2:C:33:PRO:HG2    | 2:C:700:GLN:CA   | 2.42                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:96:ILE:N     | 2:C:105:LEU:O    | 2.45                     | 0.49              |
| 2:C:212:LEU:N    | 2:C:212:LEU:HD23 | 2.26                     | 0.49              |
| 2:C:224:VAL:O    | 2:C:226:ILE:N    | 2.45                     | 0.49              |
| 2:C:756:GLU:OE2  | 2:C:868:LEU:HD11 | 2.12                     | 0.49              |
| 3:D:164:ASP:N    | 3:D:164:ASP:OD1  | 2.45                     | 0.49              |
| 3:D:240:LEU:O    | 3:D:244:LEU:HG   | 2.12                     | 0.49              |
| 5:F:242:ASN:OD1  | 5:F:245:GLU:HG3  | 2.12                     | 0.49              |
| 5:F:427:ILE:HG23 | 5:F:427:ILE:O    | 2.12                     | 0.49              |
| 7:O:28:DT:H2''   | 7:O:29:DA:C8     | 2.47                     | 0.49              |
| 8:P:18:DT:C2'    | 8:P:19:DT:H71    | 2.38                     | 0.49              |
| 8:P:24:DA:H2''   | 8:P:25:DG:O4'    | 2.12                     | 0.49              |
| 1:A:127:THR:C    | 1:A:128:LEU:HD12 | 2.37                     | 0.49              |
| 1:B:6:ARG:HG3    | 1:B:234:ILE:HG23 | 1.94                     | 0.49              |
| 2:C:97:GLU:O     | 2:C:401:ARG:NH2  | 2.42                     | 0.49              |
| 2:C:225:ARG:HD3  | 2:C:230:ARG:C    | 2.37                     | 0.49              |
| 2:C:751:HIS:CD2  | 2:C:877:ARG:HD2  | 2.47                     | 0.49              |
| 2:C:1074:TRP:HH2 | 3:D:875:ARG:HG3  | 1.77                     | 0.49              |
| 3:D:287:GLN:N    | 3:D:287:GLN:OE1  | 2.46                     | 0.49              |
| 3:D:588:LEU:O    | 3:D:588:LEU:HD22 | 2.12                     | 0.49              |
| 3:D:1070:ASP:HB2 | 3:D:1071:GLY:C   | 2.38                     | 0.49              |
| 5:F:379:LEU:HD23 | 5:F:379:LEU:C    | 2.37                     | 0.49              |
| 5:F:496:TYR:O    | 5:F:498:VAL:HG13 | 2.12                     | 0.49              |
| 5:F:501:GLU:O    | 5:F:505:GLN:HG2  | 2.12                     | 0.49              |
| 7:O:5:DG:H2'     | 7:O:6:DA:H8      | 1.74                     | 0.49              |
| 2:C:65:ILE:HD11  | 2:C:159:MET:SD   | 2.52                     | 0.49              |
| 2:C:216:VAL:HG23 | 2:C:345:LEU:HD11 | 1.94                     | 0.49              |
| 2:C:222:VAL:CG2  | 2:C:234:VAL:HG13 | 2.43                     | 0.49              |
| 2:C:806:VAL:CG2  | 2:C:832:VAL:HB   | 2.43                     | 0.49              |
| 3:D:865:LEU:HD13 | 3:D:865:LEU:C    | 2.38                     | 0.49              |
| 5:F:386:LEU:HD11 | 5:F:398:GLU:OE1  | 2.12                     | 0.49              |
| 2:C:199:LEU:HD23 | 2:C:199:LEU:N    | 2.27                     | 0.49              |
| 2:C:418:ILE:HG22 | 2:C:420:ILE:HG22 | 1.93                     | 0.49              |
| 2:C:568:VAL:HG13 | 3:D:847:LEU:HD23 | 1.94                     | 0.49              |
| 2:C:659:THR:HG22 | 2:C:669:THR:CG2  | 2.32                     | 0.49              |
| 3:D:449:LEU:O    | 3:D:449:LEU:HD13 | 2.12                     | 0.49              |
| 1:B:7:PRO:HA     | 1:B:24:GLU:O     | 2.13                     | 0.49              |
| 1:B:136:VAL:HG12 | 1:B:138:LEU:CD1  | 2.42                     | 0.49              |
| 2:C:421:ARG:O    | 2:C:424:VAL:HG12 | 2.11                     | 0.49              |
| 3:D:333:GLY:O    | 5:F:415:GLN:NE2  | 2.45                     | 0.49              |
| 3:D:579:LEU:CD2  | 3:D:808:THR:HB   | 2.40                     | 0.49              |
| 3:D:745:ILE:HD13 | 3:D:784:GLU:HG2  | 1.95                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:D:824:VAL:HG11 | 3:D:852:ASN:HA    | 1.93                     | 0.49              |
| 3:D:876:ARG:HH22 | 3:D:1032:GLN:HG3  | 1.78                     | 0.49              |
| 5:F:280:ASP:OD1  | 5:F:281:MET:N     | 2.46                     | 0.49              |
| 1:B:233:GLU:OE1  | 1:B:233:GLU:HA    | 2.13                     | 0.49              |
| 2:C:44:LEU:N     | 2:C:44:LEU:HD12   | 2.28                     | 0.49              |
| 2:C:222:VAL:HB   | 2:C:234:VAL:HG13  | 1.94                     | 0.49              |
| 2:C:223:GLY:O    | 2:C:225:ARG:N     | 2.43                     | 0.49              |
| 2:C:275:LEU:HD13 | 2:C:279:ARG:HE    | 1.77                     | 0.49              |
| 2:C:548:ILE:CD1  | 2:C:579:MET:HE1   | 2.38                     | 0.49              |
| 2:C:741:LEU:HA   | 2:C:746:VAL:HG12  | 1.94                     | 0.49              |
| 2:C:948:ALA:HB1  | 2:C:952:VAL:HA    | 1.94                     | 0.49              |
| 3:D:277:LEU:HD23 | 3:D:296:LEU:HB2   | 1.95                     | 0.49              |
| 3:D:527:LEU:CD1  | 3:D:713:VAL:HG12  | 2.42                     | 0.49              |
| 3:D:642:PRO:HB3  | 3:D:662:TRP:CE3   | 2.48                     | 0.49              |
| 3:D:1189:GLU:O   | 3:D:1192:ARG:HB3  | 2.12                     | 0.49              |
| 3:D:1193:VAL:O   | 3:D:1193:VAL:HG22 | 2.13                     | 0.49              |
| 3:D:1230:THR:O   | 3:D:1234:THR:HG22 | 2.13                     | 0.49              |
| 1:A:223:ARG:CD   | 1:A:224:GLU:H     | 2.23                     | 0.49              |
| 1:B:183:VAL:O    | 1:B:187:THR:HA    | 2.12                     | 0.49              |
| 2:C:93:LEU:CD1   | 2:C:96:ILE:HD11   | 2.43                     | 0.49              |
| 3:D:173:ARG:HB2  | 3:D:173:ARG:CZ    | 2.42                     | 0.49              |
| 2:C:771:ARG:NE   | 2:C:781:LEU:HD21  | 2.27                     | 0.49              |
| 3:D:25:TYR:HD2   | 3:D:91:ARG:HD3    | 1.78                     | 0.49              |
| 3:D:55:THR:HG22  | 6:J:12:GLY:CA     | 2.43                     | 0.49              |
| 3:D:436:LEU:HD22 | 3:D:515:MET:CE    | 2.43                     | 0.49              |
| 1:B:105:VAL:HG12 | 1:B:125:ILE:HG21  | 1.94                     | 0.49              |
| 2:C:500:LEU:HD23 | 2:C:501:SER:H     | 1.78                     | 0.49              |
| 2:C:532:THR:OG1  | 2:C:533:ALA:N     | 2.46                     | 0.49              |
| 2:C:719:LEU:CD2  | 2:C:1030:ILE:HD11 | 2.28                     | 0.49              |
| 3:D:67:ARG:NE    | 6:J:17:GLU:OE2    | 2.45                     | 0.49              |
| 3:D:717:LYS:HG3  | 3:D:718:ASP:N     | 2.28                     | 0.49              |
| 3:D:822:GLY:O    | 3:D:835:PRO:HB2   | 2.13                     | 0.49              |
| 3:D:885:ILE:HD11 | 3:D:887:ARG:HH12  | 1.76                     | 0.49              |
| 6:J:45:ALA:HB3   | 6:J:48:ALA:HB2    | 1.95                     | 0.49              |
| 1:A:161:ARG:NH1  | 1:A:161:ARG:HB2   | 2.26                     | 0.48              |
| 3:D:899:VAL:HG12 | 3:D:900:GLU:N     | 2.27                     | 0.48              |
| 2:C:222:VAL:CG2  | 2:C:224:VAL:HG23  | 2.43                     | 0.48              |
| 2:C:230:ARG:HH11 | 2:C:230:ARG:CA    | 2.23                     | 0.48              |
| 2:C:238:LEU:HD11 | 2:C:243:TRP:CD2   | 2.48                     | 0.48              |
| 2:C:601:ASP:OD1  | 2:C:602:ALA:N     | 2.45                     | 0.48              |
| 2:C:992:THR:CG2  | 2:C:1000:VAL:HG13 | 2.44                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:237:ASP:OD2   | 3:D:240:LEU:N     | 2.37                     | 0.48              |
| 3:D:513:GLU:HG3   | 3:D:513:GLU:O     | 2.13                     | 0.48              |
| 3:D:642:PRO:HD3   | 3:D:657:GLN:HG2   | 1.94                     | 0.48              |
| 3:D:1050:THR:HG23 | 3:D:1107:VAL:CG2  | 2.42                     | 0.48              |
| 1:A:59:VAL:CG1    | 1:A:66:VAL:HG22   | 2.44                     | 0.48              |
| 1:A:97:LEU:HD21   | 1:A:105:VAL:HG11  | 1.94                     | 0.48              |
| 1:B:146:TYR:CE2   | 3:D:621:ALA:HB2   | 2.48                     | 0.48              |
| 1:B:150:VAL:HG13  | 1:B:150:VAL:O     | 2.14                     | 0.48              |
| 2:C:238:LEU:CD2   | 2:C:248:ILE:HG12  | 2.43                     | 0.48              |
| 2:C:396:MET:HB2   | 2:C:422:PRO:HG2   | 1.94                     | 0.48              |
| 2:C:995:ASN:OD1   | 2:C:995:ASN:N     | 2.46                     | 0.48              |
| 3:D:1070:ASP:HB2  | 3:D:1071:GLY:O    | 2.13                     | 0.48              |
| 3:D:1243:ASP:OD1  | 3:D:1244:LYS:N    | 2.45                     | 0.48              |
| 5:F:505:GLN:HG3   | 5:F:506:ILE:N     | 2.29                     | 0.48              |
| 1:B:78:LEU:C      | 1:B:78:LEU:HD12   | 2.39                     | 0.48              |
| 1:B:170:PRO:HB2   | 1:B:202:ILE:HD11  | 1.96                     | 0.48              |
| 2:C:215:ASP:CA    | 2:C:223:GLY:HA3   | 2.43                     | 0.48              |
| 2:C:723:ILE:O     | 2:C:723:ILE:HG22  | 2.14                     | 0.48              |
| 2:C:767:GLU:HB3   | 2:C:805:LYS:HZ2   | 1.78                     | 0.48              |
| 5:F:286:ARG:CZ    | 5:F:286:ARG:HA    | 2.42                     | 0.48              |
| 5:F:306:LEU:O     | 5:F:306:LEU:HD23  | 2.13                     | 0.48              |
| 6:J:78:PRO:O      | 6:J:80:THR:HG23   | 2.13                     | 0.48              |
| 1:A:2:LEU:HD12    | 1:A:2:LEU:O       | 2.13                     | 0.48              |
| 1:B:42:LEU:HD12   | 1:B:211:ALA:CB    | 2.43                     | 0.48              |
| 2:C:1040:LYS:HD3  | 3:D:540:GLN:NE2   | 2.28                     | 0.48              |
| 2:C:1076:MET:HE1  | 3:D:559:MET:SD    | 2.53                     | 0.48              |
| 3:D:148:LEU:O     | 3:D:152:GLU:HG3   | 2.14                     | 0.48              |
| 3:D:463:LEU:O     | 3:D:465:HIS:N     | 2.43                     | 0.48              |
| 2:C:465:ARG:HD2   | 2:C:493:ASN:OD1   | 2.13                     | 0.48              |
| 2:C:556:GLU:HB2   | 2:C:557:PRO:HD2   | 1.96                     | 0.48              |
| 3:D:992:GLY:HA2   | 3:D:1264:ILE:HD11 | 1.95                     | 0.48              |
| 3:D:1249:LYS:O    | 3:D:1253:ILE:HG13 | 2.13                     | 0.48              |
| 7:O:8:DA:H2"      | 7:O:9:DA:H8       | 1.76                     | 0.48              |
| 1:A:144:ARG:CZ    | 1:B:232:ILE:HD11  | 2.43                     | 0.48              |
| 1:B:19:SER:OG     | 1:B:204:PRO:HG2   | 2.13                     | 0.48              |
| 1:B:102:PRO:CB    | 1:B:130:ASP:HA    | 2.44                     | 0.48              |
| 2:C:274:LEU:HD23  | 2:C:292:ALA:HB1   | 1.94                     | 0.48              |
| 2:C:945:LYS:HB2   | 2:C:945:LYS:NZ    | 2.29                     | 0.48              |
| 3:D:25:TYR:HE2    | 3:D:91:ARG:HG2    | 1.79                     | 0.48              |
| 3:D:263:LYS:HB2   | 3:D:263:LYS:HZ2   | 1.74                     | 0.48              |
| 3:D:1154:ILE:O    | 3:D:1158:VAL:HG23 | 2.13                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:3:ILE:HD11    | 1:B:27:GLU:CG     | 2.43                     | 0.48              |
| 2:C:117:ALA:HB3   | 2:C:122:CYS:SG    | 2.54                     | 0.48              |
| 2:C:167:ILE:N     | 2:C:167:ILE:HD12  | 2.29                     | 0.48              |
| 2:C:222:VAL:HG11  | 2:C:234:VAL:HG22  | 1.96                     | 0.48              |
| 2:C:254:PHE:H     | 2:C:255:SER:CB    | 2.21                     | 0.48              |
| 2:C:587:VAL:HG12  | 2:C:588:SER:O     | 2.14                     | 0.48              |
| 2:C:1040:LYS:HA   | 2:C:1040:LYS:HE2  | 1.95                     | 0.48              |
| 2:C:1135:VAL:CG1  | 3:D:12:ILE:HG12   | 2.34                     | 0.48              |
| 3:D:598:GLU:HG2   | 3:D:599:TYR:H     | 1.77                     | 0.48              |
| 3:D:641:ARG:HA    | 3:D:657:GLN:CB    | 2.43                     | 0.48              |
| 3:D:1052:ARG:NH2  | 3:D:1102:GLY:HA2  | 2.28                     | 0.48              |
| 3:D:1080:ILE:CG2  | 3:D:1112:MET:HG3  | 2.42                     | 0.48              |
| 5:F:483:ASP:OD1   | 5:F:483:ASP:N     | 2.45                     | 0.48              |
| 2:C:1087:GLU:HG3  | 2:C:1091:ILE:HD11 | 1.96                     | 0.48              |
| 3:D:141:GLU:OE1   | 3:D:141:GLU:HA    | 2.14                     | 0.48              |
| 3:D:323:GLU:OE1   | 3:D:323:GLU:HA    | 2.13                     | 0.48              |
| 3:D:475:MET:HG3   | 3:D:480:ARG:HG3   | 1.95                     | 0.48              |
| 3:D:545:LEU:HD12  | 3:D:546:PRO:HD2   | 1.96                     | 0.48              |
| 3:D:834:ARG:CB    | 3:D:835:PRO:HA    | 2.44                     | 0.48              |
| 5:F:474:VAL:HG22  | 5:F:496:TYR:CE2   | 2.48                     | 0.48              |
| 7:O:7:DC:H2"      | 7:O:8:DA:C8       | 2.48                     | 0.48              |
| 2:C:1037:VAL:HG12 | 3:D:429:VAL:HG11  | 1.96                     | 0.48              |
| 3:D:459:ARG:NH1   | 3:D:463:LEU:HD23  | 2.29                     | 0.48              |
| 7:O:4:DT:H2"      | 7:O:5:DG:H8       | 1.79                     | 0.48              |
| 2:C:317:ASN:HA    | 2:C:322:LEU:HB2   | 1.96                     | 0.47              |
| 2:C:763:LYS:NZ    | 3:D:332:GLY:H     | 2.11                     | 0.47              |
| 2:C:967:GLN:CD    | 2:C:968:PRO:HD2   | 2.39                     | 0.47              |
| 3:D:117:LEU:O     | 3:D:117:LEU:HD13  | 2.13                     | 0.47              |
| 3:D:121:ALA:HB3   | 3:D:124:ASP:CG    | 2.38                     | 0.47              |
| 3:D:578:ARG:O     | 3:D:582:VAL:HG23  | 2.13                     | 0.47              |
| 3:D:1047:ALA:HB2  | 3:D:1111:LEU:HD11 | 1.95                     | 0.47              |
| 3:D:1251:ASN:ND2  | 3:D:1259:PRO:HD3  | 2.29                     | 0.47              |
| 3:D:1251:ASN:CG   | 3:D:1259:PRO:HD3  | 2.39                     | 0.47              |
| 5:F:386:LEU:HD22  | 5:F:394:PRO:HB3   | 1.96                     | 0.47              |
| 1:A:225:LEU:C     | 1:A:225:LEU:HD13  | 2.38                     | 0.47              |
| 2:C:206:PRO:HG3   | 2:C:306:TYR:CZ    | 2.49                     | 0.47              |
| 2:C:584:ARG:HG3   | 2:C:584:ARG:O     | 2.14                     | 0.47              |
| 2:C:814:LEU:HD22  | 2:C:814:LEU:H     | 1.79                     | 0.47              |
| 3:D:117:LEU:HD13  | 3:D:117:LEU:C     | 2.39                     | 0.47              |
| 3:D:240:LEU:HD23  | 3:D:244:LEU:HG    | 1.95                     | 0.47              |
| 3:D:627:LEU:HD22  | 3:D:628:SER:O     | 2.14                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:965:VAL:CG1   | 3:D:979:TYR:HA    | 2.44                     | 0.47              |
| 4:E:85:PRO:HB3    | 4:E:94:ILE:HD11   | 1.94                     | 0.47              |
| 1:A:27:GLU:OE1    | 1:A:27:GLU:HA     | 2.13                     | 0.47              |
| 1:B:96:TYR:CE1    | 1:B:137:GLU:HG2   | 2.48                     | 0.47              |
| 2:C:308:LEU:H     | 2:C:308:LEU:CD2   | 2.26                     | 0.47              |
| 2:C:560:LEU:HD23  | 2:C:569:GLU:O     | 2.15                     | 0.47              |
| 3:D:357:LEU:HD23  | 3:D:357:LEU:O     | 2.15                     | 0.47              |
| 3:D:1118:PRO:O    | 3:D:1121:VAL:HG13 | 2.13                     | 0.47              |
| 5:F:244:GLU:O     | 5:F:247:VAL:HB    | 2.14                     | 0.47              |
| 6:J:92:GLU:OE1    | 6:J:92:GLU:HA     | 2.14                     | 0.47              |
| 2:C:542:ALA:HB2   | 2:C:576:VAL:HG11  | 1.94                     | 0.47              |
| 2:C:737:LEU:HD11  | 2:C:895:ILE:CD1   | 2.44                     | 0.47              |
| 2:C:861:LEU:HB2   | 2:C:862:PRO:CD    | 2.41                     | 0.47              |
| 2:C:1040:LYS:HE2  | 2:C:1040:LYS:CA   | 2.44                     | 0.47              |
| 3:D:149:SER:O     | 3:D:152:GLU:HG3   | 2.14                     | 0.47              |
| 3:D:460:LEU:C     | 3:D:460:LEU:HD12  | 2.38                     | 0.47              |
| 3:D:940:ARG:NH1   | 3:D:963:ARG:NH2   | 2.62                     | 0.47              |
| 3:D:1051:GLY:CA   | 3:D:1069:ASP:HB2  | 2.44                     | 0.47              |
| 3:D:1106:GLU:HA   | 3:D:1106:GLU:OE1  | 2.14                     | 0.47              |
| 1:B:70:LYS:NZ     | 1:B:70:LYS:CB     | 2.78                     | 0.47              |
| 2:C:741:LEU:HA    | 2:C:746:VAL:CG1   | 2.44                     | 0.47              |
| 3:D:431:VAL:HG13  | 3:D:521:ALA:HB1   | 1.97                     | 0.47              |
| 3:D:932:GLU:O     | 3:D:933:ALA:C     | 2.56                     | 0.47              |
| 3:D:1055:LEU:HD23 | 3:D:1055:LEU:C    | 2.39                     | 0.47              |
| 3:D:1152:LYS:O    | 3:D:1156:VAL:HG23 | 2.14                     | 0.47              |
| 4:E:47:VAL:HG21   | 4:E:53:LEU:HB2    | 1.95                     | 0.47              |
| 5:F:467:LEU:CD2   | 5:F:519:ARG:NH1   | 2.78                     | 0.47              |
| 2:C:374:GLY:HA3   | 2:C:534:ASP:OD1   | 2.14                     | 0.47              |
| 2:C:419:ASN:O     | 2:C:422:PRO:HD2   | 2.15                     | 0.47              |
| 2:C:776:ILE:HD11  | 2:C:780:VAL:HG21  | 1.95                     | 0.47              |
| 2:C:928:ILE:HD12  | 2:C:929:GLY:N     | 2.30                     | 0.47              |
| 3:D:157:VAL:HA    | 3:D:160:LYS:HG2   | 1.95                     | 0.47              |
| 3:D:360:LEU:H     | 3:D:360:LEU:CD1   | 2.28                     | 0.47              |
| 3:D:387:ARG:NH1   | 5:F:225:ALA:HB1   | 2.30                     | 0.47              |
| 3:D:704:TYR:HB3   | 3:D:705:PRO:HD2   | 1.96                     | 0.47              |
| 5:F:482:THR:HG23  | 5:F:483:ASP:N     | 2.30                     | 0.47              |
| 1:A:9:LEU:HD23    | 1:A:9:LEU:O       | 2.15                     | 0.47              |
| 1:A:18:ARG:HH21   | 2:C:996:ARG:HH12  | 1.61                     | 0.47              |
| 1:A:128:LEU:HD12  | 1:A:128:LEU:N     | 2.29                     | 0.47              |
| 2:C:105:LEU:HD12  | 2:C:138:GLU:O     | 2.14                     | 0.47              |
| 2:C:329:THR:O     | 2:C:329:THR:HG23  | 2.14                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:395:ARG:O     | 2:C:399:VAL:HG23  | 2.14                     | 0.47              |
| 2:C:486:ILE:CD1   | 3:D:849:TYR:HE2   | 2.27                     | 0.47              |
| 2:C:623:ALA:HB2   | 2:C:709:ASP:OD2   | 2.14                     | 0.47              |
| 2:C:767:GLU:CD    | 2:C:805:LYS:HZ1   | 2.09                     | 0.47              |
| 2:C:771:ARG:HE    | 2:C:781:LEU:HD21  | 1.79                     | 0.47              |
| 2:C:792:ILE:HD12  | 2:C:792:ILE:H     | 1.79                     | 0.47              |
| 2:C:905:PRO:HD2   | 2:C:916:ILE:HD11  | 1.96                     | 0.47              |
| 2:C:942:SER:O     | 2:C:968:PRO:HB3   | 2.15                     | 0.47              |
| 2:C:1045:SER:HB3  | 3:D:450:GLU:O     | 2.14                     | 0.47              |
| 2:C:1088:LEU:HD23 | 2:C:1092:LYS:HD2  | 1.97                     | 0.47              |
| 3:D:20:ILE:HD13   | 3:D:318:PRO:HD3   | 1.96                     | 0.47              |
| 3:D:166:ARG:HG3   | 3:D:212:ALA:CB    | 2.44                     | 0.47              |
| 3:D:230:ALA:O     | 3:D:233:GLN:HG3   | 2.14                     | 0.47              |
| 3:D:557:ILE:CD1   | 4:E:54:VAL:HG22   | 2.44                     | 0.47              |
| 3:D:757:GLU:OE1   | 3:D:770:ARG:HD3   | 2.15                     | 0.47              |
| 4:E:47:VAL:HG12   | 4:E:48:SER:N      | 2.30                     | 0.47              |
| 5:F:378:LYS:O     | 5:F:382:ILE:HD13  | 2.15                     | 0.47              |
| 5:F:386:LEU:HD23  | 5:F:386:LEU:O     | 2.15                     | 0.47              |
| 5:F:387:LEU:HG    | 5:F:392:ARG:O     | 2.15                     | 0.47              |
| 6:J:4:ARG:HA      | 6:J:4:ARG:HE      | 1.80                     | 0.47              |
| 7:O:20:DT:H2"     | 7:O:21:DT:H71     | 1.96                     | 0.47              |
| 1:A:106:THR:HB    | 1:A:123:MET:O     | 2.15                     | 0.47              |
| 2:C:265:ASP:OD1   | 2:C:266:ASN:N     | 2.48                     | 0.47              |
| 2:C:736:ILE:HG12  | 2:C:916:ILE:HB    | 1.96                     | 0.47              |
| 3:D:340:LEU:HD21  | 3:D:402:LEU:HD23  | 1.95                     | 0.47              |
| 3:D:360:LEU:HD12  | 3:D:360:LEU:N     | 2.29                     | 0.47              |
| 3:D:579:LEU:HD23  | 3:D:807:ALA:O     | 2.14                     | 0.47              |
| 3:D:823:LEU:CD2   | 3:D:835:PRO:HB3   | 2.33                     | 0.47              |
| 3:D:1252:VAL:HG23 | 3:D:1258:ILE:HG22 | 1.97                     | 0.47              |
| 1:A:66:VAL:O      | 1:A:69:VAL:HG22   | 2.13                     | 0.47              |
| 2:C:229:LYS:HZ2   | 2:C:281:LEU:CB    | 2.27                     | 0.47              |
| 2:C:235:THR:HG21  | 2:C:265:ASP:HB3   | 1.96                     | 0.47              |
| 3:D:207:GLN:OE1   | 3:D:208:ILE:HD12  | 2.15                     | 0.47              |
| 3:D:444:PRO:HD2   | 3:D:447:MET:HE2   | 1.96                     | 0.47              |
| 3:D:1189:GLU:HG3  | 3:D:1190:ASN:N    | 2.30                     | 0.47              |
| 3:D:1243:ASP:OD1  | 3:D:1245:LEU:N    | 2.25                     | 0.47              |
| 5:F:281:MET:HG3   | 5:F:282:MET:N     | 2.30                     | 0.47              |
| 5:F:460:LEU:O     | 5:F:464:LEU:HD13  | 2.15                     | 0.47              |
| 2:C:205:ILE:HG22  | 2:C:211:TRP:CD2   | 2.50                     | 0.47              |
| 2:C:279:ARG:O     | 2:C:283:PRO:HA    | 2.15                     | 0.47              |
| 2:C:561:VAL:HG22  | 2:C:562:ARG:N     | 2.30                     | 0.47              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:1051:MET:SD   | 3:D:328:VAL:HG21 | 2.54                     | 0.47              |
| 3:D:19:ASP:O      | 3:D:22:GLN:N     | 2.33                     | 0.47              |
| 3:D:76:GLU:H      | 3:D:76:GLU:CD    | 2.23                     | 0.47              |
| 3:D:1272:VAL:HG13 | 4:E:56:TYR:CE1   | 2.50                     | 0.47              |
| 5:F:241:LEU:HA    | 5:F:245:GLU:OE1  | 2.14                     | 0.47              |
| 5:F:482:THR:HG23  | 5:F:483:ASP:H    | 1.80                     | 0.47              |
| 1:A:153:ARG:NE    | 2:C:797:ARG:HG2  | 2.31                     | 0.46              |
| 1:B:60:LEU:H      | 1:B:60:LEU:CD2   | 2.28                     | 0.46              |
| 1:B:68:GLY:O      | 1:B:129:ASN:N    | 2.38                     | 0.46              |
| 2:C:141:ASN:OD1   | 2:C:142:ASN:N    | 2.48                     | 0.46              |
| 2:C:646:GLU:HB3   | 2:C:662:HIS:HD1  | 1.81                     | 0.46              |
| 3:D:384:ASN:HB2   | 3:D:401:SER:HB3  | 1.97                     | 0.46              |
| 3:D:765:LEU:HD23  | 3:D:765:LEU:N    | 2.29                     | 0.46              |
| 3:D:1194:VAL:O    | 3:D:1195:ALA:C   | 2.58                     | 0.46              |
| 5:F:386:LEU:HD22  | 5:F:394:PRO:CB   | 2.44                     | 0.46              |
| 1:A:49:ALA:CB     | 1:A:87:SER:H     | 2.28                     | 0.46              |
| 1:B:100:GLN:HA    | 1:B:133:LYS:HA   | 1.97                     | 0.46              |
| 2:C:480:TYR:CD2   | 2:C:562:ARG:NH1  | 2.83                     | 0.46              |
| 2:C:814:LEU:HD22  | 2:C:814:LEU:N    | 2.30                     | 0.46              |
| 3:D:173:ARG:NE    | 3:D:205:MET:HG2  | 2.29                     | 0.46              |
| 3:D:577:PRO:HA    | 3:D:581:MET:HE2  | 1.98                     | 0.46              |
| 4:E:64:ILE:O      | 4:E:67:TYR:HB3   | 2.16                     | 0.46              |
| 5:F:372:MET:O     | 5:F:375:VAL:HG22 | 2.16                     | 0.46              |
| 6:J:99:LYS:O      | 6:J:102:LEU:HB3  | 2.16                     | 0.46              |
| 8:P:10:DT:H2''    | 8:P:11:DA:H8     | 1.79                     | 0.46              |
| 1:A:84:VAL:HG13   | 1:A:84:VAL:O     | 2.16                     | 0.46              |
| 1:A:220:GLY:HA2   | 1:A:223:ARG:HB2  | 1.97                     | 0.46              |
| 2:C:274:LEU:HD21  | 2:C:292:ALA:C    | 2.40                     | 0.46              |
| 2:C:677:ARG:HG2   | 2:C:678:SER:O    | 2.15                     | 0.46              |
| 2:C:883:ASP:O     | 2:C:895:ILE:HG13 | 2.16                     | 0.46              |
| 2:C:1009:MET:HA   | 2:C:1009:MET:CE  | 2.45                     | 0.46              |
| 2:C:1049:TYR:CD1  | 2:C:1099:ARG:NH1 | 2.83                     | 0.46              |
| 3:D:73:ILE:CG2    | 6:J:27:ARG:NH1   | 2.78                     | 0.46              |
| 3:D:1089:PHE:CD2  | 3:D:1099:LEU:HB2 | 2.49                     | 0.46              |
| 3:D:1110:GLN:NE2  | 3:D:1112:MET:O   | 2.48                     | 0.46              |
| 5:F:333:GLU:HA    | 6:J:81:HIS:NE2   | 2.31                     | 0.46              |
| 8:P:11:DA:C2'     | 8:P:12:DA:H5'    | 2.38                     | 0.46              |
| 1:A:24:GLU:OE1    | 1:A:191:LYS:HD2  | 2.15                     | 0.46              |
| 2:C:161:THR:OG1   | 2:C:165:THR:O    | 2.33                     | 0.46              |
| 2:C:351:GLY:O     | 2:C:352:GLN:HG2  | 2.15                     | 0.46              |
| 2:C:406:THR:O     | 2:C:406:THR:OG1  | 2.30                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:633:ARG:O     | 2:C:633:ARG:HG3   | 2.15                     | 0.46              |
| 3:D:39:LEU:HD22   | 3:D:335:PHE:CZ    | 2.50                     | 0.46              |
| 3:D:186:ALA:HB3   | 3:D:187:GLU:OE1   | 2.15                     | 0.46              |
| 3:D:246:ASP:OD1   | 3:D:247:ARG:N     | 2.49                     | 0.46              |
| 3:D:453:LYS:HG3   | 3:D:476:VAL:HG11  | 1.97                     | 0.46              |
| 3:D:1176:LEU:HD12 | 3:D:1176:LEU:N    | 2.29                     | 0.46              |
| 2:C:185:VAL:HG12  | 2:C:204:VAL:HG22  | 1.96                     | 0.46              |
| 2:C:854:SER:H     | 2:C:859:ASP:HB2   | 1.79                     | 0.46              |
| 3:D:587:TYR:HE1   | 3:D:630:ARG:NH1   | 2.14                     | 0.46              |
| 3:D:1030:ARG:NH2  | 3:D:1034:LEU:HD21 | 2.31                     | 0.46              |
| 3:D:1089:PHE:HE2  | 3:D:1103:ASP:OD2  | 1.91                     | 0.46              |
| 3:D:1207:LEU:C    | 3:D:1207:LEU:HD13 | 2.41                     | 0.46              |
| 5:F:489:LEU:HG    | 8:P:20:DG:OP2     | 2.15                     | 0.46              |
| 2:C:48:LEU:HB2    | 2:C:528:ILE:CD1   | 2.46                     | 0.46              |
| 2:C:326:GLU:C     | 2:C:328:ILE:H     | 2.24                     | 0.46              |
| 2:C:532:THR:HG23  | 2:C:535:GLU:HG2   | 1.98                     | 0.46              |
| 2:C:792:ILE:HD12  | 2:C:792:ILE:N     | 2.30                     | 0.46              |
| 2:C:922:VAL:HG22  | 2:C:930:GLN:HE21  | 1.80                     | 0.46              |
| 3:D:339:ASP:OD2   | 5:F:424:ASP:OD2   | 2.33                     | 0.46              |
| 3:D:453:LYS:HB3   | 3:D:453:LYS:HZ2   | 1.80                     | 0.46              |
| 3:D:572:ARG:HB2   | 3:D:573:PRO:HD2   | 1.98                     | 0.46              |
| 3:D:708:VAL:HG22  | 4:E:29:TYR:HB3    | 1.97                     | 0.46              |
| 5:F:407:PRO:O     | 5:F:410:VAL:HG12  | 2.16                     | 0.46              |
| 1:B:34:LEU:C      | 1:B:34:LEU:HD12   | 2.41                     | 0.46              |
| 1:B:162:ILE:CG2   | 3:D:607:PRO:HG3   | 2.46                     | 0.46              |
| 2:C:344:TYR:OH    | 2:C:365:VAL:HA    | 2.16                     | 0.46              |
| 2:C:571:VAL:HG13  | 2:C:572:PRO:N     | 2.30                     | 0.46              |
| 3:D:139:VAL:HG12  | 3:D:231:PRO:HD3   | 1.98                     | 0.46              |
| 3:D:963:ARG:HD2   | 3:D:978:CYS:HA    | 1.96                     | 0.46              |
| 3:D:1086:LEU:CD2  | 3:D:1112:MET:HE1  | 2.46                     | 0.46              |
| 5:F:292:LYS:O     | 5:F:296:LEU:HG    | 2.14                     | 0.46              |
| 5:F:381:ARG:HA    | 5:F:384:ARG:NH2   | 2.30                     | 0.46              |
| 1:A:218:LEU:HD21  | 1:B:34:LEU:CD2    | 2.46                     | 0.46              |
| 3:D:165:GLN:O     | 3:D:169:GLU:HG2   | 2.15                     | 0.46              |
| 5:F:257:LEU:HD21  | 6:J:81:HIS:CE1    | 2.50                     | 0.46              |
| 7:O:5:DG:H2''     | 7:O:6:DA:O4'      | 2.14                     | 0.46              |
| 1:B:3:ILE:HG23    | 1:B:5:GLN:O       | 2.15                     | 0.46              |
| 1:B:96:TYR:HD1    | 1:B:137:GLU:HG2   | 1.78                     | 0.46              |
| 1:B:151:GLN:HE22  | 1:B:155:SER:HA    | 1.81                     | 0.46              |
| 2:C:278:TYR:CE1   | 2:C:291:SER:HB2   | 2.51                     | 0.46              |
| 2:C:400:VAL:O     | 2:C:404:MET:N     | 2.49                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:D:57:ASP:HB3   | 3:D:58:TRP:CE3    | 2.50                     | 0.46              |
| 3:D:414:ARG:HB2  | 3:D:414:ARG:HH21  | 1.80                     | 0.46              |
| 3:D:449:LEU:O    | 3:D:449:LEU:HD22  | 2.16                     | 0.46              |
| 3:D:1128:ARG:NH1 | 3:D:1132:ILE:CG1  | 2.67                     | 0.46              |
| 4:E:102:ASP:C    | 4:E:103:LEU:HD12  | 2.41                     | 0.46              |
| 1:A:35:GLY:HA2   | 1:A:192:LEU:HD21  | 1.98                     | 0.46              |
| 1:A:84:VAL:HG12  | 1:A:120:ASN:CG    | 2.42                     | 0.46              |
| 2:C:421:ARG:N    | 2:C:422:PRO:HD2   | 2.31                     | 0.46              |
| 2:C:484:CYS:HB2  | 2:C:588:SER:HB3   | 1.97                     | 0.46              |
| 2:C:737:LEU:HD23 | 2:C:915:ILE:HG22  | 1.97                     | 0.46              |
| 2:C:877:ARG:NH1  | 2:C:1036:LEU:HD12 | 2.20                     | 0.46              |
| 2:C:961:ASP:C    | 2:C:962:GLU:HG3   | 2.41                     | 0.46              |
| 2:C:1135:VAL:HA  | 3:D:11:ARG:O      | 2.16                     | 0.46              |
| 3:D:170:LEU:C    | 3:D:170:LEU:HD13  | 2.41                     | 0.46              |
| 5:F:300:LEU:O    | 5:F:304:VAL:HG23  | 2.16                     | 0.46              |
| 6:J:32:TYR:OH    | 6:J:51:PRO:HG2    | 2.15                     | 0.46              |
| 6:J:76:LYS:H     | 6:J:76:LYS:HD2    | 1.80                     | 0.46              |
| 6:J:101:ARG:HH11 | 6:J:101:ARG:CA    | 2.29                     | 0.46              |
| 6:J:104:LEU:HD23 | 6:J:104:LEU:C     | 2.41                     | 0.46              |
| 1:A:184:GLU:OE1  | 1:A:184:GLU:HA    | 2.16                     | 0.45              |
| 1:A:187:THR:O    | 1:A:187:THR:HG23  | 2.16                     | 0.45              |
| 1:B:80:LEU:CD2   | 1:B:125:ILE:HD13  | 2.46                     | 0.45              |
| 1:B:196:VAL:O    | 1:B:196:VAL:HG22  | 2.15                     | 0.45              |
| 2:C:442:GLN:O    | 2:C:442:GLN:HG3   | 2.16                     | 0.45              |
| 2:C:444:ASN:HD22 | 2:C:715:LEU:HD22  | 1.81                     | 0.45              |
| 2:C:519:VAL:HG12 | 2:C:577:ASP:C     | 2.41                     | 0.45              |
| 2:C:643:VAL:HG13 | 2:C:699:GLY:O     | 2.16                     | 0.45              |
| 2:C:1068:PHE:CE1 | 2:C:1072:GLU:HB3  | 2.51                     | 0.45              |
| 3:D:49:GLU:OE2   | 3:D:55:THR:OG1    | 2.23                     | 0.45              |
| 3:D:234:LEU:HD23 | 3:D:235:ILE:N     | 2.31                     | 0.45              |
| 3:D:243:GLU:O    | 3:D:247:ARG:HB3   | 2.17                     | 0.45              |
| 3:D:778:TRP:NE1  | 3:D:835:PRO:HD3   | 2.31                     | 0.45              |
| 4:E:81:PRO:HB3   | 4:E:94:ILE:HG21   | 1.98                     | 0.45              |
| 6:J:6:LEU:H      | 6:J:6:LEU:HD12    | 1.81                     | 0.45              |
| 1:A:147:VAL:HG12 | 1:A:168:TYR:CE2   | 2.50                     | 0.45              |
| 1:B:14:LEU:HB2   | 1:B:18:ARG:O      | 2.16                     | 0.45              |
| 2:C:298:ASN:HA   | 2:C:302:LYS:HE3   | 1.99                     | 0.45              |
| 2:C:581:VAL:H    | 2:C:585:GLN:NE2   | 2.14                     | 0.45              |
| 1:B:2:LEU:HD22   | 1:B:4:SER:H       | 1.80                     | 0.45              |
| 2:C:229:LYS:HZ2  | 2:C:281:LEU:CG    | 2.27                     | 0.45              |
| 2:C:482:ARG:NH1  | 2:C:533:ALA:HA    | 2.32                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:959:LEU:HD12 | 2:C:959:LEU:H    | 1.81                     | 0.45              |
| 3:D:466:ALA:HB1  | 3:D:471:SER:OG   | 2.16                     | 0.45              |
| 5:F:274:PRO:HD2  | 5:F:277:GLN:HG2  | 1.98                     | 0.45              |
| 3:D:262:GLN:HE21 | 3:D:310:MET:CE   | 2.29                     | 0.45              |
| 3:D:263:LYS:NZ   | 3:D:263:LYS:CB   | 2.78                     | 0.45              |
| 3:D:557:ILE:HD13 | 4:E:53:LEU:HD23  | 1.98                     | 0.45              |
| 3:D:1085:ARG:HG2 | 3:D:1113:GLU:OE1 | 2.17                     | 0.45              |
| 5:F:350:TRP:HH2  | 7:O:25:DC:OP2    | 1.99                     | 0.45              |
| 1:A:133:LYS:C    | 1:A:133:LYS:HD3  | 2.42                     | 0.45              |
| 1:A:144:ARG:CG   | 1:B:1:MET:HE2    | 2.38                     | 0.45              |
| 1:B:95:MET:HG2   | 1:B:113:PRO:HD3  | 1.99                     | 0.45              |
| 1:B:107:ALA:HB3  | 1:B:121:PRO:O    | 2.16                     | 0.45              |
| 2:C:211:TRP:O    | 2:C:227:ASP:N    | 2.44                     | 0.45              |
| 2:C:254:PHE:N    | 2:C:255:SER:CB   | 2.77                     | 0.45              |
| 2:C:571:VAL:CG2  | 2:C:572:PRO:HD2  | 2.29                     | 0.45              |
| 3:D:453:LYS:HB3  | 3:D:454:PRO:HD3  | 1.98                     | 0.45              |
| 3:D:915:TYR:CE1  | 3:D:1143:ARG:HD3 | 2.51                     | 0.45              |
| 5:F:395:THR:HG1  | 5:F:398:GLU:HB2  | 1.81                     | 0.45              |
| 1:B:59:VAL:HG12  | 1:B:59:VAL:O     | 2.17                     | 0.45              |
| 1:B:70:LYS:NZ    | 1:B:70:LYS:HB2   | 2.31                     | 0.45              |
| 2:C:71:ARG:O     | 2:C:75:ALA:HB2   | 2.16                     | 0.45              |
| 2:C:622:GLU:OE2  | 2:C:718:ASN:ND2  | 2.50                     | 0.45              |
| 2:C:668:ARG:HD3  | 2:C:669:THR:N    | 2.32                     | 0.45              |
| 2:C:1012:ASP:HB2 | 2:C:1019:PHE:CE1 | 2.52                     | 0.45              |
| 3:D:287:GLN:CD   | 3:D:287:GLN:H    | 2.25                     | 0.45              |
| 3:D:387:ARG:NH2  | 5:F:225:ALA:HA   | 2.32                     | 0.45              |
| 3:D:459:ARG:HH21 | 4:E:88:GLN:CD    | 2.25                     | 0.45              |
| 3:D:1129:GLU:HA  | 3:D:1129:GLU:OE1 | 2.16                     | 0.45              |
| 1:B:84:VAL:CG2   | 1:B:119:HIS:HB2  | 2.45                     | 0.45              |
| 2:C:740:ARG:HH21 | 2:C:914:ASP:CG   | 2.23                     | 0.45              |
| 2:C:757:ILE:HG22 | 2:C:869:VAL:HG13 | 1.98                     | 0.45              |
| 2:C:805:LYS:HB3  | 2:C:835:THR:O    | 2.17                     | 0.45              |
| 2:C:868:LEU:C    | 2:C:868:LEU:HD13 | 2.42                     | 0.45              |
| 3:D:151:LEU:HD21 | 3:D:251:TYR:HE2  | 1.82                     | 0.45              |
| 3:D:365:ILE:HD12 | 3:D:365:ILE:N    | 2.26                     | 0.45              |
| 3:D:469:ILE:HD13 | 3:D:469:ILE:C    | 2.41                     | 0.45              |
| 3:D:1101:ASP:OD1 | 3:D:1102:GLY:N   | 2.50                     | 0.45              |
| 5:F:378:LYS:CG   | 5:F:403:MET:HE3  | 2.44                     | 0.45              |
| 5:F:429:ASP:O    | 5:F:431:GLY:HA2  | 2.16                     | 0.45              |
| 1:B:66:VAL:HG23  | 1:B:73:VAL:HG22  | 1.99                     | 0.45              |
| 2:C:400:VAL:CG1  | 2:C:417:LEU:HB3  | 2.37                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:471:GLU:OE1  | 2:C:471:GLU:N     | 2.50                     | 0.45              |
| 3:D:177:LEU:HD23 | 3:D:178:GLU:N     | 2.32                     | 0.45              |
| 3:D:313:VAL:O    | 3:D:313:VAL:HG23  | 2.16                     | 0.45              |
| 3:D:900:GLU:N    | 3:D:900:GLU:OE1   | 2.50                     | 0.45              |
| 5:F:329:ILE:O    | 5:F:333:GLU:HG3   | 2.17                     | 0.45              |
| 6:J:36:ASN:ND2   | 6:J:60:MET:SD     | 2.90                     | 0.45              |
| 8:P:1:DA:H2''    | 8:P:2:DG:O4'      | 2.17                     | 0.45              |
| 2:C:188:ASP:OD1  | 2:C:188:ASP:N     | 2.50                     | 0.45              |
| 2:C:203:LYS:HB2  | 2:C:203:LYS:NZ    | 2.32                     | 0.45              |
| 3:D:449:LEU:HD13 | 3:D:449:LEU:C     | 2.41                     | 0.45              |
| 3:D:641:ARG:HA   | 3:D:657:GLN:HB2   | 1.98                     | 0.45              |
| 3:D:864:ALA:O    | 3:D:867:THR:HG22  | 2.17                     | 0.45              |
| 5:F:232:LEU:O    | 5:F:235:ILE:HG12  | 2.16                     | 0.45              |
| 5:F:511:MET:CB   | 5:F:515:ARG:HH12  | 2.30                     | 0.45              |
| 6:J:101:ARG:HH11 | 6:J:101:ARG:CB    | 2.29                     | 0.45              |
| 1:A:102:PRO:HD3  | 1:A:130:ASP:HA    | 1.98                     | 0.45              |
| 1:B:77:ILE:HG23  | 1:B:164:VAL:CG1   | 2.47                     | 0.45              |
| 2:C:848:ILE:HD12 | 2:C:874:ALA:HB2   | 1.98                     | 0.45              |
| 3:D:574:LEU:HD12 | 3:D:574:LEU:HA    | 1.81                     | 0.45              |
| 3:D:930:VAL:HA   | 3:D:937:ILE:HG22  | 1.98                     | 0.45              |
| 3:D:1051:GLY:O   | 3:D:1104:HIS:HA   | 2.17                     | 0.45              |
| 3:D:1148:SER:O   | 3:D:1149:ILE:HD13 | 2.17                     | 0.45              |
| 3:D:1175:PHE:CZ  | 3:D:1189:GLU:HG2  | 2.52                     | 0.45              |
| 4:E:32:PRO:C     | 4:E:33:LEU:HD12   | 2.42                     | 0.45              |
| 5:F:279:ARG:NH2  | 5:F:279:ARG:HB3   | 2.32                     | 0.45              |
| 5:F:387:LEU:HD23 | 5:F:387:LEU:C     | 2.42                     | 0.45              |
| 5:F:516:HIS:HD2  | 5:F:518:SER:OG    | 1.99                     | 0.45              |
| 1:A:55:ARG:HH21  | 1:A:161:ARG:HH12  | 1.64                     | 0.44              |
| 1:A:97:LEU:HD21  | 1:A:105:VAL:CG1   | 2.47                     | 0.44              |
| 1:B:166:SER:HB3  | 1:B:168:TYR:CE1   | 2.52                     | 0.44              |
| 2:C:787:ARG:HD3  | 2:C:787:ARG:C     | 2.42                     | 0.44              |
| 3:D:113:ARG:HG2  | 3:D:1238:ILE:HD11 | 1.99                     | 0.44              |
| 3:D:155:MET:HE1  | 3:D:219:LEU:CD1   | 2.43                     | 0.44              |
| 3:D:487:LEU:HD12 | 3:D:491:ILE:HG13  | 1.99                     | 0.44              |
| 3:D:576:MET:HG3  | 3:D:697:ILE:HD12  | 1.99                     | 0.44              |
| 4:E:53:LEU:HD23  | 4:E:53:LEU:C      | 2.42                     | 0.44              |
| 1:A:215:LEU:HG   | 1:B:219:PHE:CE1   | 2.52                     | 0.44              |
| 2:C:952:VAL:CG1  | 2:C:957:ALA:HA    | 2.44                     | 0.44              |
| 3:D:111:PRO:HB2  | 3:D:116:TYR:HE2   | 1.79                     | 0.44              |
| 3:D:392:THR:HG22 | 3:D:397:ARG:C     | 2.42                     | 0.44              |
| 1:A:56:ILE:HG12  | 1:A:136:VAL:HB    | 1.98                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:61:PHE:C      | 2:C:63:TRP:H      | 2.12                     | 0.44              |
| 2:C:112:PHE:CD1   | 2:C:159:MET:HE1   | 2.52                     | 0.44              |
| 2:C:231:ARG:CG    | 2:C:232:GLN:N     | 2.80                     | 0.44              |
| 3:D:1226:PHE:CE2  | 3:D:1249:LYS:NZ   | 2.85                     | 0.44              |
| 5:F:438:PHE:HB3   | 6:J:4:ARG:O       | 2.17                     | 0.44              |
| 6:J:33:ARG:HD3    | 6:J:34:THR:O      | 2.17                     | 0.44              |
| 2:C:323:HIS:O     | 2:C:326:GLU:HB2   | 2.17                     | 0.44              |
| 3:D:948:GLU:H     | 3:D:948:GLU:CD    | 2.25                     | 0.44              |
| 4:E:31:THR:HG23   | 4:E:31:THR:O      | 2.18                     | 0.44              |
| 1:A:40:ARG:NE     | 1:B:33:THR:HG22   | 2.32                     | 0.44              |
| 1:B:99:LYS:C      | 1:B:133:LYS:HG3   | 2.43                     | 0.44              |
| 2:C:224:VAL:HG22  | 2:C:234:VAL:HG12  | 1.98                     | 0.44              |
| 2:C:274:LEU:HG    | 2:C:292:ALA:CB    | 2.48                     | 0.44              |
| 3:D:211:ARG:HA    | 3:D:214:ARG:NH2   | 2.33                     | 0.44              |
| 3:D:456:VAL:O     | 3:D:460:LEU:HG    | 2.18                     | 0.44              |
| 3:D:1053:VAL:CG1  | 3:D:1103:ASP:H    | 2.31                     | 0.44              |
| 7:O:23:DT:H2"     | 7:O:24:DG:H8      | 1.83                     | 0.44              |
| 1:B:65:THR:HG22   | 1:B:66:VAL:N      | 2.32                     | 0.44              |
| 3:D:58:TRP:CA     | 3:D:82:VAL:HG23   | 2.46                     | 0.44              |
| 3:D:223:TRP:O     | 3:D:227:THR:HG23  | 2.17                     | 0.44              |
| 3:D:341:ASN:O     | 3:D:345:ARG:HG3   | 2.18                     | 0.44              |
| 3:D:1069:ASP:OD2  | 3:D:1104:HIS:HE1  | 2.01                     | 0.44              |
| 4:E:43:LEU:HB3    | 4:E:53:LEU:HD11   | 1.99                     | 0.44              |
| 1:A:226:ASN:HB2   | 1:B:9:LEU:HD23    | 1.99                     | 0.44              |
| 1:B:38:LEU:HD13   | 1:B:38:LEU:HA     | 1.74                     | 0.44              |
| 1:B:74:THR:OG1    | 3:D:608:GLU:OE2   | 2.33                     | 0.44              |
| 1:B:112:PRO:HB2   | 1:B:116:VAL:HG23  | 2.00                     | 0.44              |
| 2:C:219:ARG:HG3   | 2:C:220:ASP:O     | 2.17                     | 0.44              |
| 2:C:672:MET:HE1   | 2:C:703:ALA:HB2   | 2.00                     | 0.44              |
| 3:D:860:LEU:HD12  | 3:D:860:LEU:HA    | 1.88                     | 0.44              |
| 3:D:909:THR:O     | 3:D:910:LEU:CB    | 2.66                     | 0.44              |
| 3:D:952:LEU:HB3   | 3:D:957:ILE:CD1   | 2.43                     | 0.44              |
| 3:D:1064:ILE:CD1  | 3:D:1080:ILE:HD12 | 2.48                     | 0.44              |
| 3:D:1221:LEU:HD23 | 3:D:1221:LEU:N    | 2.33                     | 0.44              |
| 1:A:1:MET:O       | 1:A:2:LEU:HD12    | 2.18                     | 0.44              |
| 1:B:161:ARG:O     | 1:B:161:ARG:HG3   | 2.18                     | 0.44              |
| 2:C:568:VAL:CG1   | 3:D:847:LEU:HD23  | 2.48                     | 0.44              |
| 2:C:619:VAL:HG23  | 2:C:620:ARG:HG2   | 2.00                     | 0.44              |
| 3:D:20:ILE:HG21   | 3:D:316:ALA:O     | 2.18                     | 0.44              |
| 3:D:148:LEU:O     | 3:D:148:LEU:HD22  | 2.18                     | 0.44              |
| 5:F:246:GLU:OE1   | 5:F:247:VAL:HG23  | 2.17                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:P:18:DT:H2''    | 8:P:19:DT:C6      | 2.53                     | 0.44              |
| 1:B:107:ALA:O     | 1:B:110:ILE:HG22  | 2.17                     | 0.44              |
| 2:C:476:HIS:H     | 2:C:479:HIS:CD2   | 2.36                     | 0.44              |
| 2:C:730:ASN:HA    | 2:C:734:ALA:HB3   | 2.00                     | 0.44              |
| 2:C:845:GLY:HA3   | 2:C:874:ALA:O     | 2.17                     | 0.44              |
| 3:D:442:GLY:HA3   | 3:D:523:GLN:HB2   | 1.99                     | 0.44              |
| 3:D:463:LEU:HD23  | 3:D:463:LEU:H     | 1.82                     | 0.44              |
| 1:B:55:ARG:HB2    | 1:B:55:ARG:CZ     | 2.47                     | 0.43              |
| 2:C:278:TYR:CD2   | 2:C:291:SER:HB2   | 2.52                     | 0.43              |
| 4:E:76:LEU:HG     | 4:E:77:GLU:N      | 2.33                     | 0.43              |
| 5:F:477:LEU:O     | 5:F:487:ARG:HG2   | 2.18                     | 0.43              |
| 1:A:9:LEU:HD12    | 1:A:23:ILE:CD1    | 2.44                     | 0.43              |
| 2:C:319:LYS:HZ3   | 2:C:368:ASP:CG    | 2.15                     | 0.43              |
| 2:C:463:LEU:HD12  | 2:C:463:LEU:C     | 2.43                     | 0.43              |
| 2:C:542:ALA:HB3   | 2:C:579:MET:CB    | 2.47                     | 0.43              |
| 2:C:612:GLN:HE21  | 2:C:888:ARG:HG3   | 1.81                     | 0.43              |
| 2:C:694:ASP:OD1   | 2:C:694:ASP:N     | 2.50                     | 0.43              |
| 2:C:817:GLU:HG2   | 5:F:457:GLN:HG2   | 2.00                     | 0.43              |
| 3:D:148:LEU:C     | 3:D:148:LEU:HD13  | 2.43                     | 0.43              |
| 3:D:236:VAL:O     | 3:D:236:VAL:HG12  | 2.19                     | 0.43              |
| 3:D:1050:THR:HG23 | 3:D:1107:VAL:HG22 | 2.00                     | 0.43              |
| 3:D:1097:ARG:NH1  | 3:D:1100:SER:HB2  | 2.26                     | 0.43              |
| 5:F:394:PRO:HB2   | 5:F:399:LEU:HD11  | 2.00                     | 0.43              |
| 1:A:62:GLU:O      | 1:A:62:GLU:HG2    | 2.17                     | 0.43              |
| 2:C:202:VAL:HG22  | 2:C:203:LYS:N     | 2.34                     | 0.43              |
| 2:C:761:ASP:HA    | 2:C:766:ALA:HA    | 1.99                     | 0.43              |
| 3:D:25:TYR:CD2    | 3:D:91:ARG:HD3    | 2.54                     | 0.43              |
| 3:D:136:ILE:HD11  | 3:D:235:ILE:HD11  | 2.00                     | 0.43              |
| 3:D:290:LEU:O     | 3:D:294:LYS:HG3   | 2.18                     | 0.43              |
| 3:D:495:PRO:HA    | 3:D:512:PHE:O     | 2.18                     | 0.43              |
| 3:D:535:ASP:OD1   | 3:D:539:ASP:OD2   | 2.36                     | 0.43              |
| 5:F:233:LYS:HE2   | 5:F:233:LYS:HB3   | 1.79                     | 0.43              |
| 5:F:258:TYR:CE2   | 6:J:98:LEU:HD13   | 2.54                     | 0.43              |
| 5:F:492:ILE:HD11  | 5:F:503:ILE:HG21  | 2.01                     | 0.43              |
| 8:P:3:DC:H2''     | 8:P:4:DA:O5'      | 2.18                     | 0.43              |
| 2:C:524:VAL:HB    | 2:C:552:GLY:HA2   | 1.99                     | 0.43              |
| 2:C:641:VAL:CG1   | 2:C:701:VAL:HG13  | 2.48                     | 0.43              |
| 2:C:760:ARG:HB3   | 2:C:864:GLY:O     | 2.18                     | 0.43              |
| 1:A:35:GLY:CA     | 1:A:192:LEU:HD21  | 2.49                     | 0.43              |
| 1:A:97:LEU:HB2    | 1:A:110:ILE:HG12  | 2.00                     | 0.43              |
| 2:C:215:ASP:N     | 2:C:223:GLY:HA3   | 2.33                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:519:VAL:HG23 | 2:C:524:VAL:N    | 2.33                     | 0.43              |
| 2:C:632:LEU:C    | 2:C:632:LEU:HD13 | 2.43                     | 0.43              |
| 2:C:636:ILE:C    | 2:C:636:ILE:HD12 | 2.43                     | 0.43              |
| 2:C:754:GLU:HB2  | 2:C:872:TYR:CE1  | 2.53                     | 0.43              |
| 2:C:762:THR:HG23 | 2:C:765:GLY:H    | 1.83                     | 0.43              |
| 2:C:774:PRO:O    | 2:C:776:ILE:HG22 | 2.19                     | 0.43              |
| 3:D:102:THR:HG22 | 3:D:313:VAL:HG12 | 2.00                     | 0.43              |
| 3:D:237:ASP:CG   | 3:D:240:LEU:H    | 2.25                     | 0.43              |
| 3:D:505:HIS:H    | 3:D:505:HIS:CD2  | 2.36                     | 0.43              |
| 3:D:647:GLU:HG3  | 3:D:648:ALA:N    | 2.33                     | 0.43              |
| 3:D:1256:LYS:HG2 | 3:D:1257:LEU:N   | 2.34                     | 0.43              |
| 5:F:278:ARG:NH2  | 5:F:278:ARG:O    | 2.52                     | 0.43              |
| 5:F:491:GLU:O    | 5:F:494:GLN:HB3  | 2.18                     | 0.43              |
| 1:B:128:LEU:N    | 1:B:128:LEU:HD12 | 2.33                     | 0.43              |
| 2:C:781:LEU:HA   | 2:C:784:LEU:HD13 | 2.01                     | 0.43              |
| 2:C:994:PRO:HB3  | 2:C:999:ASP:N    | 2.16                     | 0.43              |
| 2:C:994:PRO:CG   | 2:C:998:GLY:HA2  | 2.48                     | 0.43              |
| 3:D:118:LEU:HB3  | 3:D:120:LEU:HD13 | 2.01                     | 0.43              |
| 3:D:513:GLU:HB2  | 4:E:35:ILE:HG13  | 2.01                     | 0.43              |
| 3:D:646:ILE:CG2  | 3:D:650:LEU:HD12 | 2.49                     | 0.43              |
| 3:D:1097:ARG:NH1 | 3:D:1100:SER:N   | 2.66                     | 0.43              |
| 4:E:50:LYS:O     | 4:E:54:VAL:HG23  | 2.19                     | 0.43              |
| 5:F:273:LEU:HB3  | 5:F:274:PRO:CD   | 2.48                     | 0.43              |
| 5:F:430:GLU:HA   | 5:F:431:GLY:HA3  | 1.63                     | 0.43              |
| 7:O:7:DC:H2''    | 7:O:8:DA:H8      | 1.83                     | 0.43              |
| 7:O:19:DA:H2''   | 7:O:20:DT:C5'    | 2.48                     | 0.43              |
| 1:B:74:THR:HG21  | 3:D:608:GLU:OE2  | 2.18                     | 0.43              |
| 2:C:113:ASP:HB2  | 2:C:132:PRO:HD2  | 2.00                     | 0.43              |
| 2:C:946:VAL:HG12 | 2:C:948:ALA:H    | 1.83                     | 0.43              |
| 3:D:125:LEU:CD1  | 3:D:261:ILE:HD11 | 2.44                     | 0.43              |
| 3:D:336:ALA:HA   | 5:F:421:ILE:O    | 2.18                     | 0.43              |
| 3:D:909:THR:C    | 3:D:910:LEU:CG   | 2.77                     | 0.43              |
| 7:O:11:DA:H2''   | 7:O:12:DG:H5''   | 2.01                     | 0.43              |
| 1:A:9:LEU:HD21   | 1:B:225:LEU:HD11 | 2.00                     | 0.43              |
| 1:A:65:THR:HG22  | 1:A:72:ASP:CB    | 2.48                     | 0.43              |
| 1:A:219:PHE:CG   | 1:B:215:LEU:HD22 | 2.54                     | 0.43              |
| 1:B:78:LEU:HD12  | 3:D:636:ARG:HH21 | 1.83                     | 0.43              |
| 2:C:77:ARG:HG3   | 2:C:77:ARG:O     | 2.18                     | 0.43              |
| 2:C:103:MET:SD   | 2:C:404:MET:HE2  | 2.59                     | 0.43              |
| 2:C:195:THR:HG21 | 2:C:218:LYS:HG3  | 1.99                     | 0.43              |
| 2:C:593:MET:HA   | 2:C:628:THR:HG21 | 2.01                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:597:LEU:HD23 | 2:C:976:VAL:CG1  | 2.48                     | 0.43              |
| 3:D:60:CYS:SG    | 3:D:63:GLY:N     | 2.89                     | 0.43              |
| 3:D:834:ARG:HA   | 3:D:834:ARG:NE   | 2.29                     | 0.43              |
| 4:E:92:LEU:O     | 4:E:92:LEU:HD13  | 2.19                     | 0.43              |
| 5:F:442:SER:HB3  | 6:J:7:ARG:CG     | 2.48                     | 0.43              |
| 1:B:182:ARG:HG3  | 1:B:186:ARG:H    | 1.84                     | 0.43              |
| 2:C:30:ASN:O     | 2:C:31:SER:OG    | 2.28                     | 0.43              |
| 2:C:79:ASP:N     | 2:C:79:ASP:OD1   | 2.51                     | 0.43              |
| 2:C:166:PHE:C    | 2:C:167:ILE:HD12 | 2.44                     | 0.43              |
| 2:C:205:ILE:O    | 2:C:205:ILE:HG13 | 2.18                     | 0.43              |
| 2:C:624:PRO:HB3  | 2:C:1029:TYR:CE1 | 2.54                     | 0.43              |
| 2:C:626:VAL:O    | 2:C:888:ARG:NH2  | 2.50                     | 0.43              |
| 2:C:830:ARG:HD2  | 2:C:832:VAL:HG22 | 2.01                     | 0.43              |
| 2:C:897:LYS:HG3  | 2:C:899:LEU:HD13 | 2.00                     | 0.43              |
| 2:C:982:GLU:HB2  | 3:D:841:ARG:NH2  | 2.33                     | 0.43              |
| 2:C:1128:LEU:CD2 | 3:D:406:LEU:HD21 | 2.48                     | 0.43              |
| 3:D:274:ALA:O    | 3:D:278:ARG:HD3  | 2.19                     | 0.43              |
| 3:D:294:LYS:O    | 3:D:297:LYS:HB3  | 2.18                     | 0.43              |
| 3:D:482:GLN:OE1  | 3:D:482:GLN:N    | 2.43                     | 0.43              |
| 3:D:905:ALA:HB2  | 3:D:911:ILE:HD12 | 2.00                     | 0.43              |
| 5:F:472:ALA:O    | 5:F:476:ARG:HG3  | 2.19                     | 0.43              |
| 1:A:47:PRO:HG3   | 1:B:230:GLU:O    | 2.18                     | 0.43              |
| 1:A:54:ILE:HD11  | 1:A:77:ILE:CD1   | 2.49                     | 0.43              |
| 1:B:181:THR:HG21 | 1:B:191:LYS:HD3  | 2.00                     | 0.43              |
| 2:C:38:ARG:HG2   | 2:C:973:SER:HB3  | 2.01                     | 0.43              |
| 2:C:762:THR:N    | 2:C:765:GLY:O    | 2.48                     | 0.43              |
| 2:C:820:LEU:HA   | 5:F:479:PHE:CE1  | 2.53                     | 0.43              |
| 2:C:1119:GLU:O   | 2:C:1119:GLU:HG2 | 2.19                     | 0.43              |
| 3:D:58:TRP:C     | 3:D:82:VAL:HG23  | 2.44                     | 0.43              |
| 3:D:262:GLN:CG   | 3:D:310:MET:HE1  | 2.49                     | 0.43              |
| 3:D:596:THR:HG22 | 3:D:626:VAL:O    | 2.19                     | 0.43              |
| 3:D:901:LEU:HD12 | 3:D:960:VAL:CG2  | 2.49                     | 0.43              |
| 3:D:975:CYS:SG   | 3:D:978:CYS:HB2  | 2.58                     | 0.43              |
| 4:E:101:ALA:CB   | 4:E:103:LEU:HD13 | 2.49                     | 0.43              |
| 5:F:418:ARG:HB2  | 5:F:418:ARG:CZ   | 2.49                     | 0.43              |
| 7:O:6:DA:H2''    | 7:O:7:DC:C5'     | 2.49                     | 0.43              |
| 1:A:46:ILE:HD12  | 1:A:210:SER:OG   | 2.18                     | 0.42              |
| 1:B:3:ILE:O      | 1:B:4:SER:OG     | 2.29                     | 0.42              |
| 2:C:196:ASP:N    | 2:C:196:ASP:OD1  | 2.50                     | 0.42              |
| 2:C:275:LEU:C    | 2:C:275:LEU:HD12 | 2.44                     | 0.42              |
| 2:C:343:GLU:HA   | 2:C:346:VAL:HG12 | 2.00                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:809:LYS:NZ    | 2:C:832:VAL:O     | 2.52                     | 0.42              |
| 2:C:881:ASP:OD1   | 2:C:881:ASP:N     | 2.52                     | 0.42              |
| 3:D:55:THR:HG22   | 6:J:12:GLY:HA2    | 2.01                     | 0.42              |
| 3:D:459:ARG:HH21  | 4:E:88:GLN:NE2    | 2.17                     | 0.42              |
| 3:D:753:ALA:HB1   | 3:D:774:LEU:CD2   | 2.48                     | 0.42              |
| 3:D:866:ARG:HH11  | 3:D:1011:THR:HA   | 1.81                     | 0.42              |
| 3:D:1008:THR:O    | 3:D:1008:THR:HG22 | 2.19                     | 0.42              |
| 3:D:1053:VAL:HG12 | 3:D:1103:ASP:N    | 2.34                     | 0.42              |
| 3:D:1070:ASP:HB2  | 3:D:1071:GLY:HA2  | 2.00                     | 0.42              |
| 5:F:456:LEU:HD13  | 5:F:526:TYR:CD2   | 2.54                     | 0.42              |
| 6:J:108:ARG:HD3   | 6:J:108:ARG:N     | 2.34                     | 0.42              |
| 1:B:50:ALA:HB3    | 1:B:168:TYR:CD1   | 2.54                     | 0.42              |
| 1:B:69:VAL:HG23   | 1:B:71:GLU:O      | 2.20                     | 0.42              |
| 2:C:93:LEU:HD12   | 2:C:96:ILE:HD11   | 2.01                     | 0.42              |
| 2:C:221:THR:OG1   | 2:C:261:THR:HG22  | 2.18                     | 0.42              |
| 2:C:476:HIS:HD2   | 2:C:478:SER:H     | 1.67                     | 0.42              |
| 2:C:820:LEU:HB2   | 5:F:479:PHE:CD1   | 2.53                     | 0.42              |
| 3:D:37:ARG:HB3    | 3:D:37:ARG:NH1    | 2.34                     | 0.42              |
| 3:D:433:GLY:O     | 3:D:436:LEU:HG    | 2.19                     | 0.42              |
| 3:D:771:ASN:OD1   | 3:D:833:PRO:HG3   | 2.19                     | 0.42              |
| 3:D:1248:LEU:HD12 | 3:D:1248:LEU:C    | 2.44                     | 0.42              |
| 8:P:2:DG:H2''     | 8:P:3:DC:O5'      | 2.19                     | 0.42              |
| 1:B:100:GLN:CB    | 1:B:133:LYS:HB2   | 2.49                     | 0.42              |
| 2:C:230:ARG:O     | 2:C:231:ARG:CB    | 2.64                     | 0.42              |
| 2:C:357:VAL:HG22  | 2:C:358:PRO:CD    | 2.49                     | 0.42              |
| 2:C:658:ILE:HD11  | 2:C:688:PRO:CB    | 2.25                     | 0.42              |
| 2:C:774:PRO:O     | 2:C:775:ASN:C     | 2.62                     | 0.42              |
| 3:D:908:GLY:C     | 3:D:910:LEU:N     | 2.59                     | 0.42              |
| 1:A:82:SER:O      | 1:A:123:MET:HE1   | 2.18                     | 0.42              |
| 1:A:183:VAL:HG13  | 1:A:185:GLN:OE1   | 2.20                     | 0.42              |
| 2:C:141:ASN:O     | 2:C:145:GLY:HA2   | 2.19                     | 0.42              |
| 2:C:353:THR:HG23  | 2:C:354:THR:N     | 2.34                     | 0.42              |
| 3:D:151:LEU:HD21  | 3:D:251:TYR:OH    | 2.18                     | 0.42              |
| 3:D:268:PHE:CZ    | 3:D:273:GLU:HG3   | 2.54                     | 0.42              |
| 3:D:444:PRO:HD2   | 3:D:447:MET:CE    | 2.49                     | 0.42              |
| 3:D:588:LEU:O     | 3:D:588:LEU:HD13  | 2.19                     | 0.42              |
| 3:D:600:GLN:O     | 3:D:601:PRO:C     | 2.61                     | 0.42              |
| 3:D:952:LEU:CB    | 3:D:957:ILE:HD11  | 2.43                     | 0.42              |
| 3:D:989:VAL:HG22  | 3:D:990:ASP:N     | 2.34                     | 0.42              |
| 3:D:1040:PRO:HB2  | 3:D:1115:SER:HB2  | 2.01                     | 0.42              |
| 3:D:1048:ASP:OD2  | 3:D:1075:VAL:HG11 | 2.20                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:1166:THR:HB  | 3:D:1206:VAL:CG2 | 2.48                     | 0.42              |
| 1:A:57:ASP:N     | 1:A:57:ASP:OD1   | 2.52                     | 0.42              |
| 1:A:217:GLU:O    | 1:B:234:ILE:HD12 | 2.19                     | 0.42              |
| 1:B:215:LEU:HD23 | 1:B:215:LEU:C    | 2.44                     | 0.42              |
| 2:C:173:ARG:NH1  | 2:C:439:PHE:CZ   | 2.87                     | 0.42              |
| 2:C:436:LEU:HD13 | 2:C:460:PRO:HD2  | 2.02                     | 0.42              |
| 3:D:638:THR:C    | 3:D:639:GLN:HE21 | 2.28                     | 0.42              |
| 3:D:834:ARG:HB2  | 3:D:835:PRO:HA   | 2.02                     | 0.42              |
| 3:D:913:ASP:N    | 3:D:916:ILE:HD11 | 2.35                     | 0.42              |
| 3:D:1117:ASP:OD1 | 3:D:1120:GLU:HB2 | 2.19                     | 0.42              |
| 1:B:6:ARG:CZ     | 1:B:237:SER:HA   | 2.49                     | 0.42              |
| 2:C:353:THR:O    | 2:C:365:VAL:N    | 2.24                     | 0.42              |
| 2:C:967:GLN:O    | 2:C:970:ALA:HB2  | 2.20                     | 0.42              |
| 3:D:64:LYS:NZ    | 3:D:65:TYR:OH    | 2.52                     | 0.42              |
| 3:D:91:ARG:O     | 3:D:321:PRO:HG3  | 2.19                     | 0.42              |
| 3:D:216:LEU:N    | 3:D:216:LEU:HD23 | 2.35                     | 0.42              |
| 3:D:657:GLN:HA   | 3:D:660:ASP:OD1  | 2.19                     | 0.42              |
| 3:D:1044:ALA:HA  | 3:D:1084:GLN:NE2 | 2.35                     | 0.42              |
| 5:F:395:THR:OG1  | 5:F:397:GLU:OE1  | 2.30                     | 0.42              |
| 5:F:470:ARG:O    | 5:F:474:VAL:HG23 | 2.19                     | 0.42              |
| 6:J:31:ARG:O     | 6:J:65:ILE:HB    | 2.19                     | 0.42              |
| 1:B:118:VAL:HG12 | 1:B:120:ASN:H    | 1.84                     | 0.42              |
| 1:B:177:LYS:O    | 1:B:177:LYS:HD3  | 2.19                     | 0.42              |
| 2:C:213:GLU:O    | 2:C:223:GLY:O    | 2.37                     | 0.42              |
| 2:C:231:ARG:HB3  | 5:F:205:ASP:OD2  | 2.19                     | 0.42              |
| 2:C:274:LEU:CG   | 2:C:292:ALA:HB1  | 2.48                     | 0.42              |
| 2:C:282:ARG:HB3  | 2:C:283:PRO:O    | 2.19                     | 0.42              |
| 2:C:308:LEU:H    | 2:C:308:LEU:HD23 | 1.84                     | 0.42              |
| 2:C:446:LEU:HD23 | 2:C:446:LEU:C    | 2.45                     | 0.42              |
| 2:C:587:VAL:HG13 | 2:C:591:THR:CG2  | 2.49                     | 0.42              |
| 2:C:797:ARG:HD3  | 2:C:798:ASP:N    | 2.35                     | 0.42              |
| 2:C:1076:MET:HA  | 2:C:1076:MET:CE  | 2.50                     | 0.42              |
| 3:D:21:ARG:HH21  | 3:D:96:GLU:CD    | 2.27                     | 0.42              |
| 3:D:363:PRO:HD3  | 5:F:296:LEU:HD12 | 2.02                     | 0.42              |
| 3:D:429:VAL:HG23 | 3:D:539:ASP:O    | 2.20                     | 0.42              |
| 3:D:1061:PHE:CB  | 3:D:1081:SER:HA  | 2.41                     | 0.42              |
| 3:D:1221:LEU:CD2 | 3:D:1243:ASP:OD2 | 2.68                     | 0.42              |
| 5:F:435:LEU:O    | 5:F:435:LEU:HD23 | 2.19                     | 0.42              |
| 6:J:98:LEU:O     | 6:J:102:LEU:HB2  | 2.20                     | 0.42              |
| 1:B:80:LEU:O     | 1:B:83:LEU:HB3   | 2.20                     | 0.42              |
| 1:B:102:PRO:HB3  | 1:B:130:ASP:CA   | 2.48                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:326:GLU:CB    | 2:C:328:ILE:HG13 | 2.50                     | 0.42              |
| 2:C:519:VAL:HG13  | 2:C:576:VAL:O    | 2.20                     | 0.42              |
| 2:C:822:ARG:NH1   | 2:C:829:ALA:CB   | 2.83                     | 0.42              |
| 2:C:891:ASN:ND2   | 2:C:930:GLN:OE1  | 2.52                     | 0.42              |
| 2:C:955:TRP:CD1   | 2:C:956:ALA:HB2  | 2.54                     | 0.42              |
| 3:D:64:LYS:HZ2    | 3:D:65:TYR:HE2   | 1.62                     | 0.42              |
| 5:F:299:ASN:HB3   | 5:F:328:LEU:HD11 | 2.00                     | 0.42              |
| 1:A:54:ILE:HD11   | 1:A:77:ILE:HD11  | 2.02                     | 0.42              |
| 1:A:61:HIS:H      | 1:A:61:HIS:CD2   | 2.38                     | 0.42              |
| 2:C:68:PRO:O      | 2:C:71:ARG:HB3   | 2.20                     | 0.42              |
| 2:C:134:PHE:CE1   | 2:C:153:PHE:HD1  | 2.37                     | 0.42              |
| 2:C:180:VAL:HG11  | 2:C:379:ARG:NH1  | 2.34                     | 0.42              |
| 2:C:540:VAL:O     | 2:C:540:VAL:HG12 | 2.20                     | 0.42              |
| 2:C:720:LEU:HD23  | 2:C:913:VAL:HA   | 2.02                     | 0.42              |
| 2:C:1044:ARG:NH2  | 2:C:1048:PRO:O   | 2.52                     | 0.42              |
| 3:D:144:ARG:O     | 3:D:144:ARG:HD2  | 2.20                     | 0.42              |
| 3:D:844:LEU:HD12  | 3:D:844:LEU:N    | 2.35                     | 0.42              |
| 3:D:1050:THR:HG22 | 3:D:1106:GLU:C   | 2.45                     | 0.42              |
| 5:F:266:LEU:HD13  | 5:F:266:LEU:C    | 2.44                     | 0.42              |
| 5:F:345:THR:HA    | 7:O:30:DC:H41    | 1.85                     | 0.42              |
| 1:A:95:MET:HG2    | 1:A:113:PRO:HD2  | 2.01                     | 0.42              |
| 1:A:186:ARG:HA    | 1:A:186:ARG:HD3  | 1.82                     | 0.42              |
| 1:A:223:ARG:C     | 1:A:225:LEU:N    | 2.77                     | 0.42              |
| 2:C:225:ARG:CB    | 2:C:231:ARG:HA   | 2.25                     | 0.42              |
| 2:C:275:LEU:HD12  | 2:C:276:ASP:N    | 2.35                     | 0.42              |
| 2:C:731:TYR:OH    | 3:D:578:ARG:HD3  | 2.19                     | 0.42              |
| 2:C:1017:GLU:HB3  | 2:C:1018:PRO:HD2 | 2.02                     | 0.42              |
| 2:C:1052:ILE:HB   | 5:F:436:GLY:O    | 2.20                     | 0.42              |
| 3:D:140:ASP:O     | 3:D:142:GLU:N    | 2.52                     | 0.42              |
| 3:D:320:ILE:HD11  | 3:D:324:LEU:CD1  | 2.50                     | 0.42              |
| 3:D:824:VAL:HG21  | 3:D:836:VAL:HG21 | 2.02                     | 0.42              |
| 3:D:933:ALA:O     | 3:D:934:GLY:C    | 2.62                     | 0.42              |
| 8:P:10:DT:H2"     | 8:P:11:DA:C8     | 2.54                     | 0.42              |
| 1:A:9:LEU:HD23    | 1:A:9:LEU:C      | 2.44                     | 0.41              |
| 1:A:95:MET:CE     | 1:A:112:PRO:HB3  | 2.44                     | 0.41              |
| 1:A:181:THR:HG21  | 1:A:189:PHE:CZ   | 2.55                     | 0.41              |
| 2:C:71:ARG:O      | 2:C:75:ALA:CB    | 2.67                     | 0.41              |
| 2:C:264:LYS:HB3   | 5:F:202:PHE:N    | 2.34                     | 0.41              |
| 2:C:558:ARG:NH2   | 2:C:572:PRO:HD3  | 2.32                     | 0.41              |
| 2:C:861:LEU:CB    | 2:C:862:PRO:HD2  | 2.44                     | 0.41              |
| 2:C:1093:SER:HB2  | 3:D:420:LYS:HD3  | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:130:TYR:OH    | 3:D:387:ARG:HG2   | 2.20                     | 0.41              |
| 3:D:345:ARG:HA    | 3:D:348:ILE:HG22  | 2.01                     | 0.41              |
| 3:D:707:ILE:O     | 3:D:707:ILE:HG12  | 2.20                     | 0.41              |
| 3:D:749:TYR:CE1   | 3:D:780:GLU:HB2   | 2.49                     | 0.41              |
| 8:P:1:DA:H2''     | 8:P:2:DG:C5'      | 2.50                     | 0.41              |
| 1:A:218:LEU:HD21  | 1:B:34:LEU:HD22   | 2.02                     | 0.41              |
| 1:B:208:LEU:HD12  | 1:B:208:LEU:O     | 2.20                     | 0.41              |
| 2:C:254:PHE:CA    | 2:C:255:SER:HB2   | 2.50                     | 0.41              |
| 2:C:612:GLN:HA    | 2:C:1031:MET:HE1  | 2.02                     | 0.41              |
| 2:C:672:MET:CE    | 2:C:703:ALA:HB2   | 2.50                     | 0.41              |
| 2:C:946:VAL:N     | 2:C:964:LEU:O     | 2.31                     | 0.41              |
| 2:C:946:VAL:HG23  | 2:C:964:LEU:O     | 2.20                     | 0.41              |
| 2:C:1103:TYR:CE2  | 2:C:1107:VAL:HG21 | 2.55                     | 0.41              |
| 2:C:1124:LEU:O    | 2:C:1128:LEU:HG   | 2.20                     | 0.41              |
| 3:D:25:TYR:CE2    | 3:D:91:ARG:HG2    | 2.56                     | 0.41              |
| 3:D:56:ARG:HB2    | 3:D:59:GLU:HB2    | 2.02                     | 0.41              |
| 3:D:118:LEU:CB    | 3:D:120:LEU:HD13  | 2.49                     | 0.41              |
| 3:D:207:GLN:NE2   | 3:D:211:ARG:NH1   | 2.67                     | 0.41              |
| 3:D:499:ASN:ND2   | 3:D:503:THR:OG1   | 2.49                     | 0.41              |
| 3:D:740:PRO:HG2   | 3:D:741:ARG:HG3   | 2.01                     | 0.41              |
| 3:D:1053:VAL:HG12 | 3:D:1103:ASP:H    | 1.85                     | 0.41              |
| 3:D:1122:LEU:HD22 | 3:D:1207:LEU:HB2  | 2.02                     | 0.41              |
| 4:E:56:TYR:CE2    | 4:E:106:HIS:HD2   | 2.37                     | 0.41              |
| 5:F:278:ARG:HH22  | 5:F:282:MET:CG    | 2.34                     | 0.41              |
| 5:F:297:GLU:HA    | 5:F:300:LEU:HG    | 2.03                     | 0.41              |
| 5:F:439:ILE:CD1   | 6:J:6:LEU:HD13    | 2.45                     | 0.41              |
| 1:B:111:VAL:O     | 1:B:111:VAL:HG13  | 2.20                     | 0.41              |
| 1:B:179:ASP:HB2   | 1:B:191:LYS:HB3   | 2.02                     | 0.41              |
| 2:C:38:ARG:NH1    | 2:C:971:ILE:CG2   | 2.84                     | 0.41              |
| 2:C:224:VAL:HB    | 2:C:232:GLN:C     | 2.46                     | 0.41              |
| 3:D:140:ASP:O     | 3:D:141:GLU:C     | 2.63                     | 0.41              |
| 1:A:223:ARG:O     | 1:A:225:LEU:N     | 2.53                     | 0.41              |
| 1:B:2:LEU:HD23    | 1:B:3:ILE:H       | 1.83                     | 0.41              |
| 1:B:69:VAL:HA     | 1:B:127:THR:O     | 2.21                     | 0.41              |
| 2:C:267:THR:HG21  | 2:C:273:ALA:CA    | 2.50                     | 0.41              |
| 2:C:338:VAL:O     | 2:C:339:VAL:C     | 2.62                     | 0.41              |
| 2:C:763:LYS:HZ3   | 3:D:332:GLY:H     | 1.66                     | 0.41              |
| 2:C:824:ILE:HG22  | 2:C:825:PHE:CD1   | 2.54                     | 0.41              |
| 3:D:244:LEU:O     | 3:D:249:GLY:N     | 2.54                     | 0.41              |
| 3:D:337:THR:OG1   | 3:D:338:SER:N     | 2.53                     | 0.41              |
| 3:D:527:LEU:HD13  | 3:D:713:VAL:CG1   | 2.50                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:F:415:GLN:NE2  | 5:F:418:ARG:HH12  | 2.18                     | 0.41              |
| 5:F:456:LEU:HD13 | 5:F:526:TYR:HD2   | 1.85                     | 0.41              |
| 5:F:487:ARG:HB2  | 5:F:492:ILE:HG23  | 2.02                     | 0.41              |
| 5:F:495:VAL:HG22 | 5:F:495:VAL:O     | 2.20                     | 0.41              |
| 8:P:23:DA:H2'    | 8:P:24:DA:H8      | 1.85                     | 0.41              |
| 1:B:21:PHE:HE2   | 1:B:196:VAL:HG11  | 1.85                     | 0.41              |
| 2:C:101:GLY:C    | 2:C:142:ASN:HD22  | 2.25                     | 0.41              |
| 2:C:317:ASN:HB3  | 2:C:324:VAL:HG12  | 2.01                     | 0.41              |
| 2:C:611:MET:O    | 2:C:1031:MET:HE1  | 2.20                     | 0.41              |
| 2:C:658:ILE:HG22 | 2:C:659:THR:N     | 2.35                     | 0.41              |
| 3:D:335:PHE:O    | 5:F:420:PRO:HA    | 2.21                     | 0.41              |
| 3:D:468:ASN:ND2  | 3:D:470:LYS:H     | 2.19                     | 0.41              |
| 3:D:627:LEU:HD23 | 3:D:628:SER:H     | 1.84                     | 0.41              |
| 3:D:923:ARG:CB   | 3:D:962:VAL:HG11  | 2.51                     | 0.41              |
| 6:J:76:LYS:HD2   | 6:J:76:LYS:O      | 2.20                     | 0.41              |
| 7:O:10:DA:H5'    | 7:O:10:DA:C8      | 2.56                     | 0.41              |
| 7:O:12:DG:H5''   | 7:O:12:DG:H8      | 1.85                     | 0.41              |
| 1:B:143:GLY:HA3  | 1:B:168:TYR:CD2   | 2.55                     | 0.41              |
| 2:C:345:LEU:O    | 2:C:345:LEU:HD22  | 2.20                     | 0.41              |
| 3:D:84:ARG:O     | 3:D:87:VAL:HG22   | 2.20                     | 0.41              |
| 3:D:370:GLU:HA   | 3:D:370:GLU:OE1   | 2.20                     | 0.41              |
| 3:D:392:THR:HA   | 3:D:399:LEU:HD12  | 2.01                     | 0.41              |
| 3:D:679:LEU:O    | 3:D:679:LEU:HD23  | 2.21                     | 0.41              |
| 3:D:820:MET:HE2  | 3:D:822:GLY:CA    | 2.45                     | 0.41              |
| 3:D:939:GLU:OE1  | 3:D:942:GLN:NE2   | 2.54                     | 0.41              |
| 3:D:1097:ARG:HD2 | 3:D:1098:VAL:N    | 2.36                     | 0.41              |
| 5:F:206:GLU:C    | 5:F:208:GLU:H     | 2.28                     | 0.41              |
| 5:F:493:GLY:O    | 5:F:497:GLY:N     | 2.54                     | 0.41              |
| 1:A:14:LEU:HD12  | 1:A:18:ARG:HD2    | 2.02                     | 0.41              |
| 1:A:177:LYS:CG   | 1:A:193:ILE:HD11  | 2.50                     | 0.41              |
| 1:B:21:PHE:HZ    | 1:B:204:PRO:O     | 2.04                     | 0.41              |
| 1:B:38:LEU:HD12  | 1:B:42:LEU:HD13   | 2.01                     | 0.41              |
| 2:C:52:GLY:O     | 2:C:54:LEU:N      | 2.53                     | 0.41              |
| 2:C:721:VAL:HG11 | 2:C:1028:MET:HB2  | 2.03                     | 0.41              |
| 2:C:862:PRO:HG2  | 2:C:865:VAL:HG21  | 2.01                     | 0.41              |
| 2:C:1020:PRO:HG2 | 2:C:1021:TYR:CD2  | 2.55                     | 0.41              |
| 3:D:123:LYS:HE3  | 3:D:123:LYS:HB2   | 1.83                     | 0.41              |
| 3:D:453:LYS:NZ   | 3:D:453:LYS:CB    | 2.83                     | 0.41              |
| 3:D:512:PHE:CE1  | 3:D:561:SER:HB2   | 2.56                     | 0.41              |
| 3:D:557:ILE:HD13 | 4:E:53:LEU:CD2    | 2.50                     | 0.41              |
| 3:D:882:GLN:HB2  | 3:D:1248:LEU:HD11 | 2.02                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:D:915:TYR:CD2  | 3:D:1143:ARG:NH1  | 2.88                     | 0.41              |
| 5:F:371:HIS:CE1  | 7:O:21:DT:OP2     | 2.74                     | 0.41              |
| 7:O:4:DT:H2''    | 7:O:5:DG:C8       | 2.54                     | 0.41              |
| 8:P:14:DA:C1'    | 8:P:15:DC:H5'     | 2.50                     | 0.41              |
| 8:P:19:DT:H2''   | 8:P:20:DG:C8      | 2.54                     | 0.41              |
| 1:A:216:VAL:HG13 | 1:B:216:VAL:HG22  | 2.03                     | 0.41              |
| 2:C:627:GLY:O    | 2:C:973:SER:HA    | 2.20                     | 0.41              |
| 3:D:638:THR:HG22 | 3:D:661:ALA:CB    | 2.50                     | 0.41              |
| 3:D:882:GLN:HG3  | 3:D:883:ASP:OD1   | 2.21                     | 0.41              |
| 3:D:1172:SER:HB3 | 3:D:1199:GLU:HB3  | 2.00                     | 0.41              |
| 1:B:95:MET:SD    | 1:B:113:PRO:HD2   | 2.61                     | 0.41              |
| 1:B:138:LEU:HD12 | 1:B:138:LEU:N     | 2.36                     | 0.41              |
| 1:B:215:LEU:HD23 | 1:B:215:LEU:O     | 2.20                     | 0.41              |
| 2:C:222:VAL:HG11 | 2:C:234:VAL:CG1   | 2.50                     | 0.41              |
| 2:C:254:PHE:CE1  | 2:C:347:ARG:NH1   | 2.85                     | 0.41              |
| 2:C:282:ARG:CB   | 2:C:283:PRO:CA    | 2.98                     | 0.41              |
| 2:C:410:GLU:HA   | 2:C:410:GLU:OE1   | 2.21                     | 0.41              |
| 2:C:518:LYS:O    | 2:C:518:LYS:HG3   | 2.19                     | 0.41              |
| 2:C:563:ARG:CG   | 2:C:564:LYS:H     | 2.34                     | 0.41              |
| 2:C:645:GLU:HA   | 2:C:645:GLU:OE1   | 2.20                     | 0.41              |
| 2:C:737:LEU:O    | 2:C:904:MET:HE1   | 2.20                     | 0.41              |
| 2:C:741:LEU:CA   | 2:C:746:VAL:HG12  | 2.51                     | 0.41              |
| 2:C:1123:VAL:O   | 2:C:1127:GLU:HG3  | 2.21                     | 0.41              |
| 2:C:1135:VAL:O   | 2:C:1135:VAL:HG23 | 2.20                     | 0.41              |
| 9:C:1201:FI8:C24 | 9:C:1201:FI8:C25  | 2.98                     | 0.41              |
| 3:D:527:LEU:HD22 | 3:D:575:ALA:O     | 2.21                     | 0.41              |
| 3:D:527:LEU:HD11 | 3:D:713:VAL:HG12  | 2.02                     | 0.41              |
| 3:D:778:TRP:CE2  | 3:D:835:PRO:HD3   | 2.55                     | 0.41              |
| 3:D:922:ALA:HB1  | 3:D:981:ARG:HB3   | 2.03                     | 0.41              |
| 3:D:981:ARG:HG2  | 3:D:982:SER:N     | 2.34                     | 0.41              |
| 3:D:1068:PRO:HG2 | 3:D:1072:GLY:H    | 1.86                     | 0.41              |
| 3:D:1089:PHE:C   | 3:D:1090:LYS:HD3  | 2.45                     | 0.41              |
| 3:D:1089:PHE:HD2 | 3:D:1099:LEU:HB2  | 1.85                     | 0.41              |
| 3:D:1217:THR:OG1 | 3:D:1218:ASP:N    | 2.54                     | 0.41              |
| 4:E:32:PRO:CB    | 4:E:36:THR:HG23   | 2.50                     | 0.41              |
| 5:F:244:GLU:CD   | 5:F:244:GLU:H     | 2.29                     | 0.41              |
| 5:F:509:LYS:HD2  | 5:F:509:LYS:HA    | 1.90                     | 0.41              |
| 6:J:98:LEU:HD23  | 6:J:98:LEU:C      | 2.46                     | 0.41              |
| 1:B:3:ILE:HG22   | 1:B:233:GLU:O     | 2.20                     | 0.41              |
| 1:B:90:ASP:OD1   | 1:B:142:ARG:HD3   | 2.20                     | 0.41              |
| 2:C:339:VAL:HA   | 2:C:342:ILE:CD1   | 2.40                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:809:LYS:HZ2  | 2:C:809:LYS:CB    | 2.27                     | 0.41              |
| 2:C:840:PRO:HD2  | 2:C:843:GLU:OE1   | 2.21                     | 0.41              |
| 3:D:345:ARG:HA   | 3:D:348:ILE:CG2   | 2.51                     | 0.41              |
| 2:C:435:GLN:CG   | 2:C:460:PRO:HD3   | 2.44                     | 0.40              |
| 2:C:455:LEU:HD23 | 2:C:455:LEU:N     | 2.36                     | 0.40              |
| 2:C:607:MET:O    | 2:C:611:MET:HG3   | 2.21                     | 0.40              |
| 2:C:1040:LYS:HB3 | 3:D:540:GLN:NE2   | 2.35                     | 0.40              |
| 3:D:293:LEU:HD23 | 3:D:293:LEU:O     | 2.20                     | 0.40              |
| 3:D:367:VAL:HG12 | 3:D:371:LYS:HE3   | 2.02                     | 0.40              |
| 3:D:606:HIS:HB2  | 3:D:607:PRO:CD    | 2.46                     | 0.40              |
| 3:D:744:GLU:HG3  | 3:D:745:ILE:N     | 2.35                     | 0.40              |
| 3:D:910:LEU:O    | 3:D:910:LEU:CD1   | 2.69                     | 0.40              |
| 4:E:32:PRO:HG2   | 4:E:37:ASN:HB2    | 2.02                     | 0.40              |
| 1:A:41:THR:OG1   | 1:A:215:LEU:HD21  | 2.22                     | 0.40              |
| 2:C:74:ALA:HB1   | 2:C:79:ASP:OD2    | 2.21                     | 0.40              |
| 2:C:224:VAL:HB   | 2:C:232:GLN:O     | 2.20                     | 0.40              |
| 2:C:231:ARG:HD2  | 5:F:205:ASP:CB    | 2.39                     | 0.40              |
| 2:C:254:PHE:CE1  | 2:C:347:ARG:HG2   | 2.54                     | 0.40              |
| 2:C:333:LEU:HD22 | 2:C:338:VAL:HG23  | 2.02                     | 0.40              |
| 2:C:336:GLU:O    | 2:C:337:ASP:C     | 2.62                     | 0.40              |
| 2:C:339:VAL:CG2  | 2:C:340:ALA:N     | 2.85                     | 0.40              |
| 2:C:542:ALA:N    | 2:C:578:TYR:O     | 2.48                     | 0.40              |
| 2:C:558:ARG:HH21 | 2:C:572:PRO:CD    | 2.30                     | 0.40              |
| 2:C:732:GLU:O    | 2:C:733:ASP:HB2   | 2.21                     | 0.40              |
| 2:C:754:GLU:HB2  | 2:C:872:TYR:CD1   | 2.56                     | 0.40              |
| 3:D:55:THR:HG22  | 3:D:55:THR:O      | 2.22                     | 0.40              |
| 3:D:327:MET:HG3  | 3:D:337:THR:HB    | 2.03                     | 0.40              |
| 3:D:467:GLN:HA   | 3:D:467:GLN:NE2   | 2.34                     | 0.40              |
| 3:D:663:MET:HE2  | 3:D:663:MET:HB3   | 1.96                     | 0.40              |
| 3:D:673:PHE:O    | 3:D:676:LEU:HB2   | 2.21                     | 0.40              |
| 3:D:746:LEU:HD23 | 3:D:746:LEU:HA    | 1.94                     | 0.40              |
| 3:D:780:GLU:HA   | 3:D:780:GLU:OE1   | 2.21                     | 0.40              |
| 3:D:820:MET:HG2  | 3:D:822:GLY:N     | 2.36                     | 0.40              |
| 3:D:1122:LEU:CA  | 3:D:1130:VAL:HG21 | 2.51                     | 0.40              |
| 5:F:386:LEU:HD11 | 5:F:398:GLU:OE2   | 2.20                     | 0.40              |
| 1:B:15:THR:O     | 1:B:17:ASN:N      | 2.54                     | 0.40              |
| 1:B:95:MET:HG2   | 1:B:113:PRO:HD2   | 2.03                     | 0.40              |
| 2:C:61:PHE:C     | 2:C:63:TRP:N      | 2.69                     | 0.40              |
| 2:C:96:ILE:O     | 2:C:104:SER:HA    | 2.21                     | 0.40              |
| 2:C:192:ASP:CG   | 2:C:195:THR:HG23  | 2.46                     | 0.40              |
| 2:C:1074:TRP:CH2 | 3:D:875:ARG:HG3   | 2.55                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:170:LEU:HA   | 3:D:173:ARG:HG2  | 2.04                     | 0.40              |
| 3:D:890:ASP:HA   | 3:D:977:THR:OG1  | 2.21                     | 0.40              |
| 3:D:1063:LYS:HD3 | 3:D:1064:ILE:H   | 1.87                     | 0.40              |
| 3:D:1063:LYS:CE  | 3:D:1078:ASP:HA  | 2.52                     | 0.40              |
| 5:F:205:ASP:CG   | 5:F:206:GLU:H    | 2.29                     | 0.40              |
| 5:F:274:PRO:HD2  | 5:F:277:GLN:HB2  | 2.03                     | 0.40              |
| 5:F:310:TYR:HD2  | 5:F:355:ILE:HG21 | 1.86                     | 0.40              |
| 5:F:415:GLN:HA   | 5:F:418:ARG:NH2  | 2.36                     | 0.40              |
| 2:C:252:PHE:O    | 2:C:255:SER:O    | 2.40                     | 0.40              |
| 2:C:373:PHE:HD2  | 2:C:482:ARG:CD   | 2.34                     | 0.40              |
| 2:C:756:GLU:HB2  | 2:C:870:ARG:HG2  | 2.03                     | 0.40              |
| 3:D:211:ARG:HA   | 3:D:214:ARG:HH21 | 1.84                     | 0.40              |
| 3:D:558:LEU:HD13 | 4:E:54:VAL:HG21  | 2.03                     | 0.40              |
| 3:D:653:HIS:CD2  | 3:D:654:SER:H    | 2.39                     | 0.40              |
| 3:D:660:ASP:OD1  | 3:D:660:ASP:N    | 2.54                     | 0.40              |
| 3:D:771:ASN:O    | 3:D:775:VAL:HG23 | 2.22                     | 0.40              |
| 3:D:834:ARG:CB   | 3:D:835:PRO:CA   | 3.00                     | 0.40              |
| 3:D:1139:GLN:HG3 | 3:D:1143:ARG:NE  | 2.34                     | 0.40              |
| 4:E:32:PRO:HB2   | 4:E:37:ASN:HB2   | 2.02                     | 0.40              |
| 5:F:488:THR:HB   | 8:P:19:DT:H3'    | 2.02                     | 0.40              |
| 1:A:218:LEU:C    | 1:A:218:LEU:HD23 | 2.46                     | 0.40              |
| 1:B:179:ASP:HB2  | 1:B:191:LYS:HE2  | 2.03                     | 0.40              |
| 2:C:280:LYS:HD3  | 2:C:280:LYS:HA   | 1.94                     | 0.40              |
| 2:C:651:GLU:OE1  | 2:C:661:MET:HE2  | 2.21                     | 0.40              |
| 2:C:931:ILE:O    | 2:C:934:THR:HB   | 2.21                     | 0.40              |
| 3:D:406:LEU:HD12 | 3:D:406:LEU:N    | 2.37                     | 0.40              |
| 3:D:627:LEU:HD23 | 3:D:628:SER:N    | 2.36                     | 0.40              |
| 3:D:911:ILE:H    | 3:D:911:ILE:CD1  | 2.26                     | 0.40              |
| 3:D:981:ARG:O    | 3:D:1152:LYS:NZ  | 2.54                     | 0.40              |
| 5:F:387:LEU:HD12 | 5:F:393:GLU:HA   | 2.03                     | 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     | 224/347 (65%)   | 206 (92%)  | 18 (8%)   | 0        | 100         | 100 |
| 1   | B     | 235/347 (68%)   | 200 (85%)  | 35 (15%)  | 0        | 100         | 100 |
| 2   | C     | 1109/1181 (94%) | 961 (87%)  | 141 (13%) | 7 (1%)   | 21          | 49  |
| 3   | D     | 1257/1324 (95%) | 1148 (91%) | 105 (8%)  | 4 (0%)   | 36          | 64  |
| 4   | E     | 81/110 (74%)    | 75 (93%)   | 6 (7%)    | 0        | 100         | 100 |
| 5   | F     | 324/531 (61%)   | 306 (94%)  | 18 (6%)   | 0        | 100         | 100 |
| 6   | J     | 105/111 (95%)   | 89 (85%)   | 15 (14%)  | 1 (1%)   | 12          | 39  |
| All | All   | 3335/3951 (84%) | 2985 (90%) | 338 (10%) | 12 (0%)  | 31          | 58  |

All (12) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | C     | 62   | GLU  |
| 2   | C     | 323  | HIS  |
| 3   | D     | 909  | THR  |
| 3   | D     | 910  | LEU  |
| 3   | D     | 904  | ARG  |
| 2   | C     | 61   | PHE  |
| 2   | C     | 225  | ARG  |
| 2   | C     | 231  | ARG  |
| 2   | C     | 959  | LEU  |
| 3   | D     | 1196 | GLU  |
| 2   | C     | 224  | VAL  |
| 6   | J     | 70   | PRO  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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     | 195/297 (66%) | 186 (95%) | 9 (5%)   | 24          | 50 |
| 1   | B     | 197/297 (66%) | 179 (91%) | 18 (9%)  | 9           | 30 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 2   | C     | 924/997 (93%)   | 865 (94%)  | 59 (6%)  | 16          | 42 |
| 3   | D     | 1041/1103 (94%) | 967 (93%)  | 74 (7%)  | 13          | 39 |
| 4   | E     | 69/89 (78%)     | 64 (93%)   | 5 (7%)   | 13          | 39 |
| 5   | F     | 272/429 (63%)   | 246 (90%)  | 26 (10%) | 8           | 28 |
| 6   | J     | 93/97 (96%)     | 80 (86%)   | 13 (14%) | 3           | 14 |
| All | All   | 2791/3309 (84%) | 2587 (93%) | 204 (7%) | 15          | 39 |

All (204) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 18  | ARG  |
| 1   | A     | 22  | VAL  |
| 1   | A     | 34  | LEU  |
| 1   | A     | 51  | VAL  |
| 1   | A     | 93  | VAL  |
| 1   | A     | 116 | VAL  |
| 1   | A     | 136 | VAL  |
| 1   | A     | 138 | LEU  |
| 1   | A     | 221 | LEU  |
| 1   | B     | 22  | VAL  |
| 1   | B     | 27  | GLU  |
| 1   | B     | 38  | LEU  |
| 1   | B     | 43  | LEU  |
| 1   | B     | 61  | HIS  |
| 1   | B     | 70  | LYS  |
| 1   | B     | 84  | VAL  |
| 1   | B     | 93  | VAL  |
| 1   | B     | 117 | THR  |
| 1   | B     | 141 | GLU  |
| 1   | B     | 147 | VAL  |
| 1   | B     | 153 | ARG  |
| 1   | B     | 172 | LEU  |
| 1   | B     | 175 | THR  |
| 1   | B     | 177 | LYS  |
| 1   | B     | 182 | ARG  |
| 1   | B     | 196 | VAL  |
| 1   | B     | 216 | VAL  |
| 2   | C     | 59  | ASP  |
| 2   | C     | 79  | ASP  |
| 2   | C     | 90  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | C     | 93  | LEU  |
| 2   | C     | 192 | ASP  |
| 2   | C     | 195 | THR  |
| 2   | C     | 196 | ASP  |
| 2   | C     | 199 | LEU  |
| 2   | C     | 203 | LYS  |
| 2   | C     | 212 | LEU  |
| 2   | C     | 215 | ASP  |
| 2   | C     | 226 | ILE  |
| 2   | C     | 230 | ARG  |
| 2   | C     | 232 | GLN  |
| 2   | C     | 258 | MET  |
| 2   | C     | 261 | THR  |
| 2   | C     | 266 | ASN  |
| 2   | C     | 313 | ARG  |
| 2   | C     | 318 | LYS  |
| 2   | C     | 328 | ILE  |
| 2   | C     | 333 | LEU  |
| 2   | C     | 343 | GLU  |
| 2   | C     | 345 | LEU  |
| 2   | C     | 373 | PHE  |
| 2   | C     | 397 | GLU  |
| 2   | C     | 406 | THR  |
| 2   | C     | 420 | ILE  |
| 2   | C     | 423 | VAL  |
| 2   | C     | 455 | LEU  |
| 2   | C     | 500 | LEU  |
| 2   | C     | 540 | VAL  |
| 2   | C     | 571 | VAL  |
| 2   | C     | 577 | ASP  |
| 2   | C     | 589 | VAL  |
| 2   | C     | 628 | THR  |
| 2   | C     | 668 | ARG  |
| 2   | C     | 694 | ASP  |
| 2   | C     | 709 | ASP  |
| 2   | C     | 787 | ARG  |
| 2   | C     | 797 | ARG  |
| 2   | C     | 809 | LYS  |
| 2   | C     | 814 | LEU  |
| 2   | C     | 835 | THR  |
| 2   | C     | 839 | VAL  |
| 2   | C     | 861 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | C     | 899  | LEU  |
| 2   | C     | 909  | ASP  |
| 2   | C     | 936  | LEU  |
| 2   | C     | 945  | LYS  |
| 2   | C     | 950  | LYS  |
| 2   | C     | 959  | LEU  |
| 2   | C     | 962  | GLU  |
| 2   | C     | 963  | LEU  |
| 2   | C     | 965  | GLU  |
| 2   | C     | 997  | ASP  |
| 2   | C     | 1009 | MET  |
| 2   | C     | 1031 | MET  |
| 2   | C     | 1057 | LEU  |
| 2   | C     | 1076 | MET  |
| 3   | D     | 12   | ILE  |
| 3   | D     | 51   | ILE  |
| 3   | D     | 67   | ARG  |
| 3   | D     | 82   | VAL  |
| 3   | D     | 86   | LYS  |
| 3   | D     | 126  | GLU  |
| 3   | D     | 135  | VAL  |
| 3   | D     | 147  | GLU  |
| 3   | D     | 152  | GLU  |
| 3   | D     | 162  | VAL  |
| 3   | D     | 164  | ASP  |
| 3   | D     | 171  | GLU  |
| 3   | D     | 173  | ARG  |
| 3   | D     | 177  | LEU  |
| 3   | D     | 207  | GLN  |
| 3   | D     | 214  | ARG  |
| 3   | D     | 216  | LEU  |
| 3   | D     | 219  | LEU  |
| 3   | D     | 222  | ILE  |
| 3   | D     | 238  | GLU  |
| 3   | D     | 263  | LYS  |
| 3   | D     | 275  | GLU  |
| 3   | D     | 330  | LEU  |
| 3   | D     | 410  | GLN  |
| 3   | D     | 414  | ARG  |
| 3   | D     | 453  | LYS  |
| 3   | D     | 463  | LEU  |
| 3   | D     | 467  | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | D     | 469  | ILE  |
| 3   | D     | 478  | ARG  |
| 3   | D     | 483  | VAL  |
| 3   | D     | 490  | VAL  |
| 3   | D     | 499  | ASN  |
| 3   | D     | 506  | ARG  |
| 3   | D     | 513  | GLU  |
| 3   | D     | 517  | VAL  |
| 3   | D     | 574  | LEU  |
| 3   | D     | 600  | GLN  |
| 3   | D     | 627  | LEU  |
| 3   | D     | 639  | GLN  |
| 3   | D     | 657  | GLN  |
| 3   | D     | 677  | LEU  |
| 3   | D     | 687  | GLN  |
| 3   | D     | 725  | THR  |
| 3   | D     | 733  | MET  |
| 3   | D     | 741  | ARG  |
| 3   | D     | 766  | ASN  |
| 3   | D     | 793  | TYR  |
| 3   | D     | 834  | ARG  |
| 3   | D     | 846  | VAL  |
| 3   | D     | 847  | LEU  |
| 3   | D     | 862  | ASP  |
| 3   | D     | 883  | ASP  |
| 3   | D     | 904  | ARG  |
| 3   | D     | 910  | LEU  |
| 3   | D     | 911  | ILE  |
| 3   | D     | 948  | GLU  |
| 3   | D     | 957  | ILE  |
| 3   | D     | 1010 | LEU  |
| 3   | D     | 1012 | MET  |
| 3   | D     | 1057 | ASP  |
| 3   | D     | 1061 | PHE  |
| 3   | D     | 1062 | TYR  |
| 3   | D     | 1088 | VAL  |
| 3   | D     | 1090 | LYS  |
| 3   | D     | 1096 | GLU  |
| 3   | D     | 1097 | ARG  |
| 3   | D     | 1098 | VAL  |
| 3   | D     | 1099 | LEU  |
| 3   | D     | 1120 | GLU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | D     | 1121 | VAL  |
| 3   | D     | 1189 | GLU  |
| 3   | D     | 1227 | GLN  |
| 3   | D     | 1231 | ARG  |
| 4   | E     | 30   | ASP  |
| 4   | E     | 65   | ASN  |
| 4   | E     | 71   | LEU  |
| 4   | E     | 78   | TYR  |
| 4   | E     | 79   | VAL  |
| 5   | F     | 206  | GLU  |
| 5   | F     | 207  | ASP  |
| 5   | F     | 214  | GLN  |
| 5   | F     | 216  | ARG  |
| 5   | F     | 240  | LEU  |
| 5   | F     | 244  | GLU  |
| 5   | F     | 246  | GLU  |
| 5   | F     | 277  | GLN  |
| 5   | F     | 282  | MET  |
| 5   | F     | 286  | ARG  |
| 5   | F     | 330  | ARG  |
| 5   | F     | 332  | VAL  |
| 5   | F     | 353  | GLN  |
| 5   | F     | 375  | VAL  |
| 5   | F     | 397  | GLU  |
| 5   | F     | 398  | GLU  |
| 5   | F     | 414  | GLN  |
| 5   | F     | 418  | ARG  |
| 5   | F     | 423  | LEU  |
| 5   | F     | 430  | GLU  |
| 5   | F     | 435  | LEU  |
| 5   | F     | 460  | LEU  |
| 5   | F     | 461  | GLN  |
| 5   | F     | 492  | ILE  |
| 5   | F     | 507  | GLU  |
| 5   | F     | 527  | LEU  |
| 6   | J     | 4    | ARG  |
| 6   | J     | 6    | LEU  |
| 6   | J     | 7    | ARG  |
| 6   | J     | 20   | ARG  |
| 6   | J     | 24   | LEU  |
| 6   | J     | 27   | ARG  |
| 6   | J     | 76   | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | J     | 86  | LEU  |
| 6   | J     | 97  | LEU  |
| 6   | J     | 98  | LEU  |
| 6   | J     | 99  | LYS  |
| 6   | J     | 101 | ARG  |
| 6   | J     | 103 | GLU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 61   | HIS  |
| 1   | A     | 226  | ASN  |
| 1   | B     | 5    | GLN  |
| 1   | B     | 79   | ASN  |
| 1   | B     | 151  | GLN  |
| 1   | B     | 152  | ASN  |
| 1   | B     | 185  | GLN  |
| 1   | B     | 226  | ASN  |
| 2   | C     | 57   | GLN  |
| 2   | C     | 169  | ASN  |
| 2   | C     | 200  | HIS  |
| 2   | C     | 317  | ASN  |
| 2   | C     | 349  | HIS  |
| 2   | C     | 388  | GLN  |
| 2   | C     | 435  | GLN  |
| 2   | C     | 442  | GLN  |
| 2   | C     | 476  | HIS  |
| 2   | C     | 479  | HIS  |
| 2   | C     | 585  | GLN  |
| 2   | C     | 612  | GLN  |
| 2   | C     | 751  | HIS  |
| 2   | C     | 891  | ASN  |
| 2   | C     | 920  | HIS  |
| 2   | C     | 986  | GLN  |
| 2   | C     | 1066 | GLN  |
| 3   | D     | 175  | GLN  |
| 3   | D     | 262  | GLN  |
| 3   | D     | 341  | ASN  |
| 3   | D     | 369  | ASN  |
| 3   | D     | 410  | GLN  |
| 3   | D     | 439  | HIS  |
| 3   | D     | 464  | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | D     | 467  | GLN  |
| 3   | D     | 468  | ASN  |
| 3   | D     | 499  | ASN  |
| 3   | D     | 540  | GLN  |
| 3   | D     | 600  | GLN  |
| 3   | D     | 639  | GLN  |
| 3   | D     | 674  | ASN  |
| 3   | D     | 693  | GLN  |
| 3   | D     | 766  | ASN  |
| 3   | D     | 813  | GLN  |
| 3   | D     | 1009 | GLN  |
| 3   | D     | 1084 | GLN  |
| 3   | D     | 1133 | HIS  |
| 3   | D     | 1139 | GLN  |
| 3   | D     | 1145 | GLN  |
| 3   | D     | 1227 | GLN  |
| 3   | D     | 1251 | ASN  |
| 4   | E     | 65   | ASN  |
| 4   | E     | 69   | ASN  |
| 4   | E     | 106  | HIS  |
| 5   | F     | 214  | GLN  |
| 5   | F     | 234  | GLN  |
| 5   | F     | 294  | HIS  |
| 5   | F     | 299  | ASN  |
| 5   | F     | 322  | GLN  |
| 5   | F     | 325  | ASN  |
| 5   | F     | 353  | GLN  |
| 5   | F     | 388  | GLN  |
| 5   | F     | 414  | GLN  |
| 5   | F     | 457  | GLN  |
| 5   | F     | 516  | HIS  |
| 6   | J     | 36   | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 9   | FI8  | C     | 1201 | -    | 74,75,75     | 1.89 | 19 (25%)    | 96,109,109  | 1.58 | 18 (18%)    |

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   |
|-----|------|-------|------|------|---------|---------------|---------|
| 9   | FI8  | C     | 1201 | -    | -       | 20/75/118/118 | 0/3/4/4 |

All (19) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 9   | C     | 1201 | FI8  | C1-C3   | 5.34  | 1.57        | 1.50     |
| 9   | C     | 1201 | FI8  | C14-C15 | 4.52  | 1.54        | 1.45     |
| 9   | C     | 1201 | FI8  | O1-C18  | -4.10 | 1.39        | 1.46     |
| 9   | C     | 1201 | FI8  | O1-C2   | 3.96  | 1.43        | 1.34     |
| 9   | C     | 1201 | FI8  | O17-C49 | 3.83  | 1.43        | 1.34     |
| 9   | C     | 1201 | FI8  | O10-C29 | -3.82 | 1.39        | 1.44     |
| 9   | C     | 1201 | FI8  | C14-C13 | 3.35  | 1.38        | 1.33     |
| 9   | C     | 1201 | FI8  | C38-CL2 | 2.99  | 1.79        | 1.72     |
| 9   | C     | 1201 | FI8  | O10-C33 | 2.92  | 1.40        | 1.34     |
| 9   | C     | 1201 | FI8  | C5-C4   | 2.84  | 1.52        | 1.43     |
| 9   | C     | 1201 | FI8  | C36-CL1 | 2.67  | 1.78        | 1.72     |
| 9   | C     | 1201 | FI8  | C2-C3   | 2.45  | 1.53        | 1.49     |
| 9   | C     | 1201 | FI8  | C10-C9  | 2.45  | 1.38        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 9   | C     | 1201 | FI8  | C11-C10 | 2.43  | 1.54        | 1.50     |
| 9   | C     | 1201 | FI8  | C17-C16 | 2.30  | 1.54        | 1.50     |
| 9   | C     | 1201 | FI8  | C7-C6   | 2.16  | 1.56        | 1.50     |
| 9   | C     | 1201 | FI8  | C11-C12 | -2.16 | 1.51        | 1.53     |
| 9   | C     | 1201 | FI8  | O13-C35 | 2.09  | 1.41        | 1.36     |
| 9   | C     | 1201 | FI8  | O14-C46 | -2.07 | 1.43        | 1.46     |

All (18) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 9   | C     | 1201 | FI8  | C18-C17-C16 | -4.88 | 104.00      | 112.94   |
| 9   | C     | 1201 | FI8  | O14-C46-C45 | 4.60  | 115.06      | 107.67   |
| 9   | C     | 1201 | FI8  | C31-C30-C29 | -4.34 | 106.94      | 113.39   |
| 9   | C     | 1201 | FI8  | O1-C2-C3    | 3.81  | 117.40      | 112.11   |
| 9   | C     | 1201 | FI8  | C7-C6-C5    | -3.73 | 120.69      | 125.44   |
| 9   | C     | 1201 | FI8  | O17-C49-C50 | 3.35  | 117.32      | 111.14   |
| 9   | C     | 1201 | FI8  | C29-O10-C33 | -3.03 | 112.40      | 117.24   |
| 9   | C     | 1201 | FI8  | C38-C37-C36 | 2.94  | 120.93      | 117.78   |
| 9   | C     | 1201 | FI8  | C17-C16-C15 | -2.88 | 121.20      | 127.50   |
| 9   | C     | 1201 | FI8  | C5-C4-C3    | -2.57 | 123.84      | 126.92   |
| 9   | C     | 1201 | FI8  | O2-C2-C3    | -2.57 | 120.30      | 124.09   |
| 9   | C     | 1201 | FI8  | C4-C5-C6    | -2.50 | 117.78      | 123.63   |
| 9   | C     | 1201 | FI8  | C28-C29-C30 | 2.46  | 113.92      | 110.30   |
| 9   | C     | 1201 | FI8  | C35-C36-CL1 | 2.43  | 121.04      | 118.09   |
| 9   | C     | 1201 | FI8  | C45-O17-C49 | -2.30 | 114.39      | 117.87   |
| 9   | C     | 1201 | FI8  | C41-C40-C39 | -2.29 | 106.83      | 112.32   |
| 9   | C     | 1201 | FI8  | C11-C12-C13 | -2.14 | 109.43      | 113.49   |
| 9   | C     | 1201 | FI8  | C24-C13-C12 | 2.06  | 120.03      | 115.96   |

There are no chirality outliers.

All (20) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 9   | C     | 1201 | FI8  | C9-C10-C11-C12  |
| 9   | C     | 1201 | FI8  | C9-C10-C11-C22  |
| 9   | C     | 1201 | FI8  | C10-C11-C22-C23 |
| 9   | C     | 1201 | FI8  | C12-C11-C22-C23 |
| 9   | C     | 1201 | FI8  | O1-C18-C19-O5A  |
| 9   | C     | 1201 | FI8  | C50-C49-O17-C45 |
| 9   | C     | 1201 | FI8  | C34-C33-O10-C29 |
| 9   | C     | 1201 | FI8  | O18-C49-O17-C45 |
| 9   | C     | 1201 | FI8  | O11-C33-O10-C29 |

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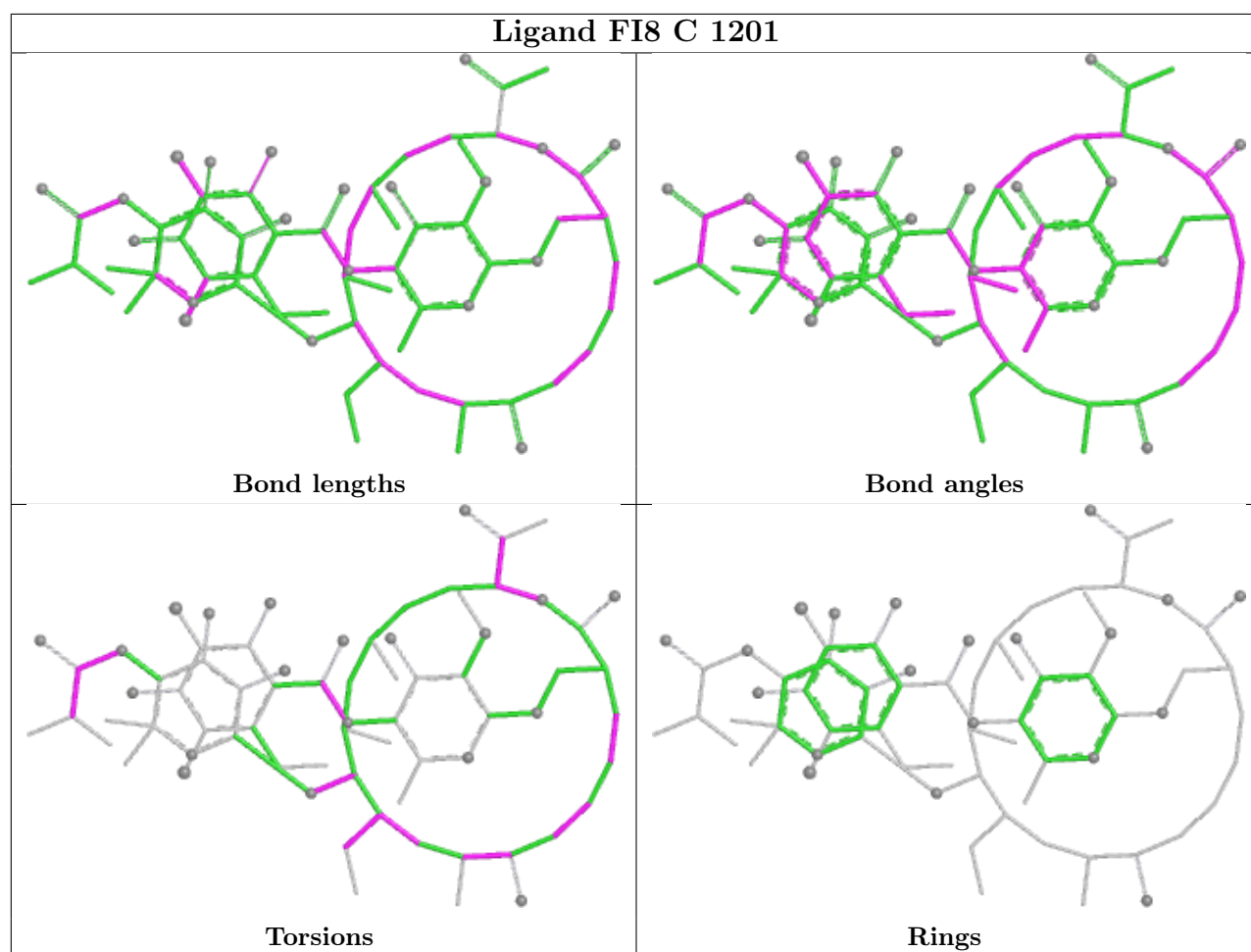
| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 9   | C     | 1201 | FI8  | C19-C18-O1-C2   |
| 9   | C     | 1201 | FI8  | C5-C6-C7-C8     |
| 9   | C     | 1201 | FI8  | C17-C18-C19-C20 |
| 9   | C     | 1201 | FI8  | O1-C18-C19-C20  |
| 9   | C     | 1201 | FI8  | C17-C18-O1-C2   |
| 9   | C     | 1201 | FI8  | C7-C8-C9-C21    |
| 9   | C     | 1201 | FI8  | C11-C12-O4-C42  |
| 9   | C     | 1201 | FI8  | C17-C18-C19-O5A |
| 9   | C     | 1201 | FI8  | O3-C8-C9-C21    |
| 9   | C     | 1201 | FI8  | O17-C49-C50-C51 |
| 9   | C     | 1201 | FI8  | C3-C4-C5-C6     |

There are no ring outliers.

1 monomer is involved in 3 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 9   | C     | 1201 | FI8  | 3       | 0            |

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



## 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.



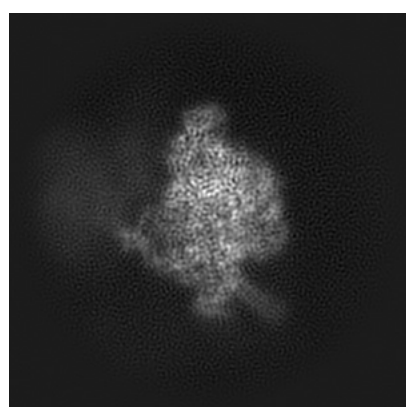
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7319. These allow visual inspection of the internal detail of the map and identification of artifacts.

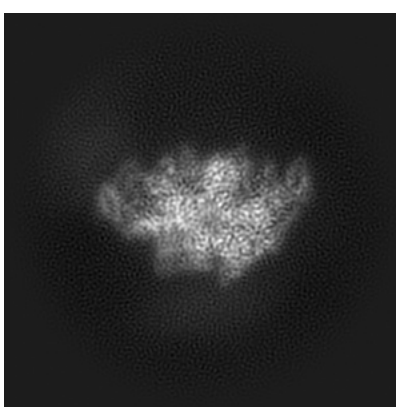
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

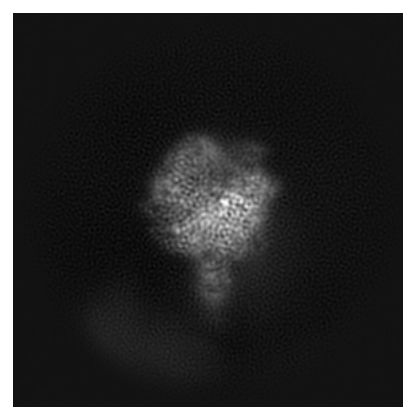
#### 6.1.1 Primary map



X



Y

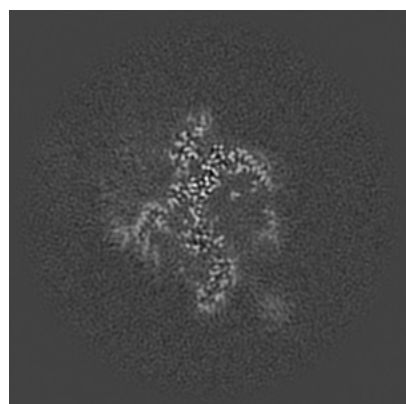


Z

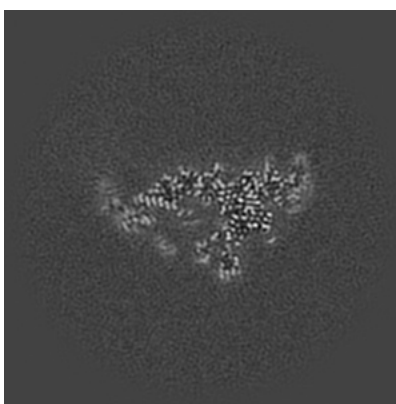
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

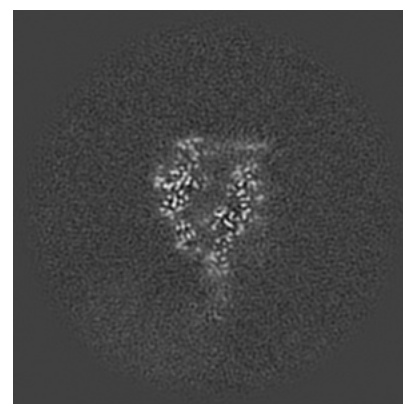
#### 6.2.1 Primary map



X Index: 150



Y Index: 150

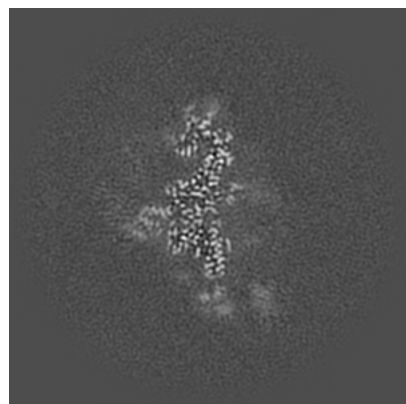


Z Index: 150

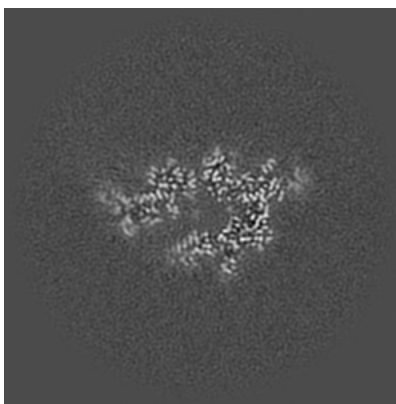
The images above show central slices of the map in three orthogonal directions.

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

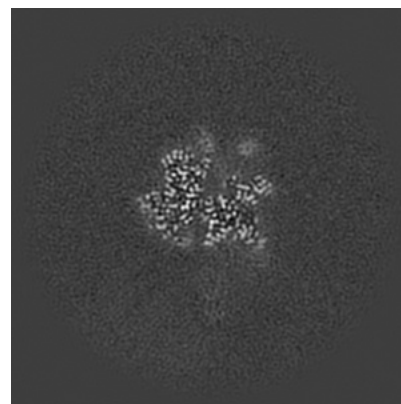
### 6.3.1 Primary map



X Index: 159



Y Index: 158

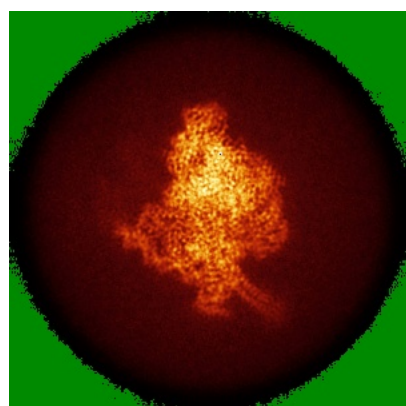


Z Index: 168

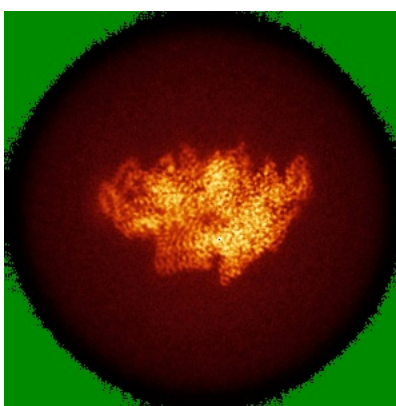
The images above show the largest variance slices of the map in three orthogonal directions.

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

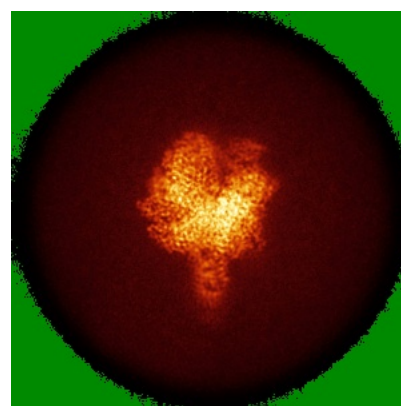
### 6.4.1 Primary map



X



Y

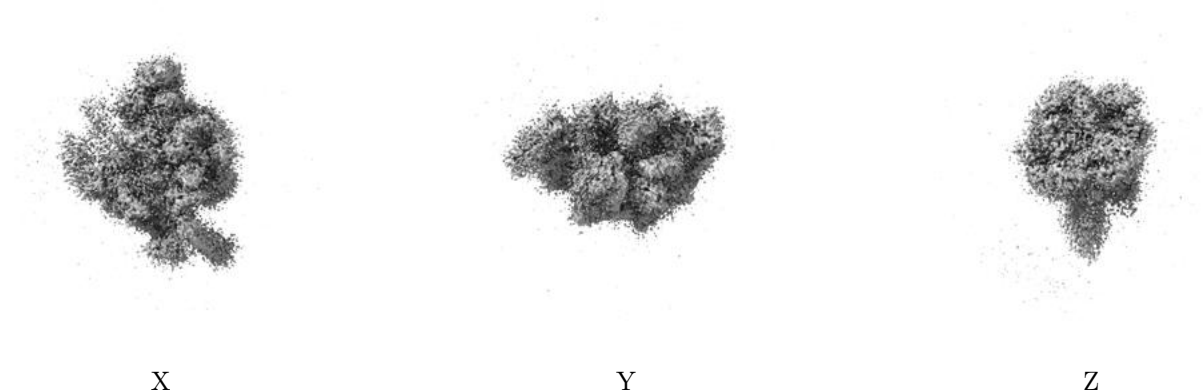


Z

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 0.347. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

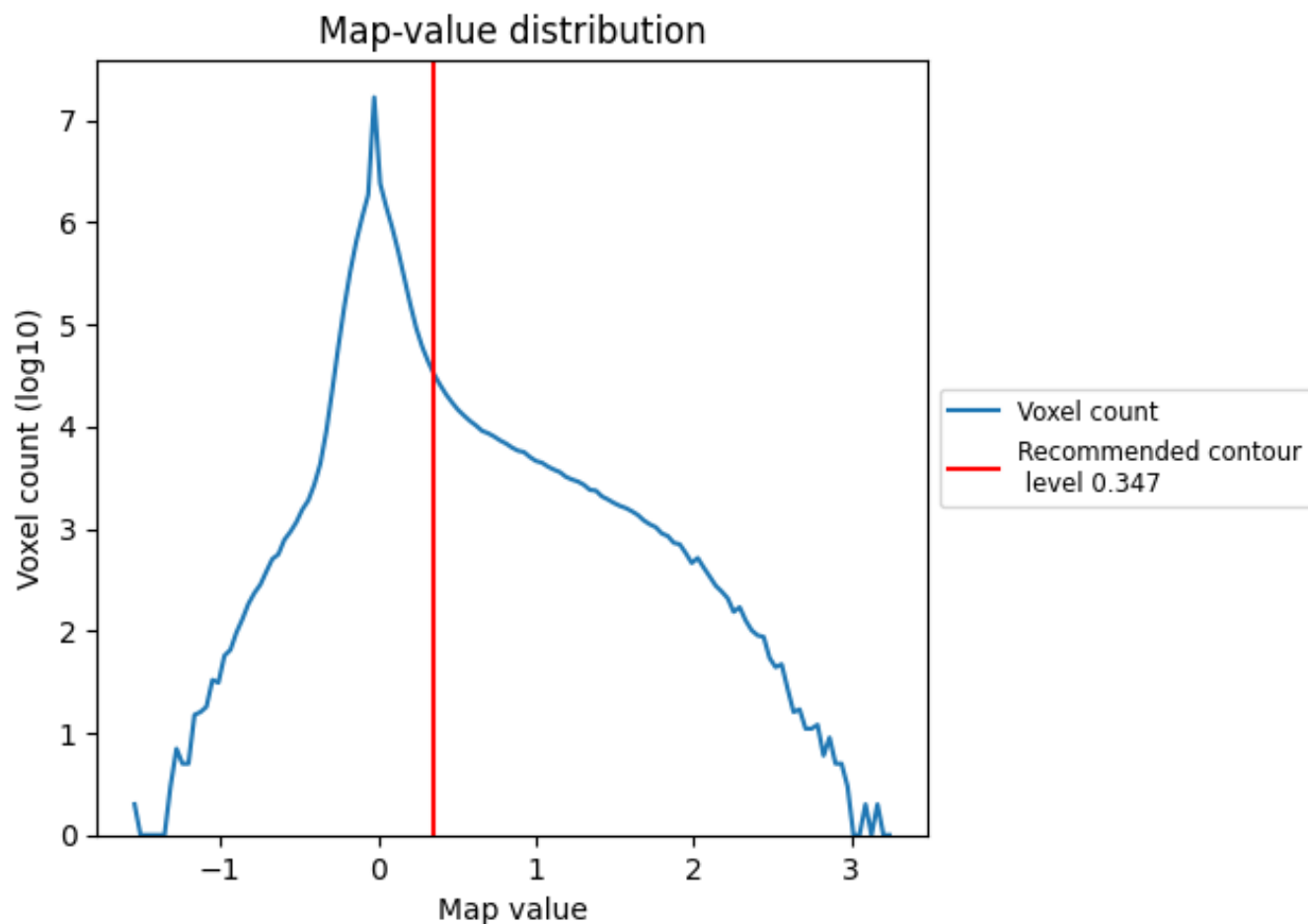
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

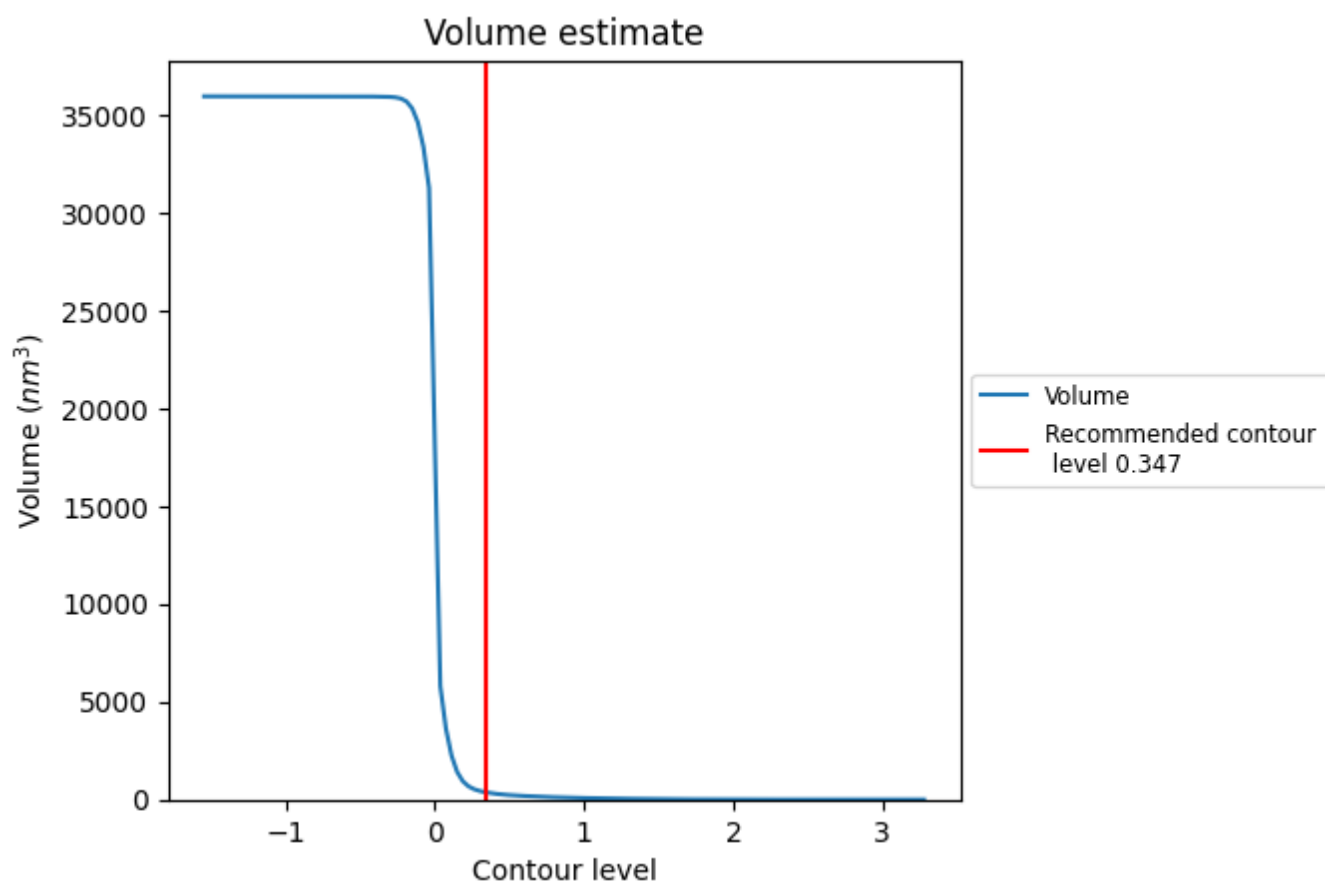
This section contains the results of statistical analysis of the map.

### 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.

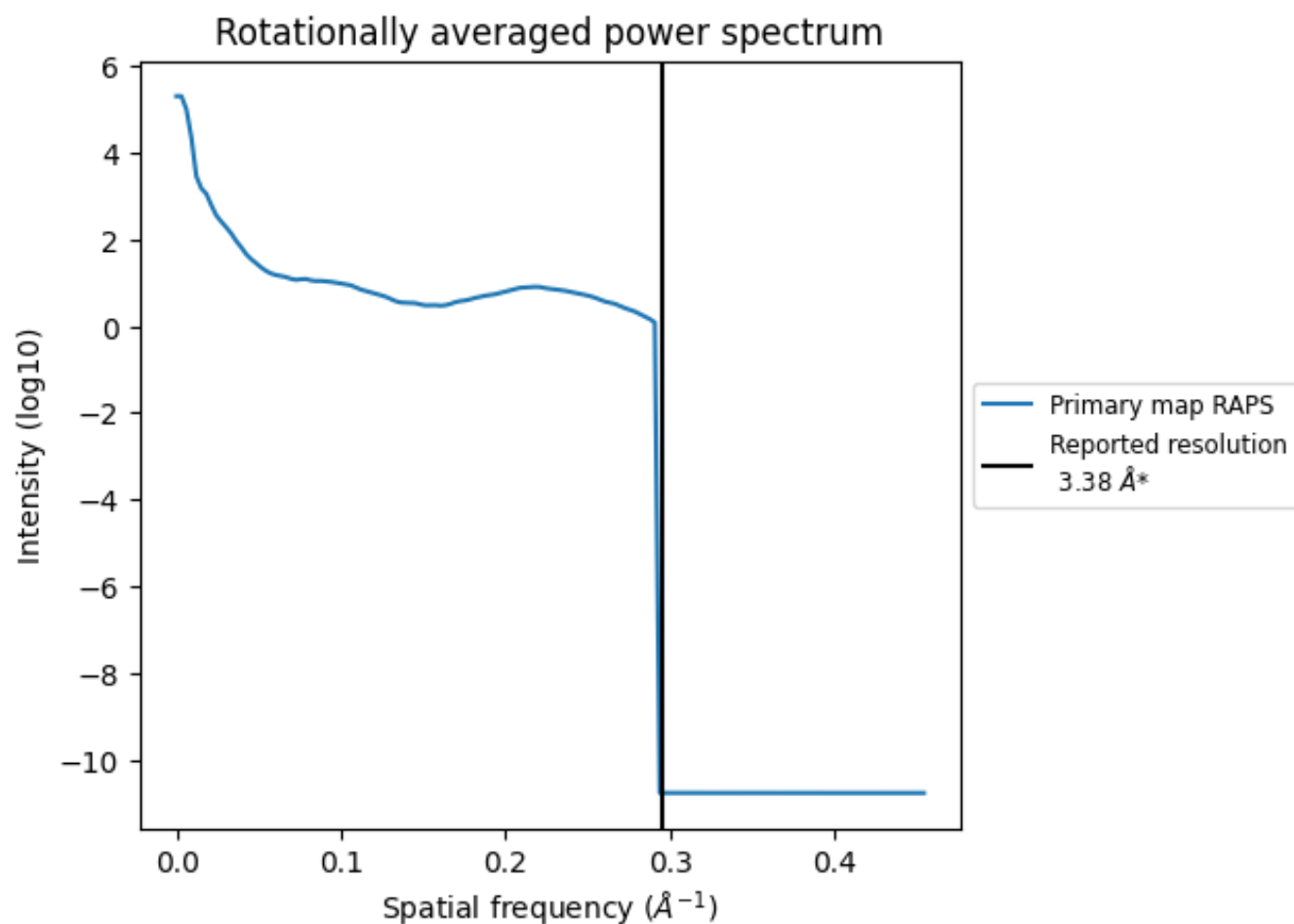
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 365  $\text{nm}^3$ ; this corresponds to an approximate mass of 329 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 0.296 Å<sup>-1</sup>

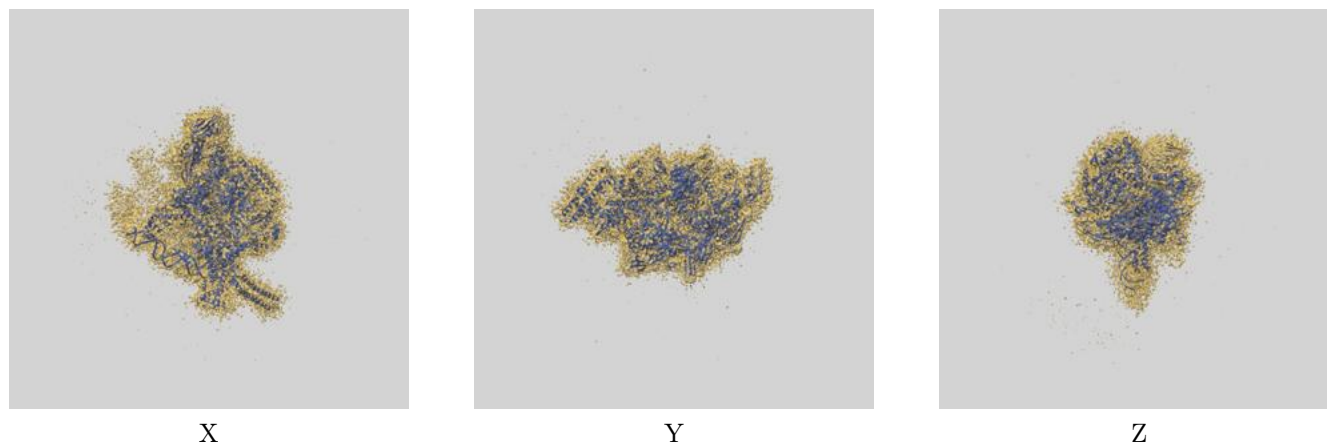
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

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

This section contains information regarding the fit between EMDB map EMD-7319 and PDB model 6BZO. Per-residue inclusion information can be found in section 3 on page 8.

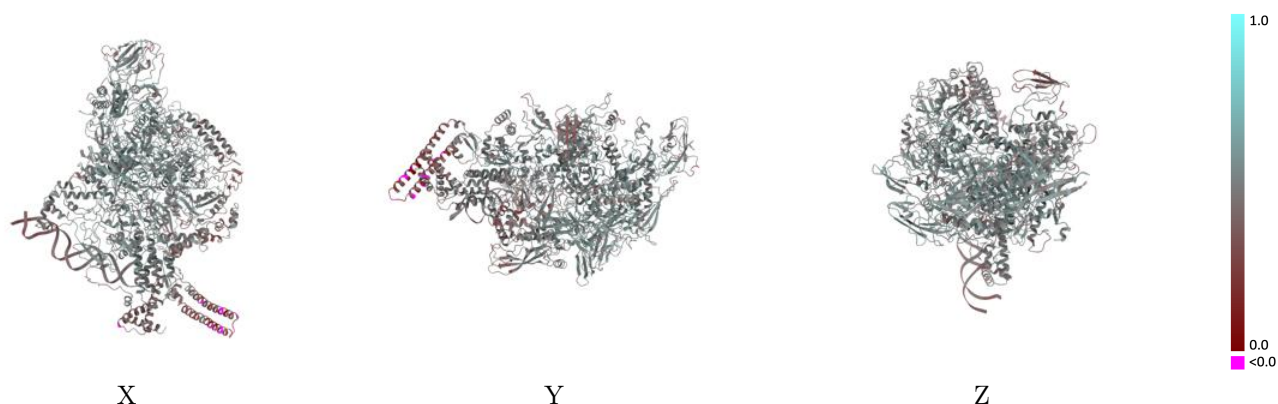
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.347 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](#)

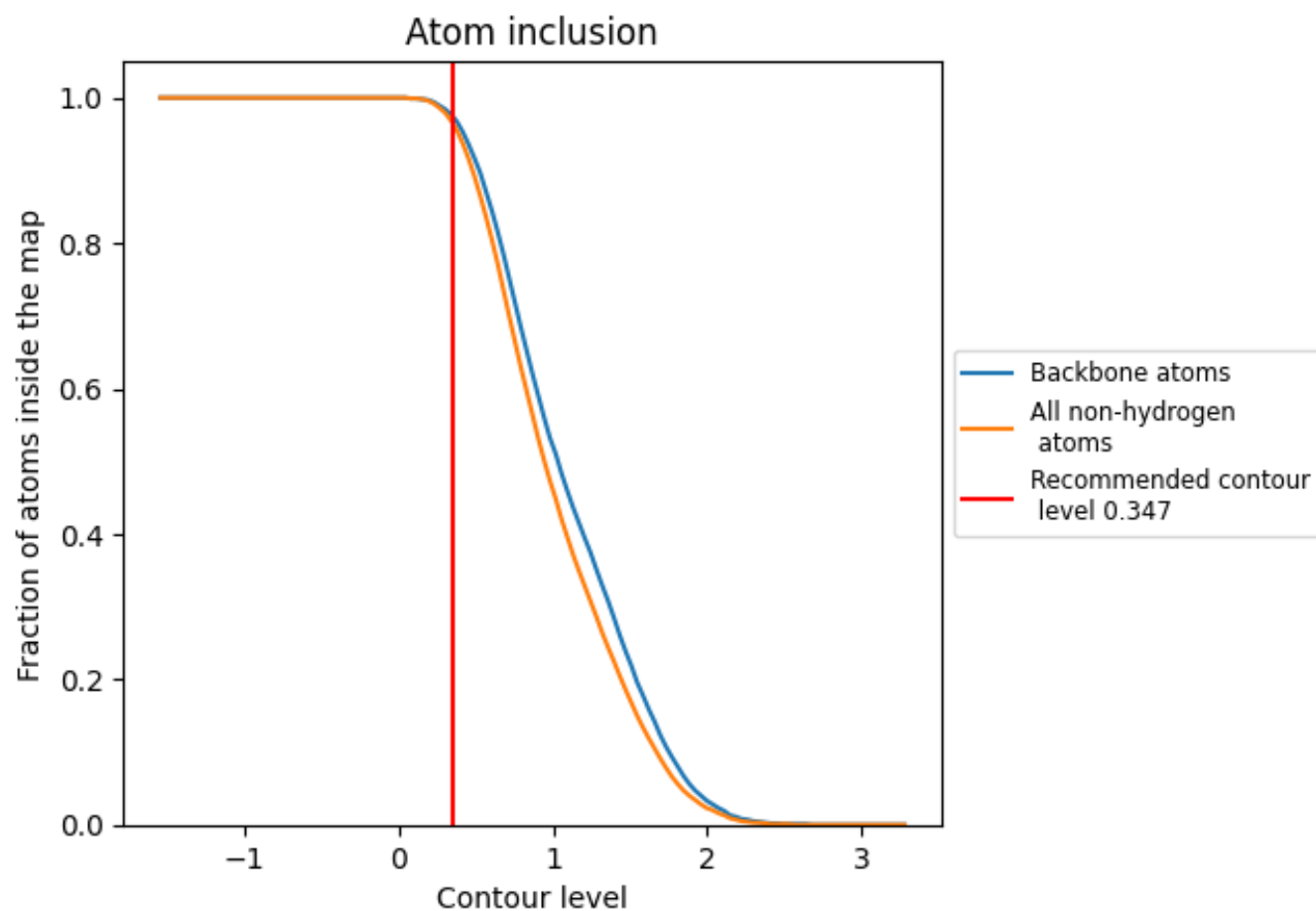


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)

This section was not generated.

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 97% 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 (0.347) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                | Q-score                       |
|-------|-------------------------------|-------------------------------|
| All   | <div><div></div></div> 0.9660 | <div><div></div></div> 0.4890 |
| A     | <div><div></div></div> 0.9750 | <div><div></div></div> 0.5130 |
| B     | <div><div></div></div> 0.9680 | <div><div></div></div> 0.4960 |
| C     | <div><div></div></div> 0.9710 | <div><div></div></div> 0.5050 |
| D     | <div><div></div></div> 0.9640 | <div><div></div></div> 0.4910 |
| E     | <div><div></div></div> 0.9610 | <div><div></div></div> 0.5010 |
| F     | <div><div></div></div> 0.9600 | <div><div></div></div> 0.4520 |
| J     | <div><div></div></div> 0.9510 | <div><div></div></div> 0.4750 |
| O     | <div><div></div></div> 0.9970 | <div><div></div></div> 0.4080 |
| P     | <div><div></div></div> 0.9910 | <div><div></div></div> 0.3890 |

1.0

0.0

<0.0