



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:49 PM UTC

PDB ID : 5W1S / pdb\_00005w1s  
Title : X-ray crystal structure of Escherichia coli RNA polymerase and TraR complex  
Authors : Murakami, K.S.; Molodtsov, V.  
Deposited on : 2017-06-04  
Resolution : 3.81 Å(reported)

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

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

A user guide is available at

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

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:

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

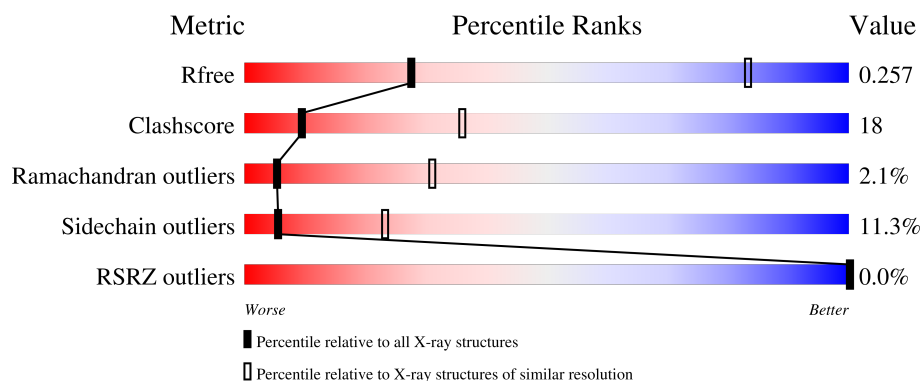
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.81 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) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1065 (3.96-3.64)                                      |
| Clashscore            | 190562                      | 1012 (3.94-3.66)                                      |
| Ramachandran outliers | 187476                      | 1048 (3.96-3.64)                                      |
| Sidechain outliers    | 187428                      | 1043 (3.96-3.64)                                      |
| RSRZ outliers         | 180081                      | 1064 (3.96-3.64)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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 electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 329    |                  |
| 1   | B     | 329    |                  |
| 1   | G     | 329    |                  |
| 1   | H     | 329    |                  |
| 2   | C     | 1342   |                  |

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| Mol | Chain | Length | Quality of chain      |
|-----|-------|--------|-----------------------|
| 2   | I     | 1342   | <br>60% 35% 5%        |
| 3   | D     | 1407   | <br>46% 32% 5% 17%    |
| 3   | J     | 1407   | <br>46% 31% 5% 18%    |
| 4   | E     | 91     | <br>62% 27% 9%        |
| 4   | K     | 91     | <br>46% 31% 1% 21%    |
| 5   | F     | 613    | <br>46% 26% 1% 24%    |
| 5   | L     | 613    | <br>47% 26% 1% 23%    |
| 6   | M     | 79     | <br>49% 33% 5% 1% 11% |
| 6   | N     | 79     | <br>43% 37% 8% 13%    |

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 56825 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 319      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2490  | 1557 | 439 | 486 | 8 |         |         |       |
| 1   | B     | 217      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1677  | 1047 | 295 | 329 | 6 |         |         |       |
| 1   | G     | 227      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1755  | 1093 | 311 | 345 | 6 |         |         |       |
| 1   | H     | 216      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1662  | 1038 | 292 | 326 | 6 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 2   | C     | 1340     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 10564 | 6628 | 1838 | 2055 | 43 |         |         |       |
| 2   | I     | 1340     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 10566 | 6629 | 1840 | 2054 | 43 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 3   | D     | 1173     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 9095  | 5718 | 1628 | 1703 | 46 |         |         |       |
| 3   | J     | 1155     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 9001  | 5659 | 1612 | 1684 | 46 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4   | E     | 89       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 691   | 421 | 129 | 140 | 1 |         |         |       |
| 4   | K     | 72       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 573   | 350 | 110 | 112 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 5   | F     | 468      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3813  | 2389 | 678 | 723 | 23 |         |         |       |
| 5   | L     | 469      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3821  | 2393 | 679 | 726 | 23 |         |         |       |

- Molecule 6 is a protein called Protein TraR.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | M     | 70       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 557   | 346 | 103 | 103 | 5 |         |         |       |
| 6   | N     | 69       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 552   | 343 | 102 | 102 | 5 |         |         |       |

There are 12 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| M     | 74      | HIS      | -      | expression tag | UNP P41065 |
| M     | 75      | HIS      | -      | expression tag | UNP P41065 |
| M     | 76      | HIS      | -      | expression tag | UNP P41065 |
| M     | 77      | HIS      | -      | expression tag | UNP P41065 |
| M     | 78      | HIS      | -      | expression tag | UNP P41065 |
| M     | 79      | HIS      | -      | expression tag | UNP P41065 |
| N     | 74      | HIS      | -      | expression tag | UNP P41065 |
| N     | 75      | HIS      | -      | expression tag | UNP P41065 |
| N     | 76      | HIS      | -      | expression tag | UNP P41065 |
| N     | 77      | HIS      | -      | expression tag | UNP P41065 |
| N     | 78      | HIS      | -      | expression tag | UNP P41065 |
| N     | 79      | HIS      | -      | expression tag | UNP P41065 |

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 7   | D     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 7   | J     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

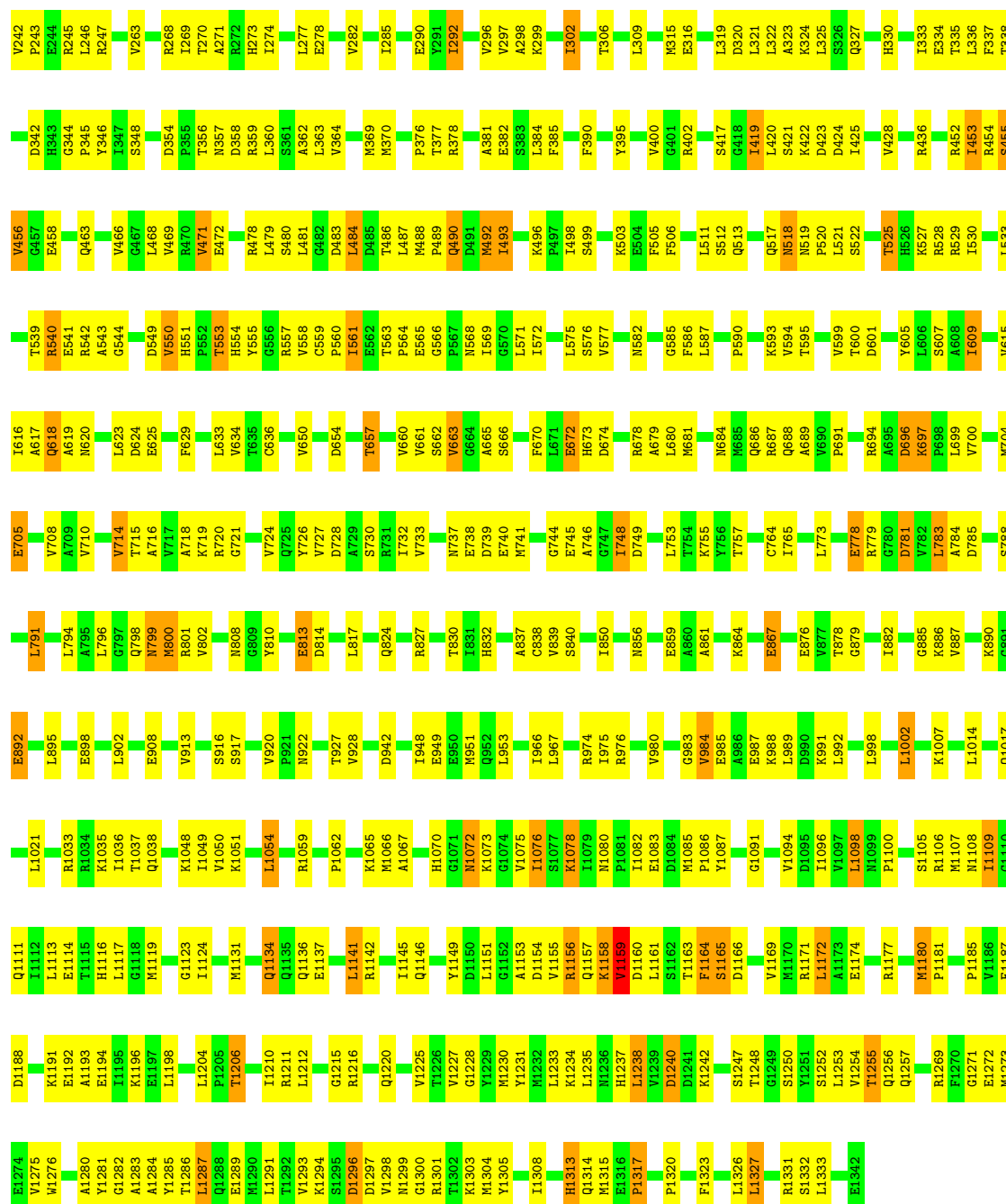
- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 8   | D     | 2        | Total<br>2 | Zn<br>2 | 0       | 0       |
| 8   | J     | 2        | Total<br>2 | Zn<br>2 | 0       | 0       |
| 8   | M     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 8   | N     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |



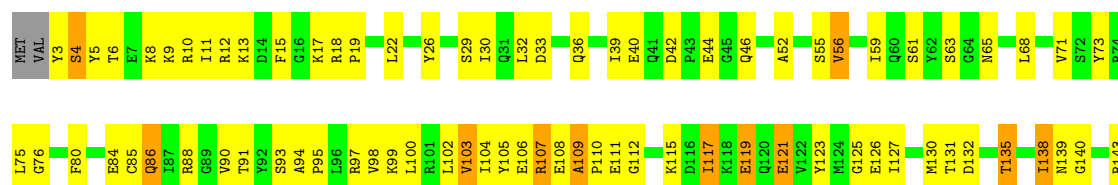






• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain I: 60% 35% 5%





|     |       |       |       |     |     |     |      |      |      |      |      |      |      |      |
|-----|-------|-------|-------|-----|-----|-----|------|------|------|------|------|------|------|------|
| GLY | L1314 | I1233 | L1155 | VAL | ASP | SER | R798 | R709 | Y609 | D505 | P427 | Y349 | T262 | F176 |
| LEU | S1318 | E1236 | I1156 | ASP | PRO | ASN | R801 | D710 | Y606 | V506 | T428 | I355 | S263 | M180 |
| GLY | F1319 | V1237 | A1157 | ALA | HIS | VAL | Q805 | Q711 | L614 | D264 | H430 | T356 | D264 | L265 |
| SER | I1320 | Q1238 | E1158 | GLN | THR | LYS | T810 | Q716 | P616 | L510 | R431 | V357 | N266 | L188 |
| ASP | S1324 | Y1241 | I1159 | ASN | PRO | VAL | E811 | W717 | A621 | Y512 | L432 | P359 | D267 | L189 |
| ASN | F1325 | R1242 | G1161 | VAL | ILE | ASN | D812 | W718 | A621 | M513 | G433 | I434 | L268 | K190 |
| GLU | Q1326 | L1243 | I1162 | LEU | THR | SER | D813 | F719 | M625 | T514 | F437 | R362 | N274 | M192 |
|     | T1329 | V1246 | S1164 | ILE | GLU | SER | W720 | W721 | M625 | R515 | E438 | H364 | R275 | D193 |
|     | L1332 | F1247 | F1165 | PRO | VAL | GLY | W721 | W722 | M625 | D516 | P439 | Q365 | L279 | L194 |
|     | T1333 | I1248 | G1166 | GLY | SER | LYS | H817 | W723 | A633 | C517 | I442 | G366 | L282 | E197 |
|     | R1341 | K1251 | K1167 | THR | PHE | VAL | T820 | W724 | M638 | V518 | I442 | G367 | L282 | C198 |
|     | D1342 | E1255 | T1169 | MET | VAL | ILE | M821 | W725 | S638 | V526 | K445 | M372 | P288 | L201 |
|     | E1343 | I1256 | K1170 | PRO | ARG | THR | R822 | W725 | V639 | L527 | A446 | A373 | L527 | R202 |
|     | L1344 | V1257 | G1171 | ALA | PHE | SER | R823 | W732 | G640 | T528 | I447 | L374 | I291 | E203 |
|     | R1345 | M1260 | R1172 | TYR | THR | ARG | W825 | W733 | I641 | G529 | Q448 | E375 | V292 | E204 |
|     | G1346 | L1261 | K1173 | PHE | ASP | ASN | W826 | W734 | P647 | E532 | L449 | L376 | L205 | L205 |
|     | L1347 | L1261 | R1174 | LEU | THR | THR | E927 | W735 | E658 | A533 | H450 | F377 | E295 | R206 |
|     | V1353 | A1264 | I1177 | LEU | GLY | LYS | G828 | W737 | E659 | E534 | P451 | K378 | K296 | E207 |
|     | G1354 | T1265 | T1178 | GLY | GLN | LYS | W831 | W738 | E660 | R535 | L452 | P379 | R297 | E207 |
|     | T1355 | I1266 | D1181 | ILE | THR | ILE | R832 | W739 | V661 | L536 | G454 | Y382 | M298 | S210 |
|     | L1356 | G1270 | G1182 | VAL | THR | ASP | E833 | L740 | I664 | A542 | D460 | G385 | D304 | K213 |
|     | P1358 | S1271 | S1183 | GLN | ARG | PHE | R834 | W742 | I664 | H545 | F461 | K384 | A305 | K214 |
|     | T1361 | D1273 | D1184 | LEU | GLN | GLY | L835 | W743 | F668 | V548 | D462 | E386 | L307 | K215 |
|     | H1366 | F1274 | P1185 | GLY | THR | ARG | W839 | W744 | F668 | K549 | G463 | L387 | G310 | I221 |
|     | R1373 | L1275 | Y1186 | ASP | THR | THR | R842 | W745 | L672 | V550 | Q465 | T392 | R311 | K222 |
|     | G1376 | M1289 | M1189 | GLY | GLU | LYS | R843 | W746 | R678 | R551 | M466 | T393 | R312 | L223 |
| GLU | ALA   | E1281 | K1192 | GLN | THR | THR | T844 | W750 | V679 | E556 | L472 | K395 | G313 | L224 |
| PRO | PRO   | Y1282 | W1193 | ILE | GLY | LYS | D847 | W754 | K681 | D558 | T473 | K398 | I394 | E225 |
| ALA | ALA   | S1283 | R1194 | SER | THR | VAL | L849 | T754 | V682 | A559 | L474 | K399 | A315 | A226 |
| ALA | ALA   | R1284 | F1199 | VAL | VAL | VAL | R850 | T754 | I685 | E562 | A476 | M400 | I316 | F227 |
| PRO | PRO   | V1285 | E1200 | ALA | ALA | PRO | T853 | T754 | V686 | E562 | Q477 | K399 | T317 | S230 |
| GLN | GLN   | K1286 | G1201 | ARG | ASP | LEU | R857 | L770 | A688 | L569 | A480 | E405 | N320 | P234 |
| VAL | VAL   | M1289 | R1203 | ILE | SER | ALA | P859 | Q771 | A689 | K570 | E479 | A406 | R321 | E235 |
| THR | THR   | A1294 | R1206 | PRO | ALA | LYS | R860 | Y772 | M690 | D571 | M484 | V407 | R322 | L238 |
| ASP | ASP   | E1294 | S1211 | GLN | GLY | ASP | T776 | T776 | V693 | T573 | T487 | V408 | L324 | L239 |
| ALA | ALA   | K1297 | E1215 | GLY | THR | GLY | L863 | T776 | S694 | R576 | N488 | D413 | K325 | T241 |
| SER | SER   | V1298 | I1220 | GLY | THR | GLY | L864 | T776 | K695 | R576 | N489 | E414 | M330 | P246 |
| ALA | ALA   | G1299 | L1221 | THR | VAL | GLN | R865 | T776 | A696 | L579 | I490 | V415 | I331 | P247 |
| SER | SER   | A1300 | R1222 | VAL | VAL | ILE | E866 | T776 | M697 | W580 | L491 | I416 | Q335 | D248 |
| LEU | LEU   | T1301 | L1223 | GLY | VAL | GLN | L872 | T776 | M698 | M581 | E491 | E418 | R337 | P251 |
| ALA | ALA   | R1304 | H1227 | LYS | THR | ASN | N875 | T776 | L701 | Q594 | A494 | E418 | L342 | L252 |
| GLY | GLY   | I1309 | A1228 | GLY | THR | LYS | R876 | T776 | Q702 | G496 | N495 | E418 | L343 | V253 |
| LEU | LEU   | T1230 | F1139 | VAL | VAL | GLY | W877 | T776 | T705 | K598 | E497 | L423 | L344 | P254 |
| LEU | LEU   | T1310 | R1140 | ALA | ALA | ILE | W882 | T776 | V705 | I601 | I500 | M424 | G344 | L255 |
| ASN | ASN   | T1310 | E1146 | LYS | ASN | LYS | R883 | T776 | T705 | I601 | I500 | R425 | K345 | K346 |
| ALA | ALA   |       |       | TRP | TRP | LEU |      |      |      | L605 | Q504 | A426 | R259 | R259 |

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

Chain J:

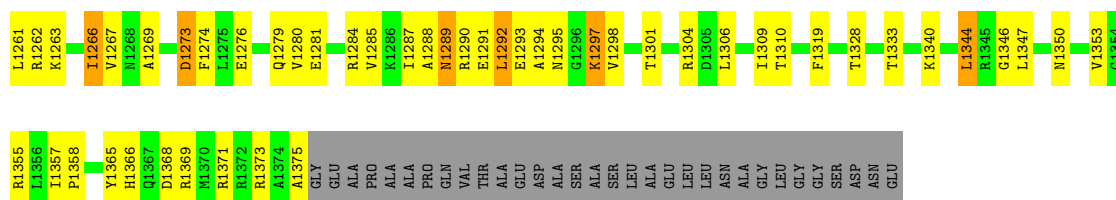
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18%

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|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| K1172 | R1173 | R1174 | P1179 | V1180 | D1181 | G1182 | S1183 | D1184 | P1185 | Y1186 | M1189 | I1190 | K1192 | W1193 | R1194 | V1198 | F1199 | E1200 | E1201 | G1202 | R1203 | V1204 | E1205 | R1206 | G1207 | D1208 | V1209 | I1210 | E1215 | L1221 | R1222 | L1223 | I1233 | V1237 | Q1238 | D1239 | R1242 | L1243 | K1247 | I1248 | K1251 | H1252 | V1255 | I1256 | V1257 | M1260 |       |       |       |       |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| LEU   | PRO   | GLY   | LYS   | ALA   | ILE   | VAL   | GLN   | LEU   | ASP   | GLY   | VAL   | GLN   | ILE   | SER   | GLY   | ASP   | THR   | LEU   | ALA   | ARG   | PRO   | GLN   | GLU   | SER   | GLY   | ALA   | THR   | LYS   | ASP   | ILE   | GLY   | L1137 | L1138 | P1139 | R1140 | E1146 | A1154 | I1155 | L1156 | A1157 | E1158 | G1161 | V1162 | S1164 | F1165 | K1167 | E1168 | T1169 | K1170 | G1171 |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| ILE   | ASP   | GLY   | GLN   | THR   | ILE   | THR   | ARG   | THR   | ASP   | GLU   | LEU   | THR   | GLY   | THR   | LYS   | HIS   | ILE   | GLY   | PRO   | VAL   | GLY   | VAL   | ALA   | LEU   | ASP   | SER   | ALA   | LYS   | GLY   | ALA   | GLY   | ASN   | THR   | GLY   | THR   | PRO   | ALA   | VAL   | ASN   | VAL   | ASN   | VAL   | THR   | GLU   | VAL   | GLY   | THR   | THR   | THR   | THR   | THR |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| GLU   | LEU   | LYS   | LEU   | ILE   | ASP   | GLU   | PHE   | GLY   | ARG   | THR   | GLY   | GLN   | THR   | SER   | THR   | THR   | VAL   | GLY   | PRO   | VAL   | GLY   | ALA   | VAL   | LEU   | ASP   | SER   | ALA   | LYS   | GLY   | ALA   | GLY   | ASP   | GLY   | ASN   | THR   | GLY   | THR   | PRO   | ALA   | VAL   | ASN   | VAL   | THR   | GLU   | VAL   | GLY   | SER   | THR   | THR   | THR   | THR |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| L835  | R836  | V839  | T844  | D847  | V848  | L849  | K850  | P851  | G852  | T853  | L857  | V858  | P859  | R860  | N861  | L863  | H865  | E866  | Q867  | L872  | E873  | V877  | V880  | R883  | S884  | V885  | V886  | F892  | G893  | V894  | H897  | C898  | R901  | D902  | L903  | A904  | R905  | G906  | H907  | I908  | I909  | N910  | K911  | G912  | E913  | A914  |       |       |       |       |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| LYS   | ASP   | THR   | THR   | THR   | GLN   | THR   | ASP   | GLY   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| I915  | I918  | I923  | G924  | E925  | P926  | L930  | T931  | MET   | ARG   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| LEU   | PRO   | GLY   | LYS   | ALA   | ILE   | VAL   | GLN   | LEU   | ASP   | GLY   | VAL   | GLN   | ILE   | SER   | GLY   | ASP   | THR   | LEU   | ALA   | ARG   | PRO   | GLN   | GLU   | SER   | GLY   | ALA   | THR   | LYS   | ASP   | ILE   | GLY   | ASN   | THR   | GLY   | THR   | PRO   | ALA   | VAL   | ASN   | VAL   | ASN   | VAL   | THR   | GLU   | VAL   | GLY   | SER   | THR   | THR   | THR   | THR | THR |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| ILE   | ASP   | GLY   | GLN   | THR   | ILE   | THR   | ARG   | THR   | ASP   | GLU   | LEU   | THR   | GLY   | THR   | LYS   | HIS   | ILE   | GLY   | PRO   | VAL   | GLY   | VAL   | ALA   | LEU   | ASP   | SER   | ALA   | LYS   | GLY   | ALA   | GLY   | ASN   | THR   | GLY   | THR   | PRO   | ALA   | VAL   | ASN   | VAL   | THR   | GLU   | VAL   | GLY   | SER   | THR   | THR   | THR   | THR   | THR   | THR | THR | THR |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| L835  | R836  | V839  | T844  | D847  | V848  | L849  | K850  | P851  | G852  | T853  | L857  | V858  | P859  | R860  | N861  | L863  | H865  | E866  | Q867  | L872  | E873  | V877  | V880  | R883  | S884  | V885  | V886  | F892  | G893  | V894  | H897  | C898  | R901  | D902  | L903  | A904  | R905  | G906  | H907  | I908  | I909  | N910  | K911  | G912  | E913  | A914  |       |       |       |       |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| LYS   | ASP   | THR   | THR   | THR   | GLN   | THR   | ASP   | GLY   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR | THR | THR |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| I915  | I918  | I923  | G924  | E925  | P926  | L930  | T931  | MET   | ARG   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR | THR | THR |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| LEU   | PRO   | GLY   | LYS   | ALA   | ILE   | VAL   | GLN   | LEU   | ASP   | GLY   | VAL   | GLN   | ILE   | SER   | GLY   | ASP   | THR   | LEU   | ALA   | ARG   | PRO   | GLN   | GLU   | SER   | GLY   | ALA   | THR   | LYS   | ASP   | ILE   | GLY   | ASN   | THR   | GLY   | THR   | PRO   | ALA   | VAL   | ASN   | VAL   | ASN   | VAL   | THR   | GLU   | VAL   | GLY   | SER   | THR   | THR   | THR   | THR | THR | THR | THR | THR |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| ILE   | ASP   | GLY   | GLN   | THR   | ILE   | THR   | ARG   | THR   | ASP   | GLU   | LEU   | THR   | GLY   | THR   | LYS   | HIS   | ILE   | GLY   | PRO   | VAL   | GLY   | VAL   | ALA   | LEU   | ASP   | SER   | ALA   | LYS   | GLY   | ALA   | GLY   | ASN   | THR   | GLY   | THR   | PRO   | ALA   | VAL   | ASN   | VAL   | THR   | GLU   | VAL   | GLY   | SER   | THR   | THR   | THR   | THR   | THR   | THR | THR | THR | THR | THR | THR |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| L835  | R836  | V839  | T844  | D847  | V848  | L849  | K850  | P851  | G852  | T853  | L857  | V858  | P859  | R860  | N861  | L863  | H865  | E866  | Q867  | L872  | E873  | V877  | V880  | R883  | S884  | V885  | V886  | F892  | G893  | V894  | H897  | C898  | R901  | D902  | L903  | A904  | R905  | G906  | H907  | I908  | I909  | N910  | K911  | G912  | E913  | A914  |       |       |       |       |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| LYS   | ASP   | THR   | THR   | THR   | GLN   | THR   | ASP   | GLY   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR | THR | THR | THR | THR | THR | THR | THR | THR |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| I915  | I918  | I923  | G924  | E925  | P926  | L930  | T931  | MET   | ARG   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR   | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |



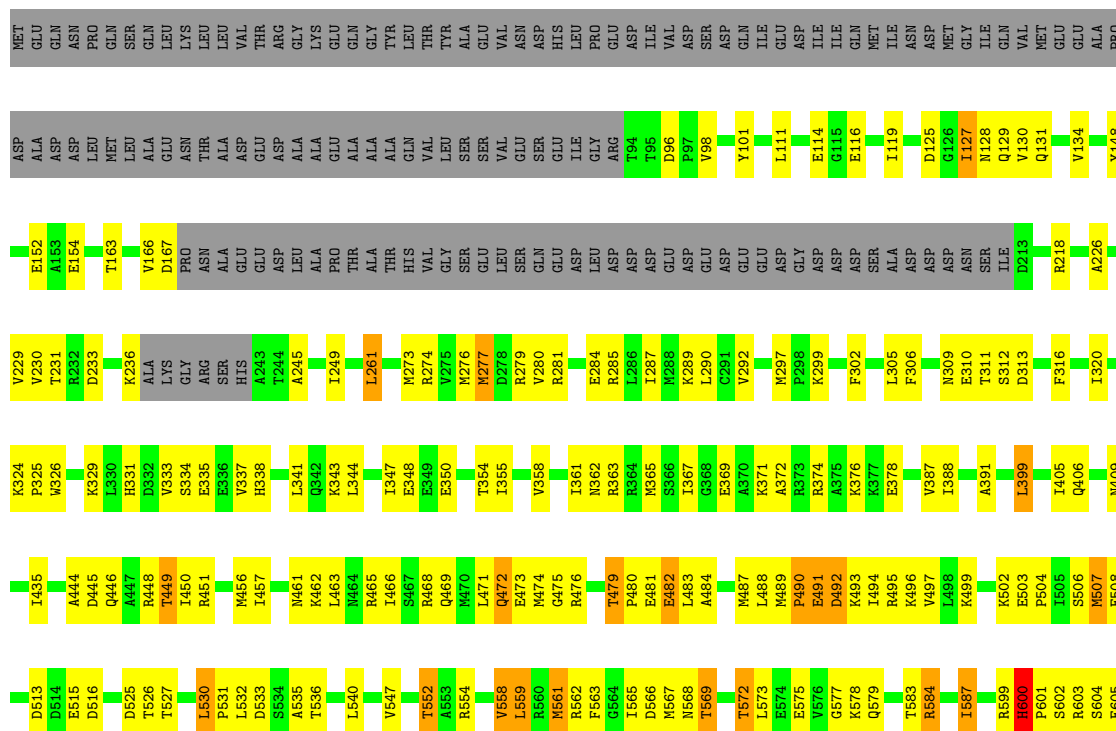
• Molecule 4: DNA-directed RNA polymerase subunit omega

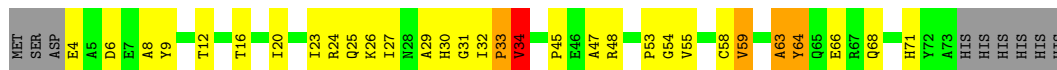
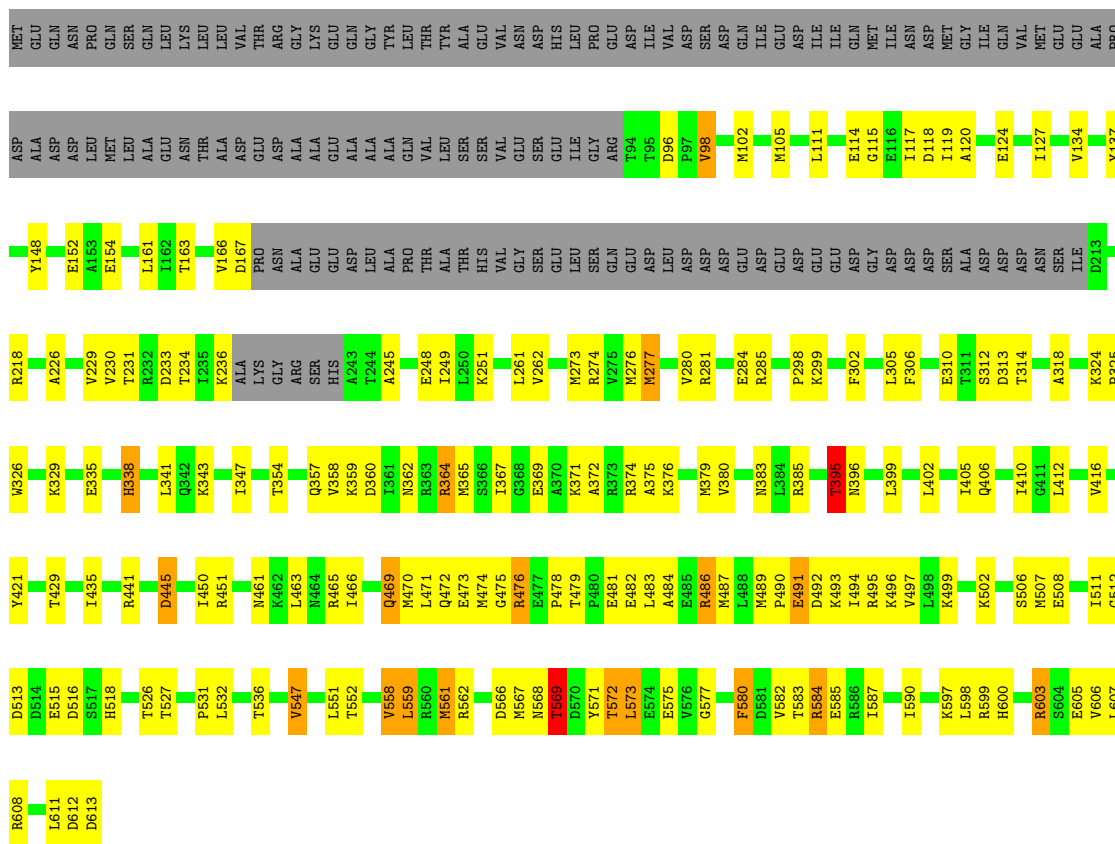


• Molecule 4: DNA-directed RNA polymerase subunit omega



• Molecule 5: RNA polymerase sigma factor RpoD





## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 186.48Å 206.04Å 310.30Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 49.84 – 3.81<br>49.84 – 3.81                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.6 (49.84-3.81)<br>86.4 (49.84-3.81)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 0.60 (at 3.77Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX (1.11.1 _2575: ???)                                  | Depositor        |
| R, $R_{free}$                                                           | 0.208 , 0.262<br>0.212 , 0.257                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2000 reflections (1.70%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 156.4                                                       | Xtriage          |
| Anisotropy                                                              | 0.169                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.30 , 217.7                                                | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.95                                                        | EDS              |
| Total number of atoms                                                   | 56825                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 239.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |             | Bond angles |                 |
|-----|-------|--------------|-------------|-------------|-----------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$     |
| 1   | A     | 0.24         | 0/2524      | 0.74        | 2/3421 (0.1%)   |
| 1   | B     | 0.22         | 0/1697      | 0.69        | 0/2300          |
| 1   | G     | 0.22         | 0/1777      | 0.63        | 0/2408          |
| 1   | H     | 0.25         | 0/1681      | 0.71        | 3/2278 (0.1%)   |
| 2   | C     | 0.24         | 0/10733     | 0.67        | 0/14482         |
| 2   | I     | 0.22         | 0/10735     | 0.63        | 3/14484 (0.0%)  |
| 3   | D     | 0.24         | 0/9235      | 0.69        | 4/12472 (0.0%)  |
| 3   | J     | 0.22         | 0/9140      | 0.65        | 0/12341         |
| 4   | E     | 0.21         | 0/693       | 0.61        | 0/935           |
| 4   | K     | 0.19         | 0/575       | 0.38        | 0/774           |
| 5   | F     | 0.21         | 0/3864      | 0.63        | 0/5194          |
| 5   | L     | 0.20         | 0/3872      | 0.61        | 0/5205          |
| 6   | M     | 0.29         | 0/567       | 0.76        | 1/766 (0.1%)    |
| 6   | N     | 0.30         | 0/562       | 0.75        | 0/759           |
| All | All   | 0.23         | 0/57655     | 0.66        | 13/77819 (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                   | 2                   |
| 2   | I     | 0                   | 2                   |
| 3   | D     | 0                   | 2                   |
| 3   | J     | 0                   | 2                   |
| 5   | F     | 0                   | 1                   |
| All | All   | 0                   | 9                   |

There are no bond length outliers.



All (13) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 1   | A     | 323  | PRO  | CA-C-N | 6.17  | 132.81      | 121.70   |
| 1   | A     | 323  | PRO  | C-N-CA | 6.17  | 132.81      | 121.70   |
| 1   | H     | 29   | GLU  | C-N-CD | -5.98 | 107.44      | 120.60   |
| 3   | D     | 746  | LEU  | CA-C-N | -5.71 | 112.79      | 122.67   |
| 3   | D     | 746  | LEU  | C-N-CA | -5.71 | 112.79      | 122.67   |
| 1   | H     | 29   | GLU  | CA-C-N | 5.61  | 140.47      | 127.00   |
| 1   | H     | 29   | GLU  | C-N-CA | 5.61  | 140.47      | 127.00   |
| 2   | I     | 1136 | GLN  | CA-C-N | 5.24  | 131.56      | 121.54   |
| 2   | I     | 1136 | GLN  | C-N-CA | 5.24  | 131.56      | 121.54   |
| 3   | D     | 1211 | SER  | CA-C-N | -5.12 | 112.70      | 123.20   |
| 3   | D     | 1211 | SER  | C-N-CA | -5.12 | 112.70      | 123.20   |
| 2   | I     | 110  | PRO  | N-CA-C | -5.06 | 102.04      | 112.47   |
| 6   | M     | 63   | ALA  | N-CA-C | -5.04 | 100.06      | 110.80   |

There are no chirality outliers.

All (9) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group   |
|-----|-------|------|------|---------|
| 2   | C     | 109  | ALA  | Peptide |
| 2   | C     | 236  | LYS  | Peptide |
| 3   | D     | 1184 | ASP  | Peptide |
| 3   | D     | 901  | ARG  | Peptide |
| 5   | F     | 600  | HIS  | Peptide |
| 2   | I     | 109  | ALA  | Peptide |
| 2   | I     | 236  | LYS  | Peptide |
| 3   | J     | 1184 | ASP  | Peptide |
| 3   | J     | 853  | THR  | Peptide |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2490  | 0        | 2542     | 121     | 0            |
| 1   | B     | 1677  | 0        | 1703     | 61      | 0            |
| 1   | G     | 1755  | 0        | 1773     | 80      | 0            |
| 1   | H     | 1662  | 0        | 1687     | 61      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | C     | 10564 | 0        | 10571    | 441     | 0            |
| 2   | I     | 10566 | 0        | 10576    | 365     | 0            |
| 3   | D     | 9095  | 0        | 9222     | 397     | 0            |
| 3   | J     | 9001  | 0        | 9167     | 385     | 0            |
| 4   | E     | 691   | 0        | 695      | 26      | 0            |
| 4   | K     | 573   | 0        | 587      | 20      | 0            |
| 5   | F     | 3813  | 0        | 3880     | 129     | 0            |
| 5   | L     | 3821  | 0        | 3884     | 116     | 0            |
| 6   | M     | 557   | 0        | 547      | 31      | 0            |
| 6   | N     | 552   | 0        | 542      | 44      | 0            |
| 7   | D     | 1     | 0        | 0        | 0       | 0            |
| 7   | J     | 1     | 0        | 0        | 0       | 0            |
| 8   | D     | 2     | 0        | 0        | 0       | 0            |
| 8   | J     | 2     | 0        | 0        | 0       | 0            |
| 8   | M     | 1     | 0        | 0        | 0       | 0            |
| 8   | N     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 56825 | 0        | 57376    | 2038    | 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 18.

All (2038) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:45:ARG:HG2   | 1:B:38:THR:HB     | 1.42                     | 1.02              |
| 1:G:190:ALA:HB2  | 1:G:200:LYS:HB2   | 1.42                     | 1.01              |
| 2:C:525:THR:HG21 | 2:C:687:ARG:HD2   | 1.38                     | 1.00              |
| 2:C:696:ASP:HB2  | 2:C:798:GLN:HG2   | 1.44                     | 0.99              |
| 2:C:10:ARG:HD3   | 2:C:1181:PRO:HG2  | 1.46                     | 0.96              |
| 2:I:1196:LYS:HD2 | 2:I:1206:THR:HG23 | 1.49                     | 0.94              |
| 2:C:65:ASN:HB3   | 2:C:105:TYR:HB2   | 1.50                     | 0.91              |
| 6:M:31:GLY:H     | 6:M:53:PRO:HB2    | 1.34                     | 0.89              |
| 3:D:35:PHE:HD1   | 3:D:101:ARG:HD3   | 1.35                     | 0.89              |
| 2:C:1116:HIS:HE1 | 3:D:641:ILE:H     | 1.19                     | 0.89              |
| 2:I:1073:LYS:HE3 | 3:J:462:ASP:HB2   | 1.55                     | 0.88              |
| 3:J:739:GLN:NE2  | 6:N:9:TYR:OH      | 2.07                     | 0.88              |
| 2:I:1116:HIS:HE1 | 3:J:641:ILE:H     | 1.16                     | 0.87              |
| 1:A:45:ARG:HH22  | 2:C:1216:ARG:HA   | 1.40                     | 0.87              |
| 2:I:696:ASP:HB2  | 2:I:798:GLN:HG2   | 1.57                     | 0.87              |
| 3:J:754:ILE:HD12 | 6:N:20:ILE:HG12   | 1.55                     | 0.86              |
| 5:L:577:GLY:HA3  | 5:L:583:THR:HG23  | 1.58                     | 0.85              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:1304:MET:HE3 | 2:C:1308:ILE:HD11 | 1.58                     | 0.85              |
| 2:C:1196:LYS:HD2 | 2:C:1206:THR:HG23 | 1.59                     | 0.84              |
| 2:C:4:SER:HB3    | 2:C:7:GLU:HG3     | 1.60                     | 0.84              |
| 2:I:550:VAL:HG11 | 3:J:776:THR:HG22  | 1.60                     | 0.84              |
| 3:J:189:LEU:HB3  | 3:J:234:PRO:HB2   | 1.58                     | 0.83              |
| 3:J:746:LEU:HD22 | 3:J:754:ILE:HD11  | 1.60                     | 0.83              |
| 3:J:325:LYS:HD3  | 5:L:508:GLU:HG2   | 1.60                     | 0.82              |
| 1:A:296:GLY:H    | 1:A:299:SER:HB2   | 1.44                     | 0.82              |
| 3:J:430:HIS:HD2  | 3:J:432:LEU:HB2   | 1.45                     | 0.82              |
| 2:C:302:ILE:HG22 | 2:C:309:LEU:HA    | 1.62                     | 0.82              |
| 5:F:134:VAL:HA   | 5:F:273:MET:HE1   | 1.61                     | 0.82              |
| 2:I:10:ARG:HD3   | 2:I:1181:PRO:HG2  | 1.62                     | 0.82              |
| 3:J:782:GLY:HA3  | 6:N:12:THR:HG22   | 1.63                     | 0.81              |
| 6:N:31:GLY:H     | 6:N:53:PRO:HB2    | 1.45                     | 0.81              |
| 1:G:48:LEU:HA    | 1:G:180:VAL:HG21  | 1.63                     | 0.80              |
| 2:C:678:ARG:NH2  | 6:M:6:ASP:OD1     | 2.13                     | 0.80              |
| 1:G:118:ASP:HB3  | 1:G:121:VAL:HB    | 1.63                     | 0.80              |
| 1:H:118:ASP:HB2  | 1:H:121:VAL:HB    | 1.61                     | 0.80              |
| 1:A:38:THR:OG1   | 1:B:45:ARG:NH1    | 2.15                     | 0.80              |
| 2:C:168:GLY:O    | 2:C:170:VAL:N     | 2.13                     | 0.79              |
| 2:C:1073:LYS:HE3 | 3:D:462:ASP:HB2   | 1.63                     | 0.79              |
| 2:C:1160:ASP:HB2 | 2:C:1161:LEU:HA   | 1.64                     | 0.79              |
| 3:D:337:ARG:HH12 | 3:D:1320:ILE:HG23 | 1.45                     | 0.79              |
| 1:B:86:LYS:HD3   | 1:B:174:ASP:HB2   | 1.63                     | 0.79              |
| 2:C:41:GLN:NE2   | 2:C:73:TYR:O      | 2.16                     | 0.79              |
| 2:C:745:GLU:HG3  | 2:C:1017:GLN:HB3  | 1.64                     | 0.78              |
| 2:I:1108:ASN:OD1 | 2:I:1111:GLN:NE2  | 2.16                     | 0.78              |
| 3:D:17:PHE:O     | 3:D:1355:ARG:NH2  | 2.15                     | 0.78              |
| 2:I:1256:GLN:HB3 | 2:I:1301:ARG:HH22 | 1.48                     | 0.78              |
| 3:D:905:ARG:HH21 | 3:D:907:HIS:HB2   | 1.49                     | 0.78              |
| 3:D:310:GLY:HA2  | 3:D:314:ARG:HD2   | 1.67                     | 0.77              |
| 3:J:114:ILE:HD12 | 3:J:304:ASP:HB3   | 1.65                     | 0.77              |
| 2:C:985:GLU:HB3  | 2:C:988:LYS:HB2   | 1.67                     | 0.77              |
| 5:F:456:MET:HE1  | 5:F:497:VAL:HG13  | 1.66                     | 0.77              |
| 1:B:14:VAL:HB    | 1:B:28:LEU:HD13   | 1.66                     | 0.77              |
| 3:D:430:HIS:HD2  | 3:D:432:LEU:HB2   | 1.50                     | 0.77              |
| 2:I:745:GLU:HG3  | 2:I:1017:GLN:HB3  | 1.66                     | 0.77              |
| 3:D:536:LEU:HD12 | 3:D:542:ALA:HB2   | 1.66                     | 0.77              |
| 3:D:325:LYS:HD3  | 5:F:508:GLU:HG2   | 1.66                     | 0.77              |
| 3:D:1238:GLN:NE2 | 3:D:1248:ILE:O    | 2.17                     | 0.77              |
| 3:D:114:ILE:HD12 | 3:D:304:ASP:HB3   | 1.67                     | 0.76              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:1116:HIS:CE1  | 3:J:641:ILE:H     | 2.02                     | 0.76              |
| 3:J:48:THR:O      | 3:J:50:LYS:N      | 2.17                     | 0.76              |
| 3:D:430:HIS:CD2   | 3:D:432:LEU:HB2   | 2.20                     | 0.76              |
| 1:G:38:THR:OG1    | 1:H:45:ARG:NH1    | 2.17                     | 0.76              |
| 1:B:82:LEU:HD22   | 1:B:173:VAL:HG22  | 1.68                     | 0.76              |
| 2:I:705:GLU:HB2   | 2:I:794:LEU:H     | 1.51                     | 0.76              |
| 1:G:226:GLU:HB3   | 1:H:10:LYS:HE3    | 1.67                     | 0.75              |
| 3:J:709:ARG:O     | 3:J:711:GLY:N     | 2.18                     | 0.75              |
| 2:C:1149:TYR:HD1  | 2:C:1159:VAL:HG11 | 1.50                     | 0.75              |
| 3:D:210:SER:HB2   | 3:D:213:LYS:HB2   | 1.69                     | 0.75              |
| 3:J:426:ALA:HB3   | 3:J:427:PRO:HD3   | 1.68                     | 0.75              |
| 2:I:1160:ASP:HB2  | 2:I:1161:LEU:HA   | 1.66                     | 0.75              |
| 2:C:61:SER:HB3    | 2:C:479:LEU:HB3   | 1.67                     | 0.74              |
| 5:L:481:GLU:OE1   | 5:L:495:ARG:NH2   | 2.20                     | 0.74              |
| 3:D:489:ASN:HA    | 3:D:904:ALA:HB1   | 1.69                     | 0.74              |
| 2:I:734:ILE:HD11  | 2:I:783:LEU:HD11  | 1.68                     | 0.74              |
| 3:J:747:MET:HB2   | 3:J:774:ILE:HG22  | 1.67                     | 0.74              |
| 3:D:126:LEU:HD13  | 3:D:223:LEU:HD21  | 1.70                     | 0.74              |
| 3:D:660:GLU:HB3   | 3:D:685:ILE:HD12  | 1.67                     | 0.74              |
| 2:I:1276:TRP:HH2  | 3:J:798:ARG:HG3   | 1.52                     | 0.74              |
| 2:I:1287:LEU:HD22 | 3:J:1357:ILE:HG13 | 1.70                     | 0.74              |
| 3:D:722:ILE:HA    | 3:D:725:MET:HE3   | 1.69                     | 0.74              |
| 2:I:525:THR:HG21  | 2:I:687:ARG:HD2   | 1.68                     | 0.74              |
| 5:L:134:VAL:HA    | 5:L:273:MET:HE1   | 1.68                     | 0.73              |
| 3:D:647:PRO:HG3   | 3:D:697:MET:HB3   | 1.68                     | 0.73              |
| 2:I:30:ILE:HD12   | 2:I:30:ILE:H      | 1.51                     | 0.73              |
| 2:C:942:ASP:OD2   | 2:C:1048:LYS:NZ   | 2.21                     | 0.73              |
| 3:J:35:PHE:HD1    | 3:J:101:ARG:HD3   | 1.52                     | 0.73              |
| 3:D:495:ASN:O     | 3:D:497:GLU:N     | 2.21                     | 0.73              |
| 2:I:976:ARG:HD2   | 2:I:989:LEU:HD23  | 1.71                     | 0.73              |
| 2:C:840:SER:HB2   | 2:C:850:ILE:HD11  | 1.70                     | 0.73              |
| 2:C:974:ARG:HD2   | 2:C:1014:LEU:HD21 | 1.71                     | 0.73              |
| 1:H:134:THR:HG23  | 1:H:135:ASP:H     | 1.53                     | 0.73              |
| 1:A:191:ARG:NH1   | 1:A:198:LEU:O     | 2.22                     | 0.73              |
| 3:D:252:LEU:HD23  | 3:D:262:THR:HB    | 1.71                     | 0.73              |
| 3:J:430:HIS:CD2   | 3:J:432:LEU:HB2   | 2.24                     | 0.73              |
| 2:C:700:VAL:HG13  | 2:C:1117:LEU:HD22 | 1.71                     | 0.73              |
| 2:C:1002:LEU:HD22 | 2:C:1007:LYS:HB2  | 1.71                     | 0.73              |
| 5:F:290:LEU:HB3   | 5:F:333:VAL:HG21  | 1.71                     | 0.72              |
| 3:D:395:LYS:HG2   | 5:F:536:THR:HG21  | 1.71                     | 0.72              |
| 5:L:231:THR:HG23  | 5:L:249:ILE:HG12  | 1.72                     | 0.72              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:460:ASP:OD1   | 3:J:462:ASP:OD1   | 2.07                     | 0.72              |
| 2:C:356:THR:HG21  | 2:C:362:ALA:HA    | 1.70                     | 0.72              |
| 3:D:418:GLU:OE1   | 4:E:3:ARG:NH2     | 2.23                     | 0.72              |
| 4:E:35:LYS:NZ     | 4:E:71:GLU:OE2    | 2.21                     | 0.72              |
| 1:G:60:GLU:HB2    | 1:G:170:ARG:HG2   | 1.71                     | 0.72              |
| 3:D:709:ARG:O     | 3:D:711:GLY:N     | 2.23                     | 0.72              |
| 1:A:66:HIS:HA     | 1:A:171:LEU:HD11  | 1.71                     | 0.71              |
| 2:C:201:ARG:NH2   | 2:C:370:MET:O     | 2.23                     | 0.71              |
| 3:J:750:PRO:HA    | 3:J:777:HIS:CE1   | 2.25                     | 0.71              |
| 3:J:1280:VAL:HG11 | 3:J:1304:ARG:HE   | 1.55                     | 0.71              |
| 3:D:739:GLN:NE2   | 6:M:9:TYR:OH      | 2.23                     | 0.71              |
| 3:J:17:PHE:O      | 3:J:1355:ARG:NH2  | 2.23                     | 0.71              |
| 1:A:226:GLU:HB3   | 1:B:10:LYS:HE2    | 1.72                     | 0.71              |
| 1:A:77:ASP:OD1    | 1:A:77:ASP:N      | 2.24                     | 0.71              |
| 1:A:47:LEU:HD23   | 1:A:51:MET:HE2    | 1.73                     | 0.71              |
| 2:C:721:GLY:N     | 2:C:740:GLU:OE1   | 2.22                     | 0.71              |
| 1:B:62:ASP:OD1    | 1:B:62:ASP:N      | 2.21                     | 0.71              |
| 1:A:14:VAL:HG22   | 1:A:15:ASP:H      | 1.56                     | 0.70              |
| 1:B:182:ARG:NH1   | 3:D:534:GLU:OE1   | 2.23                     | 0.70              |
| 2:C:69:GLN:HE21   | 2:C:101:ARG:HD2   | 1.55                     | 0.70              |
| 3:D:746:LEU:HB2   | 3:D:754:ILE:HD11  | 1.72                     | 0.70              |
| 5:F:479:THR:HG22  | 5:F:482:GLU:HB2   | 1.72                     | 0.70              |
| 3:D:362:ARG:H     | 3:D:365:GLN:HE21  | 1.39                     | 0.70              |
| 3:D:853:THR:HG21  | 3:J:1375:ALA:HB1  | 1.74                     | 0.70              |
| 1:G:35:PHE:HE1    | 1:H:46:ILE:HG12   | 1.56                     | 0.70              |
| 2:I:1116:HIS:HE1  | 3:J:641:ILE:N     | 1.89                     | 0.70              |
| 2:I:1131:MET:HE2  | 2:I:1141:LEU:HD12 | 1.73                     | 0.70              |
| 3:D:490:ILE:H     | 3:D:490:ILE:HD13  | 1.55                     | 0.70              |
| 3:D:430:HIS:ND1   | 3:D:925:GLU:HG3   | 2.07                     | 0.70              |
| 2:I:674:ASP:OD2   | 2:I:1070:HIS:ND1  | 2.23                     | 0.70              |
| 5:L:479:THR:HG22  | 5:L:482:GLU:HB2   | 1.74                     | 0.70              |
| 2:C:196:VAL:HG12  | 2:C:206:ALA:HA    | 1.74                     | 0.70              |
| 2:C:143:ARG:NH2   | 2:C:512:SER:O     | 2.25                     | 0.70              |
| 3:J:1199:PHE:HB2  | 3:J:1202:GLU:HB2  | 1.74                     | 0.70              |
| 3:J:1238:GLN:NE2  | 3:J:1248:ILE:O    | 2.24                     | 0.70              |
| 2:C:1160:ASP:CB   | 2:C:1161:LEU:HA   | 2.22                     | 0.70              |
| 2:I:528:ARG:NH2   | 2:I:576:SER:O     | 2.25                     | 0.70              |
| 5:L:573:LEU:HD23  | 5:L:573:LEU:H     | 1.57                     | 0.69              |
| 3:J:746:LEU:HG    | 3:J:758:PRO:HB3   | 1.74                     | 0.69              |
| 3:D:786:THR:HG21  | 6:M:8:ALA:HA      | 1.72                     | 0.69              |
| 1:G:83:LEU:HD23   | 2:I:694:ARG:HE    | 1.57                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:227:GLN:HG3   | 1:B:39:LEU:HD11   | 1.74                     | 0.69              |
| 3:D:363:LEU:HD23  | 3:D:487:THR:HG22  | 1.74                     | 0.69              |
| 2:I:168:GLY:O     | 2:I:170:VAL:N     | 2.24                     | 0.69              |
| 3:D:1289:ASN:O    | 3:D:1289:ASN:ND2  | 2.26                     | 0.69              |
| 2:I:9:LYS:HD2     | 2:I:791:LEU:HD21  | 1.75                     | 0.69              |
| 3:D:473:THR:HG23  | 3:D:476:ALA:H     | 1.58                     | 0.69              |
| 3:D:1233:ILE:O    | 3:D:1237:VAL:HG12 | 1.93                     | 0.69              |
| 4:E:38:LEU:HB3    | 4:E:58:LEU:HD22   | 1.74                     | 0.69              |
| 3:J:473:THR:HG23  | 3:J:476:ALA:H     | 1.57                     | 0.68              |
| 2:C:798:GLN:OE1   | 2:C:827:ARG:HB2   | 1.94                     | 0.68              |
| 3:D:35:PHE:CD1    | 3:D:101:ARG:HD3   | 2.25                     | 0.68              |
| 3:J:808:VAL:HG13  | 3:J:914:ALA:HA    | 1.76                     | 0.68              |
| 3:D:367:GLY:HA3   | 3:D:448:GLN:HB2   | 1.75                     | 0.68              |
| 2:C:839:VAL:HG12  | 2:C:1049:ILE:HG12 | 1.74                     | 0.68              |
| 3:D:120:LEU:HB3   | 3:D:121:PRO:HD3   | 1.76                     | 0.68              |
| 3:D:1298:VAL:H    | 3:D:1299:GLY:HA3  | 1.57                     | 0.68              |
| 4:E:4:VAL:HG13    | 4:E:5:THR:H       | 1.59                     | 0.68              |
| 1:G:150:ARG:NH1   | 1:H:7:GLU:O       | 2.20                     | 0.68              |
| 2:C:1161:LEU:HD21 | 2:C:1165:SER:HB3  | 1.76                     | 0.68              |
| 3:D:749:LYS:HB2   | 3:D:750:PRO:HD2   | 1.75                     | 0.68              |
| 3:J:418:GLU:HG3   | 4:K:45:LYS:H      | 1.59                     | 0.68              |
| 3:J:1169:THR:HG23 | 3:J:1192:LYS:HD3  | 1.76                     | 0.68              |
| 2:C:810:TYR:CE2   | 3:D:359:PRO:HD2   | 2.29                     | 0.68              |
| 3:J:367:GLY:HA3   | 3:J:448:GLN:HB2   | 1.74                     | 0.68              |
| 4:E:32:VAL:O      | 4:E:34:GLY:N      | 2.26                     | 0.67              |
| 3:J:683:ILE:HD13  | 6:N:23:ILE:HG21   | 1.76                     | 0.67              |
| 5:F:309:ASN:HD21  | 5:F:312:SER:HB3   | 1.59                     | 0.67              |
| 6:N:33:PRO:HG3    | 6:N:54:GLY:HA2    | 1.77                     | 0.67              |
| 2:C:898:GLU:HB3   | 5:F:540:LEU:HD22  | 1.74                     | 0.67              |
| 5:L:484:ALA:HB1   | 5:L:491:GLU:HB2   | 1.76                     | 0.67              |
| 2:I:739:ASP:OD1   | 2:I:739:ASP:N     | 2.26                     | 0.67              |
| 5:L:277:MET:HG3   | 5:L:362:ASN:HD21  | 1.60                     | 0.67              |
| 5:F:444:ALA:HB1   | 5:F:457:ILE:HD13  | 1.76                     | 0.67              |
| 2:I:596:ASP:CG    | 2:I:597:GLY:H     | 2.03                     | 0.67              |
| 2:I:678:ARG:HG3   | 2:I:1108:ASN:HD22 | 1.60                     | 0.67              |
| 2:I:559:CYS:HB2   | 2:I:662:SER:HB3   | 1.77                     | 0.67              |
| 3:J:1154:ALA:HB3  | 3:J:1215:GLU:HB3  | 1.77                     | 0.67              |
| 2:I:1160:ASP:CB   | 2:I:1161:LEU:HA   | 2.24                     | 0.67              |
| 2:I:1333:LEU:HD23 | 3:J:307:LEU:HD22  | 1.76                     | 0.67              |
| 3:J:722:ILE:HA    | 3:J:725:MET:HE3   | 1.75                     | 0.67              |
| 1:A:145:LYS:NZ    | 1:A:147:GLN:OE1   | 2.28                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:1087:TYR:HE1  | 2:I:1215:GLY:HA2  | 1.60                     | 0.67              |
| 1:B:29:GLU:HB3    | 1:B:200:LYS:HG3   | 1.76                     | 0.66              |
| 2:I:86:GLN:HA     | 2:I:140:GLY:HA2   | 1.76                     | 0.66              |
| 3:J:268:LEU:HD13  | 3:J:306:LEU:HA    | 1.75                     | 0.66              |
| 3:D:48:THR:O      | 3:D:50:LYS:N      | 2.28                     | 0.66              |
| 3:D:664:ILE:HG22  | 3:D:678:ARG:HG2   | 1.77                     | 0.66              |
| 5:F:487:MET:HA    | 5:F:487:MET:HE2   | 1.76                     | 0.66              |
| 2:I:148:GLN:NE2   | 2:I:535:PRO:O     | 2.28                     | 0.66              |
| 2:I:678:ARG:NH2   | 6:N:6:ASP:OD1     | 2.29                     | 0.66              |
| 2:I:1129:ASN:HB2  | 2:I:1177:ARG:HB2  | 1.77                     | 0.66              |
| 3:J:1233:ILE:O    | 3:J:1237:VAL:HG12 | 1.94                     | 0.66              |
| 5:L:561:MET:HA    | 5:L:567:MET:HE1   | 1.78                     | 0.66              |
| 1:A:45:ARG:NH2    | 2:C:1216:ARG:HA   | 2.11                     | 0.66              |
| 3:D:668:PHE:HB2   | 3:D:678:ARG:HG3   | 1.78                     | 0.66              |
| 3:D:690:ASN:ND2   | 3:D:745:GLY:HA2   | 2.10                     | 0.66              |
| 3:J:517:CYS:HA    | 3:J:716:GLN:HE22  | 1.60                     | 0.66              |
| 3:J:1198:VAL:HB   | 3:J:1210:ILE:HG23 | 1.78                     | 0.66              |
| 2:C:1191:LYS:HD3  | 2:C:1193:ALA:H    | 1.60                     | 0.66              |
| 2:C:1142:ARG:HH12 | 2:C:1169:VAL:HG21 | 1.60                     | 0.66              |
| 3:D:268:LEU:HD13  | 3:D:306:LEU:HA    | 1.77                     | 0.66              |
| 3:D:1227:HIS:CD2  | 3:J:1293:GLU:HG2  | 2.30                     | 0.66              |
| 3:J:1179:PRO:HD2  | 3:J:1184:ASP:HA   | 1.76                     | 0.66              |
| 5:L:493:LYS:O     | 5:L:497:VAL:N     | 2.22                     | 0.66              |
| 1:B:35:PHE:HA     | 1:B:38:THR:HG22   | 1.77                     | 0.66              |
| 3:J:885:VAL:HG12  | 3:J:894:VAL:HG11  | 1.78                     | 0.66              |
| 3:D:746:LEU:CB    | 3:D:754:ILE:HD11  | 2.25                     | 0.66              |
| 5:F:493:LYS:HG2   | 5:F:496:LYS:HE2   | 1.78                     | 0.66              |
| 2:I:65:ASN:HB3    | 2:I:105:TYR:HB2   | 1.78                     | 0.66              |
| 3:J:901:ARG:HD2   | 3:J:906:GLY:O     | 1.96                     | 0.66              |
| 2:C:1149:TYR:CD1  | 2:C:1159:VAL:HG11 | 2.30                     | 0.65              |
| 2:I:95:PRO:HA     | 2:I:126:GLU:HG2   | 1.78                     | 0.65              |
| 3:J:591:ILE:HG23  | 3:J:604:MET:HE2   | 1.78                     | 0.65              |
| 2:C:814:ASP:OD2   | 2:C:1106:ARG:NH1  | 2.16                     | 0.65              |
| 1:G:9:LEU:O       | 1:H:227:GLN:NE2   | 2.29                     | 0.65              |
| 2:I:1327:LEU:O    | 2:I:1331:ARG:HB2  | 1.97                     | 0.65              |
| 2:I:985:GLU:HB3   | 2:I:988:LYS:HB2   | 1.78                     | 0.65              |
| 5:L:313:ASP:OD1   | 5:L:338:HIS:NE2   | 2.30                     | 0.65              |
| 2:C:557:ARG:HB3   | 2:C:587:LEU:HD13  | 1.78                     | 0.65              |
| 3:D:28:ASP:OD1    | 3:D:31:ARG:NH1    | 2.30                     | 0.65              |
| 2:C:705:GLU:HB2   | 2:C:794:LEU:H     | 1.61                     | 0.65              |
| 2:I:409:LEU:HD11  | 2:I:428:VAL:HG23  | 1.79                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:746:LEU:HG    | 3:D:758:PRO:HB3   | 1.79                     | 0.65              |
| 3:D:559:ALA:HB3   | 3:D:562:GLU:HB3   | 1.77                     | 0.65              |
| 2:I:990:ASP:HA    | 2:I:997:TRP:HZ2   | 1.62                     | 0.65              |
| 3:D:885:VAL:HG12  | 3:D:894:VAL:HG11  | 1.79                     | 0.64              |
| 3:D:848:VAL:HG12  | 3:D:858:VAL:HG22  | 1.80                     | 0.64              |
| 2:I:885:GLY:HA2   | 2:I:917:SER:HB3   | 1.78                     | 0.64              |
| 2:I:470:ARG:HE    | 2:I:497:PRO:HB3   | 1.61                     | 0.64              |
| 2:I:1176:LEU:HD13 | 2:I:1180:MET:HG3  | 1.78                     | 0.64              |
| 3:J:384:LYS:NZ    | 3:J:414:GLU:OE1   | 2.28                     | 0.64              |
| 1:H:82:LEU:HD22   | 1:H:173:VAL:HG22  | 1.79                     | 0.64              |
| 2:I:452:ARG:NH1   | 2:I:584:TYR:O     | 2.31                     | 0.64              |
| 1:A:97:GLU:HB3    | 1:A:147:GLN:HG2   | 1.80                     | 0.64              |
| 2:C:297:VAL:HG12  | 2:C:315:MET:O     | 1.97                     | 0.64              |
| 3:D:262:THR:OG1   | 3:D:266:ASN:ND2   | 2.29                     | 0.64              |
| 3:D:708:ASN:OD1   | 3:D:708:ASN:N     | 2.31                     | 0.64              |
| 3:D:378:LYS:NZ    | 3:D:382:TYR:OH    | 2.28                     | 0.64              |
| 3:J:259:ARG:HD3   | 5:L:502:LYS:HD2   | 1.79                     | 0.64              |
| 3:J:395:LYS:HG2   | 5:L:536:THR:HG21  | 1.78                     | 0.64              |
| 2:C:563:THR:HG22  | 2:C:680:LEU:HD11  | 1.77                     | 0.64              |
| 1:G:45:ARG:HG2    | 1:H:38:THR:HB     | 1.80                     | 0.64              |
| 3:J:797:THR:O     | 3:J:801:VAL:HG12  | 1.98                     | 0.64              |
| 3:D:43:THR:OG1    | 5:F:449:THR:O     | 2.10                     | 0.64              |
| 2:I:732:ILE:HG21  | 2:I:783:LEU:HD12  | 1.80                     | 0.64              |
| 2:C:800:MET:HG3   | 2:C:1096:ILE:HD11 | 1.79                     | 0.64              |
| 3:J:813:ASP:OD1   | 3:J:883:ARG:NH2   | 2.30                     | 0.64              |
| 5:L:493:LYS:HG2   | 5:L:496:LYS:HE2   | 1.79                     | 0.64              |
| 2:C:93:SER:OG     | 2:C:126:GLU:OE1   | 2.12                     | 0.63              |
| 1:A:289:LEU:HD13  | 1:A:300:LEU:HD21  | 1.78                     | 0.63              |
| 2:C:297:VAL:HG23  | 2:C:333:ILE:HG23  | 1.80                     | 0.63              |
| 2:C:673:HIS:HB3   | 2:C:1109:ILE:HG22 | 1.80                     | 0.63              |
| 3:J:844:THR:OG1   | 3:J:860:ARG:O     | 2.11                     | 0.63              |
| 2:I:1106:ARG:HD2  | 2:I:1106:ARG:H    | 1.62                     | 0.63              |
| 1:A:16:ILE:HG12   | 1:A:26:VAL:HB     | 1.79                     | 0.63              |
| 2:I:30:ILE:HD11   | 2:I:575:LEU:HD22  | 1.80                     | 0.63              |
| 2:C:105:TYR:HD1   | 2:C:112:GLY:H     | 1.45                     | 0.63              |
| 2:C:708:VAL:HG11  | 2:C:794:LEU:HD22  | 1.81                     | 0.63              |
| 3:D:426:ALA:HB3   | 3:D:427:PRO:HD3   | 1.80                     | 0.63              |
| 2:I:560:PRO:O     | 3:J:780:ARG:NH2   | 2.30                     | 0.63              |
| 3:J:833:GLU:OE2   | 3:J:1247:LYS:NZ   | 2.30                     | 0.63              |
| 2:C:617:ALA:HA    | 2:C:636:CYS:SG    | 2.38                     | 0.63              |
| 2:C:724:VAL:HG11  | 2:C:727:VAL:HG22  | 1.79                     | 0.63              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:I:992:LEU:HD11 | 2:I:1000:LEU:HD11 | 1.81                     | 0.63              |
| 3:D:62:PHE:CD1   | 3:D:247:PRO:HD3   | 2.34                     | 0.63              |
| 3:J:331:ILE:HG22 | 3:J:1328:THR:HG21 | 1.81                     | 0.63              |
| 3:J:747:MET:HE2  | 3:J:775:SER:HA    | 1.79                     | 0.63              |
| 2:I:363:LEU:HB3  | 2:I:381:ALA:HB1   | 1.79                     | 0.62              |
| 2:I:1082:ILE:H   | 2:I:1082:ILE:HD12 | 1.64                     | 0.62              |
| 2:C:1256:GLN:HB3 | 2:C:1301:ARG:HH22 | 1.62                     | 0.62              |
| 3:J:866:GLU:OE2  | 3:J:901:ARG:NH2   | 2.30                     | 0.62              |
| 5:L:105:MET:HE1  | 5:L:385:ARG:HG2   | 1.80                     | 0.62              |
| 2:C:119:GLU:HG3  | 2:C:489:PRO:HD2   | 1.82                     | 0.62              |
| 2:C:246:LEU:HB2  | 2:C:269:ILE:HG21  | 1.81                     | 0.62              |
| 1:G:14:VAL:HG13  | 1:G:15:ASP:H      | 1.62                     | 0.62              |
| 1:A:184:ALA:HB2  | 2:C:1091:GLY:HA3  | 1.81                     | 0.62              |
| 1:B:63:GLY:HA3   | 1:B:71:LYS:HE3    | 1.81                     | 0.62              |
| 5:F:479:THR:HG23 | 5:F:481:GLU:H     | 1.64                     | 0.62              |
| 2:I:748:ILE:HD11 | 2:I:966:ILE:HG22  | 1.81                     | 0.62              |
| 2:I:206:ALA:O    | 2:I:209:ILE:HG22  | 1.99                     | 0.62              |
| 3:J:126:LEU:HD13 | 3:J:223:LEU:HD21  | 1.81                     | 0.62              |
| 3:J:317:THR:HG23 | 3:J:320:ASN:HB3   | 1.81                     | 0.62              |
| 1:G:161:SER:O    | 1:G:163:GLU:N     | 2.33                     | 0.62              |
| 1:H:59:VAL:HG22  | 1:H:144:ILE:HG13  | 1.81                     | 0.62              |
| 2:I:1222:GLU:OE1 | 3:J:512:TYR:OH    | 2.09                     | 0.62              |
| 3:J:79:LYS:HB2   | 5:L:569:THR:H     | 1.64                     | 0.62              |
| 3:J:378:LYS:NZ   | 3:J:382:TYR:OH    | 2.29                     | 0.62              |
| 1:B:118:ASP:HB2  | 1:B:121:VAL:HB    | 1.81                     | 0.61              |
| 3:D:609:TYR:HE2  | 3:D:614:LEU:HD12  | 1.63                     | 0.61              |
| 2:I:4:SER:OG     | 2:I:5:TYR:N       | 2.26                     | 0.61              |
| 2:I:1240:ASP:OD1 | 2:I:1240:ASP:N    | 2.25                     | 0.61              |
| 2:I:1304:MET:HE3 | 2:I:1308:ILE:HD11 | 1.82                     | 0.61              |
| 2:C:138:ILE:HD11 | 2:C:506:PHE:HB3   | 1.82                     | 0.61              |
| 2:C:550:VAL:HG11 | 3:D:776:THR:HG22  | 1.81                     | 0.61              |
| 1:G:12:ARG:H     | 1:G:30:PRO:HD2    | 1.64                     | 0.61              |
| 3:J:495:ASN:O    | 3:J:497:GLU:N     | 2.32                     | 0.61              |
| 3:J:1365:TYR:OH  | 3:J:1369:ARG:NH1  | 2.32                     | 0.61              |
| 1:A:251:PRO:HD2  | 5:F:605:GLU:HG3   | 1.83                     | 0.61              |
| 2:C:1164:PHE:O   | 2:C:1166:ASP:N    | 2.33                     | 0.61              |
| 2:I:6:THR:OG1    | 2:I:781:ASP:OD2   | 2.10                     | 0.61              |
| 2:I:557:ARG:HB3  | 2:I:587:LEU:HD13  | 1.82                     | 0.61              |
| 3:D:317:THR:HG23 | 3:D:320:ASN:HB3   | 1.81                     | 0.61              |
| 3:D:474:LEU:HD12 | 3:D:477:GLN:HE21  | 1.64                     | 0.61              |
| 5:F:492:ASP:HB2  | 5:F:495:ARG:HH12  | 1.65                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:L:562:ARG:NH2   | 5:L:573:LEU:HD22  | 2.16                     | 0.61              |
| 1:B:191:ARG:NH2   | 3:D:410:ASP:OD2   | 2.33                     | 0.61              |
| 2:C:86:GLN:HA     | 2:C:140:GLY:HA2   | 1.81                     | 0.61              |
| 2:C:125:GLY:HA3   | 2:C:499:SER:HB2   | 1.81                     | 0.61              |
| 1:H:73:GLY:HA2    | 1:H:134:THR:HG22  | 1.83                     | 0.61              |
| 2:I:618:GLN:HG3   | 3:J:770:LEU:HD21  | 1.82                     | 0.61              |
| 2:I:168:GLY:C     | 2:I:170:VAL:H     | 2.08                     | 0.61              |
| 3:J:190:LYS:HD3   | 3:J:235:GLU:HG2   | 1.83                     | 0.61              |
| 3:D:57:PHE:HB3    | 3:D:98:ARG:HH22   | 1.66                     | 0.61              |
| 3:D:355:ILE:HG22  | 3:D:447:ILE:HB    | 1.83                     | 0.61              |
| 3:D:1169:THR:HG23 | 3:D:1192:LYS:HD3  | 1.83                     | 0.61              |
| 3:J:16:GLU:HG3    | 3:J:17:PHE:H      | 1.66                     | 0.61              |
| 3:J:786:THR:HG21  | 6:N:8:ALA:HA      | 1.82                     | 0.61              |
| 6:N:46:GLU:HB3    | 6:N:49:ARG:HH21   | 1.66                     | 0.61              |
| 2:I:998:LEU:H     | 2:I:998:LEU:HD12  | 1.65                     | 0.60              |
| 2:I:1117:LEU:HD12 | 2:I:1195:ILE:HG12 | 1.83                     | 0.60              |
| 3:J:460:ASP:OD1   | 6:N:4:GLU:OE2     | 2.19                     | 0.60              |
| 4:E:39:VAL:HG22   | 4:E:40:PRO:HD2    | 1.83                     | 0.60              |
| 1:G:45:ARG:HH21   | 2:I:1216:ARG:HA   | 1.65                     | 0.60              |
| 3:D:424:ASN:HB2   | 3:D:434:ILE:HG12  | 1.83                     | 0.60              |
| 3:D:1158:GLU:HA   | 3:D:1223:LEU:HD11 | 1.82                     | 0.60              |
| 3:J:137:ARG:HG2   | 3:J:142:GLU:HB2   | 1.83                     | 0.60              |
| 4:K:26:ARG:HD3    | 4:K:64:LEU:HD21   | 1.84                     | 0.60              |
| 2:C:618:GLN:HG3   | 3:D:770:LEU:HD21  | 1.84                     | 0.60              |
| 2:C:744:GLY:C     | 2:C:746:ALA:H     | 2.09                     | 0.60              |
| 2:C:1100:PRO:HB3  | 3:D:639:VAL:HG12  | 1.83                     | 0.60              |
| 2:C:1253:LEU:HD11 | 3:D:253:VAL:HG11  | 1.82                     | 0.60              |
| 2:I:138:ILE:HD11  | 2:I:506:PHE:HB3   | 1.82                     | 0.60              |
| 2:C:1106:ARG:H    | 2:C:1106:ARG:HD2  | 1.65                     | 0.60              |
| 3:J:489:ASN:HA    | 3:J:904:ALA:HB1   | 1.83                     | 0.60              |
| 1:A:135:ASP:O     | 1:A:137:ASN:N     | 2.35                     | 0.60              |
| 2:C:1085:MET:HA   | 2:C:1085:MET:HE2  | 1.82                     | 0.60              |
| 3:D:1167:LYS:NZ   | 3:D:1168:GLU:O    | 2.34                     | 0.60              |
| 2:I:310:ILE:HG21  | 2:I:325:LEU:HB3   | 1.82                     | 0.60              |
| 2:I:972:PHE:HE2   | 2:I:998:LEU:HD11  | 1.67                     | 0.60              |
| 3:J:430:HIS:ND1   | 3:J:925:GLU:HG3   | 2.17                     | 0.60              |
| 3:J:491:LEU:HB2   | 3:J:904:ALA:HA    | 1.84                     | 0.60              |
| 2:C:718:ALA:HB2   | 2:C:783:LEU:HD23  | 1.84                     | 0.60              |
| 3:J:892:PHE:H     | 3:J:1281:GLU:HG2  | 1.66                     | 0.60              |
| 3:D:842:ARG:HB3   | 3:D:882:VAL:HG11  | 1.82                     | 0.60              |
| 1:G:228:LEU:HD21  | 1:H:224:LEU:HB3   | 1.83                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:L:489:MET:HE2   | 5:L:493:LYS:HB2   | 1.84                     | 0.60              |
| 2:C:1142:ARG:HD3  | 2:C:1161:LEU:HD22 | 1.83                     | 0.60              |
| 1:G:38:THR:HG1    | 1:H:45:ARG:NH1    | 2.00                     | 0.60              |
| 2:I:119:GLU:HG3   | 2:I:489:PRO:HD2   | 1.83                     | 0.60              |
| 3:J:658:GLU:O     | 3:J:661:VAL:HG22  | 2.01                     | 0.60              |
| 6:M:31:GLY:O      | 6:M:32:ILE:HG13   | 2.02                     | 0.60              |
| 6:M:45:PRO:HD2    | 6:M:48:ARG:CZ     | 2.32                     | 0.60              |
| 2:C:290:GLU:HG2   | 2:C:319:LEU:HD12  | 1.84                     | 0.59              |
| 3:D:1181:ASP:OD1  | 3:D:1182:GLY:N    | 2.34                     | 0.59              |
| 2:C:976:ARG:HD2   | 2:C:989:LEU:HD23  | 1.83                     | 0.59              |
| 2:C:980:VAL:HG13  | 2:C:984:VAL:HB    | 1.85                     | 0.59              |
| 3:D:849:LEU:H     | 3:D:849:LEU:HD22  | 1.67                     | 0.59              |
| 3:J:761:ALA:H     | 3:J:771:GLN:HE22  | 1.50                     | 0.59              |
| 3:J:1183:SER:C    | 3:J:1185:PRO:HD3  | 2.28                     | 0.59              |
| 2:C:519:ASN:ND2   | 2:C:689:ALA:HB3   | 2.17                     | 0.59              |
| 3:D:786:THR:HA    | 3:D:789:LYS:HG3   | 1.82                     | 0.59              |
| 3:J:612:LEU:HB3   | 3:J:616:PRO:HG2   | 1.83                     | 0.59              |
| 2:C:360:LEU:HD11  | 2:C:378:ARG:HA    | 1.83                     | 0.59              |
| 2:C:1087:TYR:HE1  | 2:C:1215:GLY:HA2  | 1.68                     | 0.59              |
| 2:C:1305:TYR:CE1  | 3:D:379:PRO:HG3   | 2.37                     | 0.59              |
| 5:F:466:ILE:HD11  | 5:F:487:MET:HE3   | 1.84                     | 0.59              |
| 1:G:41:ASN:ND2    | 2:I:1216:ARG:O    | 2.31                     | 0.59              |
| 3:J:863:LEU:HD11  | 3:J:901:ARG:HB3   | 1.84                     | 0.59              |
| 5:L:470:MET:HB2   | 5:L:478:PRO:HG3   | 1.82                     | 0.59              |
| 1:A:310:ARG:O     | 5:F:608:ARG:NH2   | 2.35                     | 0.59              |
| 1:B:112:ALA:HB3   | 1:B:126:PRO:HA    | 1.85                     | 0.59              |
| 1:B:215:GLU:HA    | 1:B:218:ARG:HG3   | 1.85                     | 0.59              |
| 2:C:209:ILE:HD11  | 2:C:425:ILE:HD13  | 1.85                     | 0.59              |
| 3:J:35:PHE:CD1    | 3:J:101:ARG:HD3   | 2.35                     | 0.59              |
| 3:J:660:GLU:HB3   | 3:J:685:ILE:HD12  | 1.83                     | 0.59              |
| 1:A:211:ILE:HG21  | 1:A:216:ALA:HB2   | 1.84                     | 0.59              |
| 2:I:1119:MET:HE3  | 2:I:1204:LEU:HD22 | 1.84                     | 0.59              |
| 2:C:519:ASN:HD21  | 2:C:796:LEU:HD23  | 1.67                     | 0.59              |
| 3:D:1183:SER:C    | 3:D:1185:PRO:HD3  | 2.27                     | 0.59              |
| 2:I:720:ARG:HE    | 2:I:736:VAL:HG11  | 1.68                     | 0.59              |
| 5:L:469:GLN:O     | 5:L:473:GLU:HB2   | 2.03                     | 0.59              |
| 2:C:1282:GLY:O    | 2:C:1284:ALA:N    | 2.35                     | 0.59              |
| 2:C:1287:LEU:HD22 | 3:D:1357:ILE:HD11 | 1.84                     | 0.59              |
| 1:H:60:GLU:OE2    | 1:H:143:ARG:NH1   | 2.35                     | 0.59              |
| 1:A:100:LEU:HD23  | 1:A:115:ILE:HG21  | 1.85                     | 0.59              |
| 2:C:1065:LYS:HD3  | 2:C:1235:LEU:HD12 | 1.85                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:1080:ASN:HB3  | 2:C:1085:MET:HE3  | 1.84                     | 0.59              |
| 3:D:515:ARG:O     | 3:D:545:HIS:HB3   | 2.02                     | 0.59              |
| 5:F:490:PRO:HB2   | 5:F:493:LYS:HG3   | 1.84                     | 0.59              |
| 1:H:89:ALA:HB3    | 1:H:124:VAL:HG12  | 1.85                     | 0.59              |
| 2:C:149:LEU:HD13  | 2:C:453:ILE:HG13  | 1.84                     | 0.59              |
| 2:C:629:PHE:CE2   | 2:C:650:VAL:HG21  | 2.38                     | 0.59              |
| 2:C:1283:ALA:HB1  | 2:C:1286:THR:HB   | 1.85                     | 0.59              |
| 1:H:48:LEU:HD21   | 3:J:535:ARG:HG3   | 1.83                     | 0.59              |
| 2:I:1013:GLN:O    | 2:I:1017:GLN:HG2  | 2.03                     | 0.59              |
| 5:F:231:THR:HG23  | 5:F:249:ILE:HG12  | 1.85                     | 0.58              |
| 2:C:802:VAL:HG11  | 2:C:1230:MET:HB3  | 1.85                     | 0.58              |
| 3:D:817:HIS:CE1   | 3:D:860:ARG:HH21  | 2.22                     | 0.58              |
| 6:M:48:ARG:NH2    | 6:M:58:CYS:HA     | 2.18                     | 0.58              |
| 2:C:143:ARG:HH21  | 2:C:513:GLN:HA    | 1.68                     | 0.58              |
| 3:D:259:ARG:HG3   | 5:F:502:LYS:HD2   | 1.86                     | 0.58              |
| 3:D:527:LEU:HB2   | 3:D:550:VAL:HG12  | 1.84                     | 0.58              |
| 2:I:1192:GLU:OE2  | 3:J:764:ARG:HD3   | 2.03                     | 0.58              |
| 2:I:1331:ARG:HG2  | 3:J:33:TRP:CZ3    | 2.39                     | 0.58              |
| 1:G:100:LEU:HD23  | 1:G:115:ILE:HG21  | 1.84                     | 0.58              |
| 2:C:810:TYR:CD2   | 3:D:359:PRO:HD2   | 2.38                     | 0.58              |
| 3:D:1167:LYS:HZ1  | 3:D:1170:LYS:HB2  | 1.68                     | 0.58              |
| 2:I:697:LYS:HD2   | 2:I:1181:PRO:HG3  | 1.85                     | 0.58              |
| 3:J:1158:GLU:HA   | 3:J:1223:LEU:HD11 | 1.84                     | 0.58              |
| 2:C:1105:SER:HB2  | 3:D:731:ARG:HG2   | 1.86                     | 0.58              |
| 3:D:1270:GLY:HA3  | 3:D:1297:LYS:C    | 2.28                     | 0.58              |
| 1:G:166:ARG:HD3   | 1:G:168:ILE:HG23  | 1.85                     | 0.58              |
| 4:K:26:ARG:NH1    | 4:K:29:GLN:OE1    | 2.36                     | 0.58              |
| 5:L:379:MET:O     | 5:L:383:ASN:ND2   | 2.36                     | 0.58              |
| 2:C:466:VAL:HA    | 2:C:469:VAL:HG22  | 1.86                     | 0.58              |
| 2:C:1124:ILE:HG21 | 2:C:1180:MET:HE2  | 1.86                     | 0.58              |
| 2:I:1105:SER:HB2  | 3:J:731:ARG:HG2   | 1.84                     | 0.58              |
| 2:C:561:ILE:HD12  | 2:C:679:ALA:HB1   | 1.85                     | 0.58              |
| 2:I:855:PRO:HG3   | 2:I:913:VAL:HG13  | 1.85                     | 0.58              |
| 2:I:949:GLU:HG2   | 2:I:1036:ILE:HG22 | 1.86                     | 0.58              |
| 3:J:504:GLN:HG3   | 3:J:505:ASP:H     | 1.69                     | 0.58              |
| 5:L:466:ILE:HB    | 5:L:483:LEU:HD23  | 1.85                     | 0.58              |
| 2:C:124:MET:HB3   | 2:C:493:ILE:HD11  | 1.85                     | 0.58              |
| 2:C:269:ILE:HG23  | 2:C:273:HIS:HB2   | 1.84                     | 0.58              |
| 3:D:839:VAL:HG12  | 3:D:864:LEU:HD12  | 1.84                     | 0.58              |
| 2:C:360:LEU:HD22  | 2:C:378:ARG:HE    | 1.68                     | 0.58              |
| 3:D:161:THR:HG22  | 3:D:164:GLN:HB2   | 1.85                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:702:GLN:HA    | 3:J:723:TYR:CE2   | 2.38                     | 0.58              |
| 3:J:1368:ASP:OD1  | 3:J:1371:ARG:NH2  | 2.30                     | 0.58              |
| 6:M:25:GLN:O      | 6:M:27:ILE:N      | 2.35                     | 0.58              |
| 1:A:66:HIS:CE1    | 1:A:69:SER:HB3    | 2.39                     | 0.57              |
| 2:C:471:VAL:HG21  | 2:C:498:ILE:HD11  | 1.85                     | 0.57              |
| 5:F:469:GLN:O     | 5:F:473:GLU:HB2   | 2.04                     | 0.57              |
| 2:I:802:VAL:HG21  | 2:I:1098:LEU:HD22 | 1.85                     | 0.57              |
| 2:C:568:ASN:HB2   | 2:C:571:LEU:HB2   | 1.86                     | 0.57              |
| 3:D:114:ILE:HD11  | 3:D:311:ARG:HB2   | 1.86                     | 0.57              |
| 3:D:264:ASP:OD2   | 5:F:506:SER:OG    | 2.17                     | 0.57              |
| 3:D:414:GLU:O     | 4:E:45:LYS:NZ     | 2.36                     | 0.57              |
| 3:D:1159:ILE:HG22 | 3:D:1177:ILE:HD12 | 1.86                     | 0.57              |
| 5:F:111:LEU:HD11  | 5:F:119:ILE:HD12  | 1.85                     | 0.57              |
| 2:I:808:ASN:H     | 3:J:633:ALA:HB2   | 1.69                     | 0.57              |
| 3:D:398:LYS:HE2   | 5:F:532:LEU:HD23  | 1.85                     | 0.57              |
| 3:D:705:THR:OG1   | 3:D:718:SER:HA    | 2.04                     | 0.57              |
| 2:I:324:LYS:O     | 2:I:327:GLN:NE2   | 2.37                     | 0.57              |
| 6:M:63:ALA:O      | 6:M:66:GLU:N      | 2.36                     | 0.57              |
| 2:C:1116:HIS:CE1  | 3:D:641:ILE:H     | 2.11                     | 0.57              |
| 2:I:338:THR:HG22  | 2:I:345:PRO:HB3   | 1.86                     | 0.57              |
| 2:I:670:PHE:HZ    | 2:I:1117:LEU:HD13 | 1.68                     | 0.57              |
| 6:N:16:THR:O      | 6:N:20:ILE:HG13   | 2.05                     | 0.57              |
| 1:A:241:GLU:HG3   | 1:A:242:VAL:H     | 1.70                     | 0.57              |
| 2:C:74:ARG:NH1    | 2:C:121:GLU:OE1   | 2.33                     | 0.57              |
| 2:C:1326:LEU:HD11 | 3:D:331:ILE:HG23  | 1.86                     | 0.57              |
| 3:D:317:THR:HG22  | 3:D:322:ARG:O     | 2.04                     | 0.57              |
| 2:I:810:TYR:CE1   | 2:I:1078:LYS:HD2  | 2.39                     | 0.57              |
| 2:C:1107:MET:HG2  | 3:D:740:LEU:HD11  | 1.85                     | 0.57              |
| 2:C:1315:MET:HE2  | 2:C:1317:PRO:HB3  | 1.85                     | 0.57              |
| 2:I:102:LEU:HB2   | 2:I:489:PRO:HG3   | 1.85                     | 0.57              |
| 2:I:109:ALA:HB1   | 2:I:111:GLU:HA    | 1.87                     | 0.57              |
| 3:J:1167:LYS:NZ   | 3:J:1168:GLU:O    | 2.38                     | 0.57              |
| 3:D:190:LYS:HD3   | 3:D:235:GLU:HG2   | 1.86                     | 0.57              |
| 2:C:97:ARG:HB3    | 2:C:121:GLU:HB3   | 1.85                     | 0.57              |
| 2:C:949:GLU:HG2   | 2:C:1036:ILE:HG22 | 1.85                     | 0.57              |
| 3:J:317:THR:HB    | 3:J:324:LEU:HB3   | 1.86                     | 0.57              |
| 2:C:26:TYR:HE2    | 2:C:32:LEU:HD12   | 1.69                     | 0.57              |
| 3:D:418:GLU:HG3   | 4:E:45:LYS:H      | 1.70                     | 0.57              |
| 2:I:736:VAL:HG23  | 2:I:748:ILE:HA    | 1.86                     | 0.57              |
| 2:I:887:VAL:HB    | 2:I:913:VAL:HG21  | 1.87                     | 0.57              |
| 3:J:120:LEU:HB3   | 3:J:121:PRO:HD3   | 1.86                     | 0.57              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:J:1319:PHE:HB3  | 3:J:1340:LYS:HD2 | 1.86                     | 0.57              |
| 5:L:148:TYR:OH    | 5:L:218:ARG:HA   | 2.05                     | 0.57              |
| 5:F:513:ASP:C     | 5:F:515:GLU:H    | 2.12                     | 0.57              |
| 4:K:39:VAL:HG22   | 4:K:40:PRO:HD2   | 1.87                     | 0.57              |
| 1:A:82:LEU:HB3    | 1:A:173:VAL:HG12 | 1.87                     | 0.56              |
| 2:C:670:PHE:CD2   | 2:C:1113:LEU:HB3 | 2.40                     | 0.56              |
| 2:C:1106:ARG:NE   | 6:M:6:ASP:OD2    | 2.36                     | 0.56              |
| 1:G:184:ALA:HB2   | 2:I:1091:GLY:HA3 | 1.86                     | 0.56              |
| 6:N:31:GLY:O      | 6:N:32:ILE:HG13  | 2.04                     | 0.56              |
| 1:B:192:VAL:O     | 1:B:194:GLN:N    | 2.38                     | 0.56              |
| 2:C:594:VAL:HG11  | 2:C:650:VAL:HG23 | 1.86                     | 0.56              |
| 1:G:49:SER:HB3    | 2:I:1083:GLU:CD  | 2.30                     | 0.56              |
| 1:H:191:ARG:HH22  | 3:J:409:TRP:HB3  | 1.69                     | 0.56              |
| 3:J:1221:LEU:HD11 | 3:J:1304:ARG:O   | 2.06                     | 0.56              |
| 1:A:47:LEU:O      | 1:A:180:VAL:HG21 | 2.04                     | 0.56              |
| 2:C:13:LYS:HD3    | 2:C:1149:TYR:HA  | 1.87                     | 0.56              |
| 2:C:324:LYS:O     | 2:C:327:GLN:NE2  | 2.38                     | 0.56              |
| 3:D:75:TYR:OH     | 3:D:86:GLU:OE1   | 2.21                     | 0.56              |
| 5:F:493:LYS:HA    | 5:F:496:LYS:HG3  | 1.85                     | 0.56              |
| 1:G:102:LEU:HD23  | 1:G:115:ILE:HG12 | 1.88                     | 0.56              |
| 2:I:169:LYS:O     | 2:I:170:VAL:HG22 | 2.05                     | 0.56              |
| 5:L:547:VAL:HG13  | 5:L:598:LEU:HD22 | 1.88                     | 0.56              |
| 1:A:16:ILE:HG23   | 1:A:26:VAL:HG12  | 1.87                     | 0.56              |
| 2:C:778:GLU:O     | 2:C:781:ASP:HB2  | 2.05                     | 0.56              |
| 1:H:133:LEU:HD11  | 1:H:140:ILE:HG21 | 1.87                     | 0.56              |
| 2:I:61:SER:HB3    | 2:I:479:LEU:HB3  | 1.87                     | 0.56              |
| 2:I:208:ILE:HG12  | 2:I:362:ALA:CB   | 2.35                     | 0.56              |
| 2:I:1243:MET:HA   | 3:J:353:SER:HB3  | 1.86                     | 0.56              |
| 1:A:83:LEU:HB3    | 2:C:694:ARG:HH21 | 1.70                     | 0.56              |
| 2:I:972:PHE:CE2   | 2:I:998:LEU:HD11 | 2.40                     | 0.56              |
| 2:I:1129:ASN:OD1  | 2:I:1177:ARG:NH2 | 2.37                     | 0.56              |
| 3:J:205:LEU:HD22  | 3:J:214:ARG:HB2  | 1.87                     | 0.56              |
| 1:A:102:LEU:HD23  | 1:A:115:ILE:HG12 | 1.88                     | 0.56              |
| 2:C:688:GLN:OE1   | 2:C:1237:HIS:HE1 | 1.87                     | 0.56              |
| 1:H:74:VAL:HG11   | 1:H:81:ILE:HD11  | 1.88                     | 0.56              |
| 2:I:798:GLN:OE1   | 2:I:827:ARG:HB2  | 2.06                     | 0.56              |
| 3:J:610:ARG:HG2   | 3:J:866:GLU:CD   | 2.31                     | 0.56              |
| 3:J:1239:ASP:OD1  | 3:J:1242:ARG:NH2 | 2.35                     | 0.56              |
| 5:L:364:ARG:HA    | 5:L:367:ILE:HD12 | 1.86                     | 0.56              |
| 2:I:746:ALA:HB2   | 2:I:974:ARG:HE   | 1.71                     | 0.56              |
| 3:J:1239:ASP:O    | 3:J:1243:LEU:HB2 | 2.06                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:1280:VAL:HG11 | 3:J:1304:ARG:NE   | 2.19                     | 0.56              |
| 1:A:137:ASN:N     | 1:A:137:ASN:OD1   | 2.36                     | 0.56              |
| 3:D:11:GLN:HG2    | 3:D:15:GLU:CD     | 2.31                     | 0.56              |
| 5:F:612:ASP:OD1   | 5:F:612:ASP:N     | 2.37                     | 0.56              |
| 2:I:395:TYR:HE2   | 2:I:397:LEU:HD12  | 1.70                     | 0.56              |
| 2:I:1192:GLU:OE1  | 3:J:764:ARG:NH1   | 2.38                     | 0.56              |
| 3:J:460:ASP:CG    | 3:J:462:ASP:OD1   | 2.48                     | 0.56              |
| 3:J:657:ALA:HA    | 3:J:660:GLU:HB2   | 1.88                     | 0.56              |
| 3:J:705:THR:HG21  | 3:J:719:PHE:H     | 1.71                     | 0.56              |
| 5:L:470:MET:O     | 5:L:478:PRO:HD3   | 2.06                     | 0.56              |
| 1:A:45:ARG:HG3    | 1:A:46:ILE:HD13   | 1.88                     | 0.56              |
| 2:I:356:THR:HG21  | 2:I:362:ALA:HA    | 1.88                     | 0.56              |
| 3:J:311:ARG:O     | 3:J:312:ARG:HD3   | 2.06                     | 0.56              |
| 3:J:761:ALA:H     | 3:J:771:GLN:NE2   | 2.04                     | 0.56              |
| 5:L:383:ASN:HB2   | 5:L:412:LEU:HD21  | 1.88                     | 0.56              |
| 2:C:269:ILE:HA    | 2:C:273:HIS:ND1   | 2.21                     | 0.56              |
| 4:E:2:ALA:HB2     | 4:E:55:GLU:CD     | 2.31                     | 0.56              |
| 3:J:68:TYR:HA     | 3:J:92:VAL:HG23   | 1.88                     | 0.56              |
| 5:L:508:GLU:HG3   | 5:L:518:HIS:ND1   | 2.21                     | 0.56              |
| 6:N:35:TYR:OH     | 6:N:49:ARG:NE     | 2.39                     | 0.56              |
| 2:C:27:LEU:HD13   | 2:C:663:VAL:HG11  | 1.88                     | 0.55              |
| 2:C:1158:LYS:O    | 2:C:1159:VAL:HG13 | 2.05                     | 0.55              |
| 2:I:59:ILE:HG23   | 2:I:476:LYS:HE3   | 1.87                     | 0.55              |
| 2:I:924:VAL:HG12  | 2:I:1058:ARG:HH21 | 1.71                     | 0.55              |
| 2:I:1247:SER:HB3  | 3:J:375:GLU:O     | 2.05                     | 0.55              |
| 2:I:1308:ILE:HG21 | 3:J:379:PRO:HB2   | 1.88                     | 0.55              |
| 3:J:304:ASP:OD2   | 3:J:312:ARG:NH2   | 2.37                     | 0.55              |
| 6:N:48:ARG:HD3    | 6:N:59:VAL:HG23   | 1.87                     | 0.55              |
| 2:C:16:GLY:O      | 2:C:1156:ARG:HG2  | 2.06                     | 0.55              |
| 3:D:844:THR:HG21  | 3:D:858:VAL:HG21  | 1.87                     | 0.55              |
| 4:K:32:VAL:O      | 4:K:34:GLY:N      | 2.38                     | 0.55              |
| 5:L:487:MET:HE2   | 5:L:487:MET:HA    | 1.88                     | 0.55              |
| 1:A:115:ILE:HG22  | 1:A:116:THR:H     | 1.69                     | 0.55              |
| 2:C:1075:VAL:HG21 | 3:D:463:GLY:HA2   | 1.88                     | 0.55              |
| 3:D:205:LEU:HD22  | 3:D:214:ARG:HB2   | 1.88                     | 0.55              |
| 5:F:600:HIS:CD2   | 5:F:601:PRO:HD3   | 2.41                     | 0.55              |
| 2:I:1106:ARG:HG3  | 6:N:6:ASP:OD1     | 2.06                     | 0.55              |
| 3:J:609:TYR:HE2   | 3:J:614:LEU:HD12  | 1.71                     | 0.55              |
| 5:F:575:GLU:O     | 5:F:579:GLN:HG2   | 2.07                     | 0.55              |
| 2:I:462:ASN:O     | 2:I:466:VAL:HG23  | 2.07                     | 0.55              |
| 3:J:91:GLU:OE1    | 3:J:93:THR:OG1    | 2.24                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:355:ILE:HG21  | 3:J:466:MET:HG3   | 1.89                     | 0.55              |
| 2:C:564:PRO:HG3   | 2:C:572:ILE:HG13  | 1.88                     | 0.55              |
| 5:F:312:SER:OG    | 5:F:313:ASP:N     | 2.40                     | 0.55              |
| 2:I:700:VAL:HG13  | 2:I:1117:LEU:HD22 | 1.88                     | 0.55              |
| 3:J:549:LYS:HD3   | 3:J:569:LEU:HD23  | 1.88                     | 0.55              |
| 1:A:77:ASP:OD2    | 2:C:755:LYS:NZ    | 2.34                     | 0.55              |
| 1:A:166:ARG:O     | 1:A:168:ILE:N     | 2.40                     | 0.55              |
| 3:D:203:GLU:O     | 3:D:207:GLU:HG2   | 2.07                     | 0.55              |
| 3:D:1165:PHE:HE1  | 3:D:1200:GLU:HB2  | 1.71                     | 0.55              |
| 3:D:1227:HIS:HB2  | 3:J:1293:GLU:OE1  | 2.07                     | 0.55              |
| 5:F:292:VAL:HG11  | 5:F:299:LYS:HG3   | 1.87                     | 0.55              |
| 1:H:83:LEU:HA     | 1:H:86:LYS:HE2    | 1.88                     | 0.55              |
| 2:I:80:PHE:HB2    | 2:I:85:CYS:SG     | 2.47                     | 0.55              |
| 1:A:44:ARG:HB2    | 1:A:183:ILE:HG21  | 1.89                     | 0.55              |
| 1:A:223:ILE:HD13  | 1:B:8:PHE:CZ      | 2.42                     | 0.55              |
| 2:C:684:ASN:HA    | 2:C:687:ARG:NH1   | 2.21                     | 0.55              |
| 2:C:1297:ASP:OD1  | 2:C:1300:GLY:N    | 2.30                     | 0.55              |
| 2:I:475:VAL:HG22  | 2:I:492:MET:HB2   | 1.89                     | 0.55              |
| 2:I:655:VAL:N     | 2:I:659:GLN:OE1   | 2.40                     | 0.55              |
| 2:I:814:ASP:HB3   | 2:I:1073:LYS:O    | 2.07                     | 0.55              |
| 2:I:985:GLU:HG2   | 2:I:988:LYS:HD2   | 1.87                     | 0.55              |
| 2:C:678:ARG:HG3   | 2:C:1108:ASN:HD22 | 1.72                     | 0.55              |
| 3:D:322:ARG:NH1   | 3:D:322:ARG:HB2   | 2.21                     | 0.55              |
| 3:D:683:ILE:HD13  | 6:M:23:ILE:HG21   | 1.87                     | 0.55              |
| 3:D:1280:VAL:HG21 | 3:D:1304:ARG:HH21 | 1.72                     | 0.55              |
| 5:F:316:PHE:CZ    | 5:F:338:HIS:HB2   | 2.41                     | 0.55              |
| 2:I:807:TRP:HE1   | 2:I:1086:PRO:HD3  | 1.71                     | 0.55              |
| 5:L:515:GLU:HG2   | 5:L:516:ASP:N     | 2.22                     | 0.55              |
| 2:C:395:TYR:HD2   | 2:C:419:ILE:HG22  | 1.71                     | 0.55              |
| 2:I:221:LEU:HD11  | 2:I:314:ASN:HB2   | 1.89                     | 0.55              |
| 3:J:1289:ASN:OD1  | 3:J:1290:ARG:NH1  | 2.40                     | 0.55              |
| 5:L:479:THR:HG23  | 5:L:481:GLU:H     | 1.72                     | 0.55              |
| 2:C:323:ALA:O     | 2:C:327:GLN:HG3   | 2.07                     | 0.55              |
| 2:C:661:VAL:HB    | 2:C:665:ALA:HB3   | 1.88                     | 0.55              |
| 2:C:1327:LEU:HD23 | 2:C:1331:ARG:HH21 | 1.72                     | 0.55              |
| 2:C:1331:ARG:HG2  | 3:D:33:TRP:CZ3    | 2.42                     | 0.55              |
| 3:D:88:CYS:O      | 3:D:90:VAL:N      | 2.39                     | 0.55              |
| 1:H:151:GLY:O     | 1:H:177:TYR:HB2   | 2.06                     | 0.55              |
| 2:I:135:THR:HG22  | 2:I:527:LYS:HE2   | 1.88                     | 0.55              |
| 2:I:678:ARG:NH1   | 2:I:1071:GLY:O    | 2.33                     | 0.55              |
| 5:L:551:LEU:HD23  | 5:L:597:LYS:HD2   | 1.88                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:268:ARG:NH2   | 2:C:270:THR:HG21  | 2.22                     | 0.54              |
| 2:C:1234:LYS:HE2  | 2:C:1238:LEU:HD23 | 1.88                     | 0.54              |
| 3:J:915:ILE:HA    | 3:J:918:ILE:HG23  | 1.89                     | 0.54              |
| 2:C:1272:GLU:H    | 3:D:342:LEU:CB    | 2.20                     | 0.54              |
| 3:D:680:ASN:OD1   | 6:M:23:ILE:HG23   | 2.07                     | 0.54              |
| 3:D:1159:ILE:HD12 | 3:D:1206:ARG:HD2  | 1.89                     | 0.54              |
| 1:H:18:GLN:HA     | 1:H:24:ALA:HA     | 1.90                     | 0.54              |
| 2:I:196:VAL:HG12  | 2:I:206:ALA:HA    | 1.89                     | 0.54              |
| 3:J:782:GLY:HA3   | 6:N:12:THR:CG2    | 2.35                     | 0.54              |
| 6:M:25:GLN:C      | 6:M:27:ILE:H      | 2.16                     | 0.54              |
| 2:C:453:ILE:HD12  | 2:C:587:LEU:HG    | 1.89                     | 0.54              |
| 3:D:661:VAL:HG12  | 3:D:685:ILE:HD11  | 1.89                     | 0.54              |
| 5:F:261:LEU:H     | 5:F:261:LEU:HD12  | 1.71                     | 0.54              |
| 5:L:612:ASP:N     | 5:L:612:ASP:OD1   | 2.39                     | 0.54              |
| 1:A:228:LEU:HA    | 1:A:231:PHE:HB2   | 1.89                     | 0.54              |
| 3:D:513:MET:HE1   | 3:D:579:LEU:HD13  | 1.89                     | 0.54              |
| 3:D:658:GLU:O     | 3:D:661:VAL:HG22  | 2.08                     | 0.54              |
| 1:B:73:GLY:HA2    | 1:B:134:THR:HG22  | 1.90                     | 0.54              |
| 2:C:1017:GLN:O    | 2:C:1021:LEU:HG   | 2.08                     | 0.54              |
| 3:D:74:LYS:HD2    | 3:D:87:LYS:HZ3    | 1.72                     | 0.54              |
| 3:D:1298:VAL:N    | 3:D:1299:GLY:HA3  | 2.22                     | 0.54              |
| 2:I:73:TYR:HB2    | 2:I:98:VAL:HG22   | 1.90                     | 0.54              |
| 2:I:887:VAL:HB    | 2:I:913:VAL:CG2   | 2.38                     | 0.54              |
| 2:C:686:GLN:HG2   | 2:C:796:LEU:HD22  | 1.90                     | 0.54              |
| 1:G:45:ARG:HH22   | 1:H:37:HIS:HB3    | 1.73                     | 0.54              |
| 3:J:436:ALA:HB3   | 3:J:485:MET:HA    | 1.90                     | 0.54              |
| 5:L:354:THR:O     | 5:L:358:VAL:HG23  | 2.08                     | 0.54              |
| 5:L:571:TYR:HD1   | 5:L:575:GLU:HG2   | 1.71                     | 0.54              |
| 2:C:227:LYS:HZ3   | 2:C:298:ALA:HB1   | 1.72                     | 0.54              |
| 5:F:128:ASN:HA    | 5:F:131:GLN:HE21  | 1.73                     | 0.54              |
| 2:I:10:ARG:NH2    | 2:I:790:ASP:OD2   | 2.28                     | 0.54              |
| 2:I:84:GLU:OE1    | 2:I:1035:LYS:HD2  | 2.08                     | 0.54              |
| 2:I:1142:ARG:HD3  | 2:I:1161:LEU:HD13 | 1.90                     | 0.54              |
| 3:J:332:LYS:HA    | 3:J:337:ARG:H     | 1.73                     | 0.54              |
| 5:L:98:VAL:HB     | 5:L:402:LEU:HD11  | 1.90                     | 0.54              |
| 5:L:362:ASN:HB2   | 5:L:365:MET:HE2   | 1.89                     | 0.54              |
| 2:C:802:VAL:HG21  | 2:C:1098:LEU:HD22 | 1.90                     | 0.54              |
| 2:C:987:GLU:HG2   | 2:C:991:LYS:HE3   | 1.89                     | 0.54              |
| 2:C:1247:SER:HB3  | 3:D:375:GLU:O     | 2.08                     | 0.54              |
| 2:C:1327:LEU:O    | 2:C:1331:ARG:HB2  | 2.08                     | 0.54              |
| 3:D:843:VAL:HG13  | 3:D:883:ARG:HD3   | 1.90                     | 0.54              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:I:1192:GLU:O   | 2:I:1196:LYS:HG2  | 2.08                     | 0.54              |
| 3:D:438:GLU:OE1  | 4:E:3:ARG:NH1     | 2.35                     | 0.54              |
| 2:I:1149:TYR:HD1 | 2:I:1159:VAL:HG11 | 1.73                     | 0.54              |
| 3:J:48:THR:C     | 3:J:50:LYS:H      | 2.12                     | 0.54              |
| 3:J:1262:ARG:HD2 | 3:J:1279:GLN:HE22 | 1.72                     | 0.54              |
| 5:L:245:ALA:O    | 5:L:249:ILE:HG13  | 2.08                     | 0.54              |
| 1:A:14:VAL:HG22  | 1:A:15:ASP:N      | 2.23                     | 0.53              |
| 1:A:45:ARG:HE    | 2:C:1083:GLU:HB3  | 1.72                     | 0.53              |
| 2:C:1255:THR:O   | 2:C:1257:GLN:N    | 2.40                     | 0.53              |
| 3:D:137:ARG:HG2  | 3:D:142:GLU:HB2   | 1.90                     | 0.53              |
| 3:D:201:LEU:HB2  | 3:D:221:ILE:HD13  | 1.90                     | 0.53              |
| 5:F:280:VAL:HG13 | 5:F:355:ILE:HD12  | 1.90                     | 0.53              |
| 2:I:590:PRO:HB2  | 2:I:655:VAL:HG21  | 1.89                     | 0.53              |
| 2:C:61:SER:O     | 2:C:63:SER:N      | 2.41                     | 0.53              |
| 2:C:243:PRO:HB3  | 2:C:277:LEU:HB3   | 1.90                     | 0.53              |
| 2:C:716:ALA:HB3  | 2:C:784:ALA:HB3   | 1.90                     | 0.53              |
| 2:C:1108:ASN:OD1 | 2:C:1111:GLN:NE2  | 2.41                     | 0.53              |
| 3:D:813:ASP:OD1  | 3:D:883:ARG:NH2   | 2.33                     | 0.53              |
| 5:F:343:LYS:H    | 5:F:343:LYS:HD2   | 1.73                     | 0.53              |
| 2:I:106:GLU:O    | 2:I:109:ALA:HB2   | 2.08                     | 0.53              |
| 2:I:201:ARG:NH2  | 2:I:370:MET:O     | 2.37                     | 0.53              |
| 2:I:810:TYR:HD2  | 3:J:359:PRO:HG2   | 1.74                     | 0.53              |
| 2:I:975:ILE:O    | 2:I:979:LEU:HB2   | 2.09                     | 0.53              |
| 3:J:492:SER:HB2  | 3:J:499:ILE:HB    | 1.90                     | 0.53              |
| 5:L:476:ARG:HB3  | 5:L:476:ARG:NH1   | 2.22                     | 0.53              |
| 6:M:63:ALA:O     | 6:M:64:TYR:C      | 2.51                     | 0.53              |
| 1:A:98:VAL:HG22  | 1:A:100:LEU:HD12  | 1.89                     | 0.53              |
| 3:D:833:GLU:OE1  | 3:D:1242:ARG:HD3  | 2.09                     | 0.53              |
| 3:D:848:VAL:HG13 | 3:D:857:LEU:HB2   | 1.89                     | 0.53              |
| 1:G:67:GLU:HB3   | 1:G:171:LEU:HG    | 1.89                     | 0.53              |
| 2:I:156:PHE:CD2  | 2:I:175:ARG:HB3   | 2.44                     | 0.53              |
| 2:I:903:ARG:HE   | 2:I:910:ALA:HB2   | 1.74                     | 0.53              |
| 3:J:128:LEU:HA   | 3:J:192:MET:HE1   | 1.91                     | 0.53              |
| 3:J:287:ALA:HB3  | 3:J:292:VAL:HG12  | 1.91                     | 0.53              |
| 1:A:57:THR:HG22  | 1:A:58:GLU:HG3    | 1.91                     | 0.53              |
| 2:C:202:ARG:HD3  | 2:C:369:MET:HG2   | 1.90                     | 0.53              |
| 2:C:953:LEU:HD11 | 2:C:1033:ARG:HG3  | 1.91                     | 0.53              |
| 3:D:325:LYS:HE2  | 3:D:330:MET:HG3   | 1.90                     | 0.53              |
| 3:D:425:ARG:HG2  | 3:D:426:ALA:H     | 1.73                     | 0.53              |
| 3:J:449:LEU:HD22 | 3:J:466:MET:SD    | 2.49                     | 0.53              |
| 5:L:357:GLN:HA   | 5:L:360:ASP:HB2   | 1.90                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:98:VAL:O      | 2:C:121:GLU:HA    | 2.09                     | 0.53              |
| 3:D:1221:LEU:HB2  | 3:D:1229:VAL:HG11 | 1.91                     | 0.53              |
| 5:F:354:THR:O     | 5:F:358:VAL:HG23  | 2.07                     | 0.53              |
| 2:I:588:GLU:HB3   | 2:I:607:SER:HA    | 1.90                     | 0.53              |
| 3:J:708:ASN:OD1   | 3:J:708:ASN:N     | 2.36                     | 0.53              |
| 2:C:228:VAL:HG22  | 2:C:245:ARG:HE    | 1.74                     | 0.53              |
| 1:G:52:PRO:HG3    | 1:H:6:THR:HG21    | 1.90                     | 0.53              |
| 2:I:125:GLY:HA3   | 2:I:499:SER:HB2   | 1.91                     | 0.53              |
| 2:I:810:TYR:CE2   | 3:J:359:PRO:HD2   | 2.43                     | 0.53              |
| 2:I:1067:ALA:HB2  | 2:I:1073:LYS:HA   | 1.91                     | 0.53              |
| 2:C:8:LYS:HE3     | 2:C:1171:ARG:NH2  | 2.24                     | 0.53              |
| 3:D:54:ASP:OD1    | 3:D:54:ASP:N      | 2.42                     | 0.53              |
| 5:F:245:ALA:O     | 5:F:249:ILE:HG13  | 2.09                     | 0.53              |
| 5:F:311:THR:HG21  | 5:F:348:GLU:OE2   | 2.08                     | 0.53              |
| 3:J:683:ILE:HD11  | 3:J:754:ILE:HD13  | 1.90                     | 0.53              |
| 3:J:865:HIS:CE1   | 3:J:867:GLN:HB2   | 2.44                     | 0.53              |
| 3:J:1280:VAL:HG11 | 3:J:1304:ARG:HH21 | 1.74                     | 0.53              |
| 1:A:237:VAL:HG12  | 1:B:14:VAL:HG12   | 1.91                     | 0.53              |
| 2:C:243:PRO:HB3   | 2:C:277:LEU:CB    | 2.38                     | 0.53              |
| 1:G:90:VAL:HG23   | 1:G:123:ILE:HD13  | 1.90                     | 0.53              |
| 2:I:149:LEU:O     | 2:I:532:ALA:HA    | 2.08                     | 0.53              |
| 2:I:409:LEU:HD21  | 2:I:428:VAL:HA    | 1.91                     | 0.53              |
| 2:I:1185:PRO:HB2  | 2:I:1188:ASP:HB3  | 1.89                     | 0.53              |
| 4:K:39:VAL:HG21   | 4:K:56:GLU:HG3    | 1.90                     | 0.53              |
| 1:A:12:ARG:H      | 1:A:30:PRO:HD2    | 1.74                     | 0.53              |
| 2:C:363:LEU:HB3   | 2:C:381:ALA:HB1   | 1.91                     | 0.53              |
| 2:C:1072:ASN:OD1  | 2:C:1072:ASN:N    | 2.40                     | 0.53              |
| 1:G:27:THR:HG23   | 1:G:202:VAL:HG22  | 1.90                     | 0.53              |
| 1:G:32:GLU:HB2    | 1:G:35:PHE:CD2    | 2.44                     | 0.53              |
| 2:I:800:MET:SD    | 2:I:1096:ILE:HD11 | 2.49                     | 0.53              |
| 3:D:872:LEU:HB3   | 3:D:877:VAL:HG11  | 1.91                     | 0.53              |
| 3:D:1160:SER:OG   | 3:D:1203:ARG:NH1  | 2.41                     | 0.53              |
| 1:G:35:PHE:CE1    | 1:H:46:ILE:HG12   | 2.40                     | 0.53              |
| 2:C:975:ILE:HG13  | 2:C:1014:LEU:HD22 | 1.92                     | 0.52              |
| 3:D:189:LEU:HB3   | 3:D:234:PRO:HB2   | 1.90                     | 0.52              |
| 2:I:143:ARG:HH21  | 2:I:513:GLN:HA    | 1.74                     | 0.52              |
| 2:I:384:LEU:O     | 2:I:388:LEU:HG    | 2.09                     | 0.52              |
| 3:J:908:ILE:HG12  | 3:J:909:ILE:N     | 2.24                     | 0.52              |
| 5:L:281:ARG:O     | 5:L:285:ARG:HG3   | 2.09                     | 0.52              |
| 1:A:318:LEU:O     | 1:A:320:ASN:N     | 2.38                     | 0.52              |
| 2:C:268:ARG:HH21  | 2:C:270:THR:HG21  | 1.73                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:483:ASP:HB2   | 2:C:486:THR:CG2   | 2.40                     | 0.52              |
| 2:I:12:ARG:NH1    | 2:I:1182:ILE:O    | 2.40                     | 0.52              |
| 2:I:26:TYR:HE2    | 2:I:32:LEU:HD12   | 1.73                     | 0.52              |
| 3:J:901:ARG:HA    | 3:J:908:ILE:HA    | 1.90                     | 0.52              |
| 5:L:395:THR:OG1   | 5:L:396:ASN:N     | 2.42                     | 0.52              |
| 3:D:820:ILE:HG22  | 3:D:1227:HIS:ND1  | 2.24                     | 0.52              |
| 3:D:1314:LEU:O    | 3:D:1326:GLN:NE2  | 2.42                     | 0.52              |
| 5:F:299:LYS:HA    | 5:F:302:PHE:HB3   | 1.91                     | 0.52              |
| 3:J:102:MET:HE3   | 3:J:246:PRO:HD3   | 1.90                     | 0.52              |
| 3:J:793:SER:O     | 3:J:797:THR:HG23  | 2.08                     | 0.52              |
| 3:J:1184:ASP:O    | 3:J:1186:TYR:N    | 2.43                     | 0.52              |
| 1:A:257:VAL:HG13  | 1:A:276:HIS:O     | 2.09                     | 0.52              |
| 2:C:582:ASN:HB3   | 2:C:586:PHE:H     | 1.74                     | 0.52              |
| 3:D:79:LYS:HG3    | 3:D:80:HIS:ND1    | 2.25                     | 0.52              |
| 3:D:426:ALA:CB    | 3:D:427:PRO:HD3   | 2.39                     | 0.52              |
| 2:I:678:ARG:NH2   | 6:N:5:ALA:HB3     | 2.24                     | 0.52              |
| 3:J:430:HIS:CE1   | 3:J:925:GLU:HG3   | 2.44                     | 0.52              |
| 3:J:513:MET:HE1   | 3:J:579:LEU:HD13  | 1.90                     | 0.52              |
| 2:C:1333:LEU:HD23 | 3:D:307:LEU:HD22  | 1.92                     | 0.52              |
| 3:D:310:GLY:HA2   | 3:D:314:ARG:CD    | 2.37                     | 0.52              |
| 3:D:863:LEU:HD11  | 3:D:901:ARG:HB3   | 1.91                     | 0.52              |
| 3:J:42:GLU:OE2    | 5:L:451:ARG:NE    | 2.31                     | 0.52              |
| 5:L:234:THR:O     | 5:L:245:ALA:HB2   | 2.09                     | 0.52              |
| 5:L:312:SER:OG    | 5:L:313:ASP:N     | 2.42                     | 0.52              |
| 3:D:147:ILE:HG22  | 3:D:188:LEU:HG    | 1.91                     | 0.52              |
| 3:D:1347:LEU:HD12 | 3:D:1358:PRO:HG2  | 1.92                     | 0.52              |
| 1:G:31:LEU:HD13   | 1:G:36:GLY:HA2    | 1.91                     | 0.52              |
| 2:I:146:VAL:HG13  | 2:I:529:ARG:HB3   | 1.90                     | 0.52              |
| 6:M:29:ALA:O      | 6:M:53:PRO:HG2    | 2.09                     | 0.52              |
| 1:A:61:ILE:HB     | 1:A:64:VAL:CG2    | 2.39                     | 0.52              |
| 1:A:86:LYS:HE2    | 1:A:174:ASP:HB2   | 1.90                     | 0.52              |
| 2:C:928:VAL:HG22  | 2:C:1054:LEU:HD11 | 1.92                     | 0.52              |
| 2:C:1131:MET:HE2  | 2:C:1141:LEU:HD12 | 1.91                     | 0.52              |
| 2:C:1211:ARG:HE   | 2:C:1220:GLN:NE2  | 2.07                     | 0.52              |
| 3:D:83:VAL:HG13   | 3:D:92:VAL:HG13   | 1.92                     | 0.52              |
| 3:J:27:PRO:HD3    | 3:J:236:TRP:CD1   | 2.44                     | 0.52              |
| 3:J:861:ASN:HD22  | 3:J:883:ARG:NH1   | 2.08                     | 0.52              |
| 3:D:48:THR:C      | 3:D:50:LYS:H      | 2.17                     | 0.52              |
| 1:G:231:PHE:HB3   | 1:H:218:ARG:HB3   | 1.92                     | 0.52              |
| 3:J:438:GLU:OE1   | 4:K:3:ARG:NH2     | 2.43                     | 0.52              |
| 2:C:363:LEU:C     | 2:C:381:ALA:HB1   | 2.35                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:594:VAL:HG22  | 2:C:599:VAL:HG22  | 1.92                     | 0.52              |
| 2:C:1256:GLN:HB3  | 2:C:1301:ARG:NH2  | 2.25                     | 0.52              |
| 3:D:1181:ASP:HA   | 3:J:202:ARG:HD3   | 1.91                     | 0.52              |
| 5:F:561:MET:HA    | 5:F:567:MET:HE1   | 1.92                     | 0.52              |
| 3:J:1174:ARG:HE   | 3:J:1189:MET:HE2  | 1.75                     | 0.52              |
| 4:K:44:ASP:HB3    | 4:K:48:VAL:HB     | 1.91                     | 0.52              |
| 2:C:657:THR:HG21  | 2:C:1188:ASP:HB2  | 1.92                     | 0.52              |
| 3:D:720:ASN:OD1   | 3:D:722:ILE:HG22  | 2.10                     | 0.52              |
| 3:D:903:LEU:HD22  | 3:D:909:ILE:HD12  | 1.91                     | 0.52              |
| 2:I:832:HIS:CE1   | 2:I:1058:ARG:HD2  | 2.46                     | 0.52              |
| 2:I:968:GLU:HG3   | 2:I:1018:TYR:CE1  | 2.45                     | 0.52              |
| 3:J:770:LEU:H     | 3:J:770:LEU:HD22  | 1.74                     | 0.52              |
| 2:C:885:GLY:HA2   | 2:C:917:SER:HB3   | 1.93                     | 0.51              |
| 2:C:1174:GLU:OE2  | 2:C:1177:ARG:NH1  | 2.43                     | 0.51              |
| 3:D:615:LYS:HB2   | 3:D:616:PRO:HD3   | 1.92                     | 0.51              |
| 3:D:909:ILE:HD11  | 3:D:913:GLU:HG2   | 1.91                     | 0.51              |
| 2:I:1065:LYS:HE2  | 3:J:462:ASP:O     | 2.10                     | 0.51              |
| 3:J:700:ASN:O     | 3:J:704:GLU:HB2   | 2.10                     | 0.51              |
| 6:N:25:GLN:C      | 6:N:27:ILE:H      | 2.18                     | 0.51              |
| 2:C:298:ALA:HB3   | 2:C:334:GLU:HB2   | 1.91                     | 0.51              |
| 2:C:1185:PRO:HB2  | 2:C:1188:ASP:HB3  | 1.92                     | 0.51              |
| 3:D:506:VAL:HG21  | 3:D:625:MET:HA    | 1.92                     | 0.51              |
| 4:E:13:ILE:HD12   | 4:E:19:LEU:HA     | 1.91                     | 0.51              |
| 3:J:72:CYS:HB3    | 3:J:88:CYS:SG     | 2.49                     | 0.51              |
| 2:C:1271:GLY:HA3  | 3:D:343:LEU:HD12  | 1.91                     | 0.51              |
| 3:D:811:GLU:OE1   | 3:D:890:THR:OG1   | 2.29                     | 0.51              |
| 2:I:156:PHE:HD2   | 2:I:175:ARG:HB3   | 1.76                     | 0.51              |
| 2:I:1211:ARG:HE   | 2:I:1220:GLN:NE2  | 2.08                     | 0.51              |
| 3:J:598:LYS:O     | 3:J:601:ILE:HG22  | 2.09                     | 0.51              |
| 3:J:903:LEU:HD22  | 3:J:909:ILE:HD12  | 1.92                     | 0.51              |
| 3:J:1157:ALA:HB3  | 3:J:1206:ARG:HA   | 1.92                     | 0.51              |
| 5:L:284:GLU:OE2   | 5:L:359:LYS:HD2   | 2.10                     | 0.51              |
| 2:C:808:ASN:H     | 3:D:633:ALA:HB2   | 1.75                     | 0.51              |
| 2:I:138:ILE:O     | 2:I:139:ASN:ND2   | 2.43                     | 0.51              |
| 2:I:1287:LEU:HD13 | 3:J:1357:ILE:HD11 | 1.92                     | 0.51              |
| 3:J:88:CYS:O      | 3:J:90:VAL:N      | 2.44                     | 0.51              |
| 3:J:517:CYS:HA    | 3:J:716:GLN:NE2   | 2.24                     | 0.51              |
| 3:J:1290:ARG:HD2  | 3:J:1298:VAL:HG12 | 1.92                     | 0.51              |
| 2:C:71:VAL:HB     | 2:C:99:LYS:HB2    | 1.93                     | 0.51              |
| 2:C:1123:GLY:HA3  | 2:C:1204:LEU:HD11 | 1.92                     | 0.51              |
| 3:D:1215:GLU:HG3  | 3:D:1220:ILE:HD11 | 1.93                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:E:15:ASN:C      | 4:E:17:PHE:H      | 2.19                     | 0.51              |
| 2:I:357:ASN:ND2   | 2:I:358:ASP:OD2   | 2.43                     | 0.51              |
| 3:J:1203:ARG:HH22 | 3:J:1205:GLU:HG2  | 1.75                     | 0.51              |
| 2:C:211:ARG:NH1   | 2:C:357:ASN:O     | 2.44                     | 0.51              |
| 2:C:338:THR:HG22  | 2:C:345:PRO:HB3   | 1.92                     | 0.51              |
| 3:D:227:PHE:O     | 3:D:230:SER:HB3   | 2.10                     | 0.51              |
| 3:D:901:ARG:HA    | 3:D:908:ILE:HA    | 1.93                     | 0.51              |
| 5:F:484:ALA:HB1   | 5:F:491:GLU:HB2   | 1.92                     | 0.51              |
| 2:I:813:GLU:HG3   | 3:J:460:ASP:HA    | 1.92                     | 0.51              |
| 2:I:942:ASP:OD2   | 2:I:1048:LYS:NZ   | 2.39                     | 0.51              |
| 2:I:1282:GLY:O    | 2:I:1284:ALA:N    | 2.44                     | 0.51              |
| 3:J:57:PHE:HB3    | 3:J:98:ARG:HH22   | 1.74                     | 0.51              |
| 3:J:363:LEU:HD23  | 3:J:487:THR:HG22  | 1.91                     | 0.51              |
| 3:J:1181:ASP:OD1  | 3:J:1182:GLY:N    | 2.43                     | 0.51              |
| 2:C:624:ASP:OD1   | 2:C:625:GLU:N     | 2.38                     | 0.51              |
| 2:C:1289:GLU:OE1  | 2:C:1294:LYS:HE2  | 2.11                     | 0.51              |
| 3:D:615:LYS:HE2   | 3:D:616:PRO:HD3   | 1.93                     | 0.51              |
| 5:F:484:ALA:HB1   | 5:F:491:GLU:CB    | 2.41                     | 0.51              |
| 2:I:75:LEU:HD11   | 2:I:127:ILE:HD11  | 1.93                     | 0.51              |
| 2:I:1289:GLU:OE2  | 3:J:473:THR:HG22  | 2.11                     | 0.51              |
| 3:J:398:LYS:HE2   | 5:L:532:LEU:HD23  | 1.93                     | 0.51              |
| 5:L:483:LEU:HD12  | 5:L:483:LEU:H     | 1.75                     | 0.51              |
| 2:C:192:ASP:OD2   | 2:C:436:ARG:NH2   | 2.43                     | 0.51              |
| 3:D:687:ALA:HB1   | 6:M:24:ARG:NE     | 2.25                     | 0.51              |
| 5:F:371:LYS:HA    | 5:F:374:ARG:NH1   | 2.26                     | 0.51              |
| 1:G:135:ASP:HB3   | 1:G:138:ALA:HB2   | 1.93                     | 0.51              |
| 2:I:673:HIS:HB3   | 2:I:1109:ILE:HG22 | 1.93                     | 0.51              |
| 2:I:1085:MET:HE2  | 2:I:1085:MET:HA   | 1.93                     | 0.51              |
| 5:L:115:GLY:HA2   | 5:L:118:ASP:HB2   | 1.92                     | 0.51              |
| 5:L:314:THR:O     | 5:L:318:ALA:HB3   | 2.11                     | 0.51              |
| 1:A:289:LEU:HD11  | 1:A:314:LEU:HD21  | 1.93                     | 0.51              |
| 2:C:344:GLY:HA3   | 2:C:346:TYR:CE2   | 2.46                     | 0.51              |
| 2:C:726:TYR:CE2   | 2:C:728:ASP:HB2   | 2.46                     | 0.51              |
| 3:D:128:LEU:HD21  | 3:D:189:LEU:HD23  | 1.93                     | 0.51              |
| 2:I:36:GLN:O      | 2:I:40:GLU:HB2    | 2.11                     | 0.51              |
| 2:I:620:ASN:O     | 2:I:620:ASN:ND2   | 2.44                     | 0.51              |
| 2:I:870:ILE:HG13  | 2:I:884:VAL:HG22  | 1.93                     | 0.51              |
| 3:J:705:THR:OG1   | 3:J:718:SER:HA    | 2.10                     | 0.51              |
| 2:C:468:LEU:HA    | 2:C:471:VAL:HG12  | 1.92                     | 0.51              |
| 2:C:810:TYR:HE2   | 3:D:359:PRO:HD2   | 1.76                     | 0.51              |
| 5:F:489:MET:O     | 5:F:491:GLU:N     | 2.44                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:I:1062:PRO:HA  | 2:I:1076:ILE:HG23 | 1.93                     | 0.51              |
| 3:J:128:LEU:HD21 | 3:J:189:LEU:HD23  | 1.93                     | 0.51              |
| 3:J:690:ASN:ND2  | 3:J:745:GLY:HA2   | 2.26                     | 0.51              |
| 1:A:44:ARG:HB2   | 1:A:183:ILE:CG2   | 2.41                     | 0.50              |
| 2:C:1086:PRO:HB3 | 2:C:1212:LEU:HD23 | 1.92                     | 0.50              |
| 1:H:107:ILE:HG23 | 1:H:134:THR:O     | 2.11                     | 0.50              |
| 2:I:208:ILE:HG12 | 2:I:362:ALA:HB1   | 1.91                     | 0.50              |
| 2:I:524:ILE:HD12 | 2:I:712:SER:HB2   | 1.93                     | 0.50              |
| 2:I:1234:LYS:HE2 | 2:I:1238:LEU:HD23 | 1.93                     | 0.50              |
| 1:A:95:LYS:O     | 1:A:148:ARG:NH2   | 2.45                     | 0.50              |
| 1:A:169:GLY:O    | 1:A:171:LEU:HD22  | 2.11                     | 0.50              |
| 1:A:225:ALA:O    | 1:A:229:GLU:N     | 2.44                     | 0.50              |
| 1:B:179:PRO:HA   | 1:B:208:ASN:ND2   | 2.26                     | 0.50              |
| 3:D:709:ARG:HD2  | 3:D:710:ASP:N     | 2.26                     | 0.50              |
| 3:D:903:LEU:HB3  | 3:D:905:ARG:HG3   | 1.94                     | 0.50              |
| 2:I:117:ILE:HD12 | 2:I:488:MET:HG2   | 1.92                     | 0.50              |
| 5:L:248:GLU:HG2  | 5:L:251:LYS:NZ    | 2.26                     | 0.50              |
| 1:B:41:ASN:OD1   | 1:B:44:ARG:NH1    | 2.44                     | 0.50              |
| 1:B:102:LEU:O    | 1:B:141:SER:HA    | 2.11                     | 0.50              |
| 2:C:463:GLN:HG3  | 2:C:505:PHE:HB2   | 1.93                     | 0.50              |
| 2:C:1111:GLN:HB2 | 2:C:1230:MET:CE   | 2.41                     | 0.50              |
| 5:F:148:TYR:OH   | 5:F:218:ARG:HA    | 2.11                     | 0.50              |
| 2:I:1256:GLN:HB3 | 2:I:1301:ARG:NH2  | 2.23                     | 0.50              |
| 3:J:682:VAL:HG13 | 3:J:685:ILE:HD11  | 1.93                     | 0.50              |
| 3:J:930:LEU:HB2  | 3:J:1138:LEU:HB2  | 1.92                     | 0.50              |
| 3:J:1161:GLY:HA3 | 3:J:1179:PRO:HA   | 1.94                     | 0.50              |
| 1:A:90:VAL:HG23  | 1:A:123:ILE:HD13  | 1.92                     | 0.50              |
| 1:B:188:GLU:O    | 1:B:200:LYS:N     | 2.37                     | 0.50              |
| 2:C:395:TYR:HB3  | 2:C:419:ILE:HG22  | 1.93                     | 0.50              |
| 2:C:1294:LYS:HB3 | 3:D:347:VAL:HG13  | 1.94                     | 0.50              |
| 3:D:491:LEU:HD22 | 3:D:496:GLY:O     | 2.11                     | 0.50              |
| 2:I:52:ALA:HB2   | 2:I:461:GLU:HG3   | 1.94                     | 0.50              |
| 2:I:629:PHE:CE2  | 2:I:650:VAL:HG21  | 2.46                     | 0.50              |
| 2:I:998:LEU:HD23 | 2:I:1015:ALA:HA   | 1.94                     | 0.50              |
| 1:A:134:THR:HG21 | 2:C:727:VAL:O     | 2.11                     | 0.50              |
| 2:C:39:ILE:HD11  | 2:C:75:LEU:HG     | 1.93                     | 0.50              |
| 3:D:258:GLY:HA3  | 5:F:499:LYS:HE2   | 1.93                     | 0.50              |
| 3:D:698:MET:HE2  | 3:D:734:ALA:HB2   | 1.93                     | 0.50              |
| 5:F:531:PRO:O    | 5:F:535:ALA:N     | 2.37                     | 0.50              |
| 1:H:100:LEU:HD21 | 1:H:121:VAL:HG11  | 1.94                     | 0.50              |
| 2:I:1296:ASP:OD2 | 2:I:1322:SER:HB3  | 2.11                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:L:299:LYS:HA   | 5:L:302:PHE:HB3  | 1.94                     | 0.50              |
| 2:C:710:VAL:HA   | 2:C:715:THR:HG21 | 1.94                     | 0.50              |
| 3:D:1170:LYS:C   | 3:D:1172:LYS:H   | 2.19                     | 0.50              |
| 5:F:292:VAL:HG13 | 5:F:297:MET:O    | 2.11                     | 0.50              |
| 5:F:391:ALA:HB3  | 5:F:405:ILE:HG22 | 1.93                     | 0.50              |
| 1:A:13:LEU:HD12  | 1:A:16:ILE:HD11  | 1.92                     | 0.50              |
| 1:A:150:ARG:NH1  | 1:B:7:GLU:O      | 2.45                     | 0.50              |
| 2:C:549:ASP:OD1  | 3:D:750:PRO:HG3  | 2.11                     | 0.50              |
| 3:D:452:LEU:HB3  | 3:D:500:ILE:HG23 | 1.92                     | 0.50              |
| 3:D:701:LEU:CD1  | 3:D:723:TYR:HB2  | 2.42                     | 0.50              |
| 5:F:111:LEU:HD13 | 5:F:116:GLU:HA   | 1.94                     | 0.50              |
| 2:I:810:TYR:HE1  | 2:I:1078:LYS:HD2 | 1.76                     | 0.50              |
| 2:I:1191:LYS:HD3 | 2:I:1193:ALA:H   | 1.77                     | 0.50              |
| 3:J:833:GLU:OE1  | 3:J:1242:ARG:HD3 | 2.11                     | 0.50              |
| 2:C:105:TYR:CD1  | 2:C:111:GLU:HB3  | 2.47                     | 0.50              |
| 2:C:225:PHE:HZ   | 2:C:348:SER:H    | 1.60                     | 0.50              |
| 3:D:478:LEU:HG   | 4:E:47:THR:HG23  | 1.94                     | 0.50              |
| 2:I:515:MET:HG2  | 2:I:517:GLN:HB2  | 1.93                     | 0.50              |
| 2:I:921:PRO:O    | 2:I:924:VAL:HG22 | 2.11                     | 0.50              |
| 2:C:208:ILE:HG13 | 2:C:354:ASP:OD1  | 2.12                     | 0.49              |
| 2:C:213:LEU:HD23 | 2:C:385:PHE:HE2  | 1.77                     | 0.49              |
| 2:C:227:LYS:NZ   | 2:C:298:ALA:HB1  | 2.26                     | 0.49              |
| 2:C:733:VAL:HG11 | 2:C:966:ILE:HG21 | 1.94                     | 0.49              |
| 2:C:748:ILE:HD11 | 2:C:967:LEU:HD12 | 1.93                     | 0.49              |
| 2:C:1116:HIS:HE1 | 3:D:641:ILE:N    | 1.99                     | 0.49              |
| 3:D:128:LEU:HB3  | 3:D:157:GLN:HE22 | 1.77                     | 0.49              |
| 5:F:310:GLU:OE2  | 5:F:355:ILE:HG21 | 2.12                     | 0.49              |
| 2:I:151:ARG:HH22 | 2:I:175:ARG:NH1  | 2.10                     | 0.49              |
| 2:I:778:GLU:O    | 2:I:781:ASP:HB2  | 2.12                     | 0.49              |
| 1:A:23:HIS:HE1   | 1:A:204:GLU:HG2  | 1.76                     | 0.49              |
| 1:A:231:PHE:HE2  | 1:B:39:LEU:HB3   | 1.78                     | 0.49              |
| 2:C:14:ASP:N     | 2:C:1157:GLN:OE1 | 2.37                     | 0.49              |
| 2:C:325:LEU:O    | 2:C:330:HIS:HB2  | 2.12                     | 0.49              |
| 3:D:421:VAL:HG13 | 3:D:439:PRO:HG3  | 1.94                     | 0.49              |
| 3:D:495:ASN:C    | 3:D:497:GLU:H    | 2.18                     | 0.49              |
| 3:D:709:ARG:HD2  | 3:D:710:ASP:H    | 1.77                     | 0.49              |
| 3:D:866:GLU:OE2  | 3:D:901:ARG:NH2  | 2.44                     | 0.49              |
| 1:G:23:HIS:HB2   | 1:G:205:MET:O    | 2.12                     | 0.49              |
| 1:G:31:LEU:HD21  | 1:G:39:LEU:HD12  | 1.94                     | 0.49              |
| 2:I:820:GLU:N    | 2:I:1080:ASN:O   | 2.45                     | 0.49              |
| 3:J:661:VAL:HG12 | 3:J:685:ILE:HD11 | 1.94                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:1289:ASN:O    | 3:J:1290:ARG:NH1  | 2.45                     | 0.49              |
| 2:C:488:MET:O     | 2:C:490:GLN:N     | 2.40                     | 0.49              |
| 2:C:1281:TYR:CD1  | 3:D:484:MET:HG2   | 2.48                     | 0.49              |
| 3:D:56:LEU:H      | 3:D:56:LEU:HD12   | 1.76                     | 0.49              |
| 1:G:11:PRO:HD3    | 1:H:227:GLN:OE1   | 2.12                     | 0.49              |
| 2:I:963:GLU:O     | 2:I:967:LEU:HB2   | 2.12                     | 0.49              |
| 2:C:1269:ARG:HG3  | 3:D:346:ARG:HG2   | 1.95                     | 0.49              |
| 1:G:140:ILE:HG13  | 1:G:140:ILE:O     | 2.12                     | 0.49              |
| 2:I:1174:GLU:OE2  | 2:I:1177:ARG:NH1  | 2.45                     | 0.49              |
| 5:L:117:ILE:HA    | 5:L:120:ALA:HB3   | 1.94                     | 0.49              |
| 5:L:161:LEU:C     | 5:L:262:VAL:HG23  | 2.37                     | 0.49              |
| 5:L:281:ARG:HG3   | 5:L:285:ARG:HH11  | 1.78                     | 0.49              |
| 2:C:10:ARG:HA     | 2:C:1172:LEU:HD23 | 1.93                     | 0.49              |
| 2:C:149:LEU:HD12  | 2:C:452:ARG:O     | 2.12                     | 0.49              |
| 2:C:296:VAL:HB    | 2:C:336:LEU:HD12  | 1.94                     | 0.49              |
| 2:C:708:VAL:CG1   | 2:C:794:LEU:HD22  | 2.42                     | 0.49              |
| 3:D:744:ARG:HG3   | 3:D:744:ARG:O     | 2.13                     | 0.49              |
| 3:D:1137:GLY:O    | 3:D:1140:ARG:HB3  | 2.12                     | 0.49              |
| 2:I:811:ASN:O     | 2:I:1099:ASN:ND2  | 2.45                     | 0.49              |
| 3:J:680:ASN:O     | 3:J:683:ILE:HG22  | 2.13                     | 0.49              |
| 5:L:513:ASP:C     | 5:L:515:GLU:H     | 2.19                     | 0.49              |
| 1:B:19:VAL:HB     | 1:B:23:HIS:HD2    | 1.78                     | 0.49              |
| 4:E:71:GLU:HA     | 4:E:74:GLU:HG3    | 1.94                     | 0.49              |
| 3:J:554:GLU:HA    | 3:J:580:TRP:HZ2   | 1.78                     | 0.49              |
| 4:K:14:GLY:C      | 4:K:16:ARG:H      | 2.20                     | 0.49              |
| 2:C:80:PHE:HB3    | 2:C:84:GLU:HB2    | 1.94                     | 0.49              |
| 2:C:298:ALA:N     | 2:C:334:GLU:O     | 2.35                     | 0.49              |
| 2:C:402:ARG:NE    | 2:C:417:SER:O     | 2.46                     | 0.49              |
| 3:D:364:HIS:HB3   | 3:D:487:THR:CG2   | 2.43                     | 0.49              |
| 3:D:392:THR:HG21  | 5:F:606:VAL:HA    | 1.95                     | 0.49              |
| 4:E:15:ASN:ND2    | 4:E:18:ASP:OD2    | 2.44                     | 0.49              |
| 2:I:1066:MET:HG2  | 2:I:1234:LYS:HA   | 1.95                     | 0.49              |
| 3:J:596:LEU:HD11  | 3:J:604:MET:HE1   | 1.94                     | 0.49              |
| 6:N:25:GLN:O      | 6:N:27:ILE:N      | 2.42                     | 0.49              |
| 1:A:279:GLY:HA3   | 1:A:321:TRP:CZ2   | 2.48                     | 0.49              |
| 1:B:35:PHE:HA     | 1:B:38:THR:CG2    | 2.43                     | 0.49              |
| 2:C:1119:MET:HB2  | 2:C:1228:GLY:HA2  | 1.94                     | 0.49              |
| 4:E:15:ASN:HB3    | 4:E:18:ASP:H      | 1.77                     | 0.49              |
| 1:G:102:LEU:HD11  | 1:G:110:VAL:HG11  | 1.95                     | 0.49              |
| 2:I:91:THR:HG21   | 2:I:503:LYS:HE3   | 1.94                     | 0.49              |
| 2:I:1248:THR:HG21 | 5:L:531:PRO:HG3   | 1.95                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:J:355:ILE:HD13 | 3:J:466:MET:HG3  | 1.95                     | 0.49              |
| 3:J:495:ASN:C    | 3:J:497:GLU:H    | 2.21                     | 0.49              |
| 3:J:615:LYS:HB2  | 3:J:616:PRO:HD3  | 1.94                     | 0.49              |
| 1:A:76:GLU:N     | 1:A:76:GLU:OE2   | 2.46                     | 0.49              |
| 1:B:89:ALA:HB3   | 1:B:124:VAL:HG12 | 1.94                     | 0.49              |
| 2:C:131:THR:OG1  | 2:C:135:THR:O    | 2.28                     | 0.49              |
| 2:C:192:ASP:HB3  | 2:C:346:TYR:CD1  | 2.48                     | 0.49              |
| 1:G:73:GLY:C     | 1:G:134:THR:HG22 | 2.37                     | 0.49              |
| 1:H:60:GLU:HA    | 1:H:171:LEU:HD12 | 1.94                     | 0.49              |
| 5:L:306:PHE:CZ   | 5:L:310:GLU:HG3  | 2.48                     | 0.49              |
| 2:C:175:ARG:HG3  | 2:C:185:ASP:OD1  | 2.13                     | 0.49              |
| 3:D:81:ARG:C     | 3:D:83:VAL:H     | 2.20                     | 0.49              |
| 3:D:1199:PHE:HB2 | 3:D:1202:GLU:HB2 | 1.95                     | 0.49              |
| 5:F:532:LEU:O    | 5:F:536:THR:HG23 | 2.13                     | 0.49              |
| 5:F:552:THR:OG1  | 5:F:554:ARG:HG2  | 2.13                     | 0.49              |
| 5:F:584:ARG:HA   | 5:F:584:ARG:HH11 | 1.78                     | 0.49              |
| 2:I:202:ARG:HB2  | 2:I:369:MET:HG2  | 1.94                     | 0.49              |
| 3:J:291:ILE:HG23 | 5:L:406:GLN:HE22 | 1.77                     | 0.49              |
| 3:J:425:ARG:HG2  | 3:J:426:ALA:H    | 1.77                     | 0.49              |
| 6:M:4:GLU:C      | 6:M:6:ASP:H      | 2.21                     | 0.49              |
| 6:M:20:ILE:HG22  | 6:M:24:ARG:HE    | 1.78                     | 0.49              |
| 6:M:48:ARG:NH1   | 6:M:59:VAL:HB    | 2.27                     | 0.49              |
| 1:A:115:ILE:HG22 | 1:A:116:THR:N    | 2.28                     | 0.48              |
| 2:C:218:GLU:HG3  | 2:C:299:LYS:HA   | 1.93                     | 0.48              |
| 2:C:555:TYR:OH   | 2:C:654:ASP:OD1  | 2.24                     | 0.48              |
| 2:C:796:LEU:H    | 2:C:796:LEU:HD12 | 1.77                     | 0.48              |
| 1:G:45:ARG:HH22  | 1:H:37:HIS:CB    | 2.25                     | 0.48              |
| 1:G:66:HIS:CE1   | 1:G:69:SER:HB3   | 2.48                     | 0.48              |
| 3:J:275:ARG:HD3  | 3:J:298:MET:HB3  | 1.95                     | 0.48              |
| 3:J:903:LEU:HD21 | 3:J:913:GLU:OE1  | 2.12                     | 0.48              |
| 5:L:166:VAL:O    | 5:L:167:ASP:HB2  | 2.13                     | 0.48              |
| 2:C:241:LEU:HD11 | 2:C:246:LEU:HD11 | 1.96                     | 0.48              |
| 2:C:520:PRO:HB3  | 2:C:714:VAL:HG21 | 1.94                     | 0.48              |
| 2:C:738:GLU:HA   | 2:C:741:MET:HE2  | 1.94                     | 0.48              |
| 2:C:998:LEU:H    | 2:C:998:LEU:HD12 | 1.79                     | 0.48              |
| 3:D:128:LEU:HA   | 3:D:192:MET:HE1  | 1.95                     | 0.48              |
| 3:D:697:MET:HE1  | 3:D:737:ILE:HG22 | 1.95                     | 0.48              |
| 5:F:326:TRP:HA   | 5:F:329:LYS:HD2  | 1.95                     | 0.48              |
| 1:H:49:SER:O     | 1:H:151:GLY:HA2  | 2.13                     | 0.48              |
| 2:I:737:ASN:O    | 2:I:741:MET:HB2  | 2.13                     | 0.48              |
| 2:I:968:GLU:HG3  | 2:I:1018:TYR:HE1 | 1.78                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:L:343:LYS:O     | 5:L:347:ILE:HG13  | 2.13                     | 0.48              |
| 1:B:6:THR:OG1     | 1:B:7:GLU:N       | 2.41                     | 0.48              |
| 3:D:114:ILE:HB    | 3:D:304:ASP:OD1   | 2.12                     | 0.48              |
| 5:F:279:ARG:HB3   | 5:F:347:ILE:HD11  | 1.95                     | 0.48              |
| 5:L:111:LEU:HD11  | 5:L:119:ILE:HD12  | 1.95                     | 0.48              |
| 2:C:838:CYS:SG    | 2:C:886:LYS:HD3   | 2.53                     | 0.48              |
| 2:C:1253:LEU:HA   | 5:F:525:ASP:HB2   | 1.95                     | 0.48              |
| 3:D:1163:VAL:HG23 | 3:D:1177:ILE:HG23 | 1.95                     | 0.48              |
| 5:F:363:ARG:O     | 5:F:367:ILE:HG13  | 2.14                     | 0.48              |
| 2:I:629:PHE:CD2   | 2:I:634:VAL:HG11  | 2.49                     | 0.48              |
| 5:L:298:PRO:HD2   | 5:L:326:TRP:CD1   | 2.48                     | 0.48              |
| 2:C:138:ILE:O     | 2:C:139:ASN:ND2   | 2.46                     | 0.48              |
| 2:C:188:PHE:CE1   | 2:C:194:LEU:HD13  | 2.48                     | 0.48              |
| 2:C:452:ARG:NH1   | 2:C:585:GLY:HA3   | 2.28                     | 0.48              |
| 1:A:266:SER:HB3   | 1:A:303:ILE:HD11  | 1.95                     | 0.48              |
| 2:C:136:PHE:CE2   | 2:C:456:VAL:HG11  | 2.49                     | 0.48              |
| 2:C:620:ASN:ND2   | 2:C:620:ASN:O     | 2.46                     | 0.48              |
| 3:D:1285:VAL:HG23 | 3:D:1286:LYS:HG3  | 1.94                     | 0.48              |
| 4:E:49:ILE:O      | 4:E:53:GLU:HG3    | 2.13                     | 0.48              |
| 1:G:45:ARG:NH2    | 2:I:1216:ARG:HA   | 2.29                     | 0.48              |
| 2:I:453:ILE:HD12  | 2:I:587:LEU:HG    | 1.96                     | 0.48              |
| 2:I:812:PHE:O     | 3:J:504:GLN:NE2   | 2.45                     | 0.48              |
| 2:I:1156:ARG:HB2  | 2:I:1156:ARG:HH11 | 1.78                     | 0.48              |
| 2:I:1253:LEU:HD11 | 3:J:253:VAL:HG11  | 1.96                     | 0.48              |
| 3:J:519:ASN:HB2   | 3:J:709:ARG:HB2   | 1.96                     | 0.48              |
| 3:J:1284:ARG:NH1  | 3:J:1288:ALA:HB2  | 2.27                     | 0.48              |
| 5:L:489:MET:O     | 5:L:491:GLU:N     | 2.47                     | 0.48              |
| 6:N:52:PHE:HB2    | 6:N:55:VAL:HG23   | 1.95                     | 0.48              |
| 2:C:149:LEU:HB2   | 2:C:530:ILE:CG2   | 2.44                     | 0.48              |
| 2:C:192:ASP:HB3   | 2:C:346:TYR:CE1   | 2.49                     | 0.48              |
| 2:C:213:LEU:HD21  | 2:C:390:PHE:CZ    | 2.48                     | 0.48              |
| 2:C:242:VAL:HB    | 2:C:245:ARG:HD2   | 1.95                     | 0.48              |
| 2:C:861:ALA:HB1   | 2:C:882:ILE:HD13  | 1.96                     | 0.48              |
| 3:D:141:PHE:HD1   | 3:D:180:MET:HG3   | 1.78                     | 0.48              |
| 3:D:275:ARG:HD3   | 3:D:298:MET:HB3   | 1.96                     | 0.48              |
| 3:D:357:VAL:HG22  | 3:D:461:PHE:CE1   | 2.49                     | 0.48              |
| 3:D:905:ARG:NH1   | 4:E:16:ARG:HB2    | 2.29                     | 0.48              |
| 3:D:1193:TRP:HB2  | 3:D:1194:ARG:NH1  | 2.28                     | 0.48              |
| 2:I:18:ARG:HH12   | 2:I:622:ASN:HA    | 1.78                     | 0.48              |
| 2:I:198:ILE:O     | 2:I:201:ARG:HB2   | 2.14                     | 0.48              |
| 3:J:148:GLU:H     | 3:J:156:ARG:HG3   | 1.79                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:J:489:ASN:HA   | 3:J:904:ALA:CB    | 2.44                     | 0.48              |
| 2:C:566:GLY:O    | 2:C:569:ILE:HG13  | 2.14                     | 0.48              |
| 2:C:1289:GLU:OE2 | 3:D:473:THR:HG22  | 2.14                     | 0.48              |
| 3:D:793:SER:O    | 3:D:797:THR:HG23  | 2.14                     | 0.48              |
| 3:D:930:LEU:HD11 | 3:D:1241:TYR:CE2  | 2.49                     | 0.48              |
| 3:D:1158:GLU:HG3 | 3:D:1186:TYR:CZ   | 2.48                     | 0.48              |
| 5:F:483:LEU:H    | 5:F:483:LEU:HD12  | 1.79                     | 0.48              |
| 1:A:112:ALA:HB3  | 1:A:126:PRO:HA    | 1.95                     | 0.48              |
| 1:A:163:GLU:O    | 1:A:164:ASP:HB2   | 2.12                     | 0.48              |
| 1:A:285:THR:OG1  | 1:A:286:GLU:N     | 2.44                     | 0.48              |
| 2:C:53:PHE:CZ    | 2:C:98:VAL:HG21   | 2.49                     | 0.48              |
| 2:C:1142:ARG:NH1 | 2:C:1169:VAL:HG21 | 2.27                     | 0.48              |
| 3:D:154:LEU:HD22 | 3:D:160:LEU:HD11  | 1.96                     | 0.48              |
| 3:D:925:GLU:HB3  | 3:D:926:PRO:HD3   | 1.96                     | 0.48              |
| 2:I:61:SER:O     | 2:I:63:SER:N      | 2.47                     | 0.48              |
| 2:I:616:ILE:HG22 | 2:I:617:ALA:O     | 2.14                     | 0.48              |
| 2:I:872:TYR:HA   | 2:I:944:ARG:HH12  | 1.79                     | 0.48              |
| 3:J:429:LEU:HD13 | 3:J:429:LEU:HA    | 1.73                     | 0.48              |
| 3:J:1137:GLY:O   | 3:J:1140:ARG:HB3  | 2.14                     | 0.48              |
| 3:J:1156:LEU:HA  | 3:J:1208:ASP:O    | 2.13                     | 0.48              |
| 5:L:338:HIS:CE1  | 5:L:341:LEU:HD13  | 2.49                     | 0.48              |
| 1:A:11:PRO:HD3   | 1:B:227:GLN:OE1   | 2.14                     | 0.48              |
| 1:A:152:TYR:CZ   | 2:C:824:GLN:HA    | 2.49                     | 0.48              |
| 1:A:315:GLY:C    | 1:A:316:MET:HG3   | 2.39                     | 0.48              |
| 1:B:81:ILE:O     | 1:B:85:LEU:HG     | 2.14                     | 0.48              |
| 2:C:42:ASP:C     | 2:C:44:GLU:H      | 2.22                     | 0.48              |
| 2:C:209:ILE:HD13 | 2:C:425:ILE:HG21  | 1.96                     | 0.48              |
| 2:C:243:PRO:HB2  | 2:C:278:GLU:HG3   | 1.94                     | 0.48              |
| 2:C:691:PRO:HA   | 2:C:788:SER:OG    | 2.14                     | 0.48              |
| 3:D:202:ARG:NH2  | 3:D:225:GLU:OE1   | 2.47                     | 0.48              |
| 3:D:678:ARG:O    | 3:D:682:VAL:HG23  | 2.14                     | 0.48              |
| 3:D:1174:ARG:HG2 | 3:D:1189:MET:HG2  | 1.96                     | 0.48              |
| 5:F:562:ARG:HH21 | 5:F:573:LEU:HD23  | 1.78                     | 0.48              |
| 1:G:89:ALA:HB1   | 1:G:210:THR:HG23  | 1.96                     | 0.48              |
| 3:J:186:GLN:HG3  | 3:J:238:ILE:HB    | 1.96                     | 0.48              |
| 6:M:68:GLN:HA    | 6:M:71:HIS:HD2    | 1.77                     | 0.48              |
| 2:C:37:LYS:HD3   | 2:C:37:LYS:HA     | 1.76                     | 0.47              |
| 3:D:598:LYS:O    | 3:D:601:ILE:HG22  | 2.14                     | 0.47              |
| 3:D:1167:LYS:HZ2 | 3:D:1168:GLU:H    | 1.61                     | 0.47              |
| 2:I:1158:LYS:O   | 2:I:1159:VAL:HG13 | 2.13                     | 0.47              |
| 3:J:883:ARG:HB3  | 3:J:898:CYS:SG    | 2.54                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:L:248:GLU:HG2  | 5:L:251:LYS:HZ2   | 1.79                     | 0.47              |
| 1:B:48:LEU:HD21  | 3:D:535:ARG:HG3   | 1.95                     | 0.47              |
| 2:C:68:LEU:HD11  | 2:C:100:LEU:HB3   | 1.95                     | 0.47              |
| 2:C:421:SER:H    | 2:C:424:ASP:HB2   | 1.79                     | 0.47              |
| 2:C:551:HIS:H    | 2:C:554:HIS:CD2   | 2.31                     | 0.47              |
| 3:D:835:LEU:O    | 3:D:839:VAL:HG23  | 2.13                     | 0.47              |
| 5:F:281:ARG:O    | 5:F:285:ARG:HG3   | 2.13                     | 0.47              |
| 5:F:584:ARG:HA   | 5:F:584:ARG:HD2   | 1.71                     | 0.47              |
| 2:I:518:ASN:OD1  | 2:I:518:ASN:N     | 2.46                     | 0.47              |
| 5:L:274:ARG:NH2  | 5:L:369:GLU:OE2   | 2.47                     | 0.47              |
| 2:C:292:ILE:HB   | 2:C:322:LEU:HD11  | 1.95                     | 0.47              |
| 2:C:719:LYS:O    | 2:C:779:ARG:HG3   | 2.14                     | 0.47              |
| 3:D:365:GLN:O    | 3:D:437:PHE:HD1   | 1.97                     | 0.47              |
| 5:F:348:GLU:HG2  | 5:F:354:THR:HA    | 1.96                     | 0.47              |
| 2:I:119:GLU:HG3  | 2:I:488:MET:HB3   | 1.96                     | 0.47              |
| 3:J:872:LEU:HD22 | 3:J:877:VAL:HG11  | 1.95                     | 0.47              |
| 5:L:476:ARG:HB3  | 5:L:476:ARG:HH11  | 1.79                     | 0.47              |
| 2:C:1164:PHE:HD1 | 2:C:1164:PHE:HA   | 1.56                     | 0.47              |
| 3:D:518:VAL:CG1  | 3:D:707:ILE:HD13  | 2.45                     | 0.47              |
| 2:I:618:GLN:CG   | 3:J:770:LEU:HD21  | 2.44                     | 0.47              |
| 3:J:342:LEU:HA   | 3:J:343:LEU:HA    | 1.66                     | 0.47              |
| 3:J:548:VAL:HG12 | 3:J:550:VAL:HG13  | 1.96                     | 0.47              |
| 3:J:649:LYS:O    | 3:J:653:ILE:HG13  | 2.14                     | 0.47              |
| 3:D:664:ILE:HG21 | 3:D:681:LYS:HB3   | 1.97                     | 0.47              |
| 1:G:44:ARG:HG3   | 1:G:183:ILE:HG22  | 1.97                     | 0.47              |
| 3:J:56:LEU:HD12  | 3:J:56:LEU:H      | 1.79                     | 0.47              |
| 3:J:1203:ARG:NH2 | 3:J:1205:GLU:HG2  | 2.30                     | 0.47              |
| 5:L:371:LYS:HA   | 5:L:374:ARG:NH1   | 2.30                     | 0.47              |
| 1:A:321:TRP:HA   | 1:A:322:PRO:HA    | 1.75                     | 0.47              |
| 2:C:468:LEU:O    | 2:C:472:GLU:N     | 2.41                     | 0.47              |
| 2:C:478:ARG:CZ   | 2:C:487:LEU:HD13  | 2.44                     | 0.47              |
| 2:C:590:PRO:HG3  | 2:C:605:TYR:CZ    | 2.49                     | 0.47              |
| 3:D:491:LEU:HB2  | 3:D:904:ALA:HA    | 1.95                     | 0.47              |
| 3:D:1257:VAL:HA  | 3:D:1260:MET:HG3  | 1.95                     | 0.47              |
| 2:I:10:ARG:HA    | 2:I:1172:LEU:HD23 | 1.95                     | 0.47              |
| 2:I:594:VAL:HG11 | 2:I:650:VAL:HG23  | 1.96                     | 0.47              |
| 2:I:1276:TRP:CH2 | 3:J:798:ARG:HG3   | 2.41                     | 0.47              |
| 3:J:664:ILE:HG21 | 3:J:681:LYS:HB3   | 1.97                     | 0.47              |
| 3:J:810:THR:CG2  | 3:J:893:GLY:HA3   | 2.45                     | 0.47              |
| 3:J:859:PRO:HG2  | 3:J:862:THR:HG21  | 1.95                     | 0.47              |
| 1:A:80:GLU:O     | 1:A:84:ASN:ND2    | 2.48                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:261:GLU:CD    | 2:C:859:GLU:HB2   | 2.39                     | 0.47              |
| 2:C:245:ARG:HG2   | 2:C:337:PHE:CE2   | 2.49                     | 0.47              |
| 2:C:1282:GLY:HA3  | 4:E:17:PHE:CE1    | 2.49                     | 0.47              |
| 3:D:322:ARG:HB2   | 3:D:322:ARG:HH11  | 1.80                     | 0.47              |
| 3:D:384:LYS:HD2   | 3:D:387:LEU:HD23  | 1.95                     | 0.47              |
| 3:D:504:GLN:HG3   | 3:D:505:ASP:H     | 1.79                     | 0.47              |
| 3:D:901:ARG:HD2   | 3:D:906:GLY:O     | 2.15                     | 0.47              |
| 5:F:608:ARG:HB2   | 5:F:608:ARG:HH11  | 1.80                     | 0.47              |
| 1:G:75:GLN:HA     | 2:I:729:ALA:N     | 2.30                     | 0.47              |
| 1:G:167:PRO:HB2   | 1:G:170:ARG:HG3   | 1.96                     | 0.47              |
| 1:H:153:VAL:HG11  | 1:H:158:ARG:HH11  | 1.79                     | 0.47              |
| 2:I:564:PRO:HA    | 2:I:684:ASN:HD21  | 1.79                     | 0.47              |
| 2:I:987:GLU:HG2   | 2:I:991:LYS:HE3   | 1.95                     | 0.47              |
| 2:I:1283:ALA:HB1  | 2:I:1286:THR:HB   | 1.97                     | 0.47              |
| 2:I:1327:LEU:HG   | 2:I:1337:ILE:HG23 | 1.96                     | 0.47              |
| 3:J:320:ASN:OD1   | 3:J:322:ARG:HB3   | 2.15                     | 0.47              |
| 4:K:19:LEU:HD13   | 4:K:54:ILE:HG21   | 1.95                     | 0.47              |
| 4:K:50:ALA:O      | 4:K:54:ILE:HG12   | 2.14                     | 0.47              |
| 2:C:104:ILE:O     | 2:C:113:THR:HA    | 2.15                     | 0.47              |
| 2:C:730:SER:O     | 2:C:753:LEU:HB2   | 2.15                     | 0.47              |
| 5:F:399:LEU:HD12  | 5:F:399:LEU:HA    | 1.76                     | 0.47              |
| 1:G:56:VAL:HG11   | 1:G:85:LEU:HB3    | 1.96                     | 0.47              |
| 1:H:102:LEU:HD11  | 1:H:130:ILE:HG21  | 1.97                     | 0.47              |
| 2:I:601:ASP:OD1   | 2:I:601:ASP:N     | 2.45                     | 0.47              |
| 2:I:617:ALA:HA    | 2:I:636:CYS:SG    | 2.55                     | 0.47              |
| 3:J:26:SER:HB2    | 3:J:236:TRP:CZ2   | 2.50                     | 0.47              |
| 3:J:1347:LEU:HD12 | 3:J:1358:PRO:HG2  | 1.97                     | 0.47              |
| 6:M:33:PRO:HG3    | 6:M:54:GLY:HA2    | 1.96                     | 0.47              |
| 6:N:48:ARG:HB3    | 6:N:55:VAL:HG11   | 1.97                     | 0.47              |
| 6:N:63:ALA:HB1    | 6:N:67:ARG:NE     | 2.30                     | 0.47              |
| 1:A:228:LEU:HD21  | 1:B:43:LEU:HD11   | 1.97                     | 0.47              |
| 2:C:15:PHE:CE1    | 2:C:1194:GLU:HB3  | 2.50                     | 0.47              |
| 2:C:105:TYR:CE1   | 2:C:111:GLU:HB3   | 2.50                     | 0.47              |
| 2:C:247:ARG:CZ    | 2:C:274:ILE:HD12  | 2.45                     | 0.47              |
| 3:D:689:ALA:O     | 3:D:693:VAL:HG23  | 2.15                     | 0.47              |
| 1:G:31:LEU:HD12   | 1:G:201:LEU:HB2   | 1.97                     | 0.47              |
| 3:J:128:LEU:HB3   | 3:J:157:GLN:HE22  | 1.80                     | 0.47              |
| 3:J:1170:LYS:C    | 3:J:1172:LYS:H    | 2.22                     | 0.47              |
| 3:J:1252:HIS:O    | 3:J:1255:VAL:HG13 | 2.14                     | 0.47              |
| 2:C:73:TYR:HB2    | 2:C:98:VAL:HG22   | 1.97                     | 0.47              |
| 2:C:169:LYS:O     | 2:C:170:VAL:HG22  | 2.15                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:609:TYR:CE2   | 3:D:614:LEU:HD12  | 2.49                     | 0.47              |
| 5:F:101:TYR:HE2   | 5:F:388:ILE:HD11  | 1.80                     | 0.47              |
| 1:G:31:LEU:HD23   | 1:G:31:LEU:HA     | 1.76                     | 0.47              |
| 2:I:68:LEU:HD11   | 2:I:100:LEU:HB3   | 1.97                     | 0.47              |
| 2:I:1142:ARG:HH22 | 2:I:1165:SER:HB2  | 1.80                     | 0.47              |
| 3:J:172:PHE:HB3   | 3:J:175:GLU:OE2   | 2.15                     | 0.47              |
| 5:L:233:ASP:O     | 5:L:236:LYS:HE2   | 2.14                     | 0.47              |
| 1:A:22:THR:O      | 1:A:207:THR:N     | 2.36                     | 0.46              |
| 3:D:53:ARG:HA     | 3:D:54:ASP:HA     | 1.58                     | 0.46              |
| 3:D:687:ALA:HB1   | 6:M:24:ARG:CZ     | 2.46                     | 0.46              |
| 1:G:83:LEU:HD23   | 2:I:694:ARG:NE    | 2.27                     | 0.46              |
| 3:J:154:LEU:HD22  | 3:J:160:LEU:HD11  | 1.97                     | 0.46              |
| 6:M:48:ARG:HD3    | 6:M:59:VAL:HG23   | 1.96                     | 0.46              |
| 2:C:5:TYR:O       | 2:C:8:LYS:HG2     | 2.15                     | 0.46              |
| 2:C:213:LEU:HD13  | 2:C:422:LYS:HG2   | 1.96                     | 0.46              |
| 2:I:88:ARG:HH11   | 2:I:88:ARG:HB2    | 1.80                     | 0.46              |
| 2:I:607:SER:OG    | 2:I:609:ILE:HG13  | 2.15                     | 0.46              |
| 2:I:1272:GLU:HB2  | 3:J:342:LEU:CB    | 2.45                     | 0.46              |
| 2:I:1285:TYR:CD1  | 3:J:475:GLU:HG2   | 2.50                     | 0.46              |
| 2:I:1287:LEU:HD22 | 3:J:1357:ILE:CG1  | 2.42                     | 0.46              |
| 3:J:518:VAL:HG12  | 3:J:707:ILE:HD13  | 1.97                     | 0.46              |
| 3:J:709:ARG:NE    | 3:J:710:ASP:OD2   | 2.48                     | 0.46              |
| 6:N:9:TYR:O       | 6:N:12:THR:OG1    | 2.18                     | 0.46              |
| 2:C:810:TYR:CE1   | 2:C:1078:LYS:HD2  | 2.51                     | 0.46              |
| 3:D:13:LYS:HA     | 3:D:13:LYS:HD3    | 1.75                     | 0.46              |
| 3:D:291:ILE:HG23  | 5:F:406:GLN:HE22  | 1.80                     | 0.46              |
| 3:D:850:LYS:HD3   | 3:D:875:ASN:ND2   | 2.31                     | 0.46              |
| 1:G:224:LEU:HD13  | 1:H:228:LEU:HD11  | 1.97                     | 0.46              |
| 2:I:1312:ASN:HD21 | 2:I:1314:GLN:HE21 | 1.63                     | 0.46              |
| 3:J:322:ARG:HB2   | 3:J:322:ARG:NH1   | 2.31                     | 0.46              |
| 3:J:716:GLN:HG3   | 3:J:717:VAL:O     | 2.16                     | 0.46              |
| 3:J:733:SER:O     | 3:J:737:ILE:HG12  | 2.15                     | 0.46              |
| 2:C:882:ILE:HD12  | 2:C:882:ILE:H     | 1.80                     | 0.46              |
| 2:C:1240:ASP:HB3  | 3:D:445:LYS:HD2   | 1.96                     | 0.46              |
| 2:C:1323:PHE:CE1  | 3:D:1353:VAL:HG23 | 2.51                     | 0.46              |
| 3:D:255:LEU:HD13  | 3:D:255:LEU:HA    | 1.79                     | 0.46              |
| 3:D:500:ILE:HG22  | 3:D:500:ILE:O     | 2.15                     | 0.46              |
| 1:G:13:LEU:HD23   | 1:G:13:LEU:H      | 1.80                     | 0.46              |
| 1:G:152:TYR:CZ    | 2:I:824:GLN:HA    | 2.50                     | 0.46              |
| 1:G:166:ARG:O     | 1:G:167:PRO:C     | 2.58                     | 0.46              |
| 2:I:465:ARG:O     | 2:I:469:VAL:HG13  | 2.16                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:615:LYS:HE2   | 3:J:616:PRO:HD3   | 1.98                     | 0.46              |
| 1:A:54:CYS:HB3    | 1:A:148:ARG:HB2   | 1.97                     | 0.46              |
| 2:C:222:ASP:HA    | 2:C:227:LYS:HE2   | 1.97                     | 0.46              |
| 2:C:225:PHE:CB    | 2:C:336:LEU:HD22  | 2.45                     | 0.46              |
| 2:C:541:GLU:OE1   | 2:C:541:GLU:N     | 2.49                     | 0.46              |
| 2:C:799:ASN:HB3   | 2:C:1231:TYR:HD1  | 1.81                     | 0.46              |
| 2:C:886:LYS:NZ    | 2:C:916:SER:HB3   | 2.30                     | 0.46              |
| 3:D:311:ARG:NH2   | 3:D:1329:THR:HG21 | 2.31                     | 0.46              |
| 3:D:820:ILE:HD11  | 3:D:822:MET:HE2   | 1.97                     | 0.46              |
| 1:H:86:LYS:HD3    | 1:H:174:ASP:HB2   | 1.96                     | 0.46              |
| 2:I:10:ARG:NH1    | 2:I:697:LYS:HD3   | 2.31                     | 0.46              |
| 2:I:215:TYR:HD1   | 2:I:219:GLN:HB3   | 1.80                     | 0.46              |
| 2:I:960:LEU:HB3   | 2:I:1025:PHE:CE2  | 2.51                     | 0.46              |
| 3:J:358:GLY:N     | 3:J:359:PRO:HD3   | 2.30                     | 0.46              |
| 3:J:559:ALA:HB3   | 3:J:562:GLU:HB3   | 1.98                     | 0.46              |
| 3:J:801:VAL:O     | 3:J:805:GLN:HB2   | 2.16                     | 0.46              |
| 3:J:1290:ARG:HD2  | 3:J:1295:ASN:HD22 | 1.81                     | 0.46              |
| 5:L:474:MET:C     | 5:L:476:ARG:H     | 2.24                     | 0.46              |
| 6:N:35:TYR:OH     | 6:N:46:GLU:HG2    | 2.16                     | 0.46              |
| 1:A:179:PRO:HA    | 1:A:208:ASN:ND2   | 2.30                     | 0.46              |
| 1:B:152:TYR:CE1   | 1:B:176:CYS:HB3   | 2.51                     | 0.46              |
| 2:C:739:ASP:N     | 2:C:739:ASP:OD1   | 2.46                     | 0.46              |
| 2:C:1314:GLN:HG2  | 4:E:28:ARG:CZ     | 2.46                     | 0.46              |
| 3:D:572:THR:OG1   | 3:D:576:ARG:HB2   | 2.16                     | 0.46              |
| 1:H:152:TYR:CE2   | 3:J:536:LEU:HD21  | 2.51                     | 0.46              |
| 2:I:971:LEU:HD22  | 2:I:1018:TYR:HB2  | 1.97                     | 0.46              |
| 3:J:580:TRP:HH2   | 3:J:587:LEU:O     | 1.97                     | 0.46              |
| 3:J:683:ILE:HD11  | 3:J:754:ILE:HG23  | 1.97                     | 0.46              |
| 2:C:296:VAL:O     | 2:C:335:THR:HA    | 2.16                     | 0.46              |
| 2:C:452:ARG:HH12  | 2:C:585:GLY:HA3   | 1.81                     | 0.46              |
| 2:C:810:TYR:HE1   | 2:C:1078:LYS:HD2  | 1.81                     | 0.46              |
| 2:C:887:VAL:HB    | 2:C:913:VAL:HG22  | 1.97                     | 0.46              |
| 3:D:1178:THR:HG23 | 3:D:1184:ASP:HB3  | 1.98                     | 0.46              |
| 2:I:617:ALA:HB3   | 2:I:653:MET:HB2   | 1.98                     | 0.46              |
| 2:I:996:ARG:NH1   | 2:I:999:GLU:OE1   | 2.39                     | 0.46              |
| 2:I:1100:PRO:HB3  | 3:J:639:VAL:HG12  | 1.98                     | 0.46              |
| 3:J:513:MET:O     | 3:J:575:GLY:HA3   | 2.16                     | 0.46              |
| 3:J:848:VAL:HG21  | 3:J:880:VAL:HG22  | 1.97                     | 0.46              |
| 3:J:1257:VAL:HA   | 3:J:1260:MET:HG3  | 1.98                     | 0.46              |
| 3:J:1350:ASN:HA   | 3:J:1353:VAL:HG12 | 1.98                     | 0.46              |
| 5:L:584:ARG:HA    | 5:L:584:ARG:HD2   | 1.78                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:56:VAL:HG21   | 1:B:144:ILE:HD11  | 1.97                     | 0.46              |
| 2:C:148:GLN:OE1   | 2:C:454:ARG:NH2   | 2.48                     | 0.46              |
| 2:C:228:VAL:HB    | 2:C:335:THR:OG1   | 2.15                     | 0.46              |
| 2:C:263:VAL:HG21  | 2:C:273:HIS:CG    | 2.51                     | 0.46              |
| 2:C:732:ILE:HG21  | 2:C:783:LEU:HD12  | 1.98                     | 0.46              |
| 3:D:405:GLU:O     | 3:D:408:VAL:HG22  | 2.15                     | 0.46              |
| 3:D:1281:GLU:O    | 3:D:1285:VAL:HG13 | 2.16                     | 0.46              |
| 2:I:13:LYS:NZ     | 2:I:1151:LEU:HB2  | 2.30                     | 0.46              |
| 2:I:688:GLN:OE1   | 2:I:1237:HIS:HE1  | 1.99                     | 0.46              |
| 3:J:587:LEU:HD23  | 3:J:591:ILE:HG21  | 1.97                     | 0.46              |
| 3:J:667:GLN:NE2   | 6:N:51:ILE:HD11   | 2.30                     | 0.46              |
| 5:L:326:TRP:HA    | 5:L:329:LYS:HD2   | 1.97                     | 0.46              |
| 6:M:45:PRO:HD2    | 6:M:48:ARG:NH2    | 2.31                     | 0.46              |
| 1:A:158:ARG:NH2   | 1:A:172:LEU:HB3   | 2.30                     | 0.46              |
| 1:A:232:VAL:O     | 1:B:218:ARG:HA    | 2.16                     | 0.46              |
| 2:C:1164:PHE:C    | 2:C:1166:ASP:H    | 2.24                     | 0.46              |
| 3:D:27:PRO:O      | 3:D:31:ARG:HG3    | 2.16                     | 0.46              |
| 3:D:310:GLY:CA    | 3:D:314:ARG:HH11  | 2.29                     | 0.46              |
| 3:D:425:ARG:HG2   | 3:D:426:ALA:N     | 2.29                     | 0.46              |
| 3:D:697:MET:SD    | 3:D:741:ALA:HB3   | 2.56                     | 0.46              |
| 3:D:1273:ASP:O    | 3:D:1275:LEU:N    | 2.47                     | 0.46              |
| 1:G:137:ASN:OD1   | 1:G:137:ASN:N     | 2.43                     | 0.46              |
| 1:H:41:ASN:OD1    | 1:H:44:ARG:NH1    | 2.46                     | 0.46              |
| 3:J:421:VAL:HG13  | 3:J:439:PRO:HG3   | 1.96                     | 0.46              |
| 3:J:515:ARG:NH2   | 3:J:717:VAL:O     | 2.48                     | 0.46              |
| 1:A:59:VAL:HG22   | 1:A:144:ILE:HG12  | 1.99                     | 0.46              |
| 1:A:195:ARG:HD2   | 1:A:196:THR:H     | 1.81                     | 0.46              |
| 2:C:395:TYR:CE2   | 2:C:420:LEU:HG    | 2.51                     | 0.46              |
| 2:C:1149:TYR:CB   | 2:C:1159:VAL:HG21 | 2.46                     | 0.46              |
| 2:C:1156:ARG:HB2  | 2:C:1156:ARG:HH11 | 1.81                     | 0.46              |
| 3:D:1167:LYS:HZ1  | 3:D:1170:LYS:CB   | 2.29                     | 0.46              |
| 5:F:277:MET:HG3   | 5:F:362:ASN:ND2   | 2.30                     | 0.46              |
| 1:G:32:GLU:HA     | 1:G:198:LEU:HD22  | 1.98                     | 0.46              |
| 1:G:62:ASP:HB2    | 1:G:141:SER:O     | 2.16                     | 0.46              |
| 1:G:219:ARG:HA    | 1:G:222:THR:HB    | 1.98                     | 0.46              |
| 2:I:1142:ARG:HH12 | 2:I:1165:SER:HA   | 1.80                     | 0.46              |
| 2:I:1280:ALA:HB3  | 3:J:431:ARG:HB3   | 1.98                     | 0.46              |
| 3:J:258:GLY:HA3   | 5:L:499:LYS:HE2   | 1.96                     | 0.46              |
| 5:L:561:MET:HA    | 5:L:567:MET:CE    | 2.45                     | 0.46              |
| 1:A:195:ARG:HG3   | 1:A:198:LEU:HD11  | 1.98                     | 0.45              |
| 1:B:194:GLN:NE2   | 3:D:406:ALA:HB2   | 2.30                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:D:80:HIS:HB3   | 3:D:83:VAL:HG11   | 1.97                     | 0.45              |
| 3:D:548:VAL:HG12 | 3:D:550:VAL:HG13  | 1.98                     | 0.45              |
| 5:F:309:ASN:ND2  | 5:F:312:SER:HB3   | 2.29                     | 0.45              |
| 1:H:62:ASP:OD1   | 1:H:62:ASP:N      | 2.31                     | 0.45              |
| 1:H:155:ALA:HB2  | 1:H:173:VAL:C     | 2.41                     | 0.45              |
| 2:I:1072:ASN:OD1 | 2:I:1072:ASN:N    | 2.44                     | 0.45              |
| 3:J:205:LEU:CD2  | 3:J:214:ARG:HB2   | 2.46                     | 0.45              |
| 3:J:322:ARG:HG3  | 3:J:323:PRO:HD2   | 1.98                     | 0.45              |
| 3:J:680:ASN:HD22 | 6:N:27:ILE:HD11   | 1.80                     | 0.45              |
| 1:A:12:ARG:HG2   | 1:A:13:LEU:H      | 1.82                     | 0.45              |
| 1:B:83:LEU:HD11  | 3:D:526:VAL:HG23  | 1.97                     | 0.45              |
| 2:C:733:VAL:CG1  | 2:C:748:ILE:HG13  | 2.45                     | 0.45              |
| 3:D:194:LEU:O    | 3:D:198:CYS:N     | 2.45                     | 0.45              |
| 3:D:746:LEU:HB3  | 3:D:754:ILE:HD11  | 1.98                     | 0.45              |
| 3:D:1227:HIS:HA  | 3:D:1230:THR:HG22 | 1.98                     | 0.45              |
| 5:F:287:ILE:HG12 | 5:F:337:VAL:HG13  | 1.97                     | 0.45              |
| 5:F:461:ASN:O    | 5:F:465:ARG:HG2   | 2.15                     | 0.45              |
| 1:G:9:LEU:HD13   | 1:G:32:GLU:HG2    | 1.98                     | 0.45              |
| 1:H:98:VAL:O     | 1:H:146:VAL:HG22  | 2.15                     | 0.45              |
| 1:H:155:ALA:HB2  | 1:H:174:ASP:N     | 2.31                     | 0.45              |
| 2:I:80:PHE:HB3   | 2:I:84:GLU:HB2    | 1.97                     | 0.45              |
| 2:I:107:ARG:HA   | 2:I:108:GLU:HA    | 1.65                     | 0.45              |
| 3:J:849:LEU:H    | 3:J:849:LEU:HD22  | 1.81                     | 0.45              |
| 2:C:60:GLN:HB3   | 2:C:67:GLU:HG3    | 1.97                     | 0.45              |
| 2:C:247:ARG:HB2  | 2:C:274:ILE:CD1   | 2.47                     | 0.45              |
| 3:D:197:GLU:O    | 3:D:201:LEU:HG    | 2.16                     | 0.45              |
| 3:D:513:MET:HE2  | 3:D:513:MET:HB3   | 1.84                     | 0.45              |
| 3:D:672:LEU:HD23 | 6:M:47:ALA:HB1    | 1.97                     | 0.45              |
| 3:D:680:ASN:O    | 3:D:683:ILE:HG22  | 2.17                     | 0.45              |
| 3:J:1287:ILE:O   | 3:J:1291:GLU:HG3  | 2.16                     | 0.45              |
| 4:K:6:VAL:O      | 4:K:10:VAL:HG23   | 2.15                     | 0.45              |
| 1:B:92:VAL:CG1   | 1:B:95:LYS:HB3    | 2.47                     | 0.45              |
| 1:B:190:ALA:HB2  | 1:B:200:LYS:HB2   | 1.99                     | 0.45              |
| 2:C:106:GLU:HG3  | 2:C:107:ARG:N     | 2.32                     | 0.45              |
| 2:C:213:LEU:HD22 | 2:C:422:LYS:HG2   | 1.99                     | 0.45              |
| 2:C:359:ARG:NH1  | 2:C:382:GLU:OE2   | 2.50                     | 0.45              |
| 2:C:492:MET:H    | 2:C:492:MET:HG2   | 1.61                     | 0.45              |
| 3:D:265:LEU:HG   | 3:D:330:MET:HE1   | 1.98                     | 0.45              |
| 3:D:316:ILE:HA   | 3:D:323:PRO:HA    | 1.99                     | 0.45              |
| 3:D:647:PRO:CG   | 3:D:697:MET:HB3   | 2.44                     | 0.45              |
| 1:H:102:LEU:HG   | 1:H:115:ILE:HG12  | 1.97                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:17:LYS:NZ     | 2:I:1154:ASP:OD1  | 2.49                     | 0.45              |
| 2:I:71:VAL:HB     | 2:I:99:LYS:HB2    | 1.97                     | 0.45              |
| 2:I:897:PRO:HB2   | 2:I:898:GLU:OE1   | 2.17                     | 0.45              |
| 3:J:812:ASP:HB2   | 3:J:911:LYS:HE3   | 1.99                     | 0.45              |
| 2:C:565:GLU:OE1   | 2:C:681:MET:HE3   | 2.17                     | 0.45              |
| 3:D:400:MET:HE2   | 3:D:400:MET:HB3   | 1.81                     | 0.45              |
| 3:D:528:THR:O     | 3:D:551:ARG:HB3   | 2.17                     | 0.45              |
| 5:F:226:ALA:O     | 5:F:229:VAL:HG22  | 2.17                     | 0.45              |
| 2:I:720:ARG:NH2   | 2:I:736:VAL:HG21  | 2.32                     | 0.45              |
| 2:I:842:ASP:N     | 2:I:1045:GLY:O    | 2.49                     | 0.45              |
| 3:J:478:LEU:HG    | 4:K:47:THR:HG23   | 1.98                     | 0.45              |
| 3:J:810:THR:HG21  | 3:J:893:GLY:HA3   | 1.98                     | 0.45              |
| 2:C:540:ARG:HB2   | 2:C:540:ARG:HH11  | 1.82                     | 0.45              |
| 1:G:166:ARG:HH11  | 1:G:168:ILE:H     | 1.65                     | 0.45              |
| 1:G:232:VAL:C     | 1:H:218:ARG:HH12  | 2.24                     | 0.45              |
| 2:I:13:LYS:HD3    | 2:I:1149:TYR:HA   | 1.99                     | 0.45              |
| 2:I:856:ASN:HB3   | 5:L:613:ASP:HA    | 1.98                     | 0.45              |
| 2:I:1149:TYR:CD1  | 2:I:1159:VAL:HG11 | 2.50                     | 0.45              |
| 3:J:1309:ILE:HG13 | 3:J:1310:THR:N    | 2.32                     | 0.45              |
| 5:L:482:GLU:HG3   | 5:L:486:ARG:HH22  | 1.81                     | 0.45              |
| 1:A:252:ILE:HG21  | 1:A:312:LEU:HD11  | 1.98                     | 0.45              |
| 1:B:98:VAL:O      | 1:B:146:VAL:HG13  | 2.17                     | 0.45              |
| 1:B:182:ARG:HD2   | 3:D:581:MET:HE1   | 1.98                     | 0.45              |
| 2:C:593:LYS:HG3   | 2:C:595:THR:HG23  | 1.97                     | 0.45              |
| 2:C:718:ALA:HB2   | 2:C:783:LEU:CD2   | 2.47                     | 0.45              |
| 2:C:741:MET:HE3   | 2:C:974:ARG:NH2   | 2.32                     | 0.45              |
| 2:C:1296:ASP:HB3  | 2:C:1320:PRO:HB3  | 1.99                     | 0.45              |
| 3:D:903:LEU:HD23  | 3:D:905:ARG:HD3   | 1.99                     | 0.45              |
| 3:D:1167:LYS:NZ   | 3:D:1170:LYS:HB2  | 2.31                     | 0.45              |
| 3:D:1301:THR:HA   | 3:J:1297:LYS:HE2  | 1.99                     | 0.45              |
| 2:I:123:TYR:OH    | 2:I:126:GLU:HG3   | 2.17                     | 0.45              |
| 2:I:1184:THR:HG23 | 2:I:1189:GLY:HA2  | 1.98                     | 0.45              |
| 3:J:474:LEU:HD12  | 3:J:474:LEU:HA    | 1.75                     | 0.45              |
| 3:J:825:VAL:C     | 3:J:826:ILE:HG13  | 2.42                     | 0.45              |
| 3:J:1173:ARG:HB2  | 3:J:1192:LYS:HB3  | 1.99                     | 0.45              |
| 3:J:1280:VAL:HG11 | 3:J:1304:ARG:NH2  | 2.32                     | 0.45              |
| 2:C:247:ARG:HH22  | 2:C:271:ALA:HA    | 1.82                     | 0.45              |
| 3:D:735:ALA:O     | 3:D:738:ARG:HB3   | 2.16                     | 0.45              |
| 3:D:770:LEU:H     | 3:D:770:LEU:HD22  | 1.80                     | 0.45              |
| 3:D:825:VAL:C     | 3:D:826:ILE:HG13  | 2.42                     | 0.45              |
| 3:D:826:ILE:HD12  | 3:D:826:ILE:O     | 2.17                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:J:69:GLU:HG3   | 3:J:76:LYS:HG2    | 1.97                     | 0.45              |
| 3:J:186:GLN:HB2  | 3:J:238:ILE:HG21  | 1.99                     | 0.45              |
| 3:J:279:LEU:HD12 | 3:J:295:GLU:HG3   | 1.99                     | 0.45              |
| 3:J:902:ASP:OD1  | 3:J:903:LEU:N     | 2.50                     | 0.45              |
| 6:N:63:ALA:O     | 6:N:64:TYR:C      | 2.60                     | 0.45              |
| 2:C:601:ASP:OD1  | 2:C:601:ASP:N     | 2.49                     | 0.45              |
| 2:I:1087:TYR:CE1 | 2:I:1215:GLY:HA2  | 2.45                     | 0.45              |
| 3:J:317:THR:HG22 | 3:J:322:ARG:O     | 2.17                     | 0.45              |
| 3:J:740:LEU:HA   | 3:J:763:PHE:HB2   | 1.99                     | 0.45              |
| 3:J:826:ILE:HD12 | 3:J:826:ILE:O     | 2.17                     | 0.45              |
| 6:N:48:ARG:CZ    | 6:N:59:VAL:H      | 2.29                     | 0.45              |
| 1:B:22:THR:OG1   | 1:B:207:THR:O     | 2.35                     | 0.45              |
| 2:C:10:ARG:NH1   | 2:C:697:LYS:HD3   | 2.31                     | 0.45              |
| 2:C:563:THR:OG1  | 2:C:564:PRO:HD2   | 2.16                     | 0.45              |
| 2:C:1187:PHE:HZ  | 3:D:772:TYR:HD2   | 1.65                     | 0.45              |
| 3:D:529:GLY:HA2  | 3:D:551:ARG:O     | 2.17                     | 0.45              |
| 5:F:608:ARG:HH11 | 5:F:608:ARG:CG    | 2.30                     | 0.45              |
| 1:G:38:THR:HG21  | 1:H:46:ILE:HG13   | 1.99                     | 0.45              |
| 2:I:548:ARG:NH2  | 2:I:567:PRO:O     | 2.50                     | 0.45              |
| 2:I:1106:ARG:O   | 2:I:1108:ASN:N    | 2.44                     | 0.45              |
| 3:J:426:ALA:CB   | 3:J:427:PRO:HD3   | 2.42                     | 0.45              |
| 3:J:1179:PRO:CD  | 3:J:1184:ASP:HA   | 2.43                     | 0.45              |
| 5:L:277:MET:HG3  | 5:L:362:ASN:ND2   | 2.30                     | 0.45              |
| 5:L:445:ASP:OD2  | 5:L:451:ARG:HD2   | 2.16                     | 0.45              |
| 2:C:94:ALA:HB2   | 2:C:129:LEU:HD11  | 1.99                     | 0.44              |
| 2:C:569:ILE:C    | 2:C:571:LEU:H     | 2.25                     | 0.44              |
| 2:C:1111:GLN:HB2 | 2:C:1230:MET:HE2  | 1.98                     | 0.44              |
| 2:I:160:ASP:HB3  | 2:I:164:THR:HG21  | 1.99                     | 0.44              |
| 2:I:1244:HIS:HD2 | 2:I:1265:PHE:HB2  | 1.82                     | 0.44              |
| 3:J:474:LEU:HD12 | 3:J:477:GLN:HE21  | 1.82                     | 0.44              |
| 2:C:395:TYR:CD2  | 2:C:419:ILE:HG22  | 2.52                     | 0.44              |
| 2:C:1062:PRO:HA  | 2:C:1076:ILE:HG13 | 1.97                     | 0.44              |
| 2:C:1134:GLN:HB3 | 2:C:1136:GLN:HG2  | 1.99                     | 0.44              |
| 3:D:45:ASN:O     | 3:D:46:TYR:HD2    | 2.00                     | 0.44              |
| 3:D:68:TYR:HA    | 3:D:92:VAL:HG23   | 1.98                     | 0.44              |
| 3:D:342:LEU:HA   | 3:D:343:LEU:HA    | 1.69                     | 0.44              |
| 3:D:416:ILE:HD13 | 3:D:416:ILE:HA    | 1.68                     | 0.44              |
| 3:D:480:ALA:HA   | 3:D:484:MET:HG3   | 1.98                     | 0.44              |
| 3:D:1167:LYS:HE3 | 3:D:1174:ARG:HD2  | 1.98                     | 0.44              |
| 1:G:71:LYS:HE2   | 1:G:139:SER:O     | 2.17                     | 0.44              |
| 1:G:97:GLU:OE2   | 1:G:145:LYS:HE2   | 2.16                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:H:85:LEU:HD23   | 1:H:85:LEU:HA     | 1.84                     | 0.44              |
| 2:I:151:ARG:HH22  | 2:I:175:ARG:HH11  | 1.64                     | 0.44              |
| 2:I:1196:LYS:HA   | 2:I:1199:LEU:HD12 | 2.00                     | 0.44              |
| 3:J:161:THR:H     | 3:J:164:GLN:HB2   | 1.82                     | 0.44              |
| 3:J:590:SER:HA    | 3:J:593:ASN:HB2   | 1.98                     | 0.44              |
| 5:L:380:VAL:HG13  | 5:L:412:LEU:HD23  | 1.99                     | 0.44              |
| 5:L:571:TYR:CD1   | 5:L:575:GLU:HG2   | 2.52                     | 0.44              |
| 1:B:71:LYS:HA     | 1:B:71:LYS:HD2    | 1.77                     | 0.44              |
| 1:B:178:SER:HA    | 1:B:179:PRO:HD3   | 1.86                     | 0.44              |
| 2:C:744:GLY:C     | 2:C:746:ALA:N     | 2.75                     | 0.44              |
| 2:C:1253:LEU:CD1  | 3:D:253:VAL:HG11  | 2.45                     | 0.44              |
| 3:D:115:TRP:CE2   | 3:D:1329:THR:HG23 | 2.52                     | 0.44              |
| 5:F:311:THR:HG21  | 5:F:348:GLU:CD    | 2.42                     | 0.44              |
| 5:F:513:ASP:C     | 5:F:515:GLU:N     | 2.75                     | 0.44              |
| 1:G:152:TYR:CG    | 2:I:824:GLN:HG2   | 2.52                     | 0.44              |
| 2:I:29:SER:O      | 2:I:33:ASP:HB2    | 2.17                     | 0.44              |
| 2:I:211:ARG:NH1   | 2:I:357:ASN:O     | 2.51                     | 0.44              |
| 2:I:245:ARG:HG2   | 2:I:337:PHE:CE2   | 2.51                     | 0.44              |
| 2:I:503:LYS:HA    | 2:I:503:LYS:HD2   | 1.74                     | 0.44              |
| 2:I:1142:ARG:NH1  | 2:I:1161:LEU:HD11 | 2.32                     | 0.44              |
| 3:J:41:PRO:HG3    | 3:J:274:ASN:OD1   | 2.17                     | 0.44              |
| 3:J:264:ASP:HB3   | 3:J:324:LEU:HB2   | 1.99                     | 0.44              |
| 3:J:650:LYS:HZ2   | 3:J:762:ASN:HD22  | 1.65                     | 0.44              |
| 3:J:689:ALA:O     | 3:J:693:VAL:HG23  | 2.16                     | 0.44              |
| 5:L:461:ASN:HB3   | 5:L:465:ARG:NH2   | 2.32                     | 0.44              |
| 5:L:515:GLU:HG2   | 5:L:516:ASP:H     | 1.82                     | 0.44              |
| 6:N:20:ILE:HG22   | 6:N:24:ARG:HE     | 1.82                     | 0.44              |
| 6:N:45:PRO:HD2    | 6:N:48:ARG:CZ     | 2.47                     | 0.44              |
| 1:B:54:CYS:SG     | 1:B:148:ARG:HG3   | 2.58                     | 0.44              |
| 2:C:117:ILE:H     | 2:C:117:ILE:HG12  | 1.61                     | 0.44              |
| 2:C:145:ILE:HA    | 2:C:511:LEU:O     | 2.18                     | 0.44              |
| 2:C:533:LEU:HD11  | 2:C:540:ARG:HD2   | 1.99                     | 0.44              |
| 2:C:737:ASN:O     | 2:C:741:MET:HB2   | 2.17                     | 0.44              |
| 2:C:1298:VAL:HG11 | 3:D:96:LYS:NZ     | 2.33                     | 0.44              |
| 3:D:9:LYS:NZ      | 3:D:11:GLN:HA     | 2.32                     | 0.44              |
| 3:D:262:THR:HG1   | 3:D:266:ASN:ND2   | 2.15                     | 0.44              |
| 1:H:84:ASN:O      | 1:H:128:HIS:HE1   | 2.01                     | 0.44              |
| 3:J:50:LYS:HD3    | 3:J:71:LEU:HD21   | 2.00                     | 0.44              |
| 3:J:620:PHE:CZ    | 3:J:624:ILE:HD11  | 2.53                     | 0.44              |
| 3:J:1266:ILE:HD12 | 3:J:1273:ASP:C    | 2.43                     | 0.44              |
| 5:L:478:PRO:HG2   | 5:L:483:LEU:HD11  | 2.00                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:188:GLU:HG3   | 1:B:200:LYS:HB3   | 1.98                     | 0.44              |
| 2:C:517:GLN:O     | 2:C:517:GLN:HG2   | 2.16                     | 0.44              |
| 2:C:672:GLU:HG2   | 2:C:1187:PHE:HA   | 1.99                     | 0.44              |
| 3:D:60:ARG:HA     | 3:D:89:GLY:O      | 2.18                     | 0.44              |
| 3:D:110:PRO:HB3   | 3:D:238:ILE:CG2   | 2.47                     | 0.44              |
| 3:D:449:LEU:HD22  | 3:D:466:MET:SD    | 2.58                     | 0.44              |
| 3:D:693:VAL:HG21  | 3:D:743:MET:HE3   | 2.00                     | 0.44              |
| 5:F:489:MET:HB2   | 5:F:490:PRO:HD2   | 1.98                     | 0.44              |
| 5:F:530:LEU:HD12  | 5:F:533:ASP:H     | 1.82                     | 0.44              |
| 1:G:191:ARG:HH12  | 1:G:197:ASP:HA    | 1.82                     | 0.44              |
| 1:H:59:VAL:HG12   | 1:H:61:ILE:HD13   | 1.98                     | 0.44              |
| 2:I:971:LEU:HG    | 2:I:1014:LEU:HD23 | 1.99                     | 0.44              |
| 2:I:974:ARG:HD2   | 2:I:1014:LEU:HD21 | 2.00                     | 0.44              |
| 2:I:1111:GLN:HB2  | 2:I:1230:MET:CE   | 2.48                     | 0.44              |
| 3:J:66:LYS:HE2    | 3:J:69:GLU:OE1    | 2.17                     | 0.44              |
| 3:J:292:VAL:O     | 3:J:296:LYS:HG3   | 2.18                     | 0.44              |
| 5:L:463:LEU:HA    | 5:L:466:ILE:HD12  | 1.99                     | 0.44              |
| 5:L:561:MET:HE3   | 5:L:561:MET:HB2   | 1.74                     | 0.44              |
| 1:A:323:PRO:CB    | 1:A:324:ALA:HB2   | 2.47                     | 0.44              |
| 2:C:666:SER:OG    | 2:C:704:MET:HG3   | 2.17                     | 0.44              |
| 2:C:1159:VAL:HB   | 2:C:1160:ASP:H    | 1.57                     | 0.44              |
| 4:E:73:GLN:HA     | 4:E:76:GLU:HB2    | 2.00                     | 0.44              |
| 1:G:77:ASP:O      | 1:G:81:ILE:HG13   | 2.17                     | 0.44              |
| 2:I:519:ASN:ND2   | 2:I:689:ALA:HB3   | 2.33                     | 0.44              |
| 2:I:871:VAL:HG11  | 2:I:883:LEU:HD22  | 2.00                     | 0.44              |
| 3:J:282:LEU:HD21  | 5:L:410:ILE:HG12  | 1.98                     | 0.44              |
| 3:J:514:THR:O     | 3:J:514:THR:OG1   | 2.35                     | 0.44              |
| 1:A:25:LYS:HG2    | 1:A:204:GLU:HG3   | 1.99                     | 0.44              |
| 1:A:102:LEU:HB3   | 1:A:142:MET:HG2   | 2.00                     | 0.44              |
| 2:C:1109:ILE:HD12 | 2:C:1109:ILE:HA   | 1.89                     | 0.44              |
| 2:C:1305:TYR:OH   | 5:F:532:LEU:HG    | 2.17                     | 0.44              |
| 3:D:27:PRO:HB3    | 3:D:241:VAL:HG23  | 1.98                     | 0.44              |
| 3:D:215:LYS:HE2   | 3:D:215:LYS:HB3   | 1.83                     | 0.44              |
| 5:F:372:ALA:O     | 5:F:376:LYS:HG3   | 2.17                     | 0.44              |
| 5:F:572:THR:HG23  | 5:F:575:GLU:HG3   | 2.00                     | 0.44              |
| 1:G:89:ALA:HB1    | 1:G:210:THR:CG2   | 2.47                     | 0.44              |
| 2:I:490:GLN:HG3   | 5:L:472:GLN:HG3   | 1.99                     | 0.44              |
| 5:L:277:MET:CG    | 5:L:362:ASN:HD21  | 2.29                     | 0.44              |
| 1:A:166:ARG:NH1   | 1:A:168:ILE:HG12  | 2.32                     | 0.44              |
| 1:A:239:GLN:HG3   | 1:A:240:PRO:HD2   | 2.00                     | 0.44              |
| 2:C:62:TYR:HD1    | 2:C:480:SER:HB2   | 1.82                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:221:LEU:HD12 | 2:C:298:ALA:O     | 2.18                     | 0.44              |
| 2:C:528:ARG:NH2  | 2:C:576:SER:O     | 2.51                     | 0.44              |
| 2:C:949:GLU:HG2  | 2:C:1036:ILE:CG2  | 2.48                     | 0.44              |
| 2:C:1192:GLU:O   | 2:C:1196:LYS:HG2  | 2.18                     | 0.44              |
| 2:C:1240:ASP:OD1 | 2:C:1240:ASP:N    | 2.51                     | 0.44              |
| 3:D:274:ASN:OD1  | 5:F:446:GLN:NE2   | 2.50                     | 0.44              |
| 3:D:1341:ARG:NH1 | 3:D:1343:GLU:OE2  | 2.51                     | 0.44              |
| 2:I:800:MET:O    | 2:I:1229:TYR:HA   | 2.18                     | 0.44              |
| 3:J:712:GLN:HB2  | 3:J:713:GLU:H     | 1.56                     | 0.44              |
| 3:J:761:ALA:N    | 3:J:771:GLN:HE22  | 2.15                     | 0.44              |
| 5:L:372:ALA:O    | 5:L:376:LYS:HG3   | 2.18                     | 0.44              |
| 6:M:68:GLN:HA    | 6:M:71:HIS:CD2    | 2.52                     | 0.44              |
| 1:A:162:GLU:HB3  | 1:A:163:GLU:H     | 1.66                     | 0.44              |
| 2:C:62:TYR:CD1   | 2:C:480:SER:HB2   | 2.53                     | 0.44              |
| 2:C:139:ASN:HD22 | 2:C:139:ASN:HA    | 1.64                     | 0.44              |
| 2:C:363:LEU:HD13 | 2:C:382:GLU:HA    | 2.00                     | 0.44              |
| 2:C:720:ARG:HH21 | 2:C:741:MET:HA    | 1.81                     | 0.44              |
| 2:C:1087:TYR:CE1 | 2:C:1215:GLY:HA2  | 2.51                     | 0.44              |
| 2:C:1187:PHE:CZ  | 3:D:772:TYR:HD2   | 2.36                     | 0.44              |
| 2:C:1304:MET:O   | 2:C:1308:ILE:HG12 | 2.18                     | 0.44              |
| 3:D:364:HIS:HB3  | 3:D:487:THR:HG23  | 2.00                     | 0.44              |
| 3:D:739:GLN:OE1  | 3:D:744:ARG:HB2   | 2.17                     | 0.44              |
| 2:I:543:ALA:HA   | 2:I:544:GLY:HA3   | 1.74                     | 0.44              |
| 2:I:700:VAL:HG21 | 2:I:1114:GLU:HG2  | 2.00                     | 0.44              |
| 2:I:975:ILE:CD1  | 2:I:998:LEU:HG    | 2.47                     | 0.44              |
| 2:I:1082:ILE:H   | 2:I:1082:ILE:CD1  | 2.27                     | 0.44              |
| 2:I:1313:HIS:HB2 | 3:J:474:LEU:HD13  | 2.00                     | 0.44              |
| 3:J:1319:PHE:HB3 | 3:J:1340:LYS:CD   | 2.48                     | 0.44              |
| 5:L:124:GLU:OE1  | 5:L:421:TYR:OH    | 2.22                     | 0.44              |
| 1:B:195:ARG:CB   | 1:B:198:LEU:HD21  | 2.48                     | 0.43              |
| 2:C:247:ARG:NH2  | 2:C:274:ILE:HD12  | 2.32                     | 0.43              |
| 2:C:800:MET:HE3  | 2:C:800:MET:HB3   | 1.69                     | 0.43              |
| 3:D:1283:SER:O   | 3:D:1286:LYS:N    | 2.50                     | 0.43              |
| 5:F:166:VAL:O    | 5:F:167:ASP:HB2   | 2.17                     | 0.43              |
| 5:F:277:MET:HG3  | 5:F:362:ASN:HD21  | 1.83                     | 0.43              |
| 5:F:324:LYS:HB3  | 5:F:325:PRO:HD2   | 2.00                     | 0.43              |
| 5:F:561:MET:HE3  | 5:F:561:MET:HB2   | 1.86                     | 0.43              |
| 1:G:76:GLU:OE2   | 1:G:76:GLU:N      | 2.51                     | 0.43              |
| 2:I:891:GLY:O    | 2:I:892:GLU:HG3   | 2.17                     | 0.43              |
| 3:J:650:LYS:NZ   | 3:J:762:ASN:HD22  | 2.17                     | 0.43              |
| 3:J:678:ARG:HG3  | 3:J:679:TYR:N     | 2.32                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:J:682:VAL:O     | 3:J:685:ILE:HG12 | 2.18                     | 0.43              |
| 3:J:1199:PHE:HB2  | 3:J:1202:GLU:CB  | 2.46                     | 0.43              |
| 5:L:489:MET:HE2   | 5:L:493:LYS:CB   | 2.47                     | 0.43              |
| 1:A:88:LEU:HA     | 1:A:128:HIS:CD2  | 2.53                     | 0.43              |
| 3:D:73:GLY:O      | 3:D:76:LYS:NZ    | 2.39                     | 0.43              |
| 3:D:147:ILE:HG13  | 3:D:147:ILE:O    | 2.18                     | 0.43              |
| 3:D:251:PRO:HD2   | 5:F:507:MET:SD   | 2.58                     | 0.43              |
| 3:D:279:LEU:HD12  | 3:D:295:GLU:HG3  | 2.00                     | 0.43              |
| 3:D:1344:LEU:O    | 3:D:1346:GLY:N   | 2.43                     | 0.43              |
| 2:I:15:PHE:CD2    | 2:I:1190:ALA:HB2 | 2.53                     | 0.43              |
| 2:I:150:HIS:CE1   | 2:I:454:ARG:HH21 | 2.36                     | 0.43              |
| 2:I:389:PHE:HA    | 2:I:395:TYR:CD1  | 2.52                     | 0.43              |
| 2:I:693:LEU:HD12  | 2:I:829:THR:HB   | 2.00                     | 0.43              |
| 2:I:705:GLU:CD    | 2:I:705:GLU:H    | 2.26                     | 0.43              |
| 2:I:1111:GLN:HB2  | 2:I:1230:MET:HE2 | 1.99                     | 0.43              |
| 3:J:53:ARG:HA     | 3:J:54:ASP:HA    | 1.55                     | 0.43              |
| 3:J:767:LEU:HD23  | 3:J:771:GLN:HB3  | 1.99                     | 0.43              |
| 3:J:779:ALA:HA    | 6:N:12:THR:HG21  | 2.00                     | 0.43              |
| 3:J:782:GLY:CA    | 6:N:12:THR:HG22  | 2.43                     | 0.43              |
| 5:L:313:ASP:CG    | 5:L:338:HIS:HE2  | 2.26                     | 0.43              |
| 1:A:112:ALA:O     | 1:A:115:ILE:HG13 | 2.18                     | 0.43              |
| 2:C:1284:ALA:N    | 3:D:479:GLU:OE1  | 2.51                     | 0.43              |
| 5:F:320:ILE:HG21  | 5:F:331:HIS:NE2  | 2.33                     | 0.43              |
| 1:G:57:THR:HG22   | 1:G:58:GLU:HG3   | 2.00                     | 0.43              |
| 2:I:42:ASP:O      | 2:I:44:GLU:N     | 2.44                     | 0.43              |
| 2:I:151:ARG:NH2   | 2:I:175:ARG:HD2  | 2.34                     | 0.43              |
| 3:J:161:THR:HG22  | 3:J:164:GLN:HB2  | 1.99                     | 0.43              |
| 5:L:280:VAL:O     | 5:L:284:GLU:HG3  | 2.18                     | 0.43              |
| 6:M:33:PRO:HB2    | 6:M:34:VAL:H     | 1.67                     | 0.43              |
| 1:A:50:SER:HB3    | 1:B:8:PHE:CZ     | 2.53                     | 0.43              |
| 1:A:316:MET:SD    | 5:F:600:HIS:CE1  | 3.12                     | 0.43              |
| 2:C:131:THR:H     | 2:C:131:THR:HG1  | 1.43                     | 0.43              |
| 2:C:577:VAL:HG23  | 2:C:661:VAL:O    | 2.18                     | 0.43              |
| 2:C:1066:MET:HG2  | 2:C:1234:LYS:HA  | 2.00                     | 0.43              |
| 2:C:1080:ASN:CB   | 2:C:1085:MET:HE3 | 2.48                     | 0.43              |
| 3:D:137:ARG:HD3   | 3:D:143:SER:HB2  | 2.00                     | 0.43              |
| 3:D:695:LYS:HA    | 3:D:695:LYS:HD3  | 1.77                     | 0.43              |
| 3:D:812:ASP:HB2   | 3:D:911:LYS:HE3  | 2.00                     | 0.43              |
| 1:H:71:LYS:HA     | 1:H:71:LYS:HD2   | 1.85                     | 0.43              |
| 2:I:1124:ILE:HG21 | 2:I:1180:MET:CE  | 2.48                     | 0.43              |
| 3:J:246:PRO:HA    | 3:J:247:PRO:HD3  | 1.89                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:J:425:ARG:HB2   | 3:J:466:MET:HG2  | 2.00                     | 0.43              |
| 4:K:31:GLN:HB2    | 4:K:46:THR:HG21  | 2.01                     | 0.43              |
| 5:L:573:LEU:H     | 5:L:573:LEU:CD2  | 2.29                     | 0.43              |
| 1:A:49:SER:O      | 1:A:51:MET:N     | 2.50                     | 0.43              |
| 1:B:104:LYS:HG2   | 1:B:110:VAL:HG13 | 2.00                     | 0.43              |
| 2:C:107:ARG:HA    | 2:C:108:GLU:HA   | 1.38                     | 0.43              |
| 2:C:1299:ASN:O    | 2:C:1303:LYS:HG2 | 2.18                     | 0.43              |
| 3:D:161:THR:HG23  | 3:D:164:GLN:H    | 1.84                     | 0.43              |
| 3:D:824:PRO:HD3   | 3:D:835:LEU:HB2  | 2.01                     | 0.43              |
| 5:F:276:MET:O     | 5:F:280:VAL:HG23 | 2.18                     | 0.43              |
| 1:H:152:TYR:CZ    | 3:J:536:LEU:HD21 | 2.53                     | 0.43              |
| 2:I:582:ASN:HB3   | 2:I:586:PHE:H    | 1.83                     | 0.43              |
| 2:I:896:THR:HB    | 2:I:897:PRO:HD2  | 2.01                     | 0.43              |
| 3:J:850:LYS:HB2   | 3:J:852:GLY:O    | 2.18                     | 0.43              |
| 5:L:230:VAL:HG22  | 5:L:248:GLU:OE2  | 2.18                     | 0.43              |
| 5:L:559:LEU:HD12  | 5:L:559:LEU:HA   | 1.81                     | 0.43              |
| 6:M:48:ARG:CZ     | 6:M:59:VAL:H     | 2.32                     | 0.43              |
| 1:B:134:THR:OG1   | 1:B:135:ASP:N    | 2.50                     | 0.43              |
| 2:C:179:TYR:OH    | 2:C:458:GLU:OE2  | 2.29                     | 0.43              |
| 3:D:19:ALA:HB2    | 3:D:1373:ARG:NH2 | 2.33                     | 0.43              |
| 3:D:489:ASN:HA    | 3:D:904:ALA:CB   | 2.44                     | 0.43              |
| 5:F:127:ILE:O     | 5:F:130:VAL:HG22 | 2.19                     | 0.43              |
| 5:F:445:ASP:OD2   | 5:F:451:ARG:HD2  | 2.18                     | 0.43              |
| 2:I:5:TYR:O       | 2:I:8:LYS:HG2    | 2.18                     | 0.43              |
| 2:I:18:ARG:HA     | 2:I:19:PRO:HD3   | 1.89                     | 0.43              |
| 2:I:149:LEU:HB2   | 2:I:530:ILE:HG22 | 2.00                     | 0.43              |
| 2:I:1080:ASN:HB3  | 2:I:1085:MET:HE3 | 2.00                     | 0.43              |
| 2:I:1129:ASN:CB   | 2:I:1177:ARG:HB2 | 2.47                     | 0.43              |
| 3:J:159:ILE:O     | 3:J:159:ILE:HG13 | 2.18                     | 0.43              |
| 3:J:1266:ILE:HD11 | 3:J:1276:GLU:HB2 | 2.01                     | 0.43              |
| 3:J:1267:VAL:HB   | 3:J:1301:THR:OG1 | 2.19                     | 0.43              |
| 3:J:1344:LEU:O    | 3:J:1346:GLY:N   | 2.43                     | 0.43              |
| 1:B:191:ARG:O     | 1:B:191:ARG:HG2  | 2.18                     | 0.43              |
| 2:C:136:PHE:HE2   | 2:C:456:VAL:HG11 | 1.83                     | 0.43              |
| 2:C:607:SER:OG    | 2:C:609:ILE:HG13 | 2.19                     | 0.43              |
| 2:C:830:THR:HG23  | 2:C:832:HIS:NE2  | 2.33                     | 0.43              |
| 3:D:81:ARG:HG3    | 3:D:82:GLY:H     | 1.84                     | 0.43              |
| 3:D:140:TYR:OH    | 3:D:312:ARG:NH1  | 2.52                     | 0.43              |
| 3:D:1166:GLY:O    | 3:D:1174:ARG:HB2 | 2.18                     | 0.43              |
| 3:D:1280:VAL:HG21 | 3:D:1304:ARG:HE  | 1.84                     | 0.43              |
| 1:H:35:PHE:HA     | 1:H:38:THR:HG22  | 2.00                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:168:GLY:C     | 2:I:170:VAL:N     | 2.73                     | 0.43              |
| 2:I:230:PHE:CE1   | 2:I:239:MET:HB2   | 2.54                     | 0.43              |
| 3:J:19:ALA:HB2    | 3:J:1373:ARG:NH2  | 2.33                     | 0.43              |
| 3:J:357:VAL:HG22  | 3:J:461:PHE:CE1   | 2.54                     | 0.43              |
| 5:L:119:ILE:HG23  | 5:L:375:ALA:HB1   | 2.00                     | 0.43              |
| 1:A:159:ILE:HG13  | 1:A:162:GLU:HG3   | 2.01                     | 0.43              |
| 2:C:178:PRO:HG3   | 2:C:395:TYR:CE1   | 2.54                     | 0.43              |
| 2:C:230:PHE:CE1   | 2:C:239:MET:HB2   | 2.54                     | 0.43              |
| 2:C:560:PRO:O     | 3:D:780:ARG:NH2   | 2.49                     | 0.43              |
| 2:C:670:PHE:CD1   | 2:C:1113:LEU:HD23 | 2.53                     | 0.43              |
| 3:D:349:TYR:CD1   | 3:D:472:LEU:HD11  | 2.53                     | 0.43              |
| 3:D:556:GLU:HG2   | 3:D:558:ASP:HB2   | 2.00                     | 0.43              |
| 3:D:733:SER:O     | 3:D:737:ILE:HG12  | 2.17                     | 0.43              |
| 3:D:860:ARG:HD2   | 3:D:860:ARG:HA    | 1.83                     | 0.43              |
| 3:D:1168:GLU:O    | 3:D:1170:LYS:N    | 2.52                     | 0.43              |
| 3:D:1356:LEU:HD23 | 3:D:1356:LEU:HA   | 1.70                     | 0.43              |
| 1:H:154:PRO:HB3   | 3:J:525:MET:HE1   | 2.01                     | 0.43              |
| 2:I:565:GLU:HG2   | 2:I:565:GLU:O     | 2.19                     | 0.43              |
| 3:J:24:LEU:HD23   | 3:J:232:ASN:ND2   | 2.34                     | 0.43              |
| 3:J:695:LYS:HA    | 3:J:695:LYS:HD3   | 1.79                     | 0.43              |
| 3:J:827:GLU:HB3   | 3:J:832:LYS:HD2   | 2.00                     | 0.43              |
| 2:C:247:ARG:HB2   | 2:C:274:ILE:HD11  | 2.01                     | 0.43              |
| 2:C:1275:VAL:HG13 | 2:C:1287:LEU:HD11 | 2.00                     | 0.43              |
| 2:I:97:ARG:HB3    | 2:I:121:GLU:HB3   | 2.00                     | 0.43              |
| 2:I:838:CYS:SG    | 2:I:886:LYS:HD3   | 2.59                     | 0.43              |
| 3:J:785:ASP:OD2   | 6:N:15:LEU:HD11   | 2.19                     | 0.43              |
| 3:J:923:ILE:O     | 3:J:926:PRO:HD2   | 2.19                     | 0.43              |
| 6:M:9:TYR:O       | 6:M:12:THR:OG1    | 2.21                     | 0.43              |
| 1:A:57:THR:O      | 1:A:158:ARG:NH2   | 2.51                     | 0.43              |
| 1:A:104:LYS:HD3   | 1:A:114:ASP:OD2   | 2.19                     | 0.43              |
| 1:A:211:ILE:CG2   | 1:A:216:ALA:HB2   | 2.48                     | 0.43              |
| 2:C:163:LYS:HE3   | 2:C:163:LYS:HB3   | 1.92                     | 0.43              |
| 2:C:856:ASN:ND2   | 2:C:908:GLU:OE1   | 2.52                     | 0.43              |
| 2:C:886:LYS:H     | 2:C:917:SER:HB3   | 1.84                     | 0.43              |
| 3:D:682:VAL:O     | 3:D:685:ILE:HG12  | 2.19                     | 0.43              |
| 3:D:1140:ARG:HH21 | 3:D:1236:GLU:HG2  | 1.83                     | 0.43              |
| 3:D:1183:SER:HA   | 3:J:206:ASN:ND2   | 2.33                     | 0.43              |
| 5:F:289:LYS:HE2   | 5:F:289:LYS:HB3   | 1.86                     | 0.43              |
| 5:F:479:THR:OG1   | 5:F:480:PRO:HD2   | 2.19                     | 0.43              |
| 2:I:93:SER:HB2    | 2:I:126:GLU:HB3   | 2.00                     | 0.43              |
| 3:J:268:LEU:HB3   | 3:J:306:LEU:HD23  | 2.00                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:J:865:HIS:HE1  | 3:J:867:GLN:HB2   | 1.84                     | 0.43              |
| 3:J:905:ARG:NH1  | 4:K:16:ARG:HB2    | 2.33                     | 0.43              |
| 3:J:1165:PHE:HE1 | 3:J:1200:GLU:HB2  | 1.83                     | 0.43              |
| 5:L:137:TYR:CD2  | 5:L:273:MET:HE2   | 2.53                     | 0.43              |
| 5:L:580:PHE:HD1  | 5:L:580:PHE:HA    | 1.68                     | 0.43              |
| 6:N:48:ARG:NH2   | 6:N:58:CYS:HA     | 2.34                     | 0.43              |
| 1:A:233:ASP:HA   | 1:B:218:ARG:HH11  | 1.84                     | 0.42              |
| 1:A:284:ARG:HG3  | 1:A:288:GLU:HG3   | 2.01                     | 0.42              |
| 2:C:209:ILE:HG13 | 2:C:385:PHE:CE1   | 2.54                     | 0.42              |
| 2:C:519:ASN:ND2  | 2:C:796:LEU:HD23  | 2.33                     | 0.42              |
| 2:C:519:ASN:HD22 | 2:C:689:ALA:HB3   | 1.83                     | 0.42              |
| 2:C:1332:SER:HB3 | 3:D:102:MET:HE1   | 2.01                     | 0.42              |
| 3:D:292:VAL:O    | 3:D:296:LYS:HG3   | 2.18                     | 0.42              |
| 3:D:702:GLN:O    | 3:D:718:SER:N     | 2.38                     | 0.42              |
| 4:E:15:ASN:O     | 4:E:16:ARG:HB3    | 2.19                     | 0.42              |
| 5:F:233:ASP:O    | 5:F:236:LYS:HE2   | 2.19                     | 0.42              |
| 1:G:22:THR:OG1   | 1:G:23:HIS:N      | 2.52                     | 0.42              |
| 1:H:183:ILE:HG23 | 1:H:205:MET:HG3   | 2.01                     | 0.42              |
| 2:I:478:ARG:HH12 | 2:I:482:GLY:HA2   | 1.83                     | 0.42              |
| 2:I:744:GLY:C    | 2:I:746:ALA:H     | 2.27                     | 0.42              |
| 3:J:279:LEU:HD23 | 3:J:283:LEU:HG    | 2.01                     | 0.42              |
| 3:J:482:ALA:HB3  | 4:K:20:VAL:HG22   | 2.01                     | 0.42              |
| 2:C:135:THR:HG22 | 2:C:527:LYS:HE2   | 2.00                     | 0.42              |
| 2:C:518:ASN:OD1  | 2:C:518:ASN:N     | 2.52                     | 0.42              |
| 2:C:801:ARG:HG2  | 2:C:1094:VAL:HG23 | 2.00                     | 0.42              |
| 5:F:125:ASP:O    | 5:F:129:GLN:HG3   | 2.19                     | 0.42              |
| 5:F:310:GLU:O    | 5:F:344:LEU:HD21  | 2.19                     | 0.42              |
| 1:H:134:THR:HG23 | 1:H:135:ASP:N     | 2.28                     | 0.42              |
| 1:H:196:THR:HG23 | 3:J:443:GLU:HG3   | 2.01                     | 0.42              |
| 2:I:55:SER:OG    | 2:I:56:VAL:N      | 2.52                     | 0.42              |
| 2:I:105:TYR:HD1  | 2:I:112:GLY:H     | 1.67                     | 0.42              |
| 2:I:151:ARG:HH12 | 2:I:175:ARG:NH1   | 2.17                     | 0.42              |
| 2:I:1164:PHE:O   | 2:I:1166:ASP:N    | 2.53                     | 0.42              |
| 2:I:1314:GLN:HG2 | 4:K:28:ARG:CZ     | 2.49                     | 0.42              |
| 3:J:528:THR:O    | 3:J:551:ARG:HB3   | 2.19                     | 0.42              |
| 6:N:20:ILE:HG22  | 6:N:24:ARG:NE     | 2.34                     | 0.42              |
| 1:A:315:GLY:O    | 1:A:316:MET:HG3   | 2.20                     | 0.42              |
| 2:C:699:LEU:HA   | 2:C:699:LEU:HD23  | 1.62                     | 0.42              |
| 2:I:32:LEU:HD23  | 2:I:130:MET:SD    | 2.59                     | 0.42              |
| 2:I:76:GLY:O     | 2:I:94:ALA:HB1    | 2.19                     | 0.42              |
| 3:J:511:TYR:CG   | 3:J:728:SER:HB3   | 2.55                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:594:GLN:HG3   | 3:J:596:LEU:HD22  | 2.00                     | 0.42              |
| 3:J:747:MET:HB2   | 3:J:774:ILE:CG2   | 2.45                     | 0.42              |
| 6:M:48:ARG:HH21   | 6:M:58:CYS:HA     | 1.83                     | 0.42              |
| 2:C:4:SER:OG      | 2:C:5:TYR:N       | 2.52                     | 0.42              |
| 2:C:202:ARG:O     | 2:C:369:MET:HE2   | 2.18                     | 0.42              |
| 2:C:697:LYS:HD2   | 2:C:1181:PRO:HG3  | 2.00                     | 0.42              |
| 2:C:1242:LYS:HD2  | 3:D:465:GLN:OE1   | 2.20                     | 0.42              |
| 3:D:511:TYR:OH    | 3:D:515:ARG:NH1   | 2.51                     | 0.42              |
| 2:I:738:GLU:HA    | 2:I:741:MET:HE2   | 2.01                     | 0.42              |
| 2:I:933:VAL:HG22  | 2:I:1050:VAL:HG13 | 2.02                     | 0.42              |
| 2:I:1124:ILE:HG21 | 2:I:1180:MET:HE3  | 2.02                     | 0.42              |
| 2:I:1191:LYS:HD3  | 2:I:1192:GLU:N    | 2.34                     | 0.42              |
| 3:J:701:LEU:HD22  | 3:J:701:LEU:HA    | 1.91                     | 0.42              |
| 5:L:547:VAL:HG22  | 5:L:603:ARG:HD3   | 2.01                     | 0.42              |
| 1:A:73:GLY:O      | 1:A:134:THR:HG22  | 2.19                     | 0.42              |
| 2:C:229:ILE:CD1   | 2:C:334:GLU:HG2   | 2.50                     | 0.42              |
| 2:C:587:LEU:HD23  | 2:C:587:LEU:HA    | 1.84                     | 0.42              |
| 2:C:813:GLU:HG3   | 3:D:460:ASP:HA    | 2.01                     | 0.42              |
| 5:F:130:VAL:HB    | 5:F:365:MET:HG3   | 2.02                     | 0.42              |
| 5:F:449:THR:OG1   | 5:F:503:GLU:OE1   | 2.37                     | 0.42              |
| 5:F:563:PHE:HB2   | 5:F:565:ILE:HG13  | 2.02                     | 0.42              |
| 1:G:89:ALA:O      | 1:G:124:VAL:HG12  | 2.20                     | 0.42              |
| 1:G:197:ASP:O     | 1:G:198:LEU:HD23  | 2.20                     | 0.42              |
| 3:J:60:ARG:HA     | 3:J:89:GLY:O      | 2.19                     | 0.42              |
| 3:J:654:ILE:O     | 3:J:658:GLU:N     | 2.50                     | 0.42              |
| 3:J:925:GLU:HB3   | 3:J:926:PRO:HD3   | 2.01                     | 0.42              |
| 1:A:48:LEU:HD23   | 1:A:48:LEU:HA     | 1.89                     | 0.42              |
| 1:A:104:LYS:HG3   | 1:A:105:SER:N     | 2.33                     | 0.42              |
| 2:C:198:ILE:O     | 2:C:201:ARG:HB2   | 2.20                     | 0.42              |
| 2:C:277:LEU:HD23  | 2:C:282:VAL:HG21  | 2.01                     | 0.42              |
| 2:C:338:THR:CG2   | 2:C:345:PRO:HB3   | 2.49                     | 0.42              |
| 2:C:1035:LYS:O    | 2:C:1038:GLN:HG2  | 2.20                     | 0.42              |
| 3:D:842:ARG:HB3   | 3:D:882:VAL:CG1   | 2.47                     | 0.42              |
| 3:D:1264:ALA:O    | 3:D:1277:GLY:HA2  | 2.20                     | 0.42              |
| 5:F:448:ARG:HE    | 5:F:448:ARG:HB3   | 1.60                     | 0.42              |
| 1:H:219:ARG:HA    | 1:H:222:THR:HB    | 2.02                     | 0.42              |
| 2:I:194:LEU:HD12  | 2:I:194:LEU:HA    | 1.79                     | 0.42              |
| 3:J:517:CYS:CA    | 3:J:716:GLN:HE22  | 2.31                     | 0.42              |
| 3:J:1260:MET:HE3  | 3:J:1306:LEU:HD21 | 2.00                     | 0.42              |
| 1:B:151:GLY:O     | 1:B:177:TYR:HB2   | 2.20                     | 0.42              |
| 2:C:69:GLN:NE2    | 2:C:101:ARG:HD2   | 2.29                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:674:ASP:OD2   | 2:C:1070:HIS:ND1  | 2.41                     | 0.42              |
| 3:D:291:ILE:HD13  | 5:F:409:ASN:HB3   | 2.01                     | 0.42              |
| 3:D:517:CYS:HA    | 3:D:716:GLN:HE22  | 1.84                     | 0.42              |
| 3:D:930:LEU:HD12  | 3:D:1138:LEU:HD13 | 2.02                     | 0.42              |
| 3:J:839:VAL:HG12  | 3:J:864:LEU:HD12  | 2.01                     | 0.42              |
| 3:J:903:LEU:HD12  | 3:J:903:LEU:HA    | 1.83                     | 0.42              |
| 3:J:1156:LEU:HB3  | 3:J:1207:GLY:HA2  | 2.02                     | 0.42              |
| 1:A:13:LEU:H      | 1:A:13:LEU:HD23   | 1.85                     | 0.42              |
| 2:C:417:SER:OG    | 2:C:419:ILE:O     | 2.31                     | 0.42              |
| 2:C:879:GLY:HA2   | 2:C:920:VAL:HG12  | 2.01                     | 0.42              |
| 3:D:16:GLU:HA     | 3:D:16:GLU:OE2    | 2.20                     | 0.42              |
| 3:D:155:GLU:HB2   | 3:D:158:GLN:HB2   | 2.01                     | 0.42              |
| 3:D:288:PRO:O     | 3:D:292:VAL:HG13  | 2.19                     | 0.42              |
| 3:D:450:HIS:HA    | 3:D:451:PRO:HD3   | 1.95                     | 0.42              |
| 3:D:451:PRO:O     | 3:D:454:CYS:HB2   | 2.20                     | 0.42              |
| 3:D:526:VAL:HA    | 3:D:549:LYS:O     | 2.20                     | 0.42              |
| 3:D:1309:ILE:HG13 | 3:D:1310:THR:N    | 2.34                     | 0.42              |
| 1:G:133:LEU:HD12  | 1:G:138:ALA:HB3   | 2.01                     | 0.42              |
| 1:H:118:ASP:HB2   | 1:H:121:VAL:CB    | 2.42                     | 0.42              |
| 2:I:820:GLU:HA    | 2:I:1079:ILE:HD11 | 2.02                     | 0.42              |
| 3:J:45:ASN:HB3    | 3:J:48:THR:O      | 2.20                     | 0.42              |
| 3:J:1291:GLU:HG2  | 3:J:1297:LYS:HD2  | 2.02                     | 0.42              |
| 5:L:226:ALA:O     | 5:L:229:VAL:HG22  | 2.19                     | 0.42              |
| 6:N:35:TYR:CE1    | 6:N:49:ARG:HD3    | 2.55                     | 0.42              |
| 1:A:54:CYS:HA     | 1:A:148:ARG:HA    | 2.00                     | 0.42              |
| 1:A:166:ARG:O     | 1:A:167:PRO:C     | 2.62                     | 0.42              |
| 1:A:257:VAL:HG12  | 1:A:278:ILE:HG22  | 2.00                     | 0.42              |
| 1:A:272:ALA:C     | 1:A:274:ALA:H     | 2.28                     | 0.42              |
| 2:C:98:VAL:C      | 2:C:121:GLU:HA    | 2.44                     | 0.42              |
| 2:C:490:GLN:HG3   | 5:F:472:GLN:CD    | 2.44                     | 0.42              |
| 2:C:533:LEU:CD1   | 2:C:540:ARG:HD2   | 2.50                     | 0.42              |
| 3:D:8:LEU:HD23    | 3:D:9:LYS:N       | 2.35                     | 0.42              |
| 3:D:347:VAL:HG12  | 3:D:348:ASP:O     | 2.19                     | 0.42              |
| 3:D:494:ALA:HA    | 3:D:922:SER:HB3   | 2.02                     | 0.42              |
| 3:D:732:GLY:HA2   | 3:D:736:GLN:OE1   | 2.19                     | 0.42              |
| 3:D:902:ASP:OD1   | 3:D:903:LEU:N     | 2.53                     | 0.42              |
| 3:D:926:PRO:CB    | 3:D:1246:VAL:HG11 | 2.50                     | 0.42              |
| 1:G:104:LYS:HG2   | 1:G:110:VAL:HG22  | 2.02                     | 0.42              |
| 2:I:1043:ALA:HB1  | 2:I:1044:PRO:HD2  | 2.01                     | 0.42              |
| 3:J:599:LYS:HA    | 3:J:599:LYS:HD3   | 1.66                     | 0.42              |
| 3:J:649:LYS:HA    | 3:J:649:LYS:HD3   | 1.84                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:J:681:LYS:HE3   | 6:N:51:ILE:CG2   | 2.50                     | 0.42              |
| 1:A:211:ILE:HD13  | 1:A:211:ILE:HA   | 1.72                     | 0.42              |
| 1:B:196:THR:HG22  | 1:B:197:ASP:N    | 2.35                     | 0.42              |
| 2:C:225:PHE:HZ    | 2:C:348:SER:N    | 2.18                     | 0.42              |
| 2:C:800:MET:HG3   | 2:C:1096:ILE:CD1 | 2.49                     | 0.42              |
| 2:C:1313:HIS:HB2  | 3:D:474:LEU:HD13 | 2.01                     | 0.42              |
| 3:D:113:HIS:CE1   | 3:D:115:TRP:HB2  | 2.54                     | 0.42              |
| 3:D:1298:VAL:H    | 3:D:1299:GLY:CA  | 2.31                     | 0.42              |
| 5:F:279:ARG:NH2   | 5:F:350:GLU:OE2  | 2.36                     | 0.42              |
| 5:F:463:LEU:HD23  | 5:F:463:LEU:HA   | 1.82                     | 0.42              |
| 2:I:538:LEU:HD13  | 2:I:543:ALA:HB3  | 2.02                     | 0.42              |
| 2:I:681:MET:HE2   | 2:I:681:MET:HB3  | 1.97                     | 0.42              |
| 2:I:1274:GLU:HA   | 3:J:428:THR:HG21 | 2.02                     | 0.42              |
| 3:J:198:CYS:O     | 3:J:202:ARG:HG3  | 2.20                     | 0.42              |
| 5:L:276:MET:O     | 5:L:280:VAL:HG23 | 2.20                     | 0.42              |
| 5:L:380:VAL:HG22  | 5:L:416:VAL:HG21 | 2.02                     | 0.42              |
| 2:C:785:ASP:OD2   | 2:C:791:LEU:N    | 2.50                     | 0.41              |
| 3:D:282:LEU:HD23  | 3:D:282:LEU:HA   | 1.89                     | 0.41              |
| 3:D:317:THR:HA    | 3:D:324:LEU:HD23 | 2.02                     | 0.41              |
| 5:F:274:ARG:NH2   | 5:F:369:GLU:OE2  | 2.52                     | 0.41              |
| 2:I:735:LYS:HA    | 2:I:748:ILE:HG22 | 2.01                     | 0.41              |
| 3:J:425:ARG:HG2   | 3:J:426:ALA:N    | 2.35                     | 0.41              |
| 3:J:441:LEU:HD13  | 3:J:441:LEU:HA   | 1.91                     | 0.41              |
| 3:J:513:MET:HE2   | 3:J:513:MET:HB3  | 1.83                     | 0.41              |
| 5:L:399:LEU:HD12  | 5:L:399:LEU:HA   | 1.77                     | 0.41              |
| 5:L:412:LEU:HD13  | 5:L:435:ILE:HD11 | 2.01                     | 0.41              |
| 5:L:441:ARG:NH1   | 5:L:445:ASP:OD1  | 2.53                     | 0.41              |
| 6:N:12:THR:OG1    | 6:N:13:GLU:N     | 2.53                     | 0.41              |
| 6:N:48:ARG:NH1    | 6:N:59:VAL:HB    | 2.35                     | 0.41              |
| 1:A:195:ARG:HD2   | 1:A:196:THR:N    | 2.35                     | 0.41              |
| 1:B:73:GLY:HA2    | 1:B:134:THR:CG2  | 2.50                     | 0.41              |
| 2:C:146:VAL:HG13  | 2:C:529:ARG:HB3  | 2.02                     | 0.41              |
| 2:C:210:LEU:HD13  | 2:C:224:PHE:HE2  | 1.86                     | 0.41              |
| 2:C:357:ASN:ND2   | 2:C:358:ASP:OD2  | 2.53                     | 0.41              |
| 2:C:487:LEU:HD23  | 2:C:487:LEU:H    | 1.85                     | 0.41              |
| 2:C:1107:MET:HG2  | 3:D:740:LEU:CD1  | 2.48                     | 0.41              |
| 3:D:119:SER:O     | 3:D:120:LEU:C    | 2.63                     | 0.41              |
| 3:D:224:LEU:O     | 3:D:227:PHE:N    | 2.53                     | 0.41              |
| 3:D:357:VAL:HB    | 3:D:358:GLY:H    | 1.71                     | 0.41              |
| 3:D:452:LEU:HD23  | 3:D:452:LEU:HA   | 1.88                     | 0.41              |
| 3:D:1361:THR:HG22 | 4:E:21:LEU:HD22  | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:F:572:THR:O     | 5:F:575:GLU:HB2   | 2.20                     | 0.41              |
| 2:I:561:ILE:HD12  | 2:I:679:ALA:HB1   | 2.02                     | 0.41              |
| 2:I:1114:GLU:OE1  | 2:I:1230:MET:HA   | 2.20                     | 0.41              |
| 2:I:1134:GLN:C    | 2:I:1135:GLN:HG2  | 2.46                     | 0.41              |
| 2:I:1140:LYS:HD2  | 2:I:1140:LYS:HA   | 1.83                     | 0.41              |
| 3:J:529:GLY:HA2   | 3:J:551:ARG:O     | 2.21                     | 0.41              |
| 1:A:23:HIS:HE1    | 1:A:204:GLU:CG    | 2.33                     | 0.41              |
| 2:C:519:ASN:HB3   | 2:C:522:SER:HB2   | 2.02                     | 0.41              |
| 2:C:559:CYS:HB2   | 2:C:662:SER:HB3   | 2.01                     | 0.41              |
| 2:C:616:ILE:HG22  | 2:C:617:ALA:O     | 2.20                     | 0.41              |
| 2:C:720:ARG:HB2   | 2:C:749:ASP:OD1   | 2.19                     | 0.41              |
| 3:D:474:LEU:HD12  | 3:D:474:LEU:HA    | 1.76                     | 0.41              |
| 3:D:888:CYS:SG    | 3:D:890:THR:HB    | 2.60                     | 0.41              |
| 5:F:284:GLU:HG2   | 5:F:310:GLU:OE1   | 2.21                     | 0.41              |
| 1:H:46:ILE:HD11   | 1:H:224:LEU:HD13  | 2.02                     | 0.41              |
| 2:I:1239:VAL:C    | 2:I:1241:ASP:H    | 2.28                     | 0.41              |
| 3:J:515:ARG:O     | 3:J:545:HIS:HB3   | 2.20                     | 0.41              |
| 3:J:517:CYS:HB3   | 3:J:719:PHE:CZ    | 2.56                     | 0.41              |
| 6:N:35:TYR:HE1    | 6:N:49:ARG:HB2    | 1.84                     | 0.41              |
| 2:C:68:LEU:HD22   | 2:C:492:MET:HE3   | 2.03                     | 0.41              |
| 2:C:543:ALA:HA    | 2:C:544:GLY:HA3   | 1.75                     | 0.41              |
| 2:C:876:GLU:HG2   | 2:C:927:THR:OG1   | 2.21                     | 0.41              |
| 2:C:1149:TYR:HB3  | 2:C:1159:VAL:HG21 | 2.03                     | 0.41              |
| 2:C:1273:MET:HE3  | 2:C:1273:MET:HB2  | 1.81                     | 0.41              |
| 3:D:801:VAL:O     | 3:D:805:GLN:HB2   | 2.21                     | 0.41              |
| 3:D:903:LEU:HD12  | 3:D:903:LEU:HA    | 1.94                     | 0.41              |
| 2:I:103:VAL:C     | 2:I:104:ILE:HD12  | 2.46                     | 0.41              |
| 2:I:541:GLU:OE1   | 2:I:541:GLU:N     | 2.52                     | 0.41              |
| 2:I:1220:GLN:HG2  | 2:I:1221:PHE:N    | 2.36                     | 0.41              |
| 2:I:1225:VAL:HG12 | 3:J:636:GLY:O     | 2.20                     | 0.41              |
| 2:I:1297:ASP:OD1  | 2:I:1300:GLY:N    | 2.41                     | 0.41              |
| 3:J:405:GLU:O     | 3:J:408:VAL:HG22  | 2.20                     | 0.41              |
| 4:K:26:ARG:HB2    | 4:K:64:LEU:HD11   | 2.02                     | 0.41              |
| 5:L:511:ILE:HD12  | 5:L:511:ILE:HA    | 1.86                     | 0.41              |
| 5:L:572:THR:HG23  | 5:L:575:GLU:HB2   | 2.03                     | 0.41              |
| 3:D:98:ARG:HB3    | 3:D:248:ASP:OD2   | 2.20                     | 0.41              |
| 3:D:253:VAL:HA    | 3:D:254:PRO:HD3   | 1.91                     | 0.41              |
| 3:D:372:MET:HE2   | 3:D:372:MET:HB3   | 1.92                     | 0.41              |
| 3:D:1221:LEU:HD11 | 3:D:1304:ARG:O    | 2.20                     | 0.41              |
| 3:D:1298:VAL:N    | 3:D:1299:GLY:CA   | 2.84                     | 0.41              |
| 4:E:58:LEU:HD12   | 4:E:58:LEU:H      | 1.85                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:F:280:VAL:HG21  | 5:F:358:VAL:HG11  | 2.03                     | 0.41              |
| 2:I:499:SER:HA    | 2:I:502:VAL:HG12  | 2.03                     | 0.41              |
| 2:I:596:ASP:CG    | 2:I:597:GLY:N     | 2.69                     | 0.41              |
| 2:I:850:ILE:O     | 2:I:850:ILE:HG22  | 2.21                     | 0.41              |
| 3:J:362:ARG:H     | 3:J:365:GLN:HE21  | 1.68                     | 0.41              |
| 3:J:416:ILE:HD12  | 3:J:416:ILE:HA    | 1.85                     | 0.41              |
| 3:J:544:LEU:O     | 3:J:574:VAL:HB    | 2.20                     | 0.41              |
| 4:K:14:GLY:O      | 4:K:16:ARG:N      | 2.50                     | 0.41              |
| 5:L:511:ILE:HG13  | 5:L:512:GLY:H     | 1.85                     | 0.41              |
| 2:C:176:ILE:HB    | 2:C:184:LEU:HB3   | 2.01                     | 0.41              |
| 2:C:681:MET:HE2   | 2:C:681:MET:HB3   | 1.91                     | 0.41              |
| 3:D:31:ARG:NH2    | 3:D:106:GLU:OE2   | 2.52                     | 0.41              |
| 3:D:262:THR:HG22  | 5:F:504:PRO:HB2   | 2.03                     | 0.41              |
| 3:D:1280:VAL:HG11 | 3:D:1304:ARG:NH2  | 2.35                     | 0.41              |
| 5:F:387:VAL:HG11  | 5:F:409:ASN:OD1   | 2.21                     | 0.41              |
| 5:F:387:VAL:HG22  | 5:F:435:ILE:HD13  | 2.01                     | 0.41              |
| 5:F:465:ARG:HD2   | 5:F:468:ARG:HH22  | 1.86                     | 0.41              |
| 5:F:577:GLY:HA3   | 5:F:583:THR:HG23  | 2.03                     | 0.41              |
| 5:F:599:ARG:O     | 5:F:604:SER:HB2   | 2.20                     | 0.41              |
| 2:I:212:ALA:HA    | 2:I:359:ARG:HG3   | 2.03                     | 0.41              |
| 2:I:607:SER:N     | 2:I:610:GLU:HB2   | 2.35                     | 0.41              |
| 2:I:908:GLU:OE2   | 5:L:611:LEU:HD13  | 2.20                     | 0.41              |
| 2:I:1323:PHE:CE1  | 3:J:1353:VAL:HG23 | 2.56                     | 0.41              |
| 3:J:268:LEU:HD11  | 3:J:324:LEU:HD13  | 2.03                     | 0.41              |
| 3:J:1167:LYS:HG2  | 3:J:1168:GLU:H    | 1.84                     | 0.41              |
| 1:A:45:ARG:NE     | 2:C:1083:GLU:HB3  | 2.33                     | 0.41              |
| 1:B:47:LEU:O      | 1:B:180:VAL:HG21  | 2.21                     | 0.41              |
| 2:C:53:PHE:HZ     | 2:C:98:VAL:HG21   | 1.85                     | 0.41              |
| 2:C:364:VAL:HG22  | 2:C:376:PRO:HB2   | 2.01                     | 0.41              |
| 2:C:499:SER:O     | 2:C:503:LYS:HB2   | 2.21                     | 0.41              |
| 3:D:101:ARG:O     | 3:D:246:PRO:HG3   | 2.20                     | 0.41              |
| 3:D:268:LEU:HD11  | 3:D:324:LEU:HD13  | 2.02                     | 0.41              |
| 5:F:559:LEU:HD12  | 5:F:559:LEU:HA    | 1.89                     | 0.41              |
| 2:I:678:ARG:CZ    | 6:N:5:ALA:HB3     | 2.51                     | 0.41              |
| 2:I:1281:TYR:CD1  | 3:J:484:MET:HG2   | 2.56                     | 0.41              |
| 3:J:686:TRP:HB3   | 3:J:758:PRO:HG2   | 2.03                     | 0.41              |
| 3:J:835:LEU:O     | 3:J:839:VAL:HG23  | 2.20                     | 0.41              |
| 4:K:21:LEU:HD12   | 4:K:21:LEU:HA     | 1.80                     | 0.41              |
| 5:L:605:GLU:HA    | 5:L:608:ARG:HH12  | 1.84                     | 0.41              |
| 2:C:119:GLU:HG3   | 2:C:488:MET:HB3   | 2.02                     | 0.41              |
| 2:C:176:ILE:HD11  | 2:C:428:VAL:HG21  | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:139:LEU:HA    | 3:D:139:LEU:HD23  | 1.86                     | 0.41              |
| 3:D:1318:SER:OG   | 3:D:1342:ASP:OD2  | 2.30                     | 0.41              |
| 5:F:561:MET:HA    | 5:F:567:MET:CE    | 2.50                     | 0.41              |
| 5:F:563:PHE:C     | 5:F:565:ILE:H     | 2.29                     | 0.41              |
| 1:G:27:THR:C      | 1:G:28:LEU:HD12   | 2.45                     | 0.41              |
| 1:G:51:MET:HE1    | 1:G:216:ALA:HA    | 2.02                     | 0.41              |
| 2:I:202:ARG:NH2   | 2:I:368:ARG:HH12  | 2.19                     | 0.41              |
| 2:I:1161:LEU:HA   | 2:I:1161:LEU:HD12 | 1.81                     | 0.41              |
| 2:I:1327:LEU:CD2  | 2:I:1331:ARG:HH21 | 2.33                     | 0.41              |
| 3:J:781:LYS:HE2   | 6:N:15:LEU:HD13   | 2.03                     | 0.41              |
| 3:J:850:LYS:HG2   | 3:J:857:LEU:CD2   | 2.51                     | 0.41              |
| 1:A:102:LEU:HD11  | 1:A:110:VAL:HG11  | 2.03                     | 0.41              |
| 1:A:135:ASP:O     | 1:A:138:ALA:N     | 2.38                     | 0.41              |
| 1:A:192:VAL:O     | 1:A:193:GLU:C     | 2.64                     | 0.41              |
| 1:B:190:ALA:O     | 1:B:198:LEU:HB2   | 2.20                     | 0.41              |
| 2:C:496:LYS:HE3   | 2:C:496:LYS:HB3   | 1.91                     | 0.41              |
| 2:C:520:PRO:HG3   | 2:C:714:VAL:HG21  | 2.02                     | 0.41              |
| 2:C:618:GLN:CG    | 3:D:770:LEU:HD21  | 2.48                     | 0.41              |
| 2:C:697:LYS:HE2   | 2:C:697:LYS:HB3   | 1.77                     | 0.41              |
| 2:C:1067:ALA:HB2  | 2:C:1073:LYS:HA   | 2.02                     | 0.41              |
| 2:C:1252:SER:HB3  | 2:C:1255:THR:O    | 2.20                     | 0.41              |
| 2:C:1276:TRP:HH2  | 3:D:798:ARG:HG3   | 1.86                     | 0.41              |
| 2:C:1280:ALA:HB3  | 3:D:431:ARG:HB3   | 2.03                     | 0.41              |
| 3:D:382:TYR:CE1   | 3:D:398:LYS:HA    | 2.55                     | 0.41              |
| 3:D:510:LEU:O     | 3:D:514:THR:HG22  | 2.21                     | 0.41              |
| 3:D:1278:GLU:OE1  | 3:D:1279:GLN:HG2  | 2.21                     | 0.41              |
| 4:E:62:GLN:O      | 4:E:66:VAL:HG23   | 2.21                     | 0.41              |
| 5:F:558:VAL:HG22  | 5:F:587:ILE:HD11  | 2.03                     | 0.41              |
| 1:G:85:LEU:HD23   | 1:G:85:LEU:HA     | 1.85                     | 0.41              |
| 2:I:147:SER:HB2   | 2:I:529:ARG:O     | 2.20                     | 0.41              |
| 2:I:660:VAL:HG11  | 3:J:769:VAL:HG13  | 2.03                     | 0.41              |
| 2:I:725:GLN:HE22  | 2:I:966:ILE:HG23  | 1.86                     | 0.41              |
| 2:I:732:ILE:HD11  | 2:I:769:PRO:HB3   | 2.01                     | 0.41              |
| 2:I:1288:GLN:HE21 | 3:J:1355:ARG:HA   | 1.86                     | 0.41              |
| 3:J:211:GLU:OE2   | 3:J:214:ARG:NH1   | 2.54                     | 0.41              |
| 3:J:514:THR:HG21  | 3:J:596:LEU:HG    | 2.03                     | 0.41              |
| 3:J:591:ILE:HD12  | 3:J:591:ILE:HA    | 1.89                     | 0.41              |
| 3:J:836:ARG:HD2   | 3:J:873:GLU:OE1   | 2.21                     | 0.41              |
| 3:J:1263:LYS:HE2  | 3:J:1279:GLN:NE2  | 2.36                     | 0.41              |
| 3:J:1292:LEU:O    | 3:J:1293:GLU:HB2  | 2.20                     | 0.41              |
| 3:J:1319:PHE:CD1  | 3:J:1319:PHE:C    | 2.98                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:N:6:ASP:OD1     | 6:N:6:ASP:N       | 2.52                     | 0.41              |
| 1:A:262:LEU:HD12  | 1:A:262:LEU:H     | 1.86                     | 0.41              |
| 2:C:867:GLU:H     | 2:C:867:GLU:HG3   | 1.46                     | 0.41              |
| 2:C:902:LEU:HD12  | 5:F:607:LEU:HD23  | 2.02                     | 0.41              |
| 2:C:1083:GLU:H    | 2:C:1083:GLU:HG3  | 1.54                     | 0.41              |
| 3:D:782:GLY:HA3   | 6:M:12:THR:CG2    | 2.51                     | 0.41              |
| 5:F:309:ASN:HB3   | 5:F:310:GLU:H     | 1.71                     | 0.41              |
| 5:F:320:ILE:HG21  | 5:F:331:HIS:CE1   | 2.56                     | 0.41              |
| 2:I:193:ASN:ND2   | 2:I:353:VAL:HG21  | 2.36                     | 0.41              |
| 2:I:425:ILE:O     | 2:I:429:MET:HG3   | 2.21                     | 0.41              |
| 2:I:714:VAL:HB    | 2:I:787:PRO:HD2   | 2.03                     | 0.41              |
| 2:I:1063:GLY:O    | 3:J:354:VAL:HG11  | 2.21                     | 0.41              |
| 2:I:1238:LEU:HD12 | 2:I:1238:LEU:H    | 1.86                     | 0.41              |
| 3:J:638:SER:OG    | 3:J:639:VAL:N     | 2.53                     | 0.41              |
| 3:J:1155:ILE:H    | 3:J:1155:ILE:HG13 | 1.75                     | 0.41              |
| 1:A:13:LEU:HD11   | 1:A:214:GLU:HG3   | 2.02                     | 0.40              |
| 1:A:31:LEU:HA     | 1:A:31:LEU:HD23   | 1.78                     | 0.40              |
| 1:B:89:ALA:HB3    | 1:B:124:VAL:CG1   | 2.51                     | 0.40              |
| 2:C:103:VAL:C     | 2:C:104:ILE:HD12  | 2.46                     | 0.40              |
| 2:C:243:PRO:O     | 2:C:274:ILE:HG12  | 2.21                     | 0.40              |
| 2:C:525:THR:HG21  | 2:C:687:ARG:CD    | 2.29                     | 0.40              |
| 2:C:1285:TYR:CD1  | 3:D:475:GLU:HG2   | 2.56                     | 0.40              |
| 3:D:336:GLY:HA3   | 3:D:1324:SER:O    | 2.21                     | 0.40              |
| 3:D:1167:LYS:HE3  | 3:D:1167:LYS:HB3  | 1.85                     | 0.40              |
| 3:D:1243:LEU:HD12 | 3:D:1243:LEU:HA   | 1.96                     | 0.40              |
| 1:G:35:PHE:HD1    | 1:G:35:PHE:HA     | 1.76                     | 0.40              |
| 2:I:238:GLN:OE1   | 2:I:284:LEU:HD21  | 2.21                     | 0.40              |
| 2:I:1086:PRO:HB3  | 2:I:1212:LEU:HD23 | 2.03                     | 0.40              |
| 3:J:114:ILE:HD11  | 3:J:311:ARG:HB2   | 2.02                     | 0.40              |
| 3:J:275:ARG:HH11  | 3:J:298:MET:HB3   | 1.86                     | 0.40              |
| 5:L:324:LYS:HB3   | 5:L:325:PRO:HD2   | 2.04                     | 0.40              |
| 5:L:558:VAL:HG11  | 5:L:590:ILE:HG22  | 2.02                     | 0.40              |
| 1:A:45:ARG:HG2    | 1:B:38:THR:CB     | 2.30                     | 0.40              |
| 2:C:88:ARG:HB2    | 2:C:88:ARG:HH11   | 1.84                     | 0.40              |
| 2:C:162:GLY:O     | 2:C:164:THR:N     | 2.54                     | 0.40              |
| 2:C:226:GLU:HB2   | 2:C:245:ARG:HH22  | 1.85                     | 0.40              |
| 2:C:837:ALA:HB2   | 2:C:1051:LYS:HG2  | 2.02                     | 0.40              |
| 3:D:556:GLU:C     | 3:D:558:ASP:H     | 2.30                     | 0.40              |
| 3:D:638:SER:OG    | 3:D:639:VAL:N     | 2.52                     | 0.40              |
| 3:D:710:ASP:OD1   | 3:D:711:GLY:N     | 2.54                     | 0.40              |
| 3:D:797:THR:O     | 3:D:801:VAL:HG12  | 2.20                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:F:316:PHE:CZ    | 5:F:334:SER:HA    | 2.57                     | 0.40              |
| 5:F:462:LYS:HD2   | 5:F:487:MET:HE1   | 2.02                     | 0.40              |
| 2:I:93:SER:OG     | 2:I:126:GLU:OE1   | 2.18                     | 0.40              |
| 2:I:157:PHE:O     | 2:I:443:ASP:N     | 2.48                     | 0.40              |
| 3:J:75:TYR:CE2    | 3:J:83:VAL:HG21   | 2.56                     | 0.40              |
| 3:J:264:ASP:OD2   | 5:L:506:SER:OG    | 2.23                     | 0.40              |
| 3:J:338:PHE:O     | 3:J:340:GLN:N     | 2.54                     | 0.40              |
| 3:J:510:LEU:HD22  | 3:J:601:ILE:HD11  | 2.02                     | 0.40              |
| 3:J:517:CYS:HB3   | 3:J:719:PHE:CE2   | 2.55                     | 0.40              |
| 3:J:1266:ILE:HD12 | 3:J:1273:ASP:O    | 2.22                     | 0.40              |
| 2:C:27:LEU:O      | 2:C:528:ARG:NH1   | 2.47                     | 0.40              |
| 2:C:1293:VAL:HG13 | 2:C:1301:ARG:HA   | 2.04                     | 0.40              |
| 3:D:45:ASN:O      | 3:D:46:TYR:CD2    | 2.74                     | 0.40              |
| 3:D:239:LEU:HD23  | 3:D:239:LEU:HA    | 1.89                     | 0.40              |
| 3:D:355:ILE:HG12  | 3:D:464:ASP:O     | 2.21                     | 0.40              |
| 3:D:430:HIS:CE1   | 3:D:925:GLU:HG3   | 2.54                     | 0.40              |
| 3:D:614:LEU:HD23  | 4:E:5:THR:HB      | 2.03                     | 0.40              |
| 5:F:119:ILE:HD13  | 5:F:378:GLU:HG2   | 2.03                     | 0.40              |
| 1:H:57:THR:HG22   | 1:H:58:GLU:OE1    | 2.22                     | 0.40              |
| 2:I:576:SER:HA    | 2:I:662:SER:HA    | 2.02                     | 0.40              |
| 2:I:742:TYR:HD2   | 2:I:743:PRO:HD2   | 1.86                     | 0.40              |
| 3:J:155:GLU:HB2   | 3:J:158:GLN:HB2   | 2.03                     | 0.40              |
| 3:J:773:PHE:O     | 3:J:776:THR:HB    | 2.20                     | 0.40              |
| 3:J:884:SER:OG    | 3:J:886:VAL:HG12  | 2.21                     | 0.40              |
| 3:J:1344:LEU:HB3  | 3:J:1350:ASN:ND2  | 2.37                     | 0.40              |
| 1:A:106:GLY:HA2   | 1:A:136:GLU:O     | 2.21                     | 0.40              |
| 2:C:14:ASP:OD2    | 2:C:1156:ARG:NE   | 2.55                     | 0.40              |
| 2:C:18:ARG:HA     | 2:C:19:PRO:HD3    | 1.92                     | 0.40              |
| 2:C:147:SER:OG    | 2:C:455:SER:HB3   | 2.21                     | 0.40              |
| 2:C:560:PRO:HB3   | 3:D:776:THR:HG21  | 2.04                     | 0.40              |
| 2:C:619:ALA:HB1   | 2:C:657:THR:HA    | 2.03                     | 0.40              |
| 2:C:887:VAL:HB    | 2:C:913:VAL:CG2   | 2.52                     | 0.40              |
| 3:D:707:ILE:HD12  | 3:D:707:ILE:H     | 1.87                     | 0.40              |
| 5:F:507:MET:HE2   | 5:F:507:MET:HB3   | 1.80                     | 0.40              |
| 1:H:125:LYS:HE2   | 1:H:128:HIS:HB2   | 2.04                     | 0.40              |
| 2:I:159:SER:O     | 2:I:160:ASP:HB2   | 2.21                     | 0.40              |
| 2:I:686:GLN:HG2   | 2:I:796:LEU:HD22  | 2.04                     | 0.40              |
| 2:I:1124:ILE:O    | 2:I:1128:ILE:HG13 | 2.21                     | 0.40              |
| 3:J:450:HIS:HA    | 3:J:451:PRO:HD3   | 1.97                     | 0.40              |
| 1:A:31:LEU:HB2    | 1:A:199:ASP:O     | 2.22                     | 0.40              |
| 2:C:551:HIS:ND1   | 2:C:553:THR:OG1   | 2.53                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:621:ALA:HA   | 3:D:624:ILE:HD12 | 2.02                     | 0.40              |
| 5:F:316:PHE:HZ   | 5:F:334:SER:HA   | 1.86                     | 0.40              |
| 5:F:474:MET:O    | 5:F:476:ARG:N    | 2.49                     | 0.40              |
| 1:G:228:LEU:HG   | 1:H:221:ALA:HB1  | 2.03                     | 0.40              |
| 2:I:95:PRO:CA    | 2:I:126:GLU:HG2  | 2.48                     | 0.40              |
| 2:I:400:VAL:HG22 | 2:I:584:TYR:HD1  | 1.86                     | 0.40              |
| 2:I:657:THR:HG21 | 2:I:1188:ASP:HB2 | 2.03                     | 0.40              |
| 2:I:1286:THR:N   | 3:J:479:GLU:OE2  | 2.42                     | 0.40              |
| 3:J:363:LEU:HA   | 3:J:450:HIS:CD2  | 2.57                     | 0.40              |
| 3:J:674:THR:HG22 | 6:N:59:VAL:HG22  | 2.03                     | 0.40              |
| 3:J:1173:ARG:N   | 3:J:1190:ILE:O   | 2.54                     | 0.40              |
| 3:J:1269:ALA:HB2 | 3:J:1274:PHE:CD1 | 2.56                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

| Mol | Chain | Analysed         | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|------------------|------------|----------|----------|-------------|----|
| 1   | A     | 317/329 (96%)    | 247 (78%)  | 52 (16%) | 18 (6%)  | 1           | 15 |
| 1   | B     | 213/329 (65%)    | 194 (91%)  | 15 (7%)  | 4 (2%)   | 6           | 32 |
| 1   | G     | 225/329 (68%)    | 199 (88%)  | 20 (9%)  | 6 (3%)   | 4           | 27 |
| 1   | H     | 212/329 (64%)    | 196 (92%)  | 12 (6%)  | 4 (2%)   | 6           | 32 |
| 2   | C     | 1338/1342 (100%) | 1201 (90%) | 118 (9%) | 19 (1%)  | 9           | 37 |
| 2   | I     | 1338/1342 (100%) | 1197 (90%) | 120 (9%) | 21 (2%)  | 7           | 35 |
| 3   | D     | 1169/1407 (83%)  | 1038 (89%) | 104 (9%) | 27 (2%)  | 5           | 30 |
| 3   | J     | 1151/1407 (82%)  | 1026 (89%) | 99 (9%)  | 26 (2%)  | 5           | 30 |
| 4   | E     | 87/91 (96%)      | 80 (92%)   | 5 (6%)   | 2 (2%)   | 5           | 30 |
| 4   | K     | 70/91 (77%)      | 61 (87%)   | 8 (11%)  | 1 (1%)   | 9           | 37 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 5   | F     | 462/613 (75%)   | 426 (92%)  | 28 (6%)  | 8 (2%)   | 7           | 34 |
| 5   | L     | 463/613 (76%)   | 425 (92%)  | 30 (6%)  | 8 (2%)   | 7           | 34 |
| 6   | M     | 68/79 (86%)     | 56 (82%)   | 7 (10%)  | 5 (7%)   | 1           | 11 |
| 6   | N     | 67/79 (85%)     | 56 (84%)   | 6 (9%)   | 5 (8%)   | 1           | 11 |
| All | All   | 7180/8380 (86%) | 6402 (89%) | 624 (9%) | 154 (2%) | 5           | 31 |

All (154) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 14   | VAL  |
| 1   | A     | 107  | ILE  |
| 1   | A     | 136  | GLU  |
| 1   | A     | 162  | GLU  |
| 1   | A     | 167  | PRO  |
| 1   | A     | 242  | VAL  |
| 1   | B     | 193  | GLU  |
| 2   | C     | 169  | LYS  |
| 2   | C     | 170  | VAL  |
| 2   | C     | 484  | LEU  |
| 2   | C     | 697  | LYS  |
| 2   | C     | 1137 | GLU  |
| 2   | C     | 1153 | ALA  |
| 2   | C     | 1154 | ASP  |
| 2   | C     | 1159 | VAL  |
| 2   | C     | 1165 | SER  |
| 3   | D     | 10   | ALA  |
| 3   | D     | 49   | PHE  |
| 3   | D     | 426  | ALA  |
| 3   | D     | 496  | GLY  |
| 3   | D     | 710  | ASP  |
| 3   | D     | 712  | GLN  |
| 3   | D     | 745  | GLY  |
| 3   | D     | 1169 | THR  |
| 3   | D     | 1294 | ALA  |
| 4   | E     | 33   | GLY  |
| 5   | F     | 490  | PRO  |
| 5   | F     | 569  | THR  |
| 1   | G     | 167  | PRO  |
| 1   | G     | 193  | GLU  |
| 2   | I     | 121  | GLU  |
| 2   | I     | 169  | LYS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | I     | 170  | VAL  |
| 2   | I     | 484  | LEU  |
| 2   | I     | 697  | LYS  |
| 2   | I     | 897  | PRO  |
| 2   | I     | 1137 | GLU  |
| 2   | I     | 1153 | ALA  |
| 2   | I     | 1159 | VAL  |
| 2   | I     | 1203 | ASP  |
| 3   | J     | 49   | PHE  |
| 3   | J     | 341  | ASN  |
| 3   | J     | 426  | ALA  |
| 3   | J     | 710  | ASP  |
| 3   | J     | 712  | GLN  |
| 3   | J     | 850  | LYS  |
| 3   | J     | 1294 | ALA  |
| 4   | K     | 33   | GLY  |
| 5   | L     | 584  | ARG  |
| 6   | M     | 26   | LYS  |
| 6   | M     | 33   | PRO  |
| 6   | M     | 64   | TYR  |
| 6   | N     | 26   | LYS  |
| 6   | N     | 33   | PRO  |
| 6   | N     | 64   | TYR  |
| 1   | A     | 50   | SER  |
| 1   | A     | 62   | ASP  |
| 1   | A     | 119  | GLY  |
| 1   | A     | 164  | ASP  |
| 1   | A     | 232  | VAL  |
| 1   | A     | 315  | GLY  |
| 1   | A     | 320  | ASN  |
| 1   | B     | 13   | LEU  |
| 2   | C     | 121  | GLU  |
| 3   | D     | 89   | GLY  |
| 3   | D     | 805  | GLN  |
| 3   | D     | 1274 | PHE  |
| 5   | F     | 566  | ASP  |
| 5   | F     | 584  | ARG  |
| 1   | G     | 162  | GLU  |
| 1   | H     | 138  | ALA  |
| 2   | I     | 1059 | ARG  |
| 2   | I     | 1165 | SER  |
| 3   | J     | 89   | GLY  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | J     | 314  | ARG  |
| 3   | J     | 339  | ARG  |
| 3   | J     | 496  | GLY  |
| 3   | J     | 745  | GLY  |
| 3   | J     | 805  | GLN  |
| 3   | J     | 826  | ILE  |
| 3   | J     | 1169 | THR  |
| 3   | J     | 1297 | LYS  |
| 5   | L     | 96   | ASP  |
| 5   | L     | 490  | PRO  |
| 5   | L     | 566  | ASP  |
| 5   | L     | 569  | THR  |
| 6   | M     | 30   | HIS  |
| 6   | N     | 30   | HIS  |
| 1   | A     | 324  | ALA  |
| 1   | B     | 136  | GLU  |
| 2   | C     | 163  | LYS  |
| 2   | C     | 696  | ASP  |
| 2   | C     | 892  | GLU  |
| 2   | C     | 1317 | PRO  |
| 3   | D     | 173  | GLY  |
| 3   | D     | 417  | ARG  |
| 3   | D     | 933  | ARG  |
| 3   | D     | 934  | THR  |
| 3   | D     | 1344 | LEU  |
| 1   | G     | 229  | GLU  |
| 1   | H     | 193  | GLU  |
| 2   | I     | 813  | GLU  |
| 2   | I     | 983  | GLY  |
| 2   | I     | 1317 | PRO  |
| 3   | J     | 332  | LYS  |
| 3   | J     | 417  | ARG  |
| 1   | A     | 319  | GLU  |
| 1   | B     | 138  | ALA  |
| 2   | C     | 813  | GLU  |
| 2   | C     | 1059 | ARG  |
| 3   | D     | 314  | ARG  |
| 3   | D     | 1297 | LYS  |
| 1   | H     | 20   | SER  |
| 2   | I     | 696  | ASP  |
| 2   | I     | 892  | GLU  |
| 3   | J     | 344  | GLY  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | J     | 1344 | LEU  |
| 1   | A     | 318  | LEU  |
| 2   | C     | 62   | TYR  |
| 2   | C     | 983  | GLY  |
| 2   | C     | 1158 | LYS  |
| 3   | D     | 46   | TYR  |
| 3   | D     | 345  | LYS  |
| 5   | F     | 602  | SER  |
| 2   | I     | 201  | ARG  |
| 3   | J     | 338  | PHE  |
| 3   | J     | 357  | VAL  |
| 5   | L     | 585  | GLU  |
| 1   | A     | 241  | GLU  |
| 3   | D     | 357  | VAL  |
| 5   | F     | 96   | ASP  |
| 1   | G     | 9    | LEU  |
| 2   | I     | 160  | ASP  |
| 2   | I     | 756  | TYR  |
| 3   | J     | 333  | GLY  |
| 5   | L     | 395  | THR  |
| 1   | A     | 19   | VAL  |
| 3   | D     | 826  | ILE  |
| 3   | J     | 173  | GLY  |
| 6   | M     | 34   | VAL  |
| 3   | D     | 828  | GLY  |
| 3   | J     | 336  | GLY  |
| 5   | L     | 475  | GLY  |
| 6   | N     | 34   | VAL  |
| 3   | D     | 831  | VAL  |
| 5   | F     | 361  | ILE  |
| 3   | J     | 639  | VAL  |
| 3   | D     | 120  | LEU  |
| 2   | I     | 1202 | GLY  |
| 3   | D     | 850  | LYS  |
| 4   | E     | 4    | VAL  |
| 5   | F     | 475  | GLY  |
| 1   | G     | 14   | VAL  |
| 1   | H     | 30   | PRO  |



### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

| Mol | Chain | Analysed         | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|------------------|------------|-----------|-------------|----|
| 1   | A     | 278/286 (97%)    | 222 (80%)  | 56 (20%)  | 1           | 8  |
| 1   | B     | 186/286 (65%)    | 163 (88%)  | 23 (12%)  | 4           | 21 |
| 1   | G     | 193/286 (68%)    | 162 (84%)  | 31 (16%)  | 2           | 14 |
| 1   | H     | 183/286 (64%)    | 167 (91%)  | 16 (9%)   | 9           | 33 |
| 2   | C     | 1154/1157 (100%) | 1022 (89%) | 132 (11%) | 5           | 23 |
| 2   | I     | 1154/1157 (100%) | 1034 (90%) | 120 (10%) | 7           | 26 |
| 3   | D     | 962/1168 (82%)   | 857 (89%)  | 105 (11%) | 6           | 25 |
| 3   | J     | 960/1168 (82%)   | 857 (89%)  | 103 (11%) | 6           | 25 |
| 4   | E     | 72/75 (96%)      | 63 (88%)   | 9 (12%)   | 4           | 21 |
| 4   | K     | 62/75 (83%)      | 56 (90%)   | 6 (10%)   | 8           | 29 |
| 5   | F     | 417/540 (77%)    | 374 (90%)  | 43 (10%)  | 7           | 27 |
| 5   | L     | 418/540 (77%)    | 373 (89%)  | 45 (11%)  | 6           | 25 |
| 6   | M     | 59/68 (87%)      | 55 (93%)   | 4 (7%)    | 14          | 40 |
| 6   | N     | 59/68 (87%)      | 55 (93%)   | 4 (7%)    | 14          | 40 |
| All | All   | 6157/7160 (86%)  | 5460 (89%) | 697 (11%) | 5           | 23 |

All (697) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 7   | GLU  |
| 1   | A     | 8   | PHE  |
| 1   | A     | 9   | LEU  |
| 1   | A     | 18  | GLN  |
| 1   | A     | 26  | VAL  |
| 1   | A     | 29  | GLU  |
| 1   | A     | 32  | GLU  |
| 1   | A     | 44  | ARG  |
| 1   | A     | 50  | SER  |
| 1   | A     | 56  | VAL  |
| 1   | A     | 70  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 71  | LYS  |
| 1   | A     | 72  | GLU  |
| 1   | A     | 74  | VAL  |
| 1   | A     | 75  | GLN  |
| 1   | A     | 77  | ASP  |
| 1   | A     | 83  | LEU  |
| 1   | A     | 90  | VAL  |
| 1   | A     | 98  | VAL  |
| 1   | A     | 99  | ILE  |
| 1   | A     | 105 | SER  |
| 1   | A     | 110 | VAL  |
| 1   | A     | 116 | THR  |
| 1   | A     | 133 | LEU  |
| 1   | A     | 137 | ASN  |
| 1   | A     | 159 | ILE  |
| 1   | A     | 165 | GLU  |
| 1   | A     | 168 | ILE  |
| 1   | A     | 171 | LEU  |
| 1   | A     | 180 | VAL  |
| 1   | A     | 183 | ILE  |
| 1   | A     | 186 | ASN  |
| 1   | A     | 192 | VAL  |
| 1   | A     | 195 | ARG  |
| 1   | A     | 207 | THR  |
| 1   | A     | 211 | ILE  |
| 1   | A     | 223 | ILE  |
| 1   | A     | 227 | GLN  |
| 1   | A     | 231 | PHE  |
| 1   | A     | 239 | GLN  |
| 1   | A     | 243 | LYS  |
| 1   | A     | 245 | GLU  |
| 1   | A     | 246 | LYS  |
| 1   | A     | 252 | ILE  |
| 1   | A     | 262 | LEU  |
| 1   | A     | 264 | VAL  |
| 1   | A     | 280 | ASP  |
| 1   | A     | 282 | VAL  |
| 1   | A     | 284 | ARG  |
| 1   | A     | 285 | THR  |
| 1   | A     | 300 | LEU  |
| 1   | A     | 302 | GLU  |
| 1   | A     | 306 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 316 | MET  |
| 1   | A     | 318 | LEU  |
| 1   | A     | 320 | ASN  |
| 1   | B     | 9   | LEU  |
| 1   | B     | 14  | VAL  |
| 1   | B     | 16  | ILE  |
| 1   | B     | 26  | VAL  |
| 1   | B     | 27  | THR  |
| 1   | B     | 50  | SER  |
| 1   | B     | 60  | GLU  |
| 1   | B     | 62  | ASP  |
| 1   | B     | 64  | VAL  |
| 1   | B     | 72  | GLU  |
| 1   | B     | 79  | LEU  |
| 1   | B     | 92  | VAL  |
| 1   | B     | 95  | LYS  |
| 1   | B     | 102 | LEU  |
| 1   | B     | 121 | VAL  |
| 1   | B     | 124 | VAL  |
| 1   | B     | 133 | LEU  |
| 1   | B     | 139 | SER  |
| 1   | B     | 146 | VAL  |
| 1   | B     | 183 | ILE  |
| 1   | B     | 191 | ARG  |
| 1   | B     | 196 | THR  |
| 1   | B     | 233 | ASP  |
| 2   | C     | 3   | TYR  |
| 2   | C     | 11  | ILE  |
| 2   | C     | 17  | LYS  |
| 2   | C     | 22  | LEU  |
| 2   | C     | 23  | ASP  |
| 2   | C     | 39  | ILE  |
| 2   | C     | 46  | GLN  |
| 2   | C     | 56  | VAL  |
| 2   | C     | 81  | ASP  |
| 2   | C     | 90  | VAL  |
| 2   | C     | 103 | VAL  |
| 2   | C     | 115 | LYS  |
| 2   | C     | 117 | ILE  |
| 2   | C     | 119 | GLU  |
| 2   | C     | 120 | GLN  |
| 2   | C     | 131 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | C     | 135 | THR  |
| 2   | C     | 138 | ILE  |
| 2   | C     | 145 | ILE  |
| 2   | C     | 164 | THR  |
| 2   | C     | 170 | VAL  |
| 2   | C     | 201 | ARG  |
| 2   | C     | 208 | ILE  |
| 2   | C     | 285 | ILE  |
| 2   | C     | 292 | ILE  |
| 2   | C     | 302 | ILE  |
| 2   | C     | 306 | THR  |
| 2   | C     | 316 | GLU  |
| 2   | C     | 320 | ASP  |
| 2   | C     | 321 | LEU  |
| 2   | C     | 342 | ASP  |
| 2   | C     | 377 | THR  |
| 2   | C     | 384 | LEU  |
| 2   | C     | 400 | VAL  |
| 2   | C     | 419 | ILE  |
| 2   | C     | 423 | ASP  |
| 2   | C     | 453 | ILE  |
| 2   | C     | 455 | SER  |
| 2   | C     | 456 | VAL  |
| 2   | C     | 471 | VAL  |
| 2   | C     | 481 | LEU  |
| 2   | C     | 484 | LEU  |
| 2   | C     | 490 | GLN  |
| 2   | C     | 492 | MET  |
| 2   | C     | 493 | ILE  |
| 2   | C     | 518 | ASN  |
| 2   | C     | 521 | LEU  |
| 2   | C     | 525 | THR  |
| 2   | C     | 539 | THR  |
| 2   | C     | 540 | ARG  |
| 2   | C     | 542 | ARG  |
| 2   | C     | 550 | VAL  |
| 2   | C     | 553 | THR  |
| 2   | C     | 558 | VAL  |
| 2   | C     | 561 | ILE  |
| 2   | C     | 575 | LEU  |
| 2   | C     | 600 | THR  |
| 2   | C     | 609 | ILE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | C     | 615  | VAL  |
| 2   | C     | 618  | GLN  |
| 2   | C     | 623  | LEU  |
| 2   | C     | 633  | LEU  |
| 2   | C     | 634  | VAL  |
| 2   | C     | 657  | THR  |
| 2   | C     | 660  | VAL  |
| 2   | C     | 663  | VAL  |
| 2   | C     | 672  | GLU  |
| 2   | C     | 705  | GLU  |
| 2   | C     | 714  | VAL  |
| 2   | C     | 748  | ILE  |
| 2   | C     | 757  | THR  |
| 2   | C     | 764  | CYS  |
| 2   | C     | 765  | ILE  |
| 2   | C     | 773  | LEU  |
| 2   | C     | 778  | GLU  |
| 2   | C     | 781  | ASP  |
| 2   | C     | 783  | LEU  |
| 2   | C     | 791  | LEU  |
| 2   | C     | 799  | ASN  |
| 2   | C     | 800  | MET  |
| 2   | C     | 817  | LEU  |
| 2   | C     | 864  | LYS  |
| 2   | C     | 867  | GLU  |
| 2   | C     | 878  | THR  |
| 2   | C     | 890  | LYS  |
| 2   | C     | 892  | GLU  |
| 2   | C     | 895  | LEU  |
| 2   | C     | 922  | ASN  |
| 2   | C     | 948  | ILE  |
| 2   | C     | 951  | MET  |
| 2   | C     | 984  | VAL  |
| 2   | C     | 992  | LEU  |
| 2   | C     | 1002 | LEU  |
| 2   | C     | 1037 | THR  |
| 2   | C     | 1050 | VAL  |
| 2   | C     | 1054 | LEU  |
| 2   | C     | 1072 | ASN  |
| 2   | C     | 1076 | ILE  |
| 2   | C     | 1078 | LYS  |
| 2   | C     | 1082 | ILE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | C     | 1098 | LEU  |
| 2   | C     | 1109 | ILE  |
| 2   | C     | 1114 | GLU  |
| 2   | C     | 1134 | GLN  |
| 2   | C     | 1141 | LEU  |
| 2   | C     | 1145 | ILE  |
| 2   | C     | 1146 | GLN  |
| 2   | C     | 1151 | LEU  |
| 2   | C     | 1155 | VAL  |
| 2   | C     | 1156 | ARG  |
| 2   | C     | 1159 | VAL  |
| 2   | C     | 1163 | THR  |
| 2   | C     | 1164 | PHE  |
| 2   | C     | 1172 | LEU  |
| 2   | C     | 1180 | MET  |
| 2   | C     | 1198 | LEU  |
| 2   | C     | 1206 | THR  |
| 2   | C     | 1210 | ILE  |
| 2   | C     | 1225 | VAL  |
| 2   | C     | 1227 | VAL  |
| 2   | C     | 1233 | LEU  |
| 2   | C     | 1238 | LEU  |
| 2   | C     | 1240 | ASP  |
| 2   | C     | 1248 | THR  |
| 2   | C     | 1250 | SER  |
| 2   | C     | 1254 | VAL  |
| 2   | C     | 1255 | THR  |
| 2   | C     | 1287 | LEU  |
| 2   | C     | 1291 | LEU  |
| 2   | C     | 1296 | ASP  |
| 2   | C     | 1313 | HIS  |
| 2   | C     | 1327 | LEU  |
| 3   | D     | 8    | LEU  |
| 3   | D     | 46   | TYR  |
| 3   | D     | 54   | ASP  |
| 3   | D     | 79   | LYS  |
| 3   | D     | 80   | HIS  |
| 3   | D     | 83   | VAL  |
| 3   | D     | 84   | ILE  |
| 3   | D     | 92   | VAL  |
| 3   | D     | 93   | THR  |
| 3   | D     | 95   | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | D     | 96  | LYS  |
| 3   | D     | 97  | VAL  |
| 3   | D     | 154 | LEU  |
| 3   | D     | 172 | PHE  |
| 3   | D     | 175 | GLU  |
| 3   | D     | 176 | PHE  |
| 3   | D     | 248 | ASP  |
| 3   | D     | 252 | LEU  |
| 3   | D     | 255 | LEU  |
| 3   | D     | 259 | ARG  |
| 3   | D     | 292 | VAL  |
| 3   | D     | 306 | LEU  |
| 3   | D     | 324 | LEU  |
| 3   | D     | 330 | MET  |
| 3   | D     | 335 | GLN  |
| 3   | D     | 343 | LEU  |
| 3   | D     | 363 | LEU  |
| 3   | D     | 374 | LEU  |
| 3   | D     | 376 | LEU  |
| 3   | D     | 386 | GLU  |
| 3   | D     | 392 | THR  |
| 3   | D     | 394 | ILE  |
| 3   | D     | 407 | VAL  |
| 3   | D     | 413 | ASP  |
| 3   | D     | 415 | VAL  |
| 3   | D     | 416 | ILE  |
| 3   | D     | 423 | LEU  |
| 3   | D     | 425 | ARG  |
| 3   | D     | 429 | LEU  |
| 3   | D     | 442 | ILE  |
| 3   | D     | 490 | ILE  |
| 3   | D     | 505 | ASP  |
| 3   | D     | 507 | VAL  |
| 3   | D     | 510 | LEU  |
| 3   | D     | 514 | THR  |
| 3   | D     | 532 | GLU  |
| 3   | D     | 536 | LEU  |
| 3   | D     | 545 | HIS  |
| 3   | D     | 569 | LEU  |
| 3   | D     | 571 | ASP  |
| 3   | D     | 573 | THR  |
| 3   | D     | 594 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | D     | 605  | LEU  |
| 3   | D     | 615  | LYS  |
| 3   | D     | 639  | VAL  |
| 3   | D     | 641  | ILE  |
| 3   | D     | 661  | VAL  |
| 3   | D     | 678  | ARG  |
| 3   | D     | 680  | ASN  |
| 3   | D     | 698  | MET  |
| 3   | D     | 701  | LEU  |
| 3   | D     | 707  | ILE  |
| 3   | D     | 708  | ASN  |
| 3   | D     | 717  | VAL  |
| 3   | D     | 721  | SER  |
| 3   | D     | 754  | ILE  |
| 3   | D     | 764  | ARG  |
| 3   | D     | 770  | LEU  |
| 3   | D     | 790  | THR  |
| 3   | D     | 797  | THR  |
| 3   | D     | 801  | VAL  |
| 3   | D     | 810  | THR  |
| 3   | D     | 844  | THR  |
| 3   | D     | 847  | ASP  |
| 3   | D     | 849  | LEU  |
| 3   | D     | 853  | THR  |
| 3   | D     | 858  | VAL  |
| 3   | D     | 860  | ARG  |
| 3   | D     | 890  | THR  |
| 3   | D     | 903  | LEU  |
| 3   | D     | 908  | ILE  |
| 3   | D     | 918  | ILE  |
| 3   | D     | 1146 | GLU  |
| 3   | D     | 1155 | ILE  |
| 3   | D     | 1156 | LEU  |
| 3   | D     | 1162 | ILE  |
| 3   | D     | 1163 | VAL  |
| 3   | D     | 1169 | THR  |
| 3   | D     | 1177 | ILE  |
| 3   | D     | 1194 | ARG  |
| 3   | D     | 1221 | LEU  |
| 3   | D     | 1251 | LYS  |
| 3   | D     | 1255 | VAL  |
| 3   | D     | 1257 | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | D     | 1261 | LEU  |
| 3   | D     | 1266 | ILE  |
| 3   | D     | 1272 | SER  |
| 3   | D     | 1279 | GLN  |
| 3   | D     | 1289 | ASN  |
| 3   | D     | 1310 | THR  |
| 3   | D     | 1332 | LEU  |
| 3   | D     | 1333 | THR  |
| 3   | D     | 1343 | GLU  |
| 3   | D     | 1361 | THR  |
| 3   | D     | 1366 | HIS  |
| 4   | E     | 3    | ARG  |
| 4   | E     | 5    | THR  |
| 4   | E     | 13   | ILE  |
| 4   | E     | 18   | ASP  |
| 4   | E     | 21   | LEU  |
| 4   | E     | 31   | GLN  |
| 4   | E     | 36   | ASP  |
| 4   | E     | 39   | VAL  |
| 4   | E     | 58   | LEU  |
| 5   | F     | 98   | VAL  |
| 5   | F     | 114  | GLU  |
| 5   | F     | 127  | ILE  |
| 5   | F     | 152  | GLU  |
| 5   | F     | 154  | GLU  |
| 5   | F     | 163  | THR  |
| 5   | F     | 230  | VAL  |
| 5   | F     | 261  | LEU  |
| 5   | F     | 277  | MET  |
| 5   | F     | 305  | LEU  |
| 5   | F     | 306  | PHE  |
| 5   | F     | 335  | GLU  |
| 5   | F     | 341  | LEU  |
| 5   | F     | 399  | LEU  |
| 5   | F     | 449  | THR  |
| 5   | F     | 450  | ILE  |
| 5   | F     | 471  | LEU  |
| 5   | F     | 472  | GLN  |
| 5   | F     | 479  | THR  |
| 5   | F     | 482  | GLU  |
| 5   | F     | 488  | LEU  |
| 5   | F     | 491  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | F     | 492 | ASP  |
| 5   | F     | 494 | ILE  |
| 5   | F     | 507 | MET  |
| 5   | F     | 516 | ASP  |
| 5   | F     | 526 | THR  |
| 5   | F     | 527 | THR  |
| 5   | F     | 530 | LEU  |
| 5   | F     | 547 | VAL  |
| 5   | F     | 552 | THR  |
| 5   | F     | 558 | VAL  |
| 5   | F     | 559 | LEU  |
| 5   | F     | 561 | MET  |
| 5   | F     | 568 | ASN  |
| 5   | F     | 569 | THR  |
| 5   | F     | 572 | THR  |
| 5   | F     | 578 | LYS  |
| 5   | F     | 587 | ILE  |
| 5   | F     | 600 | HIS  |
| 5   | F     | 603 | ARG  |
| 5   | F     | 606 | VAL  |
| 5   | F     | 608 | ARG  |
| 1   | G     | 9   | LEU  |
| 1   | G     | 12  | ARG  |
| 1   | G     | 19  | VAL  |
| 1   | G     | 23  | HIS  |
| 1   | G     | 26  | VAL  |
| 1   | G     | 27  | THR  |
| 1   | G     | 33  | ARG  |
| 1   | G     | 50  | SER  |
| 1   | G     | 64  | VAL  |
| 1   | G     | 65  | LEU  |
| 1   | G     | 70  | THR  |
| 1   | G     | 79  | LEU  |
| 1   | G     | 90  | VAL  |
| 1   | G     | 101 | THR  |
| 1   | G     | 121 | VAL  |
| 1   | G     | 124 | VAL  |
| 1   | G     | 129 | VAL  |
| 1   | G     | 133 | LEU  |
| 1   | G     | 137 | ASN  |
| 1   | G     | 145 | LYS  |
| 1   | G     | 156 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 166 | ARG  |
| 1   | G     | 178 | SER  |
| 1   | G     | 183 | ILE  |
| 1   | G     | 187 | VAL  |
| 1   | G     | 192 | VAL  |
| 1   | G     | 200 | LYS  |
| 1   | G     | 207 | THR  |
| 1   | G     | 211 | ILE  |
| 1   | G     | 217 | ILE  |
| 1   | G     | 219 | ARG  |
| 1   | H     | 16  | ILE  |
| 1   | H     | 27  | THR  |
| 1   | H     | 58  | GLU  |
| 1   | H     | 61  | ILE  |
| 1   | H     | 62  | ASP  |
| 1   | H     | 64  | VAL  |
| 1   | H     | 65  | LEU  |
| 1   | H     | 66  | HIS  |
| 1   | H     | 75  | GLN  |
| 1   | H     | 95  | LYS  |
| 1   | H     | 102 | LEU  |
| 1   | H     | 121 | VAL  |
| 1   | H     | 124 | VAL  |
| 1   | H     | 133 | LEU  |
| 1   | H     | 171 | LEU  |
| 1   | H     | 183 | ILE  |
| 2   | I     | 3   | TYR  |
| 2   | I     | 4   | SER  |
| 2   | I     | 11  | ILE  |
| 2   | I     | 22  | LEU  |
| 2   | I     | 39  | ILE  |
| 2   | I     | 46  | GLN  |
| 2   | I     | 56  | VAL  |
| 2   | I     | 86  | GLN  |
| 2   | I     | 90  | VAL  |
| 2   | I     | 103 | VAL  |
| 2   | I     | 107 | ARG  |
| 2   | I     | 115 | LYS  |
| 2   | I     | 117 | ILE  |
| 2   | I     | 119 | GLU  |
| 2   | I     | 131 | THR  |
| 2   | I     | 132 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | I     | 135 | THR  |
| 2   | I     | 138 | ILE  |
| 2   | I     | 156 | PHE  |
| 2   | I     | 164 | THR  |
| 2   | I     | 170 | VAL  |
| 2   | I     | 208 | ILE  |
| 2   | I     | 285 | ILE  |
| 2   | I     | 292 | ILE  |
| 2   | I     | 302 | ILE  |
| 2   | I     | 316 | GLU  |
| 2   | I     | 320 | ASP  |
| 2   | I     | 321 | LEU  |
| 2   | I     | 342 | ASP  |
| 2   | I     | 343 | HIS  |
| 2   | I     | 360 | LEU  |
| 2   | I     | 384 | LEU  |
| 2   | I     | 423 | ASP  |
| 2   | I     | 445 | ILE  |
| 2   | I     | 453 | ILE  |
| 2   | I     | 455 | SER  |
| 2   | I     | 456 | VAL  |
| 2   | I     | 471 | VAL  |
| 2   | I     | 481 | LEU  |
| 2   | I     | 484 | LEU  |
| 2   | I     | 492 | MET  |
| 2   | I     | 493 | ILE  |
| 2   | I     | 518 | ASN  |
| 2   | I     | 521 | LEU  |
| 2   | I     | 524 | ILE  |
| 2   | I     | 525 | THR  |
| 2   | I     | 530 | ILE  |
| 2   | I     | 538 | LEU  |
| 2   | I     | 542 | ARG  |
| 2   | I     | 550 | VAL  |
| 2   | I     | 553 | THR  |
| 2   | I     | 558 | VAL  |
| 2   | I     | 561 | ILE  |
| 2   | I     | 575 | LEU  |
| 2   | I     | 596 | ASP  |
| 2   | I     | 600 | THR  |
| 2   | I     | 604 | HIS  |
| 2   | I     | 609 | ILE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | I     | 615  | VAL  |
| 2   | I     | 623  | LEU  |
| 2   | I     | 633  | LEU  |
| 2   | I     | 635  | THR  |
| 2   | I     | 660  | VAL  |
| 2   | I     | 663  | VAL  |
| 2   | I     | 672  | GLU  |
| 2   | I     | 705  | GLU  |
| 2   | I     | 714  | VAL  |
| 2   | I     | 724  | VAL  |
| 2   | I     | 739  | ASP  |
| 2   | I     | 748  | ILE  |
| 2   | I     | 765  | ILE  |
| 2   | I     | 781  | ASP  |
| 2   | I     | 782  | VAL  |
| 2   | I     | 800  | MET  |
| 2   | I     | 817  | LEU  |
| 2   | I     | 828  | PHE  |
| 2   | I     | 878  | THR  |
| 2   | I     | 890  | LYS  |
| 2   | I     | 892  | GLU  |
| 2   | I     | 895  | LEU  |
| 2   | I     | 922  | ASN  |
| 2   | I     | 951  | MET  |
| 2   | I     | 984  | VAL  |
| 2   | I     | 1002 | LEU  |
| 2   | I     | 1037 | THR  |
| 2   | I     | 1050 | VAL  |
| 2   | I     | 1054 | LEU  |
| 2   | I     | 1078 | LYS  |
| 2   | I     | 1082 | ILE  |
| 2   | I     | 1083 | GLU  |
| 2   | I     | 1109 | ILE  |
| 2   | I     | 1114 | GLU  |
| 2   | I     | 1134 | GLN  |
| 2   | I     | 1141 | LEU  |
| 2   | I     | 1146 | GLN  |
| 2   | I     | 1151 | LEU  |
| 2   | I     | 1156 | ARG  |
| 2   | I     | 1159 | VAL  |
| 2   | I     | 1163 | THR  |
| 2   | I     | 1164 | PHE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | I     | 1172 | LEU  |
| 2   | I     | 1180 | MET  |
| 2   | I     | 1198 | LEU  |
| 2   | I     | 1206 | THR  |
| 2   | I     | 1210 | ILE  |
| 2   | I     | 1225 | VAL  |
| 2   | I     | 1227 | VAL  |
| 2   | I     | 1233 | LEU  |
| 2   | I     | 1238 | LEU  |
| 2   | I     | 1240 | ASP  |
| 2   | I     | 1248 | THR  |
| 2   | I     | 1250 | SER  |
| 2   | I     | 1254 | VAL  |
| 2   | I     | 1287 | LEU  |
| 2   | I     | 1296 | ASP  |
| 2   | I     | 1299 | ASN  |
| 2   | I     | 1313 | HIS  |
| 2   | I     | 1327 | LEU  |
| 2   | I     | 1341 | ASP  |
| 2   | I     | 1342 | GLU  |
| 3   | J     | 20   | ILE  |
| 3   | J     | 46   | TYR  |
| 3   | J     | 54   | ASP  |
| 3   | J     | 79   | LYS  |
| 3   | J     | 84   | ILE  |
| 3   | J     | 92   | VAL  |
| 3   | J     | 93   | THR  |
| 3   | J     | 95   | THR  |
| 3   | J     | 96   | LYS  |
| 3   | J     | 97   | VAL  |
| 3   | J     | 154  | LEU  |
| 3   | J     | 162  | GLU  |
| 3   | J     | 172  | PHE  |
| 3   | J     | 175  | GLU  |
| 3   | J     | 176  | PHE  |
| 3   | J     | 218  | THR  |
| 3   | J     | 235  | GLU  |
| 3   | J     | 244  | VAL  |
| 3   | J     | 248  | ASP  |
| 3   | J     | 252  | LEU  |
| 3   | J     | 255  | LEU  |
| 3   | J     | 283  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | J     | 292 | VAL  |
| 3   | J     | 306 | LEU  |
| 3   | J     | 324 | LEU  |
| 3   | J     | 343 | LEU  |
| 3   | J     | 357 | VAL  |
| 3   | J     | 363 | LEU  |
| 3   | J     | 374 | LEU  |
| 3   | J     | 376 | LEU  |
| 3   | J     | 386 | GLU  |
| 3   | J     | 392 | THR  |
| 3   | J     | 394 | ILE  |
| 3   | J     | 415 | VAL  |
| 3   | J     | 416 | ILE  |
| 3   | J     | 423 | LEU  |
| 3   | J     | 425 | ARG  |
| 3   | J     | 429 | LEU  |
| 3   | J     | 505 | ASP  |
| 3   | J     | 506 | VAL  |
| 3   | J     | 507 | VAL  |
| 3   | J     | 510 | LEU  |
| 3   | J     | 514 | THR  |
| 3   | J     | 532 | GLU  |
| 3   | J     | 536 | LEU  |
| 3   | J     | 545 | HIS  |
| 3   | J     | 567 | THR  |
| 3   | J     | 569 | LEU  |
| 3   | J     | 571 | ASP  |
| 3   | J     | 573 | THR  |
| 3   | J     | 591 | ILE  |
| 3   | J     | 594 | GLN  |
| 3   | J     | 605 | LEU  |
| 3   | J     | 615 | LYS  |
| 3   | J     | 639 | VAL  |
| 3   | J     | 641 | ILE  |
| 3   | J     | 661 | VAL  |
| 3   | J     | 678 | ARG  |
| 3   | J     | 680 | ASN  |
| 3   | J     | 698 | MET  |
| 3   | J     | 701 | LEU  |
| 3   | J     | 707 | ILE  |
| 3   | J     | 708 | ASN  |
| 3   | J     | 717 | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | J     | 754  | ILE  |
| 3   | J     | 764  | ARG  |
| 3   | J     | 797  | THR  |
| 3   | J     | 801  | VAL  |
| 3   | J     | 810  | THR  |
| 3   | J     | 826  | ILE  |
| 3   | J     | 827  | GLU  |
| 3   | J     | 847  | ASP  |
| 3   | J     | 848  | VAL  |
| 3   | J     | 849  | LEU  |
| 3   | J     | 853  | THR  |
| 3   | J     | 857  | LEU  |
| 3   | J     | 858  | VAL  |
| 3   | J     | 897  | HIS  |
| 3   | J     | 898  | CYS  |
| 3   | J     | 903  | LEU  |
| 3   | J     | 908  | ILE  |
| 3   | J     | 910  | ASN  |
| 3   | J     | 913  | GLU  |
| 3   | J     | 918  | ILE  |
| 3   | J     | 1146 | GLU  |
| 3   | J     | 1155 | ILE  |
| 3   | J     | 1162 | ILE  |
| 3   | J     | 1163 | VAL  |
| 3   | J     | 1169 | THR  |
| 3   | J     | 1194 | ARG  |
| 3   | J     | 1204 | VAL  |
| 3   | J     | 1221 | LEU  |
| 3   | J     | 1251 | LYS  |
| 3   | J     | 1255 | VAL  |
| 3   | J     | 1257 | VAL  |
| 3   | J     | 1261 | LEU  |
| 3   | J     | 1266 | ILE  |
| 3   | J     | 1273 | ASP  |
| 3   | J     | 1285 | VAL  |
| 3   | J     | 1289 | ASN  |
| 3   | J     | 1292 | LEU  |
| 3   | J     | 1333 | THR  |
| 3   | J     | 1366 | HIS  |
| 4   | K     | 3    | ARG  |
| 4   | K     | 4    | VAL  |
| 4   | K     | 13   | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | K     | 18  | ASP  |
| 4   | K     | 39  | VAL  |
| 4   | K     | 58  | LEU  |
| 5   | L     | 98  | VAL  |
| 5   | L     | 102 | MET  |
| 5   | L     | 114 | GLU  |
| 5   | L     | 127 | ILE  |
| 5   | L     | 152 | GLU  |
| 5   | L     | 154 | GLU  |
| 5   | L     | 163 | THR  |
| 5   | L     | 261 | LEU  |
| 5   | L     | 277 | MET  |
| 5   | L     | 305 | LEU  |
| 5   | L     | 335 | GLU  |
| 5   | L     | 338 | HIS  |
| 5   | L     | 364 | ARG  |
| 5   | L     | 395 | THR  |
| 5   | L     | 405 | ILE  |
| 5   | L     | 429 | THR  |
| 5   | L     | 445 | ASP  |
| 5   | L     | 450 | ILE  |
| 5   | L     | 469 | GLN  |
| 5   | L     | 471 | LEU  |
| 5   | L     | 476 | ARG  |
| 5   | L     | 486 | ARG  |
| 5   | L     | 491 | GLU  |
| 5   | L     | 492 | ASP  |
| 5   | L     | 494 | ILE  |
| 5   | L     | 507 | MET  |
| 5   | L     | 526 | THR  |
| 5   | L     | 527 | THR  |
| 5   | L     | 547 | VAL  |
| 5   | L     | 552 | THR  |
| 5   | L     | 558 | VAL  |
| 5   | L     | 559 | LEU  |
| 5   | L     | 561 | MET  |
| 5   | L     | 568 | ASN  |
| 5   | L     | 569 | THR  |
| 5   | L     | 572 | THR  |
| 5   | L     | 573 | LEU  |
| 5   | L     | 580 | PHE  |
| 5   | L     | 582 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | L     | 587 | ILE  |
| 5   | L     | 599 | ARG  |
| 5   | L     | 600 | HIS  |
| 5   | L     | 603 | ARG  |
| 5   | L     | 606 | VAL  |
| 5   | L     | 607 | LEU  |
| 6   | M     | 16  | THR  |
| 6   | M     | 34  | VAL  |
| 6   | M     | 55  | VAL  |
| 6   | M     | 59  | VAL  |
| 6   | N     | 16  | THR  |
| 6   | N     | 34  | VAL  |
| 6   | N     | 55  | VAL  |
| 6   | N     | 59  | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (103) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 18   | GLN  |
| 1   | A     | 23   | HIS  |
| 1   | A     | 128  | HIS  |
| 1   | B     | 84   | ASN  |
| 1   | B     | 117  | HIS  |
| 1   | B     | 128  | HIS  |
| 1   | B     | 132  | HIS  |
| 2   | C     | 46   | GLN  |
| 2   | C     | 139  | ASN  |
| 2   | C     | 406  | ASN  |
| 2   | C     | 510  | GLN  |
| 2   | C     | 513  | GLN  |
| 2   | C     | 517  | GLN  |
| 2   | C     | 618  | GLN  |
| 2   | C     | 620  | ASN  |
| 2   | C     | 686  | GLN  |
| 2   | C     | 725  | GLN  |
| 2   | C     | 760  | ASN  |
| 2   | C     | 1017 | GLN  |
| 2   | C     | 1023 | HIS  |
| 2   | C     | 1116 | HIS  |
| 2   | C     | 1146 | GLN  |
| 2   | C     | 1209 | GLN  |
| 2   | C     | 1220 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | C     | 1236 | ASN  |
| 2   | C     | 1237 | HIS  |
| 2   | C     | 1288 | GLN  |
| 2   | C     | 1299 | ASN  |
| 2   | C     | 1314 | GLN  |
| 3   | D     | 200  | GLN  |
| 3   | D     | 276  | ASN  |
| 3   | D     | 320  | ASN  |
| 3   | D     | 365  | GLN  |
| 3   | D     | 424  | ASN  |
| 3   | D     | 489  | ASN  |
| 3   | D     | 667  | GLN  |
| 3   | D     | 690  | ASN  |
| 3   | D     | 700  | ASN  |
| 3   | D     | 716  | GLN  |
| 3   | D     | 739  | GLN  |
| 3   | D     | 865  | HIS  |
| 3   | D     | 910  | ASN  |
| 3   | D     | 1235 | ASN  |
| 3   | D     | 1366 | HIS  |
| 5   | F     | 129  | GLN  |
| 5   | F     | 131  | GLN  |
| 5   | F     | 147  | GLN  |
| 5   | F     | 294  | GLN  |
| 5   | F     | 383  | ASN  |
| 5   | F     | 406  | GLN  |
| 5   | F     | 446  | GLN  |
| 5   | F     | 455  | HIS  |
| 5   | F     | 472  | GLN  |
| 5   | F     | 579  | GLN  |
| 1   | G     | 66   | HIS  |
| 1   | G     | 186  | ASN  |
| 1   | H     | 128  | HIS  |
| 2   | I     | 139  | ASN  |
| 2   | I     | 150  | HIS  |
| 2   | I     | 343  | HIS  |
| 2   | I     | 357  | ASN  |
| 2   | I     | 618  | GLN  |
| 2   | I     | 620  | ASN  |
| 2   | I     | 628  | HIS  |
| 2   | I     | 725  | GLN  |
| 2   | I     | 766  | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | I     | 1008 | GLN  |
| 2   | I     | 1013 | GLN  |
| 2   | I     | 1108 | ASN  |
| 2   | I     | 1111 | GLN  |
| 2   | I     | 1116 | HIS  |
| 2   | I     | 1146 | GLN  |
| 2   | I     | 1220 | GLN  |
| 2   | I     | 1237 | HIS  |
| 2   | I     | 1288 | GLN  |
| 2   | I     | 1314 | GLN  |
| 3   | J     | 157  | GLN  |
| 3   | J     | 158  | GLN  |
| 3   | J     | 200  | GLN  |
| 3   | J     | 206  | ASN  |
| 3   | J     | 435  | GLN  |
| 3   | J     | 450  | HIS  |
| 3   | J     | 489  | ASN  |
| 3   | J     | 594  | GLN  |
| 3   | J     | 667  | GLN  |
| 3   | J     | 690  | ASN  |
| 3   | J     | 716  | GLN  |
| 3   | J     | 771  | GLN  |
| 3   | J     | 817  | HIS  |
| 3   | J     | 861  | ASN  |
| 3   | J     | 1235 | ASN  |
| 3   | J     | 1295 | ASN  |
| 3   | J     | 1366 | HIS  |
| 4   | K     | 62   | GLN  |
| 5   | L     | 128  | ASN  |
| 5   | L     | 131  | GLN  |
| 5   | L     | 294  | GLN  |
| 5   | L     | 362  | ASN  |
| 5   | L     | 406  | GLN  |
| 5   | L     | 446  | GLN  |
| 5   | L     | 579  | GLN  |
| 6   | M     | 71   | HIS  |
| 6   | N     | 71   | HIS  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 1   | A     | 319/329 (96%)   | -0.93  | 0 100 100      | 152, 220, 344, 468    | 0     |
| 1   | B     | 217/329 (65%)   | -0.94  | 0 100 100      | 140, 238, 332, 383    | 0     |
| 1   | G     | 227/329 (68%)   | -0.98  | 0 100 100      | 204, 264, 358, 416    | 0     |
| 1   | H     | 216/329 (65%)   | -0.86  | 1 (0%) 87 71   | 204, 298, 387, 432    | 0     |
| 2   | C     | 1340/1342 (99%) | -0.90  | 1 (0%) 92 87   | 104, 197, 403, 528    | 0     |
| 2   | I     | 1340/1342 (99%) | -0.95  | 1 (0%) 92 87   | 127, 264, 377, 485    | 0     |
| 3   | D     | 1173/1407 (83%) | -0.87  | 0 100 100      | 101, 174, 294, 419    | 0     |
| 3   | J     | 1155/1407 (82%) | -0.95  | 0 100 100      | 125, 213, 329, 431    | 0     |
| 4   | E     | 89/91 (97%)     | -1.06  | 0 100 100      | 160, 216, 269, 393    | 0     |
| 4   | K     | 72/91 (79%)     | -1.03  | 0 100 100      | 227, 323, 429, 470    | 0     |
| 5   | F     | 468/613 (76%)   | -0.93  | 0 100 100      | 137, 239, 365, 477    | 0     |
| 5   | L     | 469/613 (76%)   | -1.01  | 0 100 100      | 162, 251, 379, 489    | 0     |
| 6   | M     | 70/79 (88%)     | -0.91  | 0 100 100      | 226, 315, 399, 479    | 0     |
| 6   | N     | 69/79 (87%)     | -0.99  | 0 100 100      | 325, 403, 501, 568    | 0     |
| All | All   | 7224/8380 (86%) | -0.93  | 3 (0%) 100 100 | 101, 230, 372, 568    | 0     |

All (3) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | C     | 209 | ILE  | 2.4  |
| 1   | H     | 28  | LEU  | 2.2  |
| 2   | I     | 836 | LEU  | 2.1  |

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 7   | MG   | D     | 2001 | 1/1   | 0.88 | 0.05 | 251,251,251,251             | 0     |
| 7   | MG   | J     | 2001 | 1/1   | 0.93 | 0.06 | 170,170,170,170             | 0     |
| 8   | ZN   | N     | 101  | 1/1   | 0.93 | 0.06 | 465,465,465,465             | 0     |
| 8   | ZN   | M     | 101  | 1/1   | 0.97 | 0.03 | 468,468,468,468             | 0     |
| 8   | ZN   | J     | 2002 | 1/1   | 0.97 | 0.05 | 229,229,229,229             | 0     |
| 8   | ZN   | D     | 2003 | 1/1   | 0.98 | 0.14 | 334,334,334,334             | 0     |
| 8   | ZN   | D     | 2002 | 1/1   | 0.98 | 0.03 | 182,182,182,182             | 0     |
| 8   | ZN   | J     | 2003 | 1/1   | 1.00 | 0.01 | 126,126,126,126             | 0     |

### 6.5 Other polymers [i](#)

There are no such residues in this entry.