



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Mar 2, 2017 – 11:23 am GMT

PDB ID : 1O1F  
EMDB ID: : EMD-1001  
Title : MOLECULAR MODELS OF AVERAGED RIGOR CROSSBRIDGES FROM  
TOMOGRAMS OF INSECT FLIGHT MUSCLE  
Authors : Chen, L.F.; Winkler, H.; Reedy, M.K.; Reedy, M.C.; Taylor, K.A.  
Deposited on : 2002-11-15  
Resolution : 70.00 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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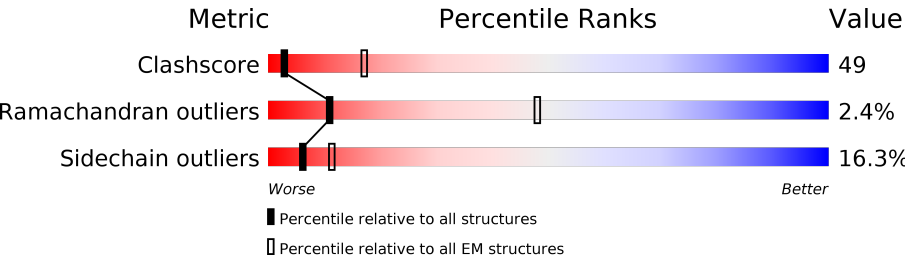
MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc29047

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 70.00 Å.

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






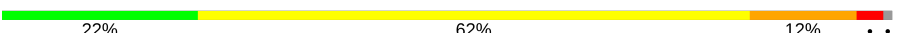
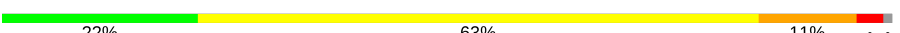
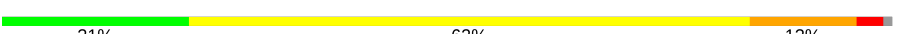









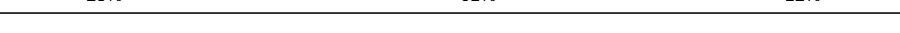
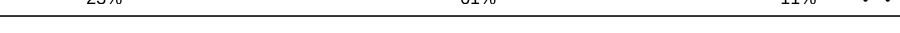
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore            | 125131                      | 1336                        |
| Ramachandran outliers | 121729                      | 1120                        |
| Sidechain outliers    | 121581                      | 1026                        |

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 840    | 26% 51% 19% .    |
| 1   | D     | 840    | 26% 51% 19% .    |
| 1   | G     | 840    | 25% 52% 19% .    |
| 1   | J     | 840    | 25% 51% 19% .    |
| 2   | B     | 145    | 66% 26% 6% .     |
| 2   | E     | 145    | 63% 28% 6% .     |
| 2   | H     | 145    | 63% 28% 6% .     |
| 2   | K     | 145    | 65% 26% 6% .     |
| 3   | C     | 147    | 61% 37% .        |

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| Mol | Chain | Length | Quality of chain                                                                                    |
|-----|-------|--------|-----------------------------------------------------------------------------------------------------|
| 3   | F     | 147    |  61% 38% .        |
| 3   | I     | 147    |  61% 37% .        |
| 3   | L     | 147    |  61% 37% .        |
| 4   | 0     | 375    |  22% 62% 12% ..   |
| 4   | 1     | 375    |  22% 63% 11% ..   |
| 4   | 2     | 375    |  21% 63% 12% ..   |
| 4   | 3     | 375    |  57% 34% 6% ..    |
| 4   | 4     | 375    |  56% 34% 8% ..    |
| 4   | 5     | 375    |  58% 32% 8% ..    |
| 4   | 6     | 375    |  56% 33% 9% ..    |
| 4   | 7     | 375    |  56% 34% 8% ..    |
| 4   | 8     | 375    |  60% 30% 7% ..    |
| 4   | V     | 375    |  59% 32% 7% ..  |
| 4   | W     | 375    |  57% 32% 8% ..  |
| 4   | X     | 375    |  23% 61% 12% .. |
| 4   | Y     | 375    |  23% 61% 11% .. |
| 4   | Z     | 375    |  23% 61% 11% .. |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 1   | MLY  | A     | 505 | -         | -        | X       | -                |
| 1   | MLY  | A     | 553 | -         | -        | X       | -                |
| 1   | MLY  | A     | 764 | -         | -        | X       | -                |
| 1   | MLY  | A     | 768 | -         | -        | X       | -                |
| 1   | MLY  | A     | 839 | -         | -        | X       | -                |
| 1   | MLY  | D     | 553 | -         | -        | X       | -                |
| 1   | MLY  | D     | 782 | -         | -        | X       | -                |
| 1   | MLY  | D     | 839 | -         | -        | X       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 1   | MLY  | G     | 553 | -         | -        | X       | -                |
| 1   | MLY  | G     | 764 | -         | -        | X       | -                |
| 1   | MLY  | G     | 768 | -         | -        | X       | -                |
| 1   | MLY  | G     | 84  | -         | -        | X       | -                |
| 1   | MLY  | J     | 553 | -         | -        | X       | -                |
| 1   | MLY  | J     | 764 | -         | -        | X       | -                |
| 1   | MLY  | J     | 768 | -         | -        | X       | -                |
| 1   | MLY  | J     | 84  | -         | -        | X       | -                |

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 76872 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called SKELETAL MUSCLE MYOSIN II.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 1   | A     | 840      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6797  | 4382 | 1135 | 1243 | 37 |         |       |
| 1   | D     | 840      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6797  | 4382 | 1135 | 1243 | 37 |         |       |
| 1   | G     | 840      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6797  | 4382 | 1135 | 1243 | 37 |         |       |
| 1   | J     | 840      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6797  | 4382 | 1135 | 1243 | 37 |         |       |

- Molecule 2 is a protein called SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2   | B     | 145      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1127  | 717 | 177 | 227 | 6 |         |       |
| 2   | E     | 145      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1127  | 717 | 177 | 227 | 6 |         |       |
| 2   | H     | 145      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1127  | 717 | 177 | 227 | 6 |         |       |
| 2   | K     | 145      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1127  | 717 | 177 | 227 | 6 |         |       |

- Molecule 3 is a protein called SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 3   | C     | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1123  | 698 | 188 | 230 | 7 |         |       |
| 3   | F     | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1123  | 698 | 188 | 230 | 7 |         |       |
| 3   | I     | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1123  | 698 | 188 | 230 | 7 |         |       |
| 3   | L     | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1123  | 698 | 188 | 230 | 7 |         |       |

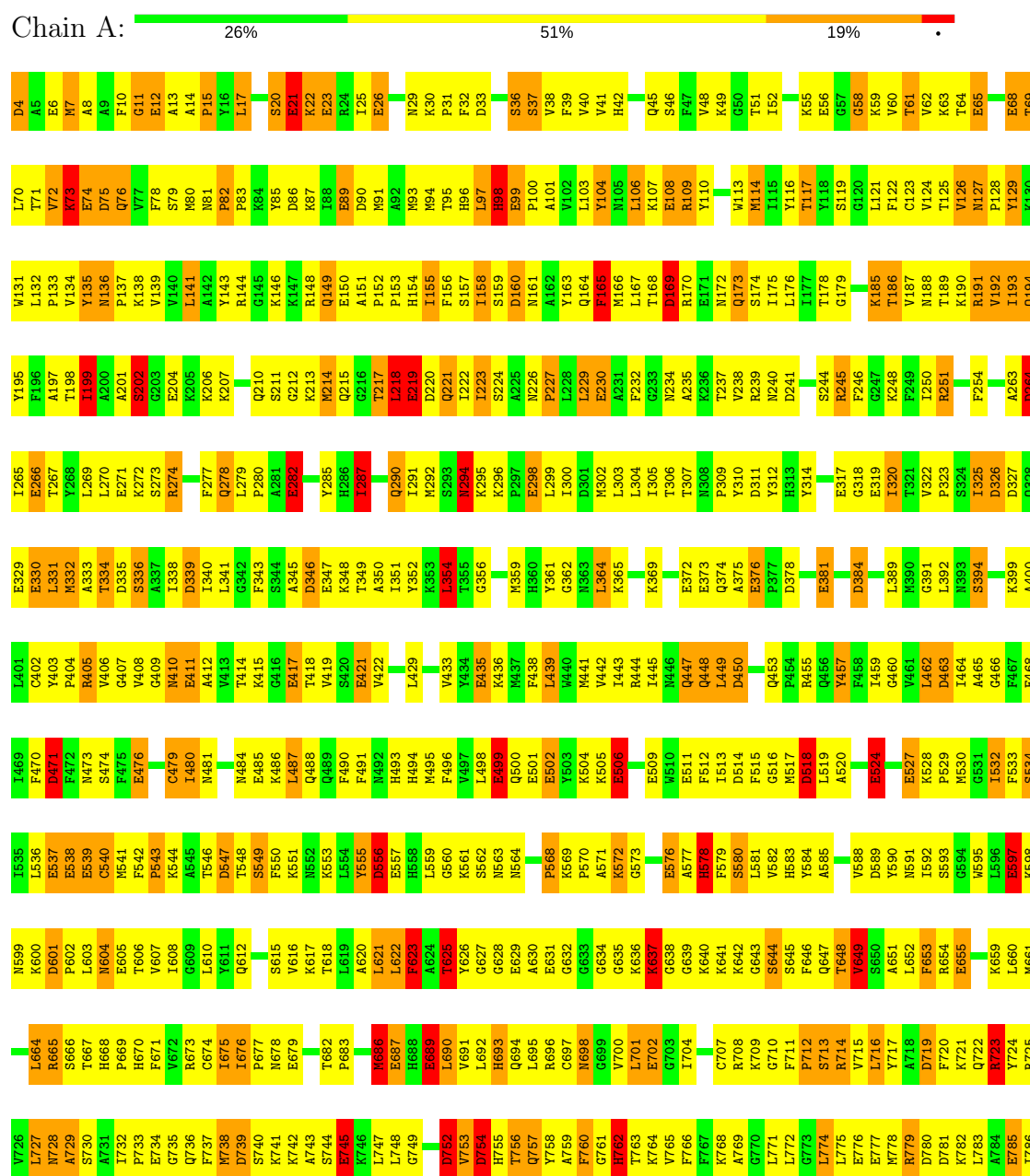
- Molecule 4 is a protein called SKELETAL MUSCLE ACTIN.

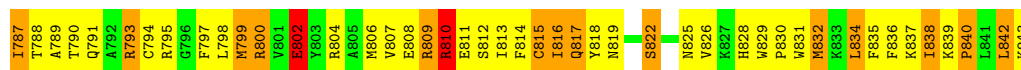
| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4   | 0     | 372      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2906  | 1836 | 489 | 561 | 20 |         |       |
| 4   | 1     | 372      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2906  | 1836 | 489 | 561 | 20 |         |       |
| 4   | 2     | 372      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2906  | 1836 | 489 | 561 | 20 |         |       |
| 4   | 3     | 372      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2906  | 1836 | 489 | 561 | 20 |         |       |
| 4   | 4     | 372      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2906  | 1836 | 489 | 561 | 20 |         |       |
| 4   | 5     | 372      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2906  | 1836 | 489 | 561 | 20 |         |       |
| 4   | 6     | 372      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2906  | 1836 | 489 | 561 | 20 |         |       |
| 4   | 7     | 372      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2906  | 1836 | 489 | 561 | 20 |         |       |
| 4   | 8     | 372      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2906  | 1836 | 489 | 561 | 20 |         |       |
| 4   | V     | 372      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2906  | 1836 | 489 | 561 | 20 |         |       |
| 4   | W     | 372      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2906  | 1836 | 489 | 561 | 20 |         |       |
| 4   | X     | 372      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2906  | 1836 | 489 | 561 | 20 |         |       |
| 4   | Y     | 372      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2906  | 1836 | 489 | 561 | 20 |         |       |
| 4   | Z     | 372      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2906  | 1836 | 489 | 561 | 20 |         |       |

### 3 Residue-property plots

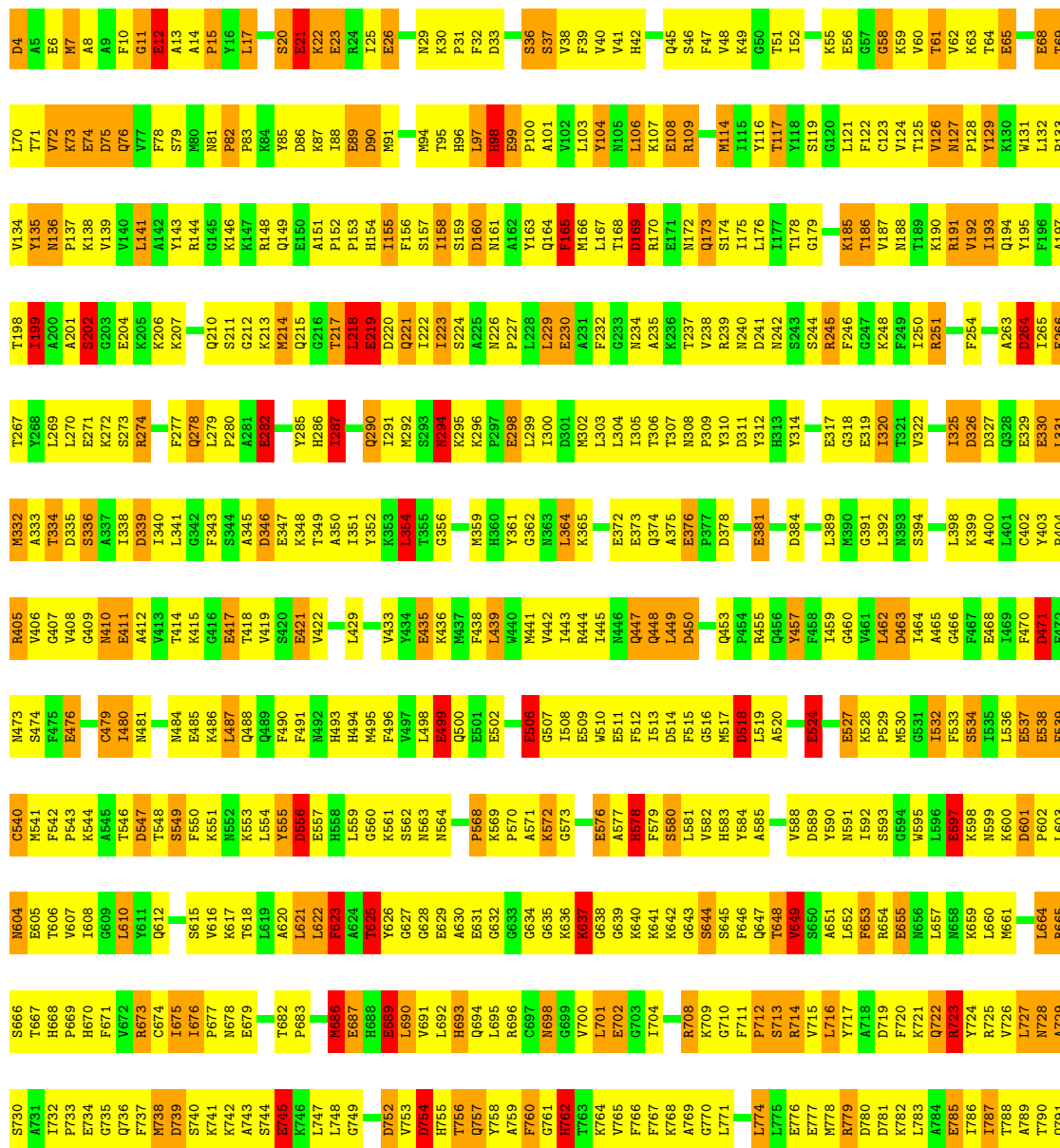
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

#### • Molecule 1: SKELETAL MUSCLE MYOSIN II





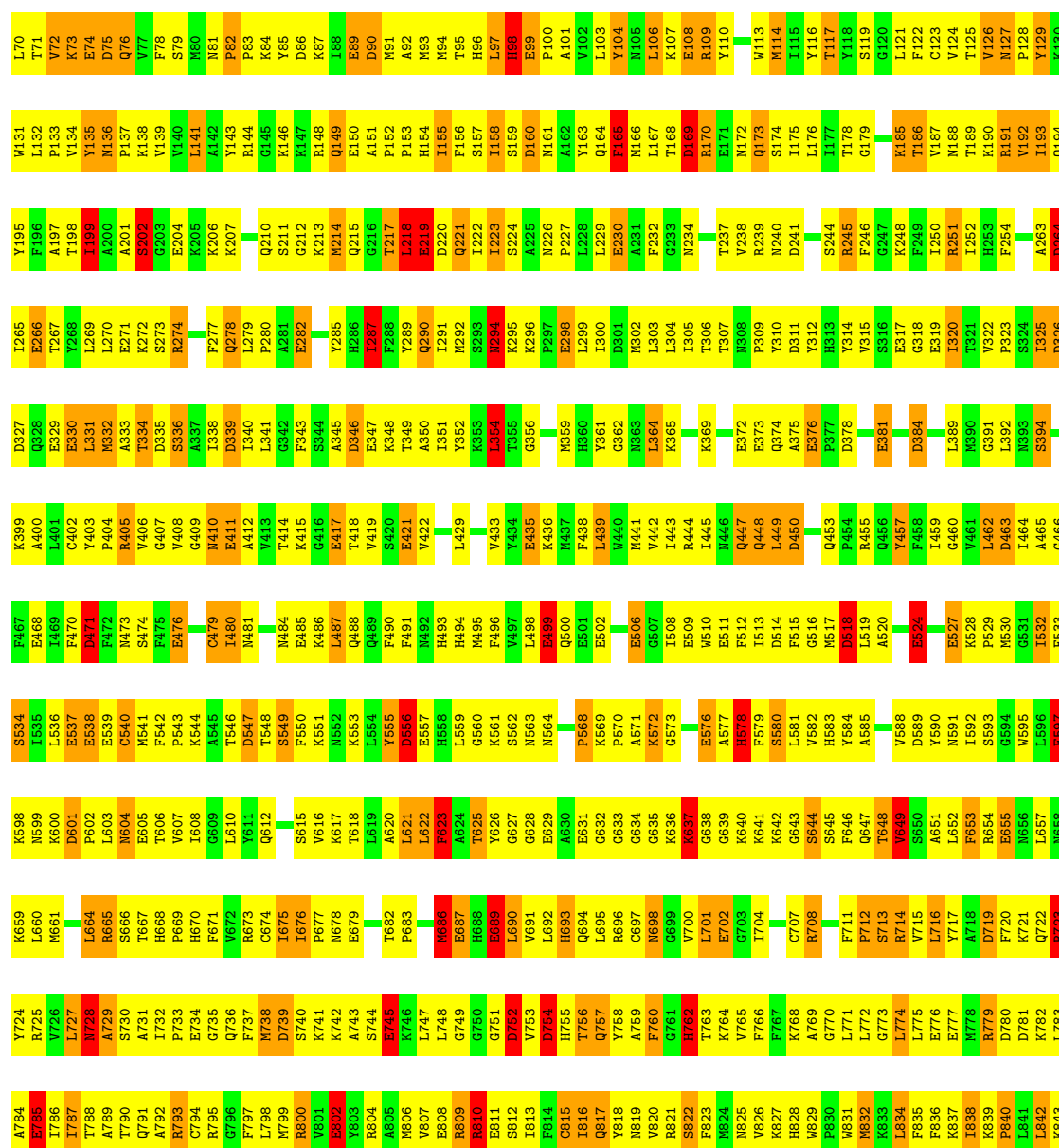
### • Molecule 1: SKELETAL MUSCLE MYOSIN II

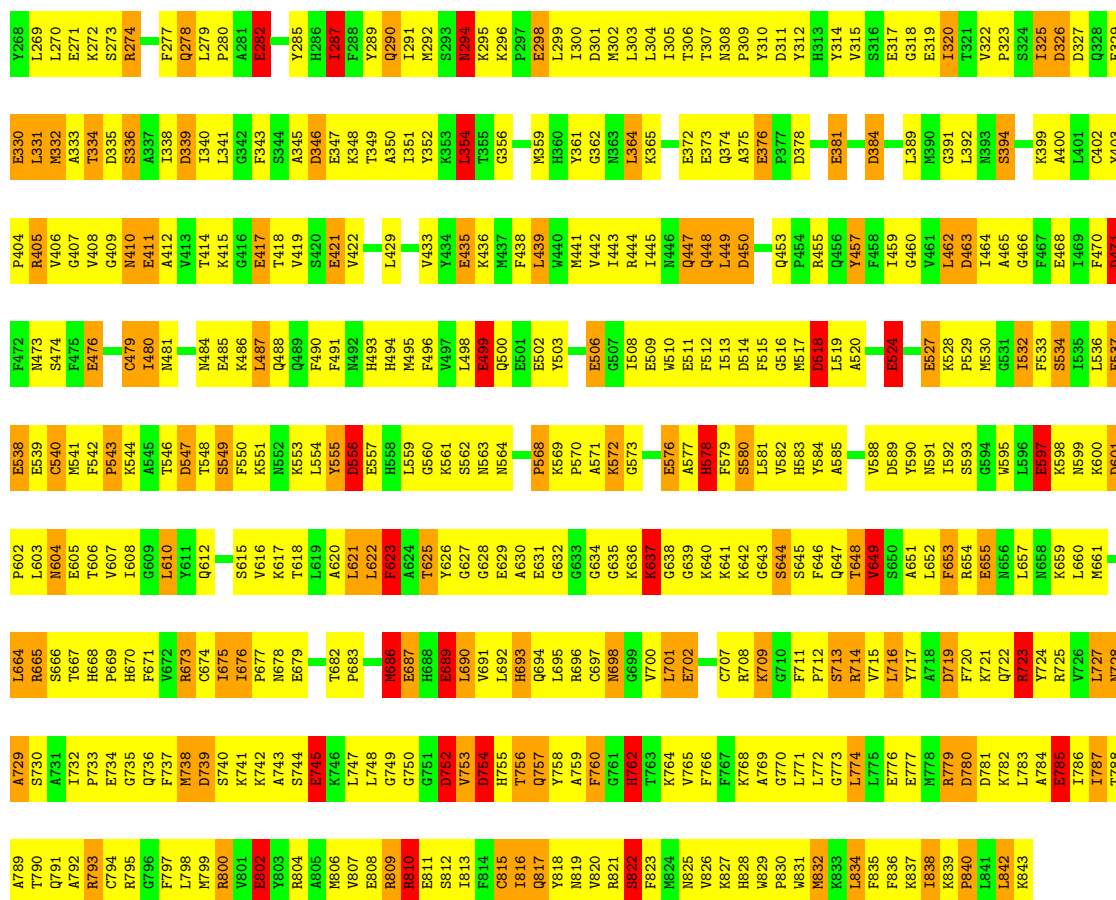


### • Molecule 1: SKELETAL MUSCLE MYOSIN II

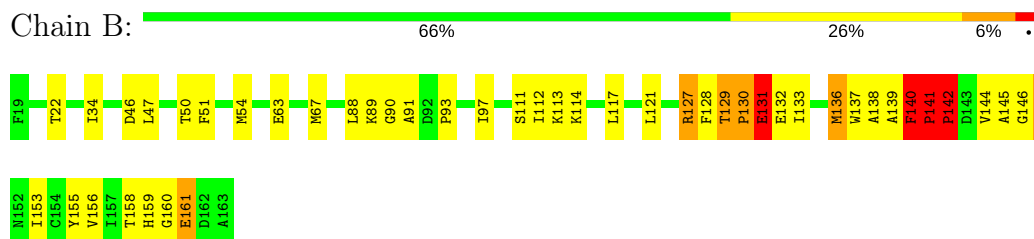




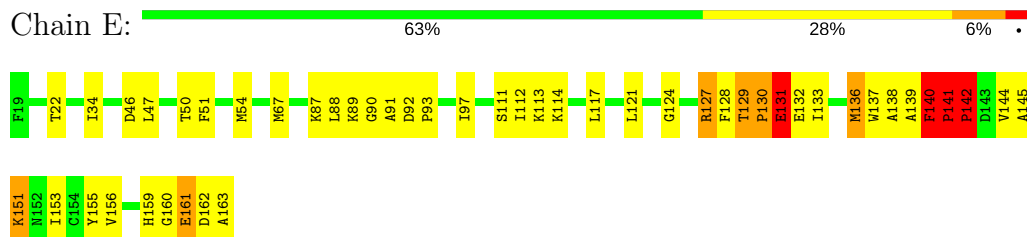




• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

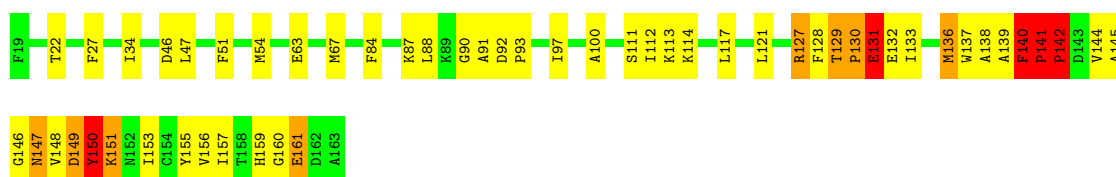


• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

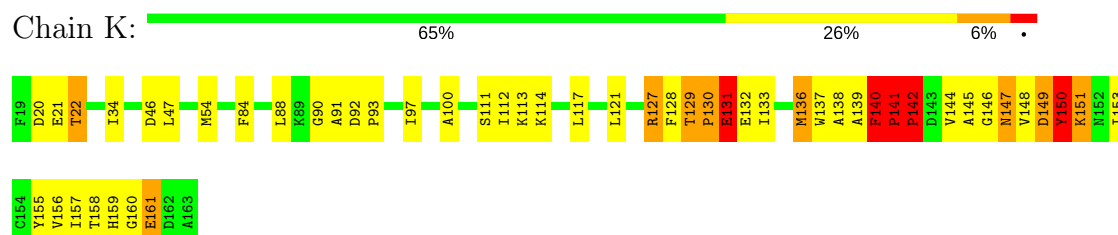


• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

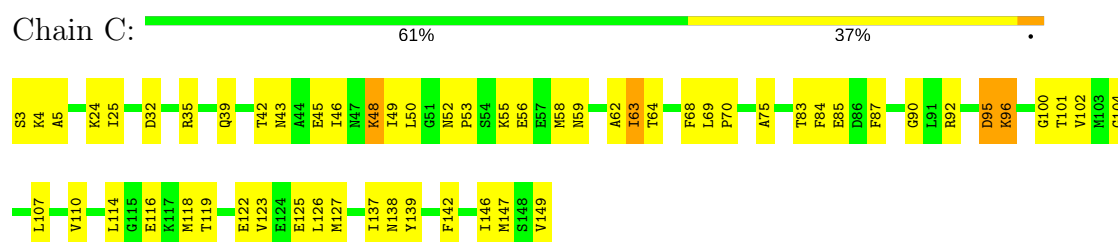




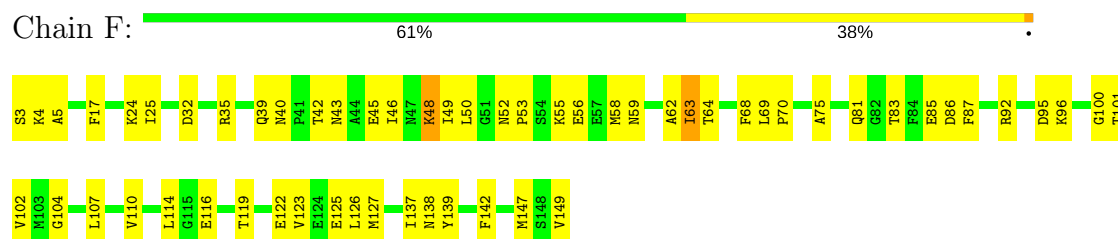
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN



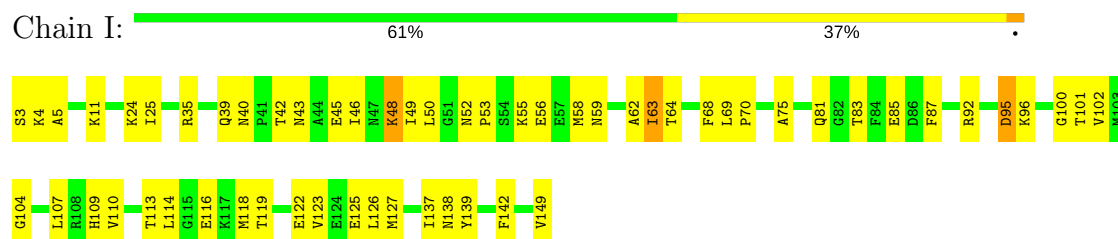
• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



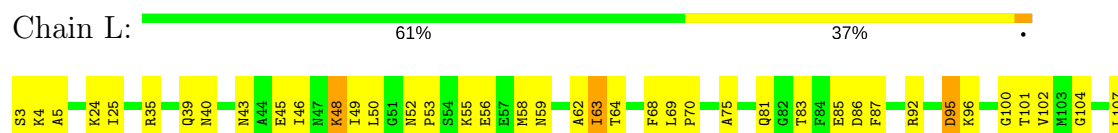
• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

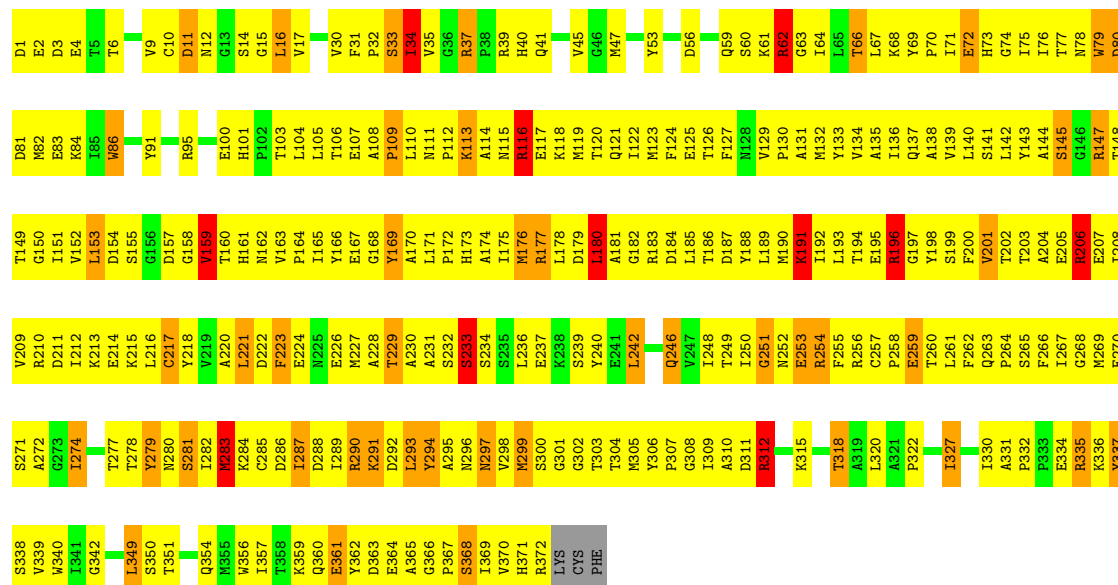


• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

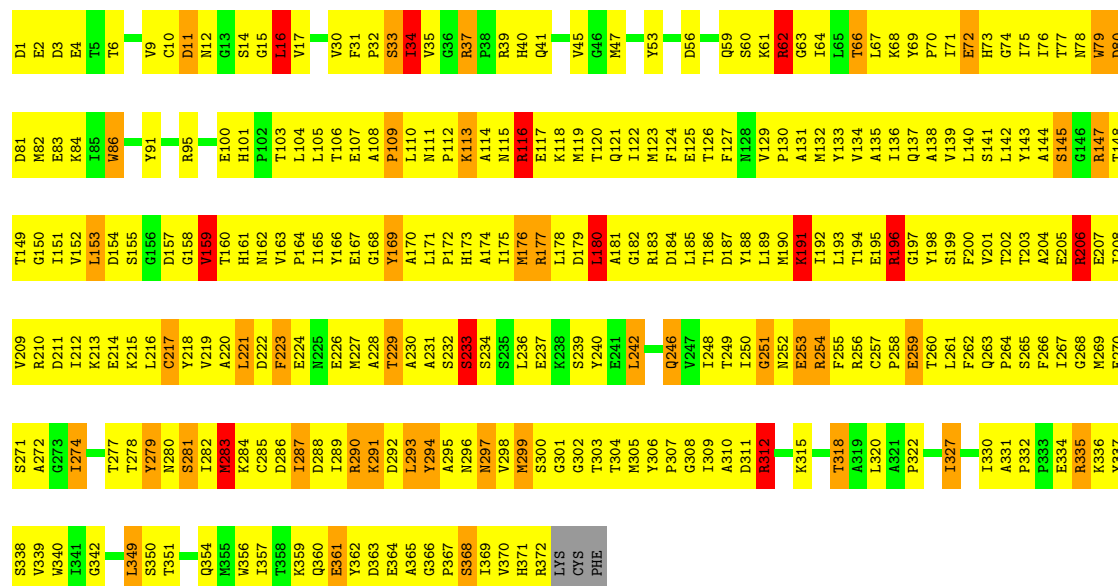




● Molecule 4: SKELETAL MUSCLE ACTIN

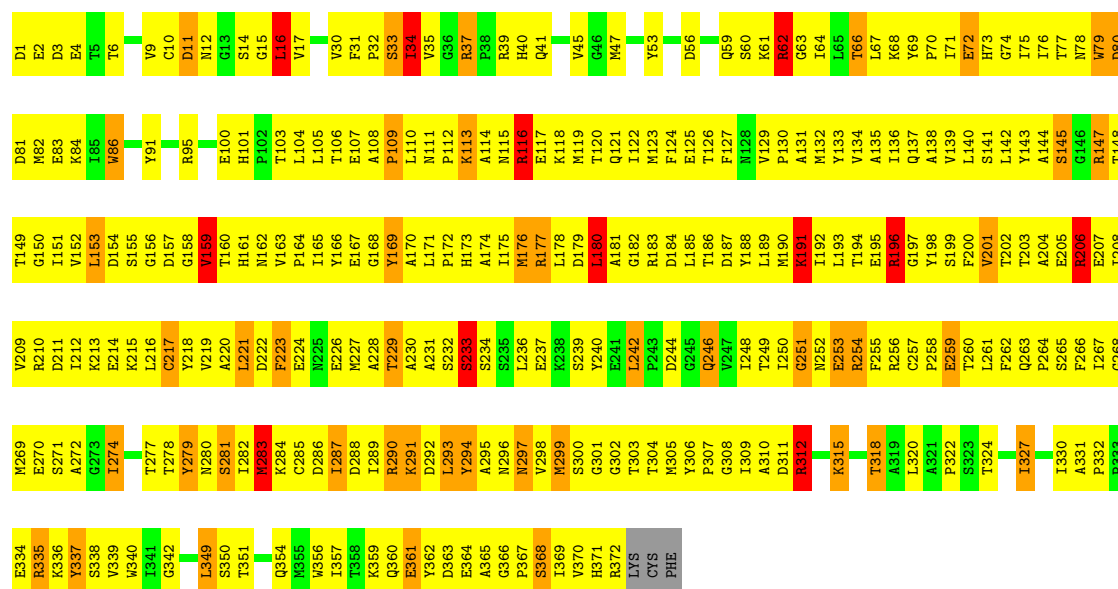


● Molecule 4: SKELETAL MUSCLE ACTIN

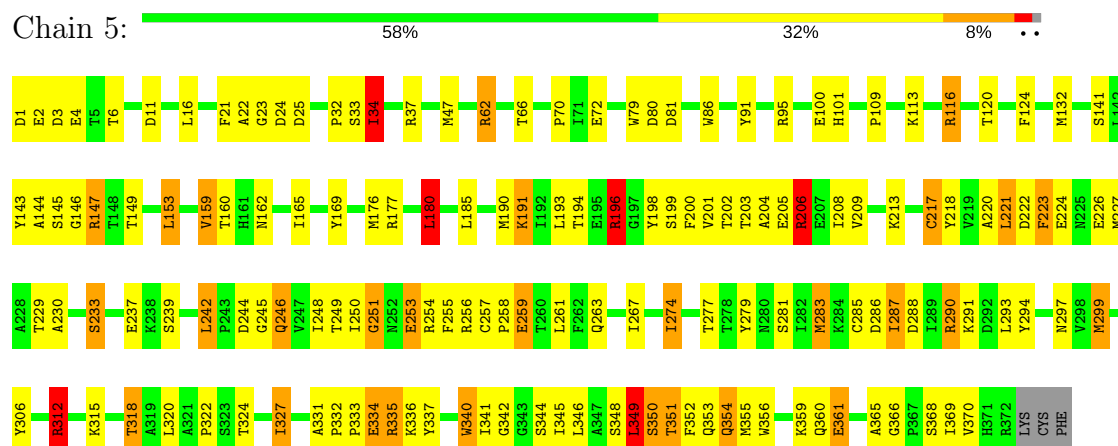


● Molecule 4: SKELETAL MUSCLE ACTIN

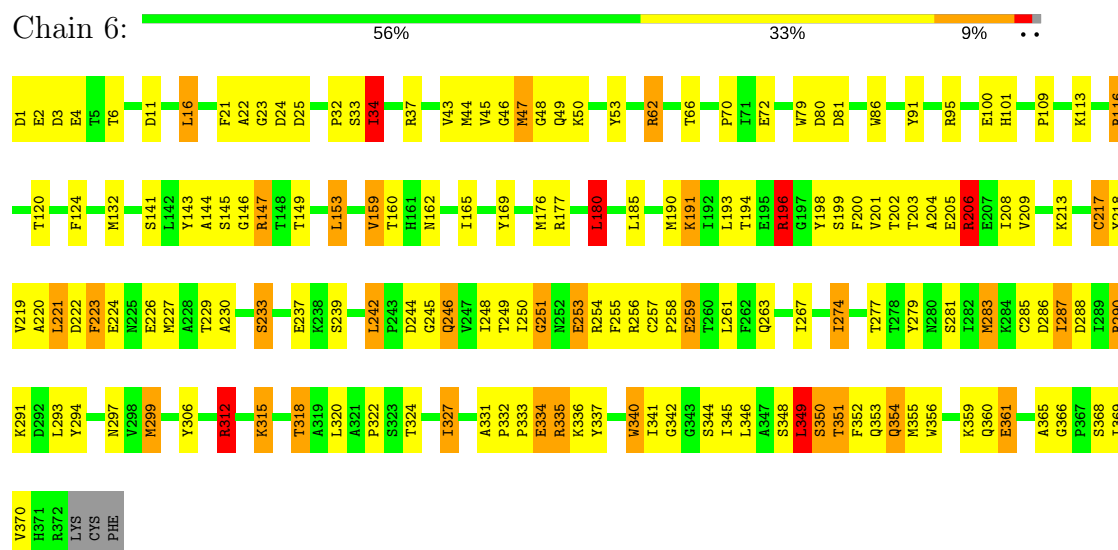




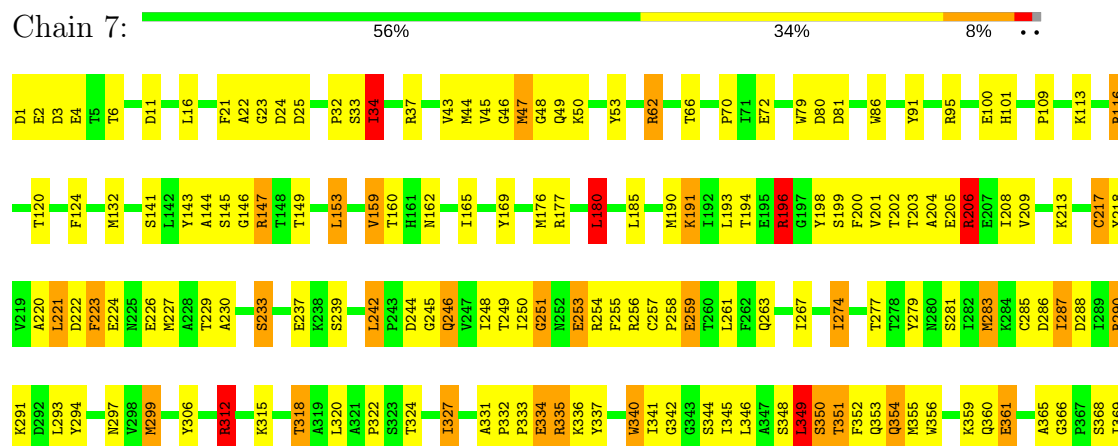
● Molecule 4: SKELETAL MUSCLE ACTIN

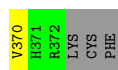


● Molecule 4: SKELETAL MUSCLE ACTIN



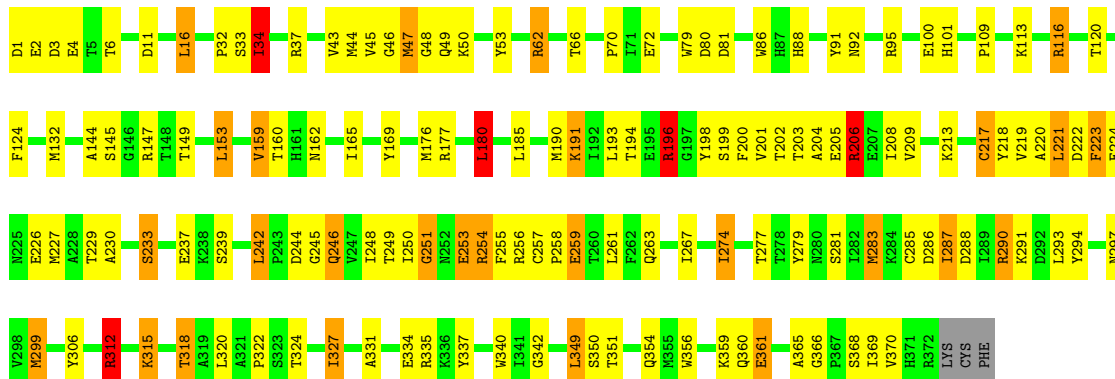
● Molecule 4: SKELETAL MUSCLE ACTIN





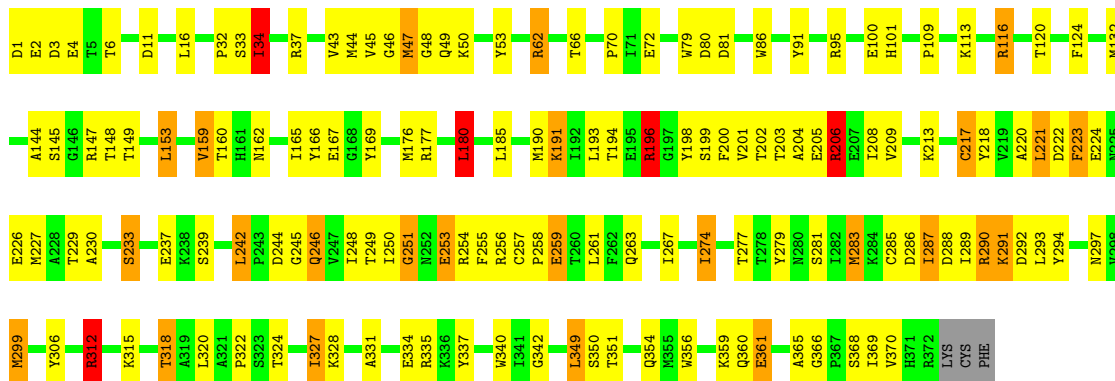
• Molecule 4: SKELETAL MUSCLE ACTIN

Chain 8:  60% 30% 7% ..



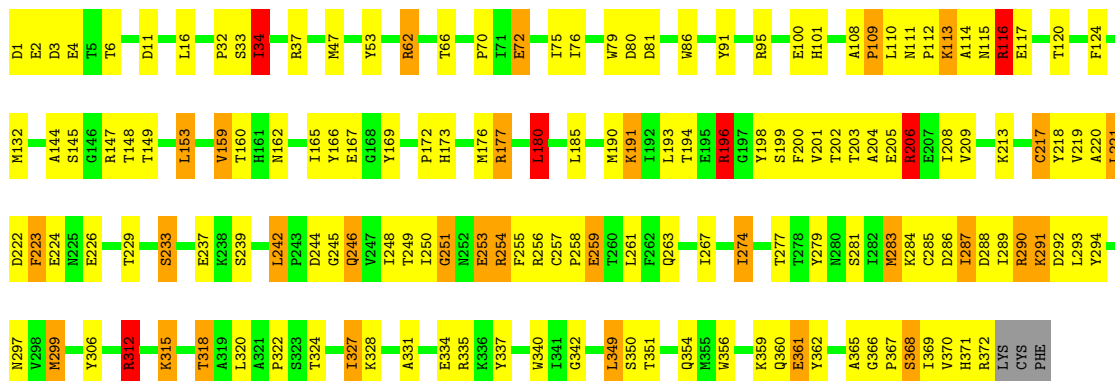
• Molecule 4: SKELETAL MUSCLE ACTIN

Chain V:  59% 32% 7% ..

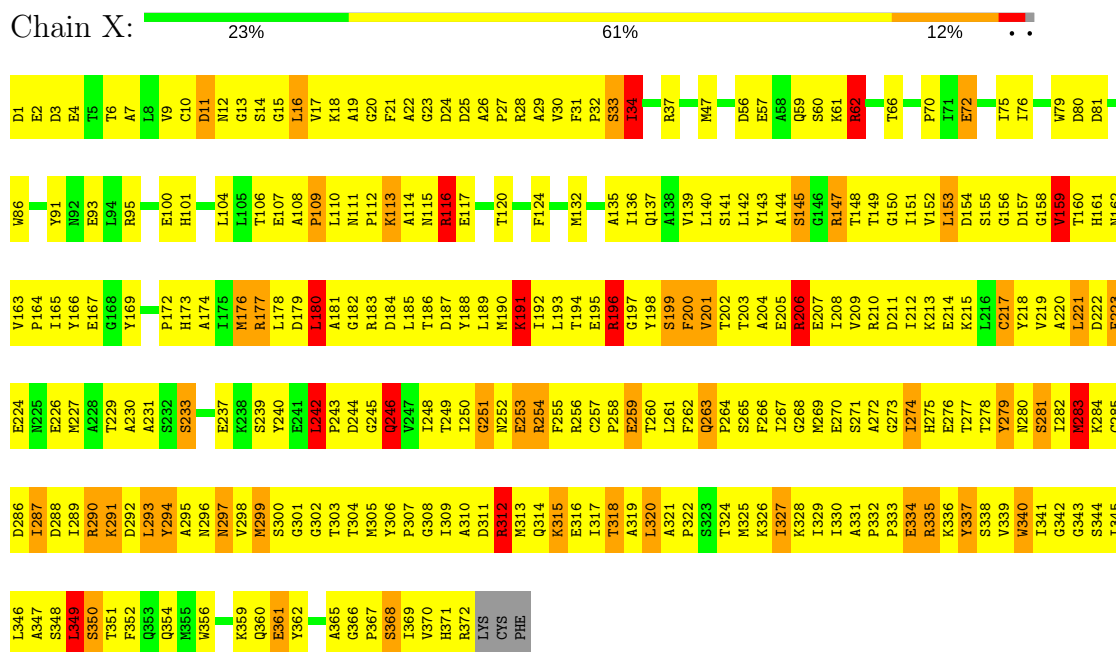


• Molecule 4: SKELETAL MUSCLE ACTIN

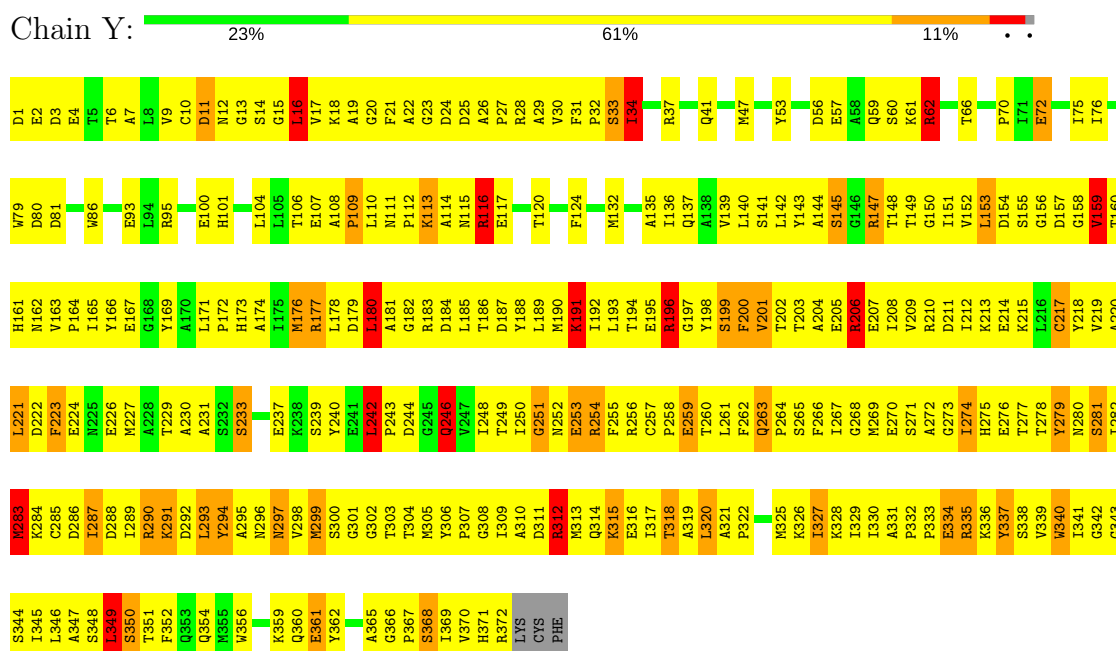
Chain W:  57% 32% 8% ..



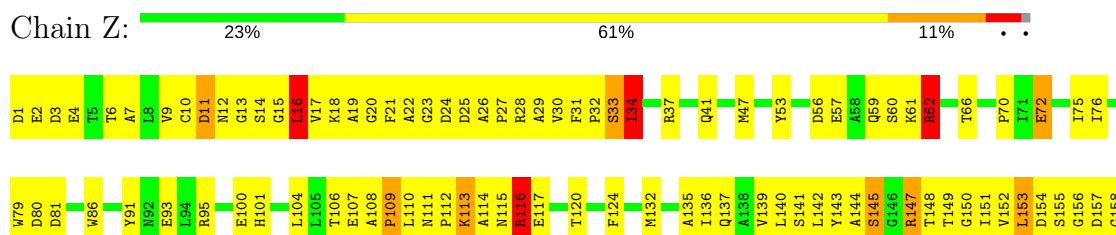
• Molecule 4: SKELETAL MUSCLE ACTIN



• Molecule 4: SKELETAL MUSCLE ACTIN



• Molecule 4: SKELETAL MUSCLE ACTIN





|      |      |      |      |
|------|------|------|------|
| G343 | I282 | A220 | N188 |
| S344 | R283 | L221 | T160 |
| I345 | K284 | D222 | H161 |
| L346 | C285 | F223 | N162 |
| A347 | D286 | E224 | P163 |
| S348 | I287 | N225 | V164 |
| L349 | D288 | E226 | I165 |
| S350 | I289 | M227 | Y166 |
| T351 | R290 | A228 | E167 |
| F352 | K291 | T229 | G168 |
| Q353 | D292 | A230 | Y169 |
| Q354 | L293 | A231 |      |
| K355 | Y294 | S232 | P172 |
| W356 | A295 | S233 | H173 |
|      | N296 |      | A174 |
|      | N297 | E237 | I175 |
| K359 | V298 | R238 | M176 |
| Q360 | M299 | S239 | R177 |
| E361 | S300 | Y240 | L178 |
| Y362 | G301 | E241 | D179 |
|      | G302 | L242 | L180 |
| A365 | T303 | P243 | A181 |
| G366 | T304 | D244 | G182 |
| P367 | N305 | G245 | R183 |
| S368 | N306 | Q246 | D184 |
| I369 | Y307 | V247 | L185 |
| V370 | G308 | I248 | T186 |
| H371 | I309 | T249 | D187 |
| R372 | A310 | I250 | Y188 |
| LYS  | D311 | G251 | L189 |
| CYS  | R312 | N252 | M190 |
| PHE  | K313 | E253 | R191 |
|      | Q314 | R254 | I192 |
|      | K315 | F255 | L193 |
|      | E316 | R256 | T194 |
|      | I317 | C257 | E195 |
|      | T318 | P258 | R196 |
|      | A319 | E259 | G197 |
|      | L320 | T260 | Y198 |
|      | A321 | L261 | S199 |
|      | P322 | F262 | F200 |
|      |      | Q263 | V201 |
|      |      | P264 | T202 |
|      | M325 | S265 | T203 |
|      | K326 | F266 | A204 |
|      | I327 | I267 | E205 |
|      | K328 | G268 | R206 |
|      | I329 | M269 | E207 |
|      | I330 | E270 | I208 |
|      | A331 | S271 | V209 |
|      | P332 | A272 | R210 |
|      | P333 | G273 | D211 |
|      | E334 | I274 | I212 |
|      | R335 | H275 | K213 |
|      | K336 | E276 | E214 |
|      | Y337 | T277 | K215 |
|      | S338 | T278 | L216 |
|      | V339 | Y279 | C217 |
|      | W340 | N280 | Y218 |
|      | I341 | S281 | V219 |
|      | G342 |      |      |

## 4 Experimental information

| Property                             | Value               | Source    |
|--------------------------------------|---------------------|-----------|
| Reconstruction method                | TOMOGRAPHY          | Depositor |
| Imposed symmetry                     | POINT, Not provided | Depositor |
| Number of tilted images used         | Not provided        | Depositor |
| Resolution determination method      | Not provided        | Depositor |
| CTF correction method                | Not provided        | Depositor |
| Microscope                           | Not provided        | Depositor |
| Voltage (kV)                         | Not provided        | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | Not provided        | Depositor |
| Minimum defocus (nm)                 | Not provided        | Depositor |
| Maximum defocus (nm)                 | Not provided        | Depositor |
| Magnification                        | Not provided        | Depositor |
| Image detector                       | KODAK S0163 FILM    | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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  >2          | RMSZ        | # Z  >2            |
| 1   | A     | 1.77         | 67/6448 (1.0%)   | 1.82        | 114/8729 (1.3%)    |
| 1   | D     | 1.77         | 65/6448 (1.0%)   | 1.82        | 114/8729 (1.3%)    |
| 1   | G     | 1.77         | 67/6448 (1.0%)   | 1.82        | 116/8729 (1.3%)    |
| 1   | J     | 1.90         | 68/6449 (1.1%)   | 1.84        | 118/8732 (1.4%)    |
| 2   | B     | 1.22         | 10/1148 (0.9%)   | 1.61        | 16/1548 (1.0%)     |
| 2   | E     | 1.22         | 10/1148 (0.9%)   | 1.61        | 16/1548 (1.0%)     |
| 2   | H     | 1.22         | 10/1148 (0.9%)   | 1.62        | 16/1548 (1.0%)     |
| 2   | K     | 1.22         | 10/1148 (0.9%)   | 1.61        | 16/1548 (1.0%)     |
| 3   | C     | 0.80         | 0/1136           | 0.95        | 4/1525 (0.3%)      |
| 3   | F     | 0.80         | 0/1136           | 0.95        | 4/1525 (0.3%)      |
| 3   | I     | 0.80         | 0/1136           | 0.95        | 4/1525 (0.3%)      |
| 3   | L     | 0.79         | 0/1136           | 0.94        | 4/1525 (0.3%)      |
| 4   | 0     | 0.89         | 1/2968 (0.0%)    | 1.64        | 52/4023 (1.3%)     |
| 4   | 1     | 0.89         | 2/2968 (0.1%)    | 1.64        | 50/4023 (1.2%)     |
| 4   | 2     | 0.89         | 1/2968 (0.0%)    | 1.64        | 52/4023 (1.3%)     |
| 4   | 3     | 0.89         | 1/2968 (0.0%)    | 1.64        | 51/4023 (1.3%)     |
| 4   | 4     | 0.89         | 1/2968 (0.0%)    | 1.64        | 51/4023 (1.3%)     |
| 4   | 5     | 0.89         | 2/2968 (0.1%)    | 1.64        | 51/4023 (1.3%)     |
| 4   | 6     | 0.89         | 2/2968 (0.1%)    | 1.64        | 52/4023 (1.3%)     |
| 4   | 7     | 0.89         | 2/2968 (0.1%)    | 1.64        | 52/4023 (1.3%)     |
| 4   | 8     | 0.89         | 2/2968 (0.1%)    | 1.64        | 51/4023 (1.3%)     |
| 4   | V     | 0.89         | 1/2968 (0.0%)    | 1.64        | 52/4023 (1.3%)     |
| 4   | W     | 0.89         | 2/2968 (0.1%)    | 1.64        | 51/4023 (1.3%)     |
| 4   | X     | 0.89         | 2/2968 (0.1%)    | 1.64        | 51/4023 (1.3%)     |
| 4   | Y     | 0.89         | 2/2968 (0.1%)    | 1.64        | 51/4023 (1.3%)     |
| 4   | Z     | 0.89         | 2/2968 (0.1%)    | 1.64        | 52/4023 (1.3%)     |
| All | All   | 1.29         | 330/76481 (0.4%) | 1.67        | 1261/103533 (1.2%) |

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

sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 1                   | 4                   |
| 1   | D     | 1                   | 4                   |
| 1   | G     | 2                   | 4                   |
| 1   | J     | 1                   | 6                   |
| 2   | B     | 0                   | 3                   |
| 2   | E     | 0                   | 3                   |
| 2   | H     | 0                   | 3                   |
| 2   | K     | 0                   | 3                   |
| 3   | C     | 0                   | 2                   |
| 3   | F     | 0                   | 2                   |
| 3   | I     | 0                   | 2                   |
| 3   | L     | 0                   | 2                   |
| 4   | 0     | 0                   | 1                   |
| 4   | 1     | 0                   | 1                   |
| 4   | 2     | 0                   | 1                   |
| 4   | 3     | 0                   | 1                   |
| 4   | 4     | 0                   | 1                   |
| 4   | 5     | 0                   | 1                   |
| 4   | 6     | 0                   | 1                   |
| 4   | 7     | 0                   | 1                   |
| 4   | 8     | 0                   | 1                   |
| 4   | V     | 0                   | 1                   |
| 4   | W     | 0                   | 1                   |
| 4   | X     | 0                   | 1                   |
| 4   | Y     | 0                   | 1                   |
| 4   | Z     | 0                   | 1                   |
| All | All   | 5                   | 52                  |

All (330) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | J     | 709 | LYS  | C-N    | -55.36 | 0.33        | 1.33     |
| 1   | J     | 649 | VAL  | CB-CG1 | 53.26  | 2.64        | 1.52     |
| 1   | G     | 649 | VAL  | CB-CG1 | 53.23  | 2.64        | 1.52     |
| 1   | D     | 649 | VAL  | CB-CG1 | 53.18  | 2.64        | 1.52     |
| 1   | A     | 649 | VAL  | CB-CG1 | 53.16  | 2.64        | 1.52     |
| 1   | D     | 623 | PHE  | CB-CG  | 48.14  | 2.33        | 1.51     |
| 1   | J     | 623 | PHE  | CB-CG  | 48.11  | 2.33        | 1.51     |
| 1   | A     | 623 | PHE  | CB-CG  | 48.09  | 2.33        | 1.51     |
| 1   | G     | 623 | PHE  | CB-CG  | 48.09  | 2.33        | 1.51     |
| 1   | A     | 649 | VAL  | CB-CG2 | 46.26  | 2.50        | 1.52     |
| 1   | G     | 649 | VAL  | CB-CG2 | 46.20  | 2.49        | 1.52     |

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| Mol | Chain | Res | Type | Atoms  | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | J     | 649 | VAL  | CB-CG2 | 46.17  | 2.49        | 1.52     |
| 1   | D     | 649 | VAL  | CB-CG2 | 46.13  | 2.49        | 1.52     |
| 1   | A     | 648 | THR  | CB-OG1 | 34.37  | 2.12        | 1.43     |
| 1   | G     | 648 | THR  | CB-OG1 | 34.36  | 2.12        | 1.43     |
| 1   | D     | 648 | THR  | CB-OG1 | 34.34  | 2.12        | 1.43     |
| 1   | J     | 648 | THR  | CB-OG1 | 34.31  | 2.11        | 1.43     |
| 1   | A     | 648 | THR  | CB-CG2 | -30.69 | 0.51        | 1.52     |
| 1   | G     | 648 | THR  | CB-CG2 | -30.68 | 0.51        | 1.52     |
| 1   | J     | 648 | THR  | CB-CG2 | -30.67 | 0.51        | 1.52     |
| 1   | D     | 648 | THR  | CB-CG2 | -30.67 | 0.51        | 1.52     |
| 1   | D     | 637 | LYS  | C-N    | -15.07 | 1.05        | 1.33     |
| 1   | J     | 637 | LYS  | C-N    | -15.00 | 1.06        | 1.33     |
| 1   | G     | 637 | LYS  | C-N    | -14.83 | 1.06        | 1.33     |
| 1   | A     | 637 | LYS  | C-N    | -14.80 | 1.06        | 1.33     |
| 1   | A     | 649 | VAL  | C-N    | -13.51 | 1.02        | 1.34     |
| 1   | G     | 649 | VAL  | C-N    | -13.49 | 1.03        | 1.34     |
| 1   | D     | 649 | VAL  | C-N    | -13.43 | 1.03        | 1.34     |
| 1   | J     | 649 | VAL  | C-N    | -13.42 | 1.03        | 1.34     |
| 2   | H     | 150 | TYR  | CB-CG  | -13.39 | 1.31        | 1.51     |
| 2   | B     | 150 | TYR  | CB-CG  | -13.36 | 1.31        | 1.51     |
| 2   | E     | 150 | TYR  | CB-CG  | -13.31 | 1.31        | 1.51     |
| 2   | K     | 150 | TYR  | CB-CG  | -13.30 | 1.31        | 1.51     |
| 2   | B     | 140 | PHE  | C-N    | -12.96 | 1.09        | 1.34     |
| 2   | E     | 140 | PHE  | C-N    | -12.96 | 1.09        | 1.34     |
| 2   | K     | 140 | PHE  | C-N    | -12.92 | 1.09        | 1.34     |
| 2   | H     | 140 | PHE  | C-N    | -12.82 | 1.09        | 1.34     |
| 2   | B     | 150 | TYR  | CG-CD2 | -11.36 | 1.24        | 1.39     |
| 2   | K     | 150 | TYR  | CG-CD2 | -11.20 | 1.24        | 1.39     |
| 2   | H     | 150 | TYR  | CG-CD2 | -11.18 | 1.24        | 1.39     |
| 2   | E     | 150 | TYR  | CG-CD2 | -11.14 | 1.24        | 1.39     |
| 2   | K     | 141 | PRO  | N-CD   | -10.60 | 1.33        | 1.47     |
| 2   | B     | 141 | PRO  | N-CD   | -10.50 | 1.33        | 1.47     |
| 2   | E     | 141 | PRO  | N-CD   | -10.45 | 1.33        | 1.47     |
| 2   | H     | 141 | PRO  | N-CD   | -10.40 | 1.33        | 1.47     |
| 1   | J     | 476 | GLU  | CD-OE1 | 8.88   | 1.35        | 1.25     |
| 1   | D     | 476 | GLU  | CD-OE1 | 8.81   | 1.35        | 1.25     |
| 1   | G     | 476 | GLU  | CD-OE1 | 8.76   | 1.35        | 1.25     |
| 1   | J     | 785 | GLU  | C-N    | 8.71   | 1.54        | 1.34     |
| 1   | A     | 622 | LEU  | C-N    | 8.68   | 1.54        | 1.34     |
| 1   | A     | 476 | GLU  | CD-OE1 | 8.66   | 1.35        | 1.25     |
| 1   | J     | 622 | LEU  | C-N    | 8.65   | 1.53        | 1.34     |
| 1   | G     | 622 | LEU  | C-N    | 8.64   | 1.53        | 1.34     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | D     | 622 | LEU  | C-N    | 8.63  | 1.53        | 1.34     |
| 1   | J     | 411 | GLU  | CD-OE1 | 8.32  | 1.34        | 1.25     |
| 1   | G     | 411 | GLU  | CD-OE1 | 8.30  | 1.34        | 1.25     |
| 2   | K     | 150 | TYR  | CA-CB  | -8.26 | 1.35        | 1.53     |
| 1   | J     | 745 | GLU  | CD-OE2 | 8.25  | 1.34        | 1.25     |
| 1   | D     | 745 | GLU  | CD-OE2 | 8.25  | 1.34        | 1.25     |
| 2   | B     | 150 | TYR  | CA-CB  | -8.23 | 1.35        | 1.53     |
| 1   | A     | 745 | GLU  | CD-OE2 | 8.15  | 1.34        | 1.25     |
| 1   | D     | 411 | GLU  | CD-OE1 | 8.11  | 1.34        | 1.25     |
| 2   | H     | 150 | TYR  | CA-CB  | -8.11 | 1.36        | 1.53     |
| 1   | G     | 745 | GLU  | CD-OE2 | 8.10  | 1.34        | 1.25     |
| 2   | E     | 150 | TYR  | CA-CB  | -8.08 | 1.36        | 1.53     |
| 1   | A     | 411 | GLU  | CD-OE1 | 8.06  | 1.34        | 1.25     |
| 1   | A     | 381 | GLU  | CD-OE1 | 8.04  | 1.34        | 1.25     |
| 1   | G     | 108 | GLU  | CD-OE1 | 7.96  | 1.34        | 1.25     |
| 1   | A     | 108 | GLU  | CD-OE1 | 7.94  | 1.34        | 1.25     |
| 1   | J     | 108 | GLU  | CD-OE1 | 7.91  | 1.34        | 1.25     |
| 1   | G     | 381 | GLU  | CD-OE1 | 7.89  | 1.34        | 1.25     |
| 1   | J     | 202 | SER  | CB-OG  | 7.84  | 1.52        | 1.42     |
| 1   | J     | 381 | GLU  | CD-OE1 | 7.83  | 1.34        | 1.25     |
| 1   | D     | 381 | GLU  | CD-OE1 | 7.81  | 1.34        | 1.25     |
| 1   | D     | 202 | SER  | CB-OG  | 7.74  | 1.52        | 1.42     |
| 1   | G     | 202 | SER  | CB-OG  | 7.72  | 1.52        | 1.42     |
| 1   | D     | 108 | GLU  | CD-OE1 | 7.65  | 1.34        | 1.25     |
| 1   | A     | 202 | SER  | CB-OG  | 7.64  | 1.52        | 1.42     |
| 1   | D     | 689 | GLU  | CD-OE2 | 7.53  | 1.33        | 1.25     |
| 1   | A     | 689 | GLU  | CD-OE2 | 7.51  | 1.33        | 1.25     |
| 1   | J     | 689 | GLU  | CD-OE2 | 7.45  | 1.33        | 1.25     |
| 1   | G     | 689 | GLU  | CD-OE2 | 7.42  | 1.33        | 1.25     |
| 1   | D     | 23  | GLU  | CD-OE1 | 7.31  | 1.33        | 1.25     |
| 1   | D     | 347 | GLU  | CD-OE1 | 7.27  | 1.33        | 1.25     |
| 1   | J     | 23  | GLU  | CD-OE1 | 7.23  | 1.33        | 1.25     |
| 1   | A     | 347 | GLU  | CD-OE1 | 7.21  | 1.33        | 1.25     |
| 1   | J     | 511 | GLU  | CD-OE1 | 7.19  | 1.33        | 1.25     |
| 1   | G     | 347 | GLU  | CD-OE1 | 7.18  | 1.33        | 1.25     |
| 1   | G     | 23  | GLU  | CD-OE1 | 7.17  | 1.33        | 1.25     |
| 1   | A     | 23  | GLU  | CD-OE1 | 7.17  | 1.33        | 1.25     |
| 1   | J     | 347 | GLU  | CD-OE1 | 7.17  | 1.33        | 1.25     |
| 1   | G     | 26  | GLU  | CD-OE1 | 7.08  | 1.33        | 1.25     |
| 1   | D     | 68  | GLU  | CD-OE2 | 7.05  | 1.33        | 1.25     |
| 1   | J     | 524 | GLU  | CD-OE1 | 7.05  | 1.33        | 1.25     |
| 1   | G     | 330 | GLU  | CD-OE1 | 7.04  | 1.33        | 1.25     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | G     | 68  | GLU  | CD-OE2  | 7.04  | 1.33        | 1.25     |
| 1   | D     | 524 | GLU  | CD-OE1  | 7.03  | 1.33        | 1.25     |
| 1   | A     | 511 | GLU  | CD-OE1  | 7.02  | 1.33        | 1.25     |
| 1   | J     | 330 | GLU  | CD-OE1  | 6.99  | 1.33        | 1.25     |
| 1   | D     | 376 | GLU  | CD-OE1  | 6.95  | 1.33        | 1.25     |
| 1   | G     | 376 | GLU  | CD-OE1  | 6.94  | 1.33        | 1.25     |
| 1   | A     | 376 | GLU  | CD-OE1  | 6.93  | 1.33        | 1.25     |
| 1   | J     | 811 | GLU  | CD-OE1  | 6.92  | 1.33        | 1.25     |
| 1   | D     | 511 | GLU  | CD-OE1  | 6.91  | 1.33        | 1.25     |
| 1   | A     | 330 | GLU  | CD-OE1  | 6.90  | 1.33        | 1.25     |
| 1   | G     | 524 | GLU  | CD-OE1  | 6.88  | 1.33        | 1.25     |
| 1   | J     | 68  | GLU  | CD-OE2  | 6.88  | 1.33        | 1.25     |
| 1   | A     | 68  | GLU  | CD-OE2  | 6.87  | 1.33        | 1.25     |
| 1   | A     | 524 | GLU  | CD-OE1  | 6.87  | 1.33        | 1.25     |
| 1   | D     | 26  | GLU  | CD-OE1  | 6.85  | 1.33        | 1.25     |
| 1   | J     | 376 | GLU  | CD-OE1  | 6.85  | 1.33        | 1.25     |
| 1   | G     | 511 | GLU  | CD-OE1  | 6.82  | 1.33        | 1.25     |
| 1   | J     | 26  | GLU  | CD-OE1  | 6.81  | 1.33        | 1.25     |
| 1   | D     | 811 | GLU  | CD-OE1  | 6.81  | 1.33        | 1.25     |
| 1   | A     | 655 | GLU  | CD-OE1  | 6.80  | 1.33        | 1.25     |
| 1   | D     | 330 | GLU  | CD-OE1  | 6.78  | 1.33        | 1.25     |
| 1   | A     | 26  | GLU  | CD-OE1  | 6.76  | 1.33        | 1.25     |
| 1   | A     | 811 | GLU  | CD-OE1  | 6.75  | 1.33        | 1.25     |
| 1   | J     | 538 | GLU  | CD-OE1  | 6.69  | 1.33        | 1.25     |
| 1   | J     | 655 | GLU  | CD-OE1  | 6.67  | 1.32        | 1.25     |
| 1   | J     | 319 | GLU  | CD-OE1  | 6.62  | 1.32        | 1.25     |
| 2   | E     | 150 | TYR  | CD2-CE2 | -6.60 | 1.29        | 1.39     |
| 1   | A     | 538 | GLU  | CD-OE1  | 6.60  | 1.32        | 1.25     |
| 1   | G     | 319 | GLU  | CD-OE1  | 6.59  | 1.32        | 1.25     |
| 1   | G     | 811 | GLU  | CD-OE1  | 6.59  | 1.32        | 1.25     |
| 1   | G     | 538 | GLU  | CD-OE1  | 6.58  | 1.32        | 1.25     |
| 1   | J     | 266 | GLU  | CD-OE2  | 6.56  | 1.32        | 1.25     |
| 1   | D     | 655 | GLU  | CD-OE1  | 6.55  | 1.32        | 1.25     |
| 1   | G     | 785 | GLU  | C-N     | 6.55  | 1.49        | 1.34     |
| 1   | G     | 89  | GLU  | CD-OE1  | 6.55  | 1.32        | 1.25     |
| 1   | G     | 655 | GLU  | CD-OE1  | 6.55  | 1.32        | 1.25     |
| 1   | A     | 319 | GLU  | CD-OE1  | 6.54  | 1.32        | 1.25     |
| 1   | A     | 266 | GLU  | CD-OE2  | 6.52  | 1.32        | 1.25     |
| 2   | B     | 150 | TYR  | CD2-CE2 | -6.52 | 1.29        | 1.39     |
| 1   | D     | 538 | GLU  | CD-OE1  | 6.50  | 1.32        | 1.25     |
| 1   | G     | 99  | GLU  | CD-OE2  | 6.48  | 1.32        | 1.25     |
| 1   | D     | 538 | GLU  | CD-OE2  | -6.46 | 1.18        | 1.25     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | D     | 266 | GLU  | CD-OE2  | 6.46  | 1.32        | 1.25     |
| 1   | A     | 538 | GLU  | CD-OE2  | -6.45 | 1.18        | 1.25     |
| 1   | D     | 319 | GLU  | CD-OE1  | 6.44  | 1.32        | 1.25     |
| 1   | J     | 89  | GLU  | CD-OE1  | 6.44  | 1.32        | 1.25     |
| 1   | D     | 99  | GLU  | CD-OE2  | 6.43  | 1.32        | 1.25     |
| 1   | A     | 89  | GLU  | CD-OE1  | 6.43  | 1.32        | 1.25     |
| 2   | K     | 150 | TYR  | CD2-CE2 | -6.42 | 1.29        | 1.39     |
| 1   | D     | 89  | GLU  | CD-OE1  | 6.41  | 1.32        | 1.25     |
| 1   | G     | 502 | GLU  | CD-OE2  | 6.41  | 1.32        | 1.25     |
| 1   | A     | 605 | GLU  | CD-OE1  | 6.40  | 1.32        | 1.25     |
| 1   | G     | 266 | GLU  | CD-OE2  | 6.38  | 1.32        | 1.25     |
| 1   | J     | 538 | GLU  | CD-OE2  | -6.38 | 1.18        | 1.25     |
| 2   | H     | 150 | TYR  | CD2-CE2 | -6.37 | 1.29        | 1.39     |
| 1   | G     | 802 | GLU  | CD-OE1  | 6.37  | 1.32        | 1.25     |
| 1   | J     | 808 | GLU  | CD-OE1  | 6.37  | 1.32        | 1.25     |
| 1   | J     | 99  | GLU  | CD-OE2  | 6.36  | 1.32        | 1.25     |
| 1   | G     | 808 | GLU  | CD-OE1  | 6.34  | 1.32        | 1.25     |
| 2   | B     | 150 | TYR  | N-CA    | -6.33 | 1.33        | 1.46     |
| 1   | J     | 6   | GLU  | CD-OE1  | 6.32  | 1.32        | 1.25     |
| 1   | G     | 605 | GLU  | CD-OE1  | 6.32  | 1.32        | 1.25     |
| 1   | G     | 538 | GLU  | CD-OE2  | -6.31 | 1.18        | 1.25     |
| 1   | D     | 808 | GLU  | CD-OE1  | 6.31  | 1.32        | 1.25     |
| 1   | A     | 808 | GLU  | CD-OE1  | 6.30  | 1.32        | 1.25     |
| 4   | 7     | 259 | GLU  | CG-CD   | 6.30  | 1.61        | 1.51     |
| 4   | 4     | 259 | GLU  | CG-CD   | 6.29  | 1.61        | 1.51     |
| 1   | D     | 502 | GLU  | CD-OE2  | 6.27  | 1.32        | 1.25     |
| 1   | J     | 502 | GLU  | CD-OE2  | 6.27  | 1.32        | 1.25     |
| 4   | X     | 259 | GLU  | CG-CD   | 6.27  | 1.61        | 1.51     |
| 1   | A     | 6   | GLU  | CD-OE1  | 6.27  | 1.32        | 1.25     |
| 4   | V     | 259 | GLU  | CG-CD   | 6.27  | 1.61        | 1.51     |
| 4   | 6     | 259 | GLU  | CG-CD   | 6.26  | 1.61        | 1.51     |
| 4   | W     | 259 | GLU  | CG-CD   | 6.25  | 1.61        | 1.51     |
| 1   | J     | 802 | GLU  | CD-OE1  | 6.25  | 1.32        | 1.25     |
| 4   | 5     | 259 | GLU  | CG-CD   | 6.24  | 1.61        | 1.51     |
| 4   | Y     | 259 | GLU  | CG-CD   | 6.24  | 1.61        | 1.51     |
| 2   | K     | 150 | TYR  | N-CA    | -6.24 | 1.33        | 1.46     |
| 1   | A     | 502 | GLU  | CD-OE2  | 6.24  | 1.32        | 1.25     |
| 1   | G     | 6   | GLU  | CD-OE1  | 6.23  | 1.32        | 1.25     |
| 4   | 2     | 259 | GLU  | CG-CD   | 6.23  | 1.61        | 1.51     |
| 4   | 8     | 259 | GLU  | CG-CD   | 6.23  | 1.61        | 1.51     |
| 2   | E     | 150 | TYR  | N-CA    | -6.22 | 1.33        | 1.46     |
| 4   | 1     | 259 | GLU  | CG-CD   | 6.22  | 1.61        | 1.51     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | D     | 6   | GLU  | CD-OE1 | 6.22  | 1.32        | 1.25     |
| 4   | 0     | 259 | GLU  | CG-CD  | 6.22  | 1.61        | 1.51     |
| 4   | Z     | 259 | GLU  | CG-CD  | 6.21  | 1.61        | 1.51     |
| 1   | D     | 605 | GLU  | CD-OE1 | 6.20  | 1.32        | 1.25     |
| 1   | J     | 605 | GLU  | CD-OE1 | 6.20  | 1.32        | 1.25     |
| 1   | A     | 99  | GLU  | CD-OE2 | 6.18  | 1.32        | 1.25     |
| 4   | 3     | 259 | GLU  | CG-CD  | 6.18  | 1.61        | 1.51     |
| 2   | H     | 150 | TYR  | N-CA   | -6.17 | 1.34        | 1.46     |
| 1   | D     | 509 | GLU  | CD-OE1 | 6.16  | 1.32        | 1.25     |
| 1   | D     | 802 | GLU  | CD-OE1 | 6.14  | 1.32        | 1.25     |
| 1   | J     | 509 | GLU  | CD-OE1 | 6.13  | 1.32        | 1.25     |
| 1   | G     | 509 | GLU  | CD-OE1 | 6.11  | 1.32        | 1.25     |
| 1   | A     | 417 | GLU  | CD-OE1 | 6.11  | 1.32        | 1.25     |
| 1   | J     | 329 | GLU  | CD-OE1 | 6.05  | 1.32        | 1.25     |
| 1   | D     | 417 | GLU  | CD-OE1 | 6.01  | 1.32        | 1.25     |
| 1   | G     | 476 | GLU  | CD-OE2 | -6.01 | 1.19        | 1.25     |
| 1   | A     | 509 | GLU  | CD-OE1 | 6.00  | 1.32        | 1.25     |
| 1   | G     | 540 | CYS  | CB-SG  | -5.98 | 1.72        | 1.81     |
| 1   | A     | 329 | GLU  | CD-OE1 | 5.97  | 1.32        | 1.25     |
| 1   | G     | 329 | GLU  | CD-OE1 | 5.96  | 1.32        | 1.25     |
| 1   | A     | 802 | GLU  | CD-OE1 | 5.96  | 1.32        | 1.25     |
| 1   | D     | 329 | GLU  | CD-OE1 | 5.91  | 1.32        | 1.25     |
| 1   | J     | 417 | GLU  | CD-OE1 | 5.89  | 1.32        | 1.25     |
| 1   | D     | 230 | GLU  | CD-OE2 | 5.88  | 1.32        | 1.25     |
| 1   | G     | 417 | GLU  | CD-OE1 | 5.88  | 1.32        | 1.25     |
| 1   | G     | 230 | GLU  | CD-OE2 | 5.86  | 1.32        | 1.25     |
| 1   | J     | 540 | CYS  | CB-SG  | -5.86 | 1.72        | 1.81     |
| 1   | D     | 468 | GLU  | CD-OE1 | 5.85  | 1.32        | 1.25     |
| 1   | J     | 230 | GLU  | CD-OE2 | 5.83  | 1.32        | 1.25     |
| 1   | J     | 476 | GLU  | CD-OE2 | -5.80 | 1.19        | 1.25     |
| 1   | G     | 597 | GLU  | CD-OE1 | 5.80  | 1.32        | 1.25     |
| 1   | J     | 527 | GLU  | CD-OE1 | 5.80  | 1.32        | 1.25     |
| 1   | D     | 476 | GLU  | CD-OE2 | -5.79 | 1.19        | 1.25     |
| 1   | G     | 218 | LEU  | CB-CG  | 5.79  | 1.69        | 1.52     |
| 1   | A     | 468 | GLU  | CD-OE1 | 5.79  | 1.32        | 1.25     |
| 1   | J     | 421 | GLU  | CD-OE2 | 5.77  | 1.32        | 1.25     |
| 1   | J     | 499 | GLU  | CD-OE2 | 5.77  | 1.31        | 1.25     |
| 1   | A     | 540 | CYS  | CB-SG  | -5.76 | 1.72        | 1.81     |
| 1   | D     | 540 | CYS  | CB-SG  | -5.76 | 1.72        | 1.81     |
| 1   | A     | 476 | GLU  | CD-OE2 | -5.76 | 1.19        | 1.25     |
| 1   | J     | 468 | GLU  | CD-OE1 | 5.75  | 1.31        | 1.25     |
| 1   | A     | 625 | THR  | CB-CG2 | 5.74  | 1.71        | 1.52     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | D     | 785 | GLU  | CD-OE2 | 5.73  | 1.31        | 1.25     |
| 1   | A     | 230 | GLU  | CD-OE2 | 5.73  | 1.31        | 1.25     |
| 1   | G     | 527 | GLU  | CD-OE1 | 5.71  | 1.31        | 1.25     |
| 1   | A     | 785 | GLU  | CD-OE2 | 5.70  | 1.31        | 1.25     |
| 1   | G     | 625 | THR  | CB-CG2 | 5.70  | 1.71        | 1.52     |
| 1   | A     | 597 | GLU  | CD-OE1 | 5.69  | 1.31        | 1.25     |
| 1   | J     | 625 | THR  | CB-CG2 | 5.69  | 1.71        | 1.52     |
| 1   | A     | 74  | GLU  | CD-OE2 | 5.67  | 1.31        | 1.25     |
| 1   | J     | 74  | GLU  | CD-OE2 | 5.67  | 1.31        | 1.25     |
| 1   | D     | 597 | GLU  | CD-OE1 | 5.67  | 1.31        | 1.25     |
| 1   | D     | 625 | THR  | CB-CG2 | 5.67  | 1.71        | 1.52     |
| 1   | J     | 785 | GLU  | CD-OE2 | 5.66  | 1.31        | 1.25     |
| 1   | J     | 218 | LEU  | CB-CG  | 5.66  | 1.69        | 1.52     |
| 1   | A     | 218 | LEU  | CB-CG  | 5.65  | 1.69        | 1.52     |
| 1   | G     | 785 | GLU  | CD-OE2 | 5.65  | 1.31        | 1.25     |
| 1   | D     | 218 | LEU  | CB-CG  | 5.63  | 1.68        | 1.52     |
| 1   | D     | 499 | GLU  | CD-OE2 | 5.62  | 1.31        | 1.25     |
| 1   | G     | 74  | GLU  | CD-OE2 | 5.61  | 1.31        | 1.25     |
| 1   | A     | 527 | GLU  | CD-OE1 | 5.61  | 1.31        | 1.25     |
| 1   | D     | 687 | GLU  | CD-OE1 | 5.60  | 1.31        | 1.25     |
| 1   | D     | 74  | GLU  | CD-OE2 | 5.58  | 1.31        | 1.25     |
| 1   | J     | 687 | GLU  | CD-OE1 | 5.56  | 1.31        | 1.25     |
| 1   | J     | 373 | GLU  | CD-OE1 | 5.56  | 1.31        | 1.25     |
| 1   | A     | 421 | GLU  | CD-OE2 | 5.54  | 1.31        | 1.25     |
| 1   | A     | 687 | GLU  | CD-OE1 | 5.54  | 1.31        | 1.25     |
| 1   | G     | 421 | GLU  | CD-OE2 | 5.54  | 1.31        | 1.25     |
| 1   | G     | 468 | GLU  | CD-OE1 | 5.53  | 1.31        | 1.25     |
| 1   | J     | 597 | GLU  | CD-OE1 | 5.52  | 1.31        | 1.25     |
| 1   | G     | 687 | GLU  | CD-OE1 | 5.51  | 1.31        | 1.25     |
| 2   | H     | 150 | TYR  | CE1-CZ | 5.51  | 1.45        | 1.38     |
| 1   | A     | 499 | GLU  | CD-OE2 | 5.50  | 1.31        | 1.25     |
| 1   | A     | 777 | GLU  | CD-OE2 | 5.50  | 1.31        | 1.25     |
| 1   | D     | 373 | GLU  | CD-OE1 | 5.50  | 1.31        | 1.25     |
| 1   | G     | 373 | GLU  | CD-OE1 | 5.49  | 1.31        | 1.25     |
| 2   | E     | 150 | TYR  | CE1-CZ | 5.48  | 1.45        | 1.38     |
| 1   | A     | 506 | GLU  | CD-OE2 | 5.48  | 1.31        | 1.25     |
| 1   | G     | 499 | GLU  | CD-OE2 | 5.48  | 1.31        | 1.25     |
| 1   | D     | 527 | GLU  | CD-OE1 | 5.47  | 1.31        | 1.25     |
| 1   | D     | 777 | GLU  | CD-OE2 | 5.47  | 1.31        | 1.25     |
| 2   | K     | 150 | TYR  | CE1-CZ | 5.46  | 1.45        | 1.38     |
| 1   | G     | 479 | CYS  | CB-SG  | -5.45 | 1.73        | 1.81     |
| 1   | A     | 373 | GLU  | CD-OE1 | 5.44  | 1.31        | 1.25     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | G     | 298 | GLU  | CD-OE2 | 5.44  | 1.31        | 1.25     |
| 1   | J     | 479 | CYS  | CB-SG  | -5.44 | 1.73        | 1.81     |
| 1   | G     | 777 | GLU  | CD-OE2 | 5.43  | 1.31        | 1.25     |
| 2   | K     | 131 | GLU  | N-CA   | 5.42  | 1.57        | 1.46     |
| 2   | E     | 131 | GLU  | N-CA   | 5.41  | 1.57        | 1.46     |
| 2   | H     | 131 | GLU  | N-CA   | 5.41  | 1.57        | 1.46     |
| 1   | A     | 479 | CYS  | CB-SG  | -5.40 | 1.73        | 1.81     |
| 1   | J     | 777 | GLU  | CD-OE2 | 5.39  | 1.31        | 1.25     |
| 1   | G     | 506 | GLU  | CD-OE2 | 5.39  | 1.31        | 1.25     |
| 2   | B     | 150 | TYR  | CE1-CZ | 5.38  | 1.45        | 1.38     |
| 1   | D     | 218 | LEU  | C-N    | -5.37 | 1.21        | 1.34     |
| 1   | A     | 218 | LEU  | C-N    | -5.36 | 1.21        | 1.34     |
| 1   | G     | 679 | GLU  | CD-OE2 | 5.36  | 1.31        | 1.25     |
| 1   | D     | 421 | GLU  | CD-OE2 | 5.35  | 1.31        | 1.25     |
| 1   | J     | 218 | LEU  | C-N    | -5.34 | 1.21        | 1.34     |
| 1   | D     | 298 | GLU  | CD-OE2 | 5.34  | 1.31        | 1.25     |
| 1   | J     | 298 | GLU  | CD-OE2 | 5.34  | 1.31        | 1.25     |
| 1   | A     | 65  | GLU  | CD-OE1 | 5.32  | 1.31        | 1.25     |
| 1   | A     | 298 | GLU  | CD-OE2 | 5.31  | 1.31        | 1.25     |
| 1   | G     | 218 | LEU  | C-N    | -5.30 | 1.21        | 1.34     |
| 2   | B     | 131 | GLU  | N-CA   | 5.29  | 1.56        | 1.46     |
| 1   | D     | 65  | GLU  | CD-OE1 | 5.29  | 1.31        | 1.25     |
| 1   | D     | 479 | CYS  | CB-SG  | -5.28 | 1.73        | 1.81     |
| 1   | J     | 679 | GLU  | CD-OE2 | 5.28  | 1.31        | 1.25     |
| 1   | J     | 527 | GLU  | CD-OE2 | -5.27 | 1.19        | 1.25     |
| 1   | D     | 679 | GLU  | CD-OE2 | 5.24  | 1.31        | 1.25     |
| 1   | J     | 65  | GLU  | CD-OE1 | 5.21  | 1.31        | 1.25     |
| 1   | D     | 282 | GLU  | CD-OE1 | 5.20  | 1.31        | 1.25     |
| 2   | K     | 149 | ASP  | CB-CG  | 5.19  | 1.62        | 1.51     |
| 1   | J     | 12  | GLU  | CD-OE2 | 5.18  | 1.31        | 1.25     |
| 1   | J     | 506 | GLU  | CD-OE2 | 5.18  | 1.31        | 1.25     |
| 1   | D     | 702 | GLU  | CD-OE2 | 5.16  | 1.31        | 1.25     |
| 2   | E     | 149 | ASP  | CB-CG  | 5.16  | 1.62        | 1.51     |
| 1   | A     | 679 | GLU  | CD-OE2 | 5.15  | 1.31        | 1.25     |
| 1   | G     | 12  | GLU  | CD-OE2 | 5.15  | 1.31        | 1.25     |
| 1   | A     | 527 | GLU  | CD-OE2 | -5.14 | 1.20        | 1.25     |
| 1   | A     | 697 | CYS  | CB-SG  | 5.14  | 1.91        | 1.82     |
| 1   | A     | 539 | GLU  | CD-OE1 | 5.13  | 1.31        | 1.25     |
| 1   | G     | 21  | GLU  | CD-OE2 | 5.13  | 1.31        | 1.25     |
| 2   | B     | 149 | ASP  | CB-CG  | 5.12  | 1.62        | 1.51     |
| 1   | A     | 702 | GLU  | CD-OE2 | 5.11  | 1.31        | 1.25     |
| 1   | D     | 506 | GLU  | CD-OE2 | 5.11  | 1.31        | 1.25     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | G     | 65  | GLU  | CD-OE1 | 5.11  | 1.31        | 1.25     |
| 1   | A     | 21  | GLU  | CD-OE2 | 5.11  | 1.31        | 1.25     |
| 1   | G     | 702 | GLU  | CD-OE2 | 5.10  | 1.31        | 1.25     |
| 1   | J     | 702 | GLU  | CD-OE2 | 5.09  | 1.31        | 1.25     |
| 1   | A     | 282 | GLU  | CD-OE1 | 5.09  | 1.31        | 1.25     |
| 1   | J     | 282 | GLU  | CD-OE1 | 5.09  | 1.31        | 1.25     |
| 1   | A     | 150 | GLU  | CD-OE1 | 5.08  | 1.31        | 1.25     |
| 1   | G     | 527 | GLU  | CD-OE2 | -5.06 | 1.20        | 1.25     |
| 1   | G     | 697 | CYS  | CB-SG  | 5.05  | 1.90        | 1.82     |
| 4   | Y     | 259 | GLU  | CB-CG  | 5.05  | 1.61        | 1.52     |
| 2   | H     | 149 | ASP  | CB-CG  | 5.05  | 1.62        | 1.51     |
| 4   | 1     | 259 | GLU  | CB-CG  | 5.05  | 1.61        | 1.52     |
| 4   | 8     | 259 | GLU  | CB-CG  | 5.05  | 1.61        | 1.52     |
| 1   | J     | 21  | GLU  | CD-OE2 | 5.05  | 1.31        | 1.25     |
| 4   | 5     | 259 | GLU  | CB-CG  | 5.04  | 1.61        | 1.52     |
| 1   | D     | 539 | GLU  | CD-OE1 | 5.04  | 1.31        | 1.25     |
| 1   | D     | 21  | GLU  | CD-OE2 | 5.03  | 1.31        | 1.25     |
| 4   | 6     | 259 | GLU  | CB-CG  | 5.03  | 1.61        | 1.52     |
| 4   | Z     | 259 | GLU  | CB-CG  | 5.03  | 1.61        | 1.52     |
| 1   | G     | 150 | GLU  | CD-OE1 | 5.02  | 1.31        | 1.25     |
| 4   | 7     | 259 | GLU  | CB-CG  | 5.02  | 1.61        | 1.52     |
| 1   | J     | 697 | CYS  | CB-SG  | 5.01  | 1.90        | 1.82     |
| 4   | W     | 259 | GLU  | CB-CG  | 5.01  | 1.61        | 1.52     |
| 4   | X     | 259 | GLU  | CB-CG  | 5.01  | 1.61        | 1.52     |
| 1   | D     | 12  | GLU  | CD-OE2 | 5.00  | 1.31        | 1.25     |

All (1261) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | G     | 637 | LYS  | O-C-N      | -58.53 | 23.69       | 123.20   |
| 1   | J     | 637 | LYS  | O-C-N      | -58.47 | 23.80       | 123.20   |
| 1   | D     | 637 | LYS  | O-C-N      | -58.47 | 23.81       | 123.20   |
| 1   | A     | 637 | LYS  | O-C-N      | -58.45 | 23.83       | 123.20   |
| 1   | J     | 649 | VAL  | CG1-CB-CG2 | -34.02 | 56.47       | 110.90   |
| 1   | D     | 649 | VAL  | CG1-CB-CG2 | -34.00 | 56.50       | 110.90   |
| 1   | A     | 649 | VAL  | CG1-CB-CG2 | -33.99 | 56.51       | 110.90   |
| 1   | G     | 649 | VAL  | CG1-CB-CG2 | -33.98 | 56.53       | 110.90   |
| 1   | J     | 648 | THR  | CA-CB-OG1  | -31.72 | 42.38       | 109.00   |
| 1   | A     | 648 | THR  | CA-CB-OG1  | -31.70 | 42.43       | 109.00   |
| 1   | D     | 648 | THR  | CA-CB-OG1  | -31.70 | 42.43       | 109.00   |
| 1   | G     | 648 | THR  | CA-CB-OG1  | -31.68 | 42.48       | 109.00   |
| 2   | H     | 150 | TYR  | CB-CG-CD2  | -28.73 | 103.76      | 121.00   |

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| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 2   | E     | 150 | TYR  | CB-CG-CD2  | -28.64 | 103.81      | 121.00   |
| 2   | K     | 150 | TYR  | CB-CG-CD2  | -28.60 | 103.84      | 121.00   |
| 2   | B     | 150 | TYR  | CB-CG-CD2  | -28.58 | 103.85      | 121.00   |
| 1   | G     | 649 | VAL  | CA-CB-CG1  | -28.52 | 68.11       | 110.90   |
| 1   | J     | 649 | VAL  | CA-CB-CG1  | -28.49 | 68.16       | 110.90   |
| 1   | D     | 649 | VAL  | CA-CB-CG1  | -28.47 | 68.19       | 110.90   |
| 1   | A     | 649 | VAL  | CA-CB-CG1  | -28.45 | 68.23       | 110.90   |
| 1   | J     | 649 | VAL  | CA-CB-CG2  | -28.18 | 68.62       | 110.90   |
| 1   | G     | 649 | VAL  | CA-CB-CG2  | -28.17 | 68.64       | 110.90   |
| 1   | A     | 649 | VAL  | CA-CB-CG2  | -28.17 | 68.64       | 110.90   |
| 1   | D     | 649 | VAL  | CA-CB-CG2  | -28.16 | 68.66       | 110.90   |
| 1   | D     | 648 | THR  | CA-CB-CG2  | -25.60 | 76.56       | 112.40   |
| 1   | J     | 648 | THR  | CA-CB-CG2  | -25.56 | 76.61       | 112.40   |
| 1   | A     | 648 | THR  | CA-CB-CG2  | -25.45 | 76.78       | 112.40   |
| 1   | G     | 648 | THR  | CA-CB-CG2  | -25.36 | 76.90       | 112.40   |
| 1   | J     | 709 | LYS  | O-C-N      | -21.06 | 87.39       | 123.20   |
| 2   | H     | 150 | TYR  | CG-CD2-CE2 | -20.84 | 104.63      | 121.30   |
| 2   | K     | 150 | TYR  | CG-CD2-CE2 | -20.66 | 104.78      | 121.30   |
| 2   | E     | 150 | TYR  | CG-CD2-CE2 | -20.54 | 104.86      | 121.30   |
| 2   | B     | 150 | TYR  | CG-CD2-CE2 | -20.43 | 104.95      | 121.30   |
| 2   | K     | 150 | TYR  | CD1-CG-CD2 | 19.49  | 139.34      | 117.90   |
| 2   | H     | 150 | TYR  | CD1-CG-CD2 | 19.45  | 139.29      | 117.90   |
| 2   | E     | 150 | TYR  | CD1-CG-CD2 | 19.40  | 139.24      | 117.90   |
| 2   | B     | 150 | TYR  | CD1-CG-CD2 | 19.38  | 139.22      | 117.90   |
| 2   | H     | 150 | TYR  | CG-CD1-CE1 | -18.44 | 106.55      | 121.30   |
| 2   | K     | 150 | TYR  | CG-CD1-CE1 | -18.44 | 106.55      | 121.30   |
| 2   | B     | 150 | TYR  | CG-CD1-CE1 | -18.39 | 106.59      | 121.30   |
| 2   | E     | 150 | TYR  | CG-CD1-CE1 | -18.38 | 106.59      | 121.30   |
| 1   | J     | 800 | ARG  | NE-CZ-NH2  | -16.61 | 112.00      | 120.30   |
| 1   | D     | 800 | ARG  | NE-CZ-NH2  | -16.48 | 112.06      | 120.30   |
| 1   | G     | 800 | ARG  | NE-CZ-NH2  | -16.31 | 112.14      | 120.30   |
| 1   | A     | 800 | ARG  | NE-CZ-NH2  | -16.29 | 112.16      | 120.30   |
| 1   | G     | 623 | PHE  | CB-CG-CD2  | -13.78 | 111.16      | 120.80   |
| 1   | J     | 623 | PHE  | CB-CG-CD2  | -13.67 | 111.23      | 120.80   |
| 1   | A     | 623 | PHE  | CB-CG-CD2  | -13.64 | 111.25      | 120.80   |
| 1   | D     | 623 | PHE  | CB-CG-CD2  | -13.64 | 111.25      | 120.80   |
| 1   | A     | 623 | PHE  | CB-CG-CD1  | 12.37  | 129.46      | 120.80   |
| 1   | G     | 623 | PHE  | CB-CG-CD1  | 12.35  | 129.45      | 120.80   |
| 1   | J     | 623 | PHE  | CB-CG-CD1  | 12.33  | 129.43      | 120.80   |
| 1   | J     | 623 | PHE  | CA-CB-CG   | -12.27 | 84.47       | 113.90   |
| 1   | A     | 623 | PHE  | CA-CB-CG   | -12.26 | 84.48       | 113.90   |
| 1   | D     | 623 | PHE  | CA-CB-CG   | -12.23 | 84.54       | 113.90   |

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| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1   | G     | 623 | PHE  | CA-CB-CG  | -12.21 | 84.59       | 113.90   |
| 1   | D     | 623 | PHE  | CB-CG-CD1 | 12.03  | 129.22      | 120.80   |
| 1   | J     | 98  | HIS  | CB-CA-C   | -11.57 | 87.27       | 110.40   |
| 1   | A     | 98  | HIS  | CB-CA-C   | -11.56 | 87.29       | 110.40   |
| 1   | G     | 98  | HIS  | CB-CA-C   | -11.55 | 87.29       | 110.40   |
| 1   | D     | 98  | HIS  | CB-CA-C   | -11.54 | 87.33       | 110.40   |
| 1   | G     | 568 | PRO  | O-C-N     | 10.71  | 139.83      | 122.70   |
| 1   | A     | 568 | PRO  | O-C-N     | 10.67  | 139.78      | 122.70   |
| 1   | D     | 568 | PRO  | O-C-N     | 10.66  | 139.76      | 122.70   |
| 1   | J     | 568 | PRO  | O-C-N     | 10.58  | 139.63      | 122.70   |
| 1   | J     | 709 | LYS  | C-N-CA    | 10.30  | 143.93      | 122.30   |
| 2   | E     | 141 | PRO  | CA-N-CD   | 10.30  | 126.11      | 111.70   |
| 2   | H     | 141 | PRO  | CA-N-CD   | 10.27  | 126.08      | 111.70   |
| 2   | K     | 141 | PRO  | CA-N-CD   | 10.21  | 125.99      | 111.70   |
| 2   | B     | 141 | PRO  | CA-N-CD   | 10.18  | 125.95      | 111.70   |
| 1   | G     | 625 | THR  | CA-CB-CG2 | -10.10 | 98.26       | 112.40   |
| 1   | A     | 327 | ASP  | CB-CG-OD1 | -10.06 | 109.24      | 118.30   |
| 1   | G     | 327 | ASP  | CB-CG-OD1 | -10.05 | 109.25      | 118.30   |
| 1   | J     | 327 | ASP  | CB-CG-OD1 | -10.04 | 109.26      | 118.30   |
| 1   | A     | 625 | THR  | CA-CB-CG2 | -10.03 | 98.35       | 112.40   |
| 1   | J     | 625 | THR  | CA-CB-CG2 | -10.03 | 98.36       | 112.40   |
| 1   | D     | 625 | THR  | CA-CB-CG2 | -10.02 | 98.38       | 112.40   |
| 1   | D     | 327 | ASP  | CB-CG-OD1 | -10.00 | 109.30      | 118.30   |
| 1   | A     | 241 | ASP  | CB-CG-OD1 | -9.85  | 109.44      | 118.30   |
| 1   | G     | 241 | ASP  | CB-CG-OD1 | -9.80  | 109.48      | 118.30   |
| 3   | C     | 63  | ILE  | O-C-N     | 9.80   | 138.38      | 122.70   |
| 1   | D     | 728 | ASN  | O-C-N     | 9.76   | 138.32      | 122.70   |
| 1   | J     | 241 | ASP  | CB-CG-OD1 | -9.73  | 109.54      | 118.30   |
| 1   | D     | 241 | ASP  | CB-CG-OD1 | -9.73  | 109.55      | 118.30   |
| 3   | I     | 63  | ILE  | O-C-N     | 9.72   | 138.25      | 122.70   |
| 3   | F     | 63  | ILE  | O-C-N     | 9.71   | 138.23      | 122.70   |
| 1   | A     | 728 | ASN  | O-C-N     | 9.68   | 138.19      | 122.70   |
| 1   | J     | 728 | ASN  | O-C-N     | 9.67   | 138.17      | 122.70   |
| 3   | L     | 63  | ILE  | O-C-N     | 9.66   | 138.16      | 122.70   |
| 1   | G     | 728 | ASN  | O-C-N     | 9.60   | 138.06      | 122.70   |
| 1   | G     | 264 | ASP  | CB-CG-OD2 | -9.50  | 109.75      | 118.30   |
| 1   | D     | 264 | ASP  | CB-CG-OD2 | -9.42  | 109.82      | 118.30   |
| 1   | A     | 264 | ASP  | CB-CG-OD2 | -9.42  | 109.82      | 118.30   |
| 1   | J     | 709 | LYS  | CA-C-N    | 9.42   | 135.04      | 116.20   |
| 2   | E     | 150 | TYR  | N-CA-CB   | -9.40  | 93.68       | 110.60   |
| 1   | J     | 264 | ASP  | CB-CG-OD2 | -9.38  | 109.86      | 118.30   |
| 2   | H     | 150 | TYR  | N-CA-CB   | -9.36  | 93.75       | 110.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | K     | 150 | TYR  | N-CA-CB    | -9.36 | 93.75       | 110.60   |
| 2   | B     | 150 | TYR  | N-CA-CB    | -9.28 | 93.90       | 110.60   |
| 4   | W     | 356 | TRP  | CD1-CG-CD2 | 9.18  | 113.64      | 106.30   |
| 4   | 8     | 356 | TRP  | CD1-CG-CD2 | 9.17  | 113.64      | 106.30   |
| 4   | Y     | 356 | TRP  | CD1-CG-CD2 | 9.17  | 113.64      | 106.30   |
| 4   | 3     | 356 | TRP  | CD1-CG-CD2 | 9.17  | 113.63      | 106.30   |
| 4   | 2     | 356 | TRP  | CD1-CG-CD2 | 9.16  | 113.63      | 106.30   |
| 4   | 5     | 356 | TRP  | CD1-CG-CD2 | 9.16  | 113.63      | 106.30   |
| 4   | 0     | 356 | TRP  | CD1-CG-CD2 | 9.14  | 113.61      | 106.30   |
| 4   | 6     | 356 | TRP  | CD1-CG-CD2 | 9.11  | 113.59      | 106.30   |
| 4   | 4     | 356 | TRP  | CD1-CG-CD2 | 9.10  | 113.58      | 106.30   |
| 4   | V     | 356 | TRP  | CD1-CG-CD2 | 9.10  | 113.58      | 106.30   |
| 4   | 7     | 356 | TRP  | CD1-CG-CD2 | 9.10  | 113.58      | 106.30   |
| 4   | X     | 356 | TRP  | CD1-CG-CD2 | 9.06  | 113.54      | 106.30   |
| 4   | Z     | 356 | TRP  | CD1-CG-CD2 | 9.04  | 113.53      | 106.30   |
| 4   | 1     | 356 | TRP  | CD1-CG-CD2 | 9.02  | 113.51      | 106.30   |
| 1   | J     | 378 | ASP  | CB-CG-OD2  | 8.98  | 126.39      | 118.30   |
| 1   | J     | 352 | TYR  | CB-CG-CD1  | 8.97  | 126.38      | 121.00   |
| 1   | D     | 378 | ASP  | CB-CG-OD2  | 8.95  | 126.35      | 118.30   |
| 1   | A     | 378 | ASP  | CB-CG-OD2  | 8.92  | 126.32      | 118.30   |
| 1   | G     | 378 | ASP  | CB-CG-OD2  | 8.91  | 126.32      | 118.30   |
| 1   | G     | 352 | TYR  | CB-CG-CD1  | 8.84  | 126.30      | 121.00   |
| 4   | 2     | 177 | ARG  | NE-CZ-NH2  | -8.80 | 115.90      | 120.30   |
| 1   | D     | 352 | TYR  | CB-CG-CD1  | 8.77  | 126.26      | 121.00   |
| 2   | K     | 138 | ALA  | O-C-N      | -8.74 | 108.72      | 122.70   |
| 2   | E     | 138 | ALA  | O-C-N      | -8.72 | 108.75      | 122.70   |
| 1   | A     | 352 | TYR  | CB-CG-CD1  | 8.72  | 126.23      | 121.00   |
| 4   | 4     | 177 | ARG  | NE-CZ-NH2  | -8.70 | 115.95      | 120.30   |
| 2   | B     | 138 | ALA  | O-C-N      | -8.70 | 108.79      | 122.70   |
| 2   | H     | 138 | ALA  | O-C-N      | -8.65 | 108.86      | 122.70   |
| 4   | 7     | 177 | ARG  | NE-CZ-NH2  | -8.64 | 115.98      | 120.30   |
| 4   | W     | 177 | ARG  | NE-CZ-NH2  | -8.57 | 116.02      | 120.30   |
| 4   | 4     | 86  | TRP  | CD1-CG-CD2 | 8.53  | 113.13      | 106.30   |
| 4   | Y     | 86  | TRP  | CD1-CG-CD2 | 8.53  | 113.12      | 106.30   |
| 1   | D     | 601 | ASP  | CB-CG-OD1  | -8.52 | 110.63      | 118.30   |
| 4   | X     | 177 | ARG  | NE-CZ-NH2  | -8.52 | 116.04      | 120.30   |
| 4   | X     | 86  | TRP  | CD1-CG-CD2 | 8.52  | 113.11      | 106.30   |
| 1   | G     | 601 | ASP  | CB-CG-OD1  | -8.51 | 110.64      | 118.30   |
| 4   | 8     | 177 | ARG  | NE-CZ-NH2  | -8.50 | 116.05      | 120.30   |
| 4   | 7     | 86  | TRP  | CD1-CG-CD2 | 8.49  | 113.09      | 106.30   |
| 1   | J     | 601 | ASP  | CB-CG-OD1  | -8.49 | 110.66      | 118.30   |
| 4   | 0     | 177 | ARG  | NE-CZ-NH2  | -8.48 | 116.06      | 120.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | 5     | 177 | ARG  | NE-CZ-NH2  | -8.47 | 116.06      | 120.30   |
| 4   | V     | 177 | ARG  | NE-CZ-NH2  | -8.47 | 116.06      | 120.30   |
| 4   | Z     | 177 | ARG  | NE-CZ-NH2  | -8.47 | 116.06      | 120.30   |
| 4   | 5     | 86  | TRP  | CD1-CG-CD2 | 8.47  | 113.08      | 106.30   |
| 4   | 6     | 86  | TRP  | CD1-CG-CD2 | 8.46  | 113.07      | 106.30   |
| 4   | Z     | 86  | TRP  | CD1-CG-CD2 | 8.46  | 113.07      | 106.30   |
| 4   | 2     | 86  | TRP  | CD1-CG-CD2 | 8.46  | 113.07      | 106.30   |
| 4   | 1     | 177 | ARG  | NE-CZ-NH2  | -8.46 | 116.07      | 120.30   |
| 4   | 3     | 177 | ARG  | NE-CZ-NH2  | -8.46 | 116.07      | 120.30   |
| 4   | 6     | 177 | ARG  | NE-CZ-NH2  | -8.46 | 116.07      | 120.30   |
| 4   | 8     | 86  | TRP  | CD1-CG-CD2 | 8.45  | 113.06      | 106.30   |
| 1   | J     | 33  | ASP  | CB-CG-OD1  | -8.44 | 110.71      | 118.30   |
| 4   | 0     | 86  | TRP  | CD1-CG-CD2 | 8.44  | 113.05      | 106.30   |
| 4   | V     | 86  | TRP  | CD1-CG-CD2 | 8.43  | 113.04      | 106.30   |
| 1   | A     | 601 | ASP  | CB-CG-OD1  | -8.42 | 110.72      | 118.30   |
| 4   | 3     | 86  | TRP  | CD1-CG-CD2 | 8.42  | 113.03      | 106.30   |
| 4   | W     | 86  | TRP  | CD1-CG-CD2 | 8.41  | 113.03      | 106.30   |
| 1   | J     | 352 | TYR  | CB-CG-CD2  | -8.38 | 115.97      | 121.00   |
| 1   | G     | 33  | ASP  | CB-CG-OD1  | -8.36 | 110.78      | 118.30   |
| 4   | 1     | 86  | TRP  | CD1-CG-CD2 | 8.36  | 112.99      | 106.30   |
| 1   | A     | 352 | TYR  | CB-CG-CD2  | -8.33 | 116.00      | 121.00   |
| 1   | D     | 33  | ASP  | CB-CG-OD1  | -8.27 | 110.85      | 118.30   |
| 4   | Y     | 177 | ARG  | NE-CZ-NH2  | -8.24 | 116.18      | 120.30   |
| 1   | A     | 33  | ASP  | CB-CG-OD1  | -8.22 | 110.90      | 118.30   |
| 1   | G     | 352 | TYR  | CB-CG-CD2  | -8.18 | 116.09      | 121.00   |
| 1   | D     | 352 | TYR  | CB-CG-CD2  | -8.10 | 116.14      | 121.00   |
| 1   | A     | 339 | ASP  | CB-CG-OD1  | -8.04 | 111.06      | 118.30   |
| 4   | 3     | 356 | TRP  | CE2-CD2-CG | -8.04 | 100.87      | 107.30   |
| 4   | Y     | 356 | TRP  | CE2-CD2-CG | -8.01 | 100.89      | 107.30   |
| 4   | 5     | 356 | TRP  | CE2-CD2-CG | -8.00 | 100.90      | 107.30   |
| 4   | V     | 356 | TRP  | CE2-CD2-CG | -8.00 | 100.90      | 107.30   |
| 4   | 8     | 356 | TRP  | CE2-CD2-CG | -7.99 | 100.91      | 107.30   |
| 4   | 0     | 356 | TRP  | CE2-CD2-CG | -7.99 | 100.91      | 107.30   |
| 4   | 7     | 356 | TRP  | CE2-CD2-CG | -7.99 | 100.91      | 107.30   |
| 4   | 6     | 356 | TRP  | CE2-CD2-CG | -7.98 | 100.92      | 107.30   |
| 4   | W     | 356 | TRP  | CE2-CD2-CG | -7.97 | 100.92      | 107.30   |
| 1   | D     | 637 | LYS  | CA-C-N     | 7.93  | 132.06      | 116.20   |
| 4   | 2     | 356 | TRP  | CE2-CD2-CG | -7.92 | 100.96      | 107.30   |
| 4   | X     | 356 | TRP  | CE2-CD2-CG | -7.92 | 100.97      | 107.30   |
| 1   | A     | 637 | LYS  | CA-C-N     | 7.91  | 132.01      | 116.20   |
| 1   | G     | 339 | ASP  | CB-CG-OD1  | -7.91 | 111.18      | 118.30   |
| 1   | J     | 637 | LYS  | CA-C-N     | 7.91  | 132.01      | 116.20   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | Z     | 356 | TRP  | CE2-CD2-CG | -7.90 | 100.98      | 107.30   |
| 2   | E     | 150 | TYR  | CD1-CE1-CZ | -7.90 | 112.69      | 119.80   |
| 1   | G     | 637 | LYS  | CA-C-N     | 7.89  | 131.97      | 116.20   |
| 1   | D     | 339 | ASP  | CB-CG-OD1  | -7.88 | 111.21      | 118.30   |
| 4   | 1     | 356 | TRP  | CE2-CD2-CG | -7.87 | 101.00      | 107.30   |
| 2   | H     | 150 | TYR  | CD1-CE1-CZ | -7.87 | 112.72      | 119.80   |
| 4   | 4     | 356 | TRP  | CE2-CD2-CG | -7.86 | 101.01      | 107.30   |
| 1   | J     | 339 | ASP  | CB-CG-OD1  | -7.84 | 111.24      | 118.30   |
| 1   | A     | 202 | SER  | CB-CA-C    | -7.78 | 95.31       | 110.10   |
| 2   | B     | 150 | TYR  | CD1-CE1-CZ | -7.76 | 112.81      | 119.80   |
| 1   | D     | 202 | SER  | CB-CA-C    | -7.76 | 95.35       | 110.10   |
| 2   | K     | 150 | TYR  | CD1-CE1-CZ | -7.74 | 112.83      | 119.80   |
| 1   | J     | 202 | SER  | CB-CA-C    | -7.73 | 95.41       | 110.10   |
| 4   | 0     | 312 | ARG  | NE-CZ-NH2  | 7.73  | 124.17      | 120.30   |
| 1   | G     | 202 | SER  | CB-CA-C    | -7.72 | 95.44       | 110.10   |
| 4   | 1     | 312 | ARG  | NE-CZ-NH2  | 7.69  | 124.15      | 120.30   |
| 1   | G     | 654 | ARG  | NE-CZ-NH1  | 7.68  | 124.14      | 120.30   |
| 4   | X     | 312 | ARG  | NE-CZ-NH2  | 7.68  | 124.14      | 120.30   |
| 4   | 5     | 312 | ARG  | NE-CZ-NH2  | 7.68  | 124.14      | 120.30   |
| 4   | 3     | 312 | ARG  | NE-CZ-NH2  | 7.66  | 124.13      | 120.30   |
| 1   | J     | 653 | PHE  | CB-CG-CD1  | -7.66 | 115.44      | 120.80   |
| 4   | Y     | 312 | ARG  | NE-CZ-NH2  | 7.65  | 124.13      | 120.30   |
| 1   | D     | 653 | PHE  | CB-CG-CD1  | -7.65 | 115.45      | 120.80   |
| 4   | X     | 86  | TRP  | CE2-CD2-CG | -7.63 | 101.19      | 107.30   |
| 4   | Z     | 312 | ARG  | NE-CZ-NH2  | 7.63  | 124.12      | 120.30   |
| 4   | 4     | 312 | ARG  | NE-CZ-NH2  | 7.63  | 124.11      | 120.30   |
| 4   | 8     | 312 | ARG  | NE-CZ-NH2  | 7.62  | 124.11      | 120.30   |
| 4   | 2     | 312 | ARG  | NE-CZ-NH2  | 7.60  | 124.10      | 120.30   |
| 4   | 8     | 86  | TRP  | CE2-CD2-CG | -7.59 | 101.22      | 107.30   |
| 4   | 4     | 86  | TRP  | CE2-CD2-CG | -7.58 | 101.24      | 107.30   |
| 4   | V     | 312 | ARG  | NE-CZ-NH2  | 7.56  | 124.08      | 120.30   |
| 4   | 7     | 86  | TRP  | CE2-CD2-CG | -7.56 | 101.25      | 107.30   |
| 4   | 0     | 86  | TRP  | CE2-CD2-CG | -7.56 | 101.25      | 107.30   |
| 4   | 6     | 312 | ARG  | NE-CZ-NH2  | 7.56  | 124.08      | 120.30   |
| 1   | A     | 654 | ARG  | NE-CZ-NH1  | 7.55  | 124.08      | 120.30   |
| 4   | Y     | 86  | TRP  | CE2-CD2-CG | -7.55 | 101.26      | 107.30   |
| 1   | G     | 653 | PHE  | CB-CG-CD1  | -7.54 | 115.52      | 120.80   |
| 4   | 7     | 312 | ARG  | NE-CZ-NH2  | 7.53  | 124.06      | 120.30   |
| 2   | E     | 127 | ARG  | NE-CZ-NH2  | 7.52  | 124.06      | 120.30   |
| 4   | 2     | 86  | TRP  | CE2-CD2-CG | -7.52 | 101.28      | 107.30   |
| 4   | V     | 86  | TRP  | CE2-CD2-CG | -7.52 | 101.28      | 107.30   |
| 3   | C     | 63  | ILE  | CG1-CB-CG2 | -7.52 | 94.86       | 111.40   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | 5     | 86  | TRP  | CE2-CD2-CG | -7.51 | 101.29      | 107.30   |
| 4   | W     | 86  | TRP  | CE2-CD2-CG | -7.51 | 101.29      | 107.30   |
| 4   | W     | 312 | ARG  | NE-CZ-NH2  | 7.49  | 124.05      | 120.30   |
| 4   | 3     | 86  | TRP  | CE2-CD2-CG | -7.49 | 101.31      | 107.30   |
| 3   | F     | 63  | ILE  | CG1-CB-CG2 | -7.48 | 94.94       | 111.40   |
| 1   | G     | 346 | ASP  | CB-CG-OD2  | -7.48 | 111.57      | 118.30   |
| 1   | J     | 654 | ARG  | NE-CZ-NH1  | 7.47  | 124.04      | 120.30   |
| 3   | L     | 63  | ILE  | CG1-CB-CG2 | -7.47 | 94.96       | 111.40   |
| 3   | I     | 63  | ILE  | CG1-CB-CG2 | -7.47 | 94.97       | 111.40   |
| 4   | 6     | 86  | TRP  | CE2-CD2-CG | -7.46 | 101.33      | 107.30   |
| 4   | Z     | 86  | TRP  | CE2-CD2-CG | -7.46 | 101.33      | 107.30   |
| 4   | 1     | 86  | TRP  | CE2-CD2-CG | -7.46 | 101.33      | 107.30   |
| 1   | A     | 653 | PHE  | CB-CG-CD1  | -7.46 | 115.58      | 120.80   |
| 1   | J     | 518 | ASP  | CB-CG-OD1  | -7.43 | 111.61      | 118.30   |
| 1   | A     | 518 | ASP  | CB-CG-OD1  | -7.40 | 111.64      | 118.30   |
| 4   | 1     | 254 | ARG  | NE-CZ-NH2  | -7.40 | 116.60      | 120.30   |
| 3   | I     | 63  | ILE  | CA-C-N     | -7.39 | 100.94      | 117.20   |
| 4   | W     | 180 | LEU  | CA-CB-CG   | 7.39  | 132.29      | 115.30   |
| 4   | 0     | 233 | SER  | CA-C-N     | -7.38 | 100.95      | 117.20   |
| 4   | W     | 233 | SER  | CA-C-N     | -7.38 | 100.96      | 117.20   |
| 4   | 6     | 233 | SER  | CA-C-N     | -7.38 | 100.97      | 117.20   |
| 4   | X     | 233 | SER  | CA-C-N     | -7.37 | 100.98      | 117.20   |
| 4   | 1     | 233 | SER  | CA-C-N     | -7.37 | 100.98      | 117.20   |
| 2   | B     | 127 | ARG  | NE-CZ-NH2  | 7.37  | 123.98      | 120.30   |
| 1   | D     | 346 | ASP  | CB-CG-OD2  | -7.37 | 111.67      | 118.30   |
| 1   | D     | 654 | ARG  | NE-CZ-NH1  | 7.37  | 123.98      | 120.30   |
| 4   | 8     | 233 | SER  | CA-C-N     | -7.37 | 101.00      | 117.20   |
| 4   | 3     | 233 | SER  | CA-C-N     | -7.36 | 101.00      | 117.20   |
| 4   | 5     | 233 | SER  | CA-C-N     | -7.36 | 101.00      | 117.20   |
| 1   | D     | 518 | ASP  | CB-CG-OD1  | -7.36 | 111.68      | 118.30   |
| 4   | 4     | 233 | SER  | CA-C-N     | -7.36 | 101.02      | 117.20   |
| 4   | 7     | 233 | SER  | CA-C-N     | -7.36 | 101.01      | 117.20   |
| 3   | C     | 63  | ILE  | CA-C-N     | -7.36 | 101.02      | 117.20   |
| 4   | V     | 233 | SER  | CA-C-N     | -7.36 | 101.02      | 117.20   |
| 4   | 7     | 180 | LEU  | CA-CB-CG   | 7.35  | 132.21      | 115.30   |
| 4   | 1     | 180 | LEU  | CA-CB-CG   | 7.35  | 132.20      | 115.30   |
| 4   | Z     | 233 | SER  | CA-C-N     | -7.35 | 101.03      | 117.20   |
| 4   | 2     | 233 | SER  | CA-C-N     | -7.35 | 101.04      | 117.20   |
| 4   | 6     | 180 | LEU  | CA-CB-CG   | 7.34  | 132.19      | 115.30   |
| 4   | 3     | 180 | LEU  | CA-CB-CG   | 7.34  | 132.19      | 115.30   |
| 4   | 5     | 180 | LEU  | CA-CB-CG   | 7.34  | 132.19      | 115.30   |
| 3   | L     | 63  | ILE  | CA-C-N     | -7.34 | 101.05      | 117.20   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | X     | 180 | LEU  | CA-CB-CG   | 7.34  | 132.18      | 115.30   |
| 4   | 0     | 180 | LEU  | CA-CB-CG   | 7.33  | 132.17      | 115.30   |
| 4   | V     | 180 | LEU  | CA-CB-CG   | 7.33  | 132.16      | 115.30   |
| 4   | Y     | 233 | SER  | CA-C-N     | -7.33 | 101.08      | 117.20   |
| 1   | A     | 346 | ASP  | CB-CG-OD2  | -7.33 | 111.71      | 118.30   |
| 4   | 4     | 180 | LEU  | CA-CB-CG   | 7.33  | 132.15      | 115.30   |
| 4   | 8     | 180 | LEU  | CA-CB-CG   | 7.32  | 132.14      | 115.30   |
| 3   | F     | 63  | ILE  | CA-C-N     | -7.31 | 101.11      | 117.20   |
| 4   | 2     | 180 | LEU  | CA-CB-CG   | 7.31  | 132.12      | 115.30   |
| 4   | Y     | 180 | LEU  | CA-CB-CG   | 7.31  | 132.10      | 115.30   |
| 4   | Z     | 180 | LEU  | CA-CB-CG   | 7.30  | 132.09      | 115.30   |
| 1   | G     | 104 | TYR  | CB-CG-CD2  | 7.30  | 125.38      | 121.00   |
| 4   | 2     | 254 | ARG  | NE-CZ-NH2  | -7.30 | 116.65      | 120.30   |
| 1   | J     | 346 | ASP  | CB-CG-OD2  | -7.29 | 111.73      | 118.30   |
| 4   | W     | 254 | ARG  | NE-CZ-NH2  | -7.29 | 116.66      | 120.30   |
| 4   | 4     | 254 | ARG  | NE-CZ-NH2  | -7.28 | 116.66      | 120.30   |
| 4   | X     | 79  | TRP  | CD1-CG-CD2 | 7.26  | 112.11      | 106.30   |
| 1   | J     | 104 | TYR  | CB-CG-CD2  | 7.26  | 125.36      | 121.00   |
| 1   | G     | 518 | ASP  | CB-CG-OD1  | -7.25 | 111.78      | 118.30   |
| 4   | V     | 254 | ARG  | NE-CZ-NH2  | -7.25 | 116.68      | 120.30   |
| 4   | 5     | 254 | ARG  | NE-CZ-NH2  | -7.23 | 116.69      | 120.30   |
| 4   | 1     | 79  | TRP  | CD1-CG-CD2 | 7.22  | 112.07      | 106.30   |
| 4   | V     | 340 | TRP  | CE2-CD2-CG | -7.21 | 101.53      | 107.30   |
| 4   | X     | 254 | ARG  | NE-CZ-NH2  | -7.21 | 116.69      | 120.30   |
| 4   | 8     | 254 | ARG  | NE-CZ-NH2  | -7.21 | 116.70      | 120.30   |
| 4   | 5     | 79  | TRP  | CD1-CG-CD2 | 7.21  | 112.06      | 106.30   |
| 4   | 6     | 340 | TRP  | CE2-CD2-CG | -7.20 | 101.54      | 107.30   |
| 4   | W     | 340 | TRP  | CE2-CD2-CG | -7.20 | 101.54      | 107.30   |
| 4   | 5     | 340 | TRP  | CE2-CD2-CG | -7.20 | 101.54      | 107.30   |
| 4   | 2     | 79  | TRP  | CD1-CG-CD2 | 7.19  | 112.06      | 106.30   |
| 4   | V     | 206 | ARG  | NE-CZ-NH1  | 7.19  | 123.90      | 120.30   |
| 4   | 3     | 340 | TRP  | CE2-CD2-CG | -7.18 | 101.55      | 107.30   |
| 4   | 0     | 79  | TRP  | CD1-CG-CD2 | 7.17  | 112.04      | 106.30   |
| 4   | 2     | 340 | TRP  | CE2-CD2-CG | -7.17 | 101.56      | 107.30   |
| 4   | 0     | 340 | TRP  | CE2-CD2-CG | -7.16 | 101.57      | 107.30   |
| 4   | 3     | 206 | ARG  | NE-CZ-NH1  | 7.16  | 123.88      | 120.30   |
| 4   | 8     | 79  | TRP  | CD1-CG-CD2 | 7.16  | 112.02      | 106.30   |
| 1   | A     | 148 | ARG  | NE-CZ-NH2  | -7.15 | 116.72      | 120.30   |
| 4   | 6     | 79  | TRP  | CD1-CG-CD2 | 7.15  | 112.02      | 106.30   |
| 4   | Y     | 340 | TRP  | CE2-CD2-CG | -7.15 | 101.58      | 107.30   |
| 4   | Z     | 340 | TRP  | CE2-CD2-CG | -7.15 | 101.58      | 107.30   |
| 4   | Y     | 254 | ARG  | NE-CZ-NH2  | -7.15 | 116.73      | 120.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | 1     | 340 | TRP  | CE2-CD2-CG | -7.15 | 101.58      | 107.30   |
| 4   | Z     | 79  | TRP  | CD1-CG-CD2 | 7.15  | 112.02      | 106.30   |
| 4   | W     | 206 | ARG  | NE-CZ-NH1  | 7.14  | 123.87      | 120.30   |
| 4   | 7     | 340 | TRP  | CE2-CD2-CG | -7.14 | 101.59      | 107.30   |
| 4   | 1     | 206 | ARG  | NE-CZ-NH1  | 7.14  | 123.87      | 120.30   |
| 4   | 4     | 79  | TRP  | CD1-CG-CD2 | 7.14  | 112.01      | 106.30   |
| 4   | 4     | 340 | TRP  | CE2-CD2-CG | -7.14 | 101.59      | 107.30   |
| 4   | V     | 79  | TRP  | CD1-CG-CD2 | 7.14  | 112.01      | 106.30   |
| 1   | G     | 568 | PRO  | CA-C-N     | -7.13 | 101.51      | 117.20   |
| 1   | A     | 104 | TYR  | CB-CG-CD2  | 7.13  | 125.28      | 121.00   |
| 4   | Y     | 79  | TRP  | CD1-CG-CD2 | 7.13  | 112.01      | 106.30   |
| 2   | K     | 150 | TYR  | CB-CG-CD1  | -7.12 | 116.73      | 121.00   |
| 4   | 7     | 79  | TRP  | CD1-CG-CD2 | 7.12  | 112.00      | 106.30   |
| 4   | W     | 79  | TRP  | CD1-CG-CD2 | 7.12  | 112.00      | 106.30   |
| 4   | X     | 340 | TRP  | CE2-CD2-CG | -7.12 | 101.61      | 107.30   |
| 4   | 6     | 254 | ARG  | NE-CZ-NH2  | -7.11 | 116.75      | 120.30   |
| 4   | 8     | 206 | ARG  | NE-CZ-NH1  | 7.11  | 123.85      | 120.30   |
| 1   | A     | 568 | PRO  | CA-C-N     | -7.10 | 101.57      | 117.20   |
| 2   | K     | 127 | ARG  | NE-CZ-NH2  | 7.10  | 123.85      | 120.30   |
| 4   | 7     | 254 | ARG  | NE-CZ-NH2  | -7.10 | 116.75      | 120.30   |
| 4   | X     | 79  | TRP  | CE2-CD2-CG | -7.10 | 101.62      | 107.30   |
| 4   | 3     | 340 | TRP  | CD1-CG-CD2 | 7.09  | 111.97      | 106.30   |
| 4   | 5     | 206 | ARG  | NE-CZ-NH1  | 7.09  | 123.84      | 120.30   |
| 4   | 3     | 79  | TRP  | CD1-CG-CD2 | 7.08  | 111.97      | 106.30   |
| 1   | D     | 568 | PRO  | CA-C-N     | -7.08 | 101.63      | 117.20   |
| 4   | 0     | 254 | ARG  | NE-CZ-NH2  | -7.08 | 116.76      | 120.30   |
| 4   | 6     | 206 | ARG  | NE-CZ-NH1  | 7.08  | 123.84      | 120.30   |
| 1   | J     | 568 | PRO  | CA-C-N     | -7.07 | 101.64      | 117.20   |
| 4   | 2     | 206 | ARG  | NE-CZ-NH1  | 7.07  | 123.84      | 120.30   |
| 4   | 4     | 206 | ARG  | NE-CZ-NH1  | 7.07  | 123.83      | 120.30   |
| 2   | H     | 127 | ARG  | NE-CZ-NH2  | 7.06  | 123.83      | 120.30   |
| 4   | X     | 206 | ARG  | NE-CZ-NH1  | 7.06  | 123.83      | 120.30   |
| 1   | D     | 218 | LEU  | CB-CG-CD1  | 7.05  | 122.99      | 111.00   |
| 4   | 1     | 47  | MET  | CA-CB-CG   | -7.05 | 101.31      | 113.30   |
| 1   | A     | 264 | ASP  | N-CA-CB    | -7.04 | 97.92       | 110.60   |
| 4   | 6     | 47  | MET  | CA-CB-CG   | -7.04 | 101.34      | 113.30   |
| 4   | 7     | 206 | ARG  | NE-CZ-NH1  | 7.04  | 123.82      | 120.30   |
| 4   | 8     | 47  | MET  | CA-CB-CG   | -7.04 | 101.34      | 113.30   |
| 4   | 0     | 47  | MET  | CA-CB-CG   | -7.03 | 101.35      | 113.30   |
| 4   | Z     | 254 | ARG  | NE-CZ-NH2  | -7.03 | 116.78      | 120.30   |
| 4   | 8     | 340 | TRP  | CE2-CD2-CG | -7.02 | 101.68      | 107.30   |
| 4   | Z     | 47  | MET  | CA-CB-CG   | -7.02 | 101.36      | 113.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | Y     | 206 | ARG  | NE-CZ-NH1  | 7.02  | 123.81      | 120.30   |
| 1   | D     | 217 | THR  | N-CA-CB    | 7.01  | 123.63      | 110.30   |
| 4   | 8     | 79  | TRP  | CE2-CD2-CG | -7.01 | 101.69      | 107.30   |
| 4   | X     | 47  | MET  | CA-CB-CG   | -7.01 | 101.38      | 113.30   |
| 4   | 0     | 206 | ARG  | NE-CZ-NH1  | 7.01  | 123.81      | 120.30   |
| 4   | 3     | 47  | MET  | CA-CB-CG   | -7.01 | 101.38      | 113.30   |
| 4   | V     | 47  | MET  | CA-CB-CG   | -7.01 | 101.38      | 113.30   |
| 4   | W     | 47  | MET  | CA-CB-CG   | -7.01 | 101.38      | 113.30   |
| 1   | J     | 264 | ASP  | N-CA-CB    | -7.01 | 97.99       | 110.60   |
| 4   | 0     | 79  | TRP  | CE2-CD2-CG | -7.01 | 101.69      | 107.30   |
| 4   | 2     | 47  | MET  | CA-CB-CG   | -7.01 | 101.39      | 113.30   |
| 1   | D     | 104 | TYR  | CB-CG-CD2  | 7.00  | 125.20      | 121.00   |
| 1   | J     | 218 | LEU  | CB-CG-CD1  | 7.00  | 122.90      | 111.00   |
| 4   | W     | 79  | TRP  | CE2-CD2-CG | -7.00 | 101.70      | 107.30   |
| 4   | 4     | 47  | MET  | CA-CB-CG   | -7.00 | 101.40      | 113.30   |
| 4   | 5     | 47  | MET  | CA-CB-CG   | -7.00 | 101.40      | 113.30   |
| 4   | 7     | 47  | MET  | CA-CB-CG   | -7.00 | 101.41      | 113.30   |
| 4   | Z     | 206 | ARG  | NE-CZ-NH1  | 7.00  | 123.80      | 120.30   |
| 1   | D     | 264 | ASP  | N-CA-CB    | -7.00 | 98.01       | 110.60   |
| 1   | G     | 217 | THR  | N-CA-CB    | 6.99  | 123.58      | 110.30   |
| 1   | G     | 218 | LEU  | CB-CG-CD1  | 6.99  | 122.89      | 111.00   |
| 4   | W     | 340 | TRP  | CD1-CG-CD2 | 6.99  | 111.89      | 106.30   |
| 4   | 5     | 79  | TRP  | CE2-CD2-CG | -6.98 | 101.71      | 107.30   |
| 4   | 1     | 79  | TRP  | CE2-CD2-CG | -6.98 | 101.72      | 107.30   |
| 1   | G     | 264 | ASP  | N-CA-CB    | -6.98 | 98.04       | 110.60   |
| 4   | 2     | 79  | TRP  | CE2-CD2-CG | -6.97 | 101.72      | 107.30   |
| 1   | J     | 148 | ARG  | NE-CZ-NH2  | -6.97 | 116.81      | 120.30   |
| 4   | Z     | 79  | TRP  | CE2-CD2-CG | -6.97 | 101.72      | 107.30   |
| 4   | Z     | 340 | TRP  | CD1-CG-CD2 | 6.97  | 111.88      | 106.30   |
| 4   | Y     | 47  | MET  | CA-CB-CG   | -6.97 | 101.45      | 113.30   |
| 1   | J     | 217 | THR  | N-CA-CB    | 6.96  | 123.52      | 110.30   |
| 1   | A     | 218 | LEU  | CB-CG-CD1  | 6.96  | 122.83      | 111.00   |
| 4   | 7     | 340 | TRP  | CD1-CG-CD2 | 6.96  | 111.86      | 106.30   |
| 2   | B     | 150 | TYR  | CB-CG-CD1  | -6.95 | 116.83      | 121.00   |
| 4   | 2     | 340 | TRP  | CD1-CG-CD2 | 6.95  | 111.86      | 106.30   |
| 4   | Y     | 340 | TRP  | CD1-CG-CD2 | 6.95  | 111.86      | 106.30   |
| 4   | 5     | 340 | TRP  | CD1-CG-CD2 | 6.95  | 111.86      | 106.30   |
| 1   | A     | 217 | THR  | N-CA-CB    | 6.94  | 123.49      | 110.30   |
| 4   | 6     | 340 | TRP  | CD1-CG-CD2 | 6.94  | 111.86      | 106.30   |
| 4   | V     | 79  | TRP  | CE2-CD2-CG | -6.94 | 101.75      | 107.30   |
| 2   | H     | 150 | TYR  | CB-CG-CD1  | -6.93 | 116.84      | 121.00   |
| 4   | 3     | 254 | ARG  | NE-CZ-NH2  | -6.93 | 116.83      | 120.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | 4     | 340 | TRP  | CD1-CG-CD2 | 6.93  | 111.85      | 106.30   |
| 4   | Y     | 79  | TRP  | CE2-CD2-CG | -6.93 | 101.75      | 107.30   |
| 4   | X     | 340 | TRP  | CD1-CG-CD2 | 6.93  | 111.84      | 106.30   |
| 4   | 1     | 340 | TRP  | CD1-CG-CD2 | 6.93  | 111.84      | 106.30   |
| 4   | 4     | 79  | TRP  | CE2-CD2-CG | -6.92 | 101.76      | 107.30   |
| 4   | 0     | 340 | TRP  | CD1-CG-CD2 | 6.92  | 111.84      | 106.30   |
| 4   | 7     | 79  | TRP  | CE2-CD2-CG | -6.92 | 101.76      | 107.30   |
| 4   | 3     | 79  | TRP  | CE2-CD2-CG | -6.92 | 101.76      | 107.30   |
| 4   | V     | 340 | TRP  | CD1-CG-CD2 | 6.92  | 111.83      | 106.30   |
| 2   | E     | 150 | TYR  | CB-CG-CD1  | -6.91 | 116.85      | 121.00   |
| 4   | 6     | 79  | TRP  | CE2-CD2-CG | -6.91 | 101.77      | 107.30   |
| 1   | A     | 75  | ASP  | N-CA-CB    | 6.91  | 123.03      | 110.60   |
| 1   | D     | 728 | ASN  | CA-C-N     | -6.90 | 102.02      | 117.20   |
| 1   | G     | 75  | ASP  | N-CA-CB    | 6.90  | 123.02      | 110.60   |
| 4   | 8     | 340 | TRP  | CD1-CG-CD2 | 6.89  | 111.81      | 106.30   |
| 1   | G     | 148 | ARG  | NE-CZ-NH2  | -6.88 | 116.86      | 120.30   |
| 1   | J     | 75  | ASP  | N-CA-CB    | 6.86  | 122.94      | 110.60   |
| 1   | J     | 728 | ASN  | CA-C-N     | -6.85 | 102.13      | 117.20   |
| 1   | G     | 728 | ASN  | CA-C-N     | -6.85 | 102.14      | 117.20   |
| 1   | G     | 450 | ASP  | CB-CG-OD2  | 6.85  | 124.46      | 118.30   |
| 1   | A     | 728 | ASN  | CA-C-N     | -6.84 | 102.14      | 117.20   |
| 1   | D     | 450 | ASP  | CB-CG-OD2  | 6.83  | 124.45      | 118.30   |
| 1   | J     | 450 | ASP  | CB-CG-OD2  | 6.83  | 124.45      | 118.30   |
| 1   | D     | 148 | ARG  | NE-CZ-NH2  | -6.81 | 116.89      | 120.30   |
| 1   | A     | 450 | ASP  | CB-CG-OD2  | 6.79  | 124.41      | 118.30   |
| 1   | D     | 75  | ASP  | N-CA-CB    | 6.76  | 122.77      | 110.60   |
| 1   | D     | 781 | ASP  | CB-CG-OD1  | -6.73 | 112.24      | 118.30   |
| 1   | J     | 75  | ASP  | CB-CG-OD2  | 6.70  | 124.33      | 118.30   |
| 1   | J     | 219 | GLU  | N-CA-C     | -6.69 | 92.94       | 111.00   |
| 1   | G     | 756 | THR  | N-CA-CB    | -6.68 | 97.61       | 110.30   |
| 1   | D     | 756 | THR  | N-CA-CB    | -6.66 | 97.64       | 110.30   |
| 1   | J     | 756 | THR  | N-CA-CB    | -6.66 | 97.64       | 110.30   |
| 4   | V     | 169 | TYR  | CB-CG-CD2  | -6.65 | 117.01      | 121.00   |
| 1   | G     | 219 | GLU  | N-CA-C     | -6.65 | 93.04       | 111.00   |
| 1   | A     | 343 | PHE  | CB-CG-CD1  | 6.65  | 125.45      | 120.80   |
| 1   | G     | 781 | ASP  | CB-CG-OD1  | -6.64 | 112.32      | 118.30   |
| 1   | G     | 555 | TYR  | CB-CG-CD2  | -6.64 | 117.01      | 121.00   |
| 1   | J     | 555 | TYR  | CB-CG-CD2  | -6.64 | 117.02      | 121.00   |
| 1   | A     | 75  | ASP  | CB-CG-OD2  | 6.63  | 124.27      | 118.30   |
| 1   | A     | 756 | THR  | N-CA-CB    | -6.63 | 97.70       | 110.30   |
| 4   | 2     | 169 | TYR  | CB-CG-CD2  | -6.63 | 117.02      | 121.00   |
| 4   | 5     | 196 | ARG  | NE-CZ-NH1  | 6.62  | 123.61      | 120.30   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | J     | 781 | ASP  | CB-CG-OD1 | -6.62 | 112.34      | 118.30   |
| 1   | A     | 781 | ASP  | CB-CG-OD1 | -6.60 | 112.36      | 118.30   |
| 1   | D     | 555 | TYR  | CB-CG-CD2 | -6.60 | 117.04      | 121.00   |
| 1   | A     | 219 | GLU  | N-CA-C    | -6.60 | 93.19       | 111.00   |
| 4   | 4     | 169 | TYR  | CB-CG-CD2 | -6.57 | 117.06      | 121.00   |
| 1   | D     | 75  | ASP  | CB-CG-OD2 | 6.57  | 124.21      | 118.30   |
| 4   | X     | 169 | TYR  | CB-CG-CD2 | -6.57 | 117.06      | 121.00   |
| 1   | A     | 332 | MET  | CG-SD-CE  | -6.56 | 89.70       | 100.20   |
| 1   | D     | 219 | GLU  | N-CA-C    | -6.56 | 93.28       | 111.00   |
| 1   | A     | 555 | TYR  | CB-CG-CD2 | -6.56 | 117.06      | 121.00   |
| 4   | 7     | 169 | TYR  | CB-CG-CD2 | -6.55 | 117.07      | 121.00   |
| 1   | G     | 169 | ASP  | CB-CG-OD1 | -6.55 | 112.40      | 118.30   |
| 1   | D     | 332 | MET  | CG-SD-CE  | -6.55 | 89.72       | 100.20   |
| 4   | W     | 283 | MET  | CG-SD-CE  | 6.54  | 110.67      | 100.20   |
| 1   | J     | 332 | MET  | CG-SD-CE  | -6.54 | 89.73       | 100.20   |
| 4   | 4     | 283 | MET  | CG-SD-CE  | 6.54  | 110.67      | 100.20   |
| 4   | 6     | 283 | MET  | CG-SD-CE  | 6.54  | 110.67      | 100.20   |
| 4   | Y     | 169 | TYR  | CB-CG-CD2 | -6.54 | 117.08      | 121.00   |
| 4   | 5     | 283 | MET  | CG-SD-CE  | 6.54  | 110.66      | 100.20   |
| 4   | W     | 196 | ARG  | NE-CZ-NH1 | 6.54  | 123.57      | 120.30   |
| 1   | G     | 332 | MET  | CG-SD-CE  | -6.54 | 89.74       | 100.20   |
| 4   | X     | 283 | MET  | CG-SD-CE  | 6.53  | 110.65      | 100.20   |
| 4   | 3     | 169 | TYR  | CB-CG-CD2 | -6.53 | 117.08      | 121.00   |
| 4   | 1     | 283 | MET  | CG-SD-CE  | 6.53  | 110.65      | 100.20   |
| 4   | 6     | 196 | ARG  | NE-CZ-NH1 | 6.53  | 123.56      | 120.30   |
| 4   | 8     | 169 | TYR  | CB-CG-CD2 | -6.52 | 117.09      | 121.00   |
| 4   | 0     | 283 | MET  | CG-SD-CE  | 6.52  | 110.63      | 100.20   |
| 4   | 2     | 283 | MET  | CG-SD-CE  | 6.52  | 110.63      | 100.20   |
| 4   | Z     | 169 | TYR  | CB-CG-CD2 | -6.52 | 117.09      | 121.00   |
| 4   | 5     | 169 | TYR  | CB-CG-CD2 | -6.52 | 117.09      | 121.00   |
| 4   | 8     | 283 | MET  | CG-SD-CE  | 6.52  | 110.63      | 100.20   |
| 1   | J     | 141 | LEU  | CB-CA-C   | -6.51 | 97.82       | 110.20   |
| 4   | 1     | 169 | TYR  | CB-CG-CD2 | -6.51 | 117.09      | 121.00   |
| 4   | 3     | 283 | MET  | CG-SD-CE  | 6.51  | 110.62      | 100.20   |
| 4   | 7     | 283 | MET  | CG-SD-CE  | 6.51  | 110.62      | 100.20   |
| 4   | Y     | 283 | MET  | CG-SD-CE  | 6.51  | 110.61      | 100.20   |
| 4   | 3     | 159 | VAL  | CB-CA-C   | -6.51 | 99.04       | 111.40   |
| 4   | 8     | 196 | ARG  | NE-CZ-NH1 | 6.51  | 123.55      | 120.30   |
| 4   | V     | 283 | MET  | CG-SD-CE  | 6.51  | 110.61      | 100.20   |
| 1   | J     | 334 | THR  | CA-CB-CG2 | -6.50 | 103.30      | 112.40   |
| 1   | G     | 590 | TYR  | CB-CG-CD2 | 6.50  | 124.90      | 121.00   |
| 1   | D     | 334 | THR  | CA-CB-CG2 | -6.50 | 103.31      | 112.40   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | G     | 141 | LEU  | CB-CA-C   | -6.50 | 97.86       | 110.20   |
| 4   | V     | 196 | ARG  | NE-CZ-NH1 | 6.50  | 123.55      | 120.30   |
| 4   | Z     | 159 | VAL  | CB-CA-C   | -6.49 | 99.07       | 111.40   |
| 4   | Z     | 283 | MET  | CG-SD-CE  | 6.49  | 110.59      | 100.20   |
| 1   | A     | 169 | ASP  | CB-CG-OD1 | -6.49 | 112.46      | 118.30   |
| 4   | 0     | 169 | TYR  | CB-CG-CD2 | -6.49 | 117.11      | 121.00   |
| 2   | E     | 141 | PRO  | N-CD-CG   | -6.49 | 93.47       | 103.20   |
| 4   | 2     | 159 | VAL  | CB-CA-C   | -6.49 | 99.08       | 111.40   |
| 4   | V     | 159 | VAL  | CB-CA-C   | -6.49 | 99.08       | 111.40   |
| 1   | J     | 169 | ASP  | CB-CG-OD1 | -6.48 | 112.47      | 118.30   |
| 4   | 5     | 159 | VAL  | CB-CA-C   | -6.48 | 99.09       | 111.40   |
| 4   | Y     | 196 | ARG  | NE-CZ-NH1 | 6.48  | 123.54      | 120.30   |
| 1   | G     | 334 | THR  | CA-CB-CG2 | -6.48 | 103.33      | 112.40   |
| 4   | 0     | 159 | VAL  | CB-CA-C   | -6.48 | 99.09       | 111.40   |
| 4   | 1     | 159 | VAL  | CB-CA-C   | -6.48 | 99.09       | 111.40   |
| 4   | 6     | 159 | VAL  | CB-CA-C   | -6.47 | 99.10       | 111.40   |
| 4   | 8     | 159 | VAL  | CB-CA-C   | -6.47 | 99.10       | 111.40   |
| 4   | 0     | 196 | ARG  | NE-CZ-NH1 | 6.47  | 123.54      | 120.30   |
| 4   | 7     | 196 | ARG  | NE-CZ-NH1 | 6.47  | 123.54      | 120.30   |
| 1   | D     | 141 | LEU  | CB-CA-C   | -6.47 | 97.91       | 110.20   |
| 2   | H     | 141 | PRO  | N-CD-CG   | -6.47 | 93.50       | 103.20   |
| 4   | 4     | 159 | VAL  | CB-CA-C   | -6.47 | 99.11       | 111.40   |
| 4   | X     | 159 | VAL  | CB-CA-C   | -6.47 | 99.11       | 111.40   |
| 4   | 6     | 169 | TYR  | CB-CG-CD2 | -6.46 | 117.12      | 121.00   |
| 4   | W     | 159 | VAL  | CB-CA-C   | -6.46 | 99.12       | 111.40   |
| 4   | 1     | 196 | ARG  | NE-CZ-NH1 | 6.46  | 123.53      | 120.30   |
| 4   | Y     | 159 | VAL  | CB-CA-C   | -6.46 | 99.13       | 111.40   |
| 1   | D     | 169 | ASP  | CB-CG-OD1 | -6.46 | 112.49      | 118.30   |
| 4   | 7     | 159 | VAL  | CB-CA-C   | -6.46 | 99.13       | 111.40   |
| 4   | W     | 169 | TYR  | CB-CG-CD2 | -6.46 | 117.13      | 121.00   |
| 4   | Z     | 196 | ARG  | NE-CZ-NH1 | 6.45  | 123.53      | 120.30   |
| 1   | A     | 334 | THR  | CA-CB-CG2 | -6.45 | 103.37      | 112.40   |
| 4   | 2     | 196 | ARG  | NE-CZ-NH1 | 6.44  | 123.52      | 120.30   |
| 1   | A     | 141 | LEU  | CB-CA-C   | -6.44 | 97.96       | 110.20   |
| 1   | D     | 343 | PHE  | CB-CG-CD1 | 6.44  | 125.31      | 120.80   |
| 4   | 0     | 34  | ILE  | CA-CB-CG2 | -6.44 | 98.03       | 110.90   |
| 1   | G     | 589 | ASP  | CB-CG-OD1 | -6.43 | 112.51      | 118.30   |
| 1   | G     | 343 | PHE  | CB-CG-CD1 | 6.42  | 125.30      | 120.80   |
| 1   | G     | 75  | ASP  | CB-CG-OD2 | 6.41  | 124.07      | 118.30   |
| 4   | W     | 34  | ILE  | CA-CB-CG2 | -6.41 | 98.07       | 110.90   |
| 1   | J     | 589 | ASP  | CB-CG-OD1 | -6.41 | 112.53      | 118.30   |
| 4   | 7     | 34  | ILE  | CA-CB-CG2 | -6.41 | 98.08       | 110.90   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 4   | 6     | 34  | ILE  | CA-CB-CG2 | -6.41 | 98.09       | 110.90   |
| 1   | A     | 589 | ASP  | CB-CG-OD1 | -6.41 | 112.54      | 118.30   |
| 4   | 4     | 34  | ILE  | CA-CB-CG2 | -6.41 | 98.09       | 110.90   |
| 4   | 8     | 34  | ILE  | CA-CB-CG2 | -6.41 | 98.09       | 110.90   |
| 4   | X     | 34  | ILE  | CA-CB-CG2 | -6.41 | 98.09       | 110.90   |
| 4   | Z     | 34  | ILE  | CA-CB-CG2 | -6.40 | 98.09       | 110.90   |
| 4   | 2     | 34  | ILE  | CA-CB-CG2 | -6.40 | 98.10       | 110.90   |
| 4   | 3     | 34  | ILE  | CA-CB-CG2 | -6.39 | 98.11       | 110.90   |
| 4   | 3     | 196 | ARG  | NE-CZ-NH1 | 6.39  | 123.50      | 120.30   |
| 4   | 1     | 34  | ILE  | CA-CB-CG2 | -6.39 | 98.13       | 110.90   |
| 1   | J     | 810 | ARG  | NE-CZ-NH1 | 6.38  | 123.49      | 120.30   |
| 4   | 4     | 196 | ARG  | NE-CZ-NH1 | 6.38  | 123.49      | 120.30   |
| 2   | K     | 141 | PRO  | N-CD-CG   | -6.37 | 93.64       | 103.20   |
| 4   | 5     | 34  | ILE  | CA-CB-CG2 | -6.37 | 98.15       | 110.90   |
| 4   | V     | 34  | ILE  | CA-CB-CG2 | -6.37 | 98.15       | 110.90   |
| 1   | D     | 129 | TYR  | CB-CG-CD2 | -6.37 | 117.18      | 121.00   |
| 1   | J     | 327 | ASP  | CB-CG-OD2 | 6.37  | 124.03      | 118.30   |
| 4   | Y     | 34  | ILE  | CA-CB-CG2 | -6.36 | 98.17       | 110.90   |
| 4   | X     | 196 | ARG  | NE-CZ-NH1 | 6.36  | 123.48      | 120.30   |
| 2   | B     | 141 | PRO  | N-CD-CG   | -6.35 | 93.68       | 103.20   |
| 1   | D     | 589 | ASP  | CB-CG-OD1 | -6.35 | 112.59      | 118.30   |
| 1   | G     | 578 | HIS  | N-CA-CB   | 6.33  | 122.00      | 110.60   |
| 1   | J     | 129 | TYR  | CB-CG-CD2 | -6.33 | 117.20      | 121.00   |
| 1   | A     | 341 | LEU  | CB-CA-C   | 6.33  | 122.23      | 110.20   |
| 1   | G     | 341 | LEU  | CB-CA-C   | 6.33  | 122.22      | 110.20   |
| 1   | J     | 341 | LEU  | CB-CA-C   | 6.32  | 122.20      | 110.20   |
| 4   | Z     | 217 | CYS  | CA-CB-SG  | -6.31 | 102.64      | 114.00   |
| 1   | J     | 779 | ARG  | NE-CZ-NH1 | 6.30  | 123.45      | 120.30   |
| 1   | G     | 129 | TYR  | CB-CG-CD2 | -6.30 | 117.22      | 121.00   |
| 4   | 3     | 217 | CYS  | CA-CB-SG  | -6.30 | 102.67      | 114.00   |
| 4   | 7     | 217 | CYS  | CA-CB-SG  | -6.30 | 102.67      | 114.00   |
| 1   | A     | 578 | HIS  | N-CA-CB   | 6.29  | 121.93      | 110.60   |
| 4   | 5     | 217 | CYS  | CA-CB-SG  | -6.29 | 102.67      | 114.00   |
| 4   | 2     | 217 | CYS  | CA-CB-SG  | -6.29 | 102.67      | 114.00   |
| 4   | 4     | 217 | CYS  | CA-CB-SG  | -6.29 | 102.68      | 114.00   |
| 4   | 0     | 217 | CYS  | CA-CB-SG  | -6.28 | 102.69      | 114.00   |
| 4   | Y     | 217 | CYS  | CA-CB-SG  | -6.28 | 102.69      | 114.00   |
| 1   | J     | 343 | PHE  | CB-CG-CD1 | 6.28  | 125.19      | 120.80   |
| 1   | J     | 578 | HIS  | N-CA-CB   | 6.28  | 121.90      | 110.60   |
| 4   | 8     | 217 | CYS  | CA-CB-SG  | -6.28 | 102.70      | 114.00   |
| 4   | W     | 217 | CYS  | CA-CB-SG  | -6.27 | 102.71      | 114.00   |
| 4   | V     | 217 | CYS  | CA-CB-SG  | -6.27 | 102.72      | 114.00   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 4   | 1     | 217 | CYS  | CA-CB-SG  | -6.27 | 102.72      | 114.00   |
| 1   | D     | 341 | LEU  | CB-CA-C   | 6.27  | 122.11      | 110.20   |
| 4   | X     | 217 | CYS  | CA-CB-SG  | -6.27 | 102.72      | 114.00   |
| 4   | 6     | 217 | CYS  | CA-CB-SG  | -6.26 | 102.73      | 114.00   |
| 1   | A     | 129 | TYR  | CB-CG-CD2 | -6.25 | 117.25      | 121.00   |
| 1   | D     | 578 | HIS  | N-CA-CB   | 6.24  | 121.83      | 110.60   |
| 1   | J     | 760 | PHE  | CB-CG-CD2 | -6.22 | 116.45      | 120.80   |
| 2   | K     | 129 | THR  | CB-CA-C   | -6.22 | 94.81       | 111.60   |
| 1   | A     | 780 | ASP  | CB-CG-OD2 | 6.21  | 123.89      | 118.30   |
| 1   | D     | 760 | PHE  | CB-CG-CD2 | -6.21 | 116.45      | 120.80   |
| 1   | A     | 463 | ASP  | CB-CG-OD2 | -6.20 | 112.72      | 118.30   |
| 1   | A     | 327 | ASP  | CB-CG-OD2 | 6.20  | 123.88      | 118.30   |
| 2   | B     | 129 | THR  | CB-CA-C   | -6.19 | 94.88       | 111.60   |
| 1   | D     | 327 | ASP  | CB-CG-OD2 | 6.19  | 123.87      | 118.30   |
| 1   | A     | 698 | ASN  | CB-CA-C   | -6.19 | 98.02       | 110.40   |
| 2   | H     | 129 | THR  | CB-CA-C   | -6.19 | 94.89       | 111.60   |
| 1   | J     | 214 | MET  | CG-SD-CE  | 6.18  | 110.10      | 100.20   |
| 2   | E     | 129 | THR  | CB-CA-C   | -6.17 | 94.94       | 111.60   |
| 1   | D     | 214 | MET  | CG-SD-CE  | 6.17  | 110.07      | 100.20   |
| 2   | K     | 141 | PRO  | N-CA-CB   | -6.17 | 95.82       | 102.60   |
| 1   | G     | 214 | MET  | CG-SD-CE  | 6.16  | 110.06      | 100.20   |
| 1   | G     | 327 | ASP  | CB-CG-OD2 | 6.16  | 123.84      | 118.30   |
| 1   | J     | 463 | ASP  | CB-CG-OD2 | -6.16 | 112.76      | 118.30   |
| 2   | H     | 141 | PRO  | N-CA-CB   | -6.15 | 95.84       | 102.60   |
| 1   | A     | 214 | MET  | CG-SD-CE  | 6.14  | 110.03      | 100.20   |
| 4   | 4     | 259 | GLU  | CA-CB-CG  | 6.14  | 126.92      | 113.40   |
| 1   | D     | 590 | TYR  | CB-CG-CD2 | 6.14  | 124.69      | 121.00   |
| 3   | F     | 58  | MET  | CG-SD-CE  | 6.14  | 110.02      | 100.20   |
| 4   | X     | 259 | GLU  | CA-CB-CG  | 6.14  | 126.91      | 113.40   |
| 1   | G     | 104 | TYR  | CB-CG-CD1 | -6.13 | 117.32      | 121.00   |
| 4   | 1     | 259 | GLU  | CA-CB-CG  | 6.13  | 126.90      | 113.40   |
| 4   | Y     | 259 | GLU  | CA-CB-CG  | 6.13  | 126.89      | 113.40   |
| 4   | 2     | 259 | GLU  | CA-CB-CG  | 6.13  | 126.89      | 113.40   |
| 4   | 3     | 259 | GLU  | CA-CB-CG  | 6.13  | 126.89      | 113.40   |
| 4   | Z     | 259 | GLU  | CA-CB-CG  | 6.13  | 126.89      | 113.40   |
| 1   | A     | 760 | PHE  | CB-CG-CD2 | -6.13 | 116.51      | 120.80   |
| 1   | D     | 698 | ASN  | CB-CA-C   | -6.13 | 98.14       | 110.40   |
| 4   | W     | 259 | GLU  | CA-CB-CG  | 6.13  | 126.88      | 113.40   |
| 4   | V     | 259 | GLU  | CA-CB-CG  | 6.13  | 126.88      | 113.40   |
| 4   | 0     | 259 | GLU  | CA-CB-CG  | 6.12  | 126.87      | 113.40   |
| 2   | E     | 129 | THR  | CA-CB-CG2 | 6.12  | 120.96      | 112.40   |
| 4   | 6     | 259 | GLU  | CA-CB-CG  | 6.12  | 126.86      | 113.40   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 590 | TYR  | CB-CG-CD2 | 6.12  | 124.67      | 121.00   |
| 1   | D     | 104 | TYR  | CB-CG-CD1 | -6.12 | 117.33      | 121.00   |
| 4   | 5     | 259 | GLU  | CA-CB-CG  | 6.12  | 126.85      | 113.40   |
| 2   | E     | 141 | PRO  | N-CA-CB   | -6.11 | 95.87       | 102.60   |
| 4   | 7     | 259 | GLU  | CA-CB-CG  | 6.11  | 126.85      | 113.40   |
| 4   | 8     | 259 | GLU  | CA-CB-CG  | 6.11  | 126.85      | 113.40   |
| 1   | J     | 752 | ASP  | CB-CG-OD2 | 6.11  | 123.80      | 118.30   |
| 1   | J     | 104 | TYR  | CB-CG-CD1 | -6.11 | 117.33      | 121.00   |
| 1   | J     | 698 | ASN  | CB-CA-C   | -6.11 | 98.18       | 110.40   |
| 3   | L     | 58  | MET  | CG-SD-CE  | 6.10  | 109.97      | 100.20   |
| 1   | G     | 779 | ARG  | NE-CZ-NH1 | 6.10  | 123.35      | 120.30   |
| 4   | 5     | 335 | ARG  | NE-CZ-NH2 | -6.10 | 117.25      | 120.30   |
| 1   | G     | 810 | ARG  | NE-CZ-NH1 | 6.09  | 123.34      | 120.30   |
| 1   | J     | 682 | THR  | CA-CB-CG2 | -6.09 | 103.87      | 112.40   |
| 1   | G     | 698 | ASN  | CB-CA-C   | -6.09 | 98.23       | 110.40   |
| 1   | G     | 346 | ASP  | CB-CG-OD1 | 6.08  | 123.78      | 118.30   |
| 4   | W     | 349 | LEU  | CA-C-N    | -6.08 | 103.82      | 117.20   |
| 1   | G     | 463 | ASP  | CB-CG-OD2 | -6.08 | 112.83      | 118.30   |
| 1   | G     | 625 | THR  | CA-CB-OG1 | 6.07  | 121.75      | 109.00   |
| 1   | D     | 346 | ASP  | CB-CG-OD1 | 6.07  | 123.76      | 118.30   |
| 2   | H     | 129 | THR  | CA-CB-CG2 | 6.07  | 120.89      | 112.40   |
| 4   | 3     | 349 | LEU  | CA-C-N    | -6.07 | 103.86      | 117.20   |
| 3   | I     | 58  | MET  | CG-SD-CE  | 6.06  | 109.90      | 100.20   |
| 4   | 2     | 349 | LEU  | CA-C-N    | -6.06 | 103.87      | 117.20   |
| 2   | B     | 141 | PRO  | N-CA-CB   | -6.06 | 95.94       | 102.60   |
| 1   | G     | 682 | THR  | CA-CB-CG2 | -6.06 | 103.92      | 112.40   |
| 1   | J     | 625 | THR  | CA-CB-OG1 | 6.06  | 121.72      | 109.00   |
| 1   | J     | 590 | TYR  | CB-CG-CD2 | 6.05  | 124.63      | 121.00   |
| 4   | 0     | 349 | LEU  | CA-C-N    | -6.05 | 103.89      | 117.20   |
| 4   | 7     | 16  | LEU  | CA-CB-CG  | 6.05  | 129.21      | 115.30   |
| 1   | D     | 810 | ARG  | NE-CZ-NH1 | 6.05  | 123.32      | 120.30   |
| 4   | 0     | 16  | LEU  | CA-CB-CG  | 6.05  | 129.21      | 115.30   |
| 4   | 4     | 349 | LEU  | CA-C-N    | -6.05 | 103.89      | 117.20   |
| 4   | 4     | 16  | LEU  | CA-CB-CG  | 6.05  | 129.21      | 115.30   |
| 4   | V     | 16  | LEU  | CA-CB-CG  | 6.05  | 129.21      | 115.30   |
| 3   | C     | 58  | MET  | CG-SD-CE  | 6.04  | 109.87      | 100.20   |
| 4   | 2     | 16  | LEU  | CA-CB-CG  | 6.04  | 129.20      | 115.30   |
| 1   | D     | 463 | ASP  | CB-CG-OD2 | -6.04 | 112.86      | 118.30   |
| 1   | J     | 450 | ASP  | CB-CG-OD1 | -6.04 | 112.86      | 118.30   |
| 4   | Y     | 349 | LEU  | CA-C-N    | -6.04 | 103.90      | 117.20   |
| 2   | K     | 129 | THR  | CA-CB-CG2 | 6.04  | 120.86      | 112.40   |
| 4   | 1     | 349 | LEU  | CA-C-N    | -6.04 | 103.91      | 117.20   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | 6     | 349 | LEU  | CA-C-N     | -6.04 | 103.91      | 117.20   |
| 4   | 5     | 16  | LEU  | CA-CB-CG   | 6.04  | 129.19      | 115.30   |
| 4   | 8     | 16  | LEU  | CA-CB-CG   | 6.04  | 129.19      | 115.30   |
| 4   | X     | 16  | LEU  | CA-CB-CG   | 6.04  | 129.19      | 115.30   |
| 4   | Y     | 16  | LEU  | CA-CB-CG   | 6.04  | 129.18      | 115.30   |
| 4   | 3     | 16  | LEU  | CA-CB-CG   | 6.03  | 129.17      | 115.30   |
| 4   | 8     | 349 | LEU  | CA-C-N     | -6.03 | 103.93      | 117.20   |
| 4   | W     | 16  | LEU  | CA-CB-CG   | 6.03  | 129.17      | 115.30   |
| 1   | J     | 192 | VAL  | CA-CB-CG1  | -6.03 | 101.85      | 110.90   |
| 4   | 1     | 16  | LEU  | CA-CB-CG   | 6.03  | 129.17      | 115.30   |
| 1   | G     | 760 | PHE  | CB-CG-CD2  | -6.03 | 116.58      | 120.80   |
| 4   | 5     | 349 | LEU  | CA-C-N     | -6.03 | 103.94      | 117.20   |
| 4   | 6     | 16  | LEU  | CA-CB-CG   | 6.03  | 129.16      | 115.30   |
| 4   | Z     | 349 | LEU  | CA-C-N     | -6.03 | 103.94      | 117.20   |
| 4   | Z     | 16  | LEU  | CA-CB-CG   | 6.02  | 129.16      | 115.30   |
| 1   | A     | 682 | THR  | CA-CB-CG2  | -6.02 | 103.97      | 112.40   |
| 1   | J     | 665 | ARG  | NE-CZ-NH2  | -6.02 | 117.29      | 120.30   |
| 4   | 7     | 349 | LEU  | CA-C-N     | -6.02 | 103.95      | 117.20   |
| 1   | A     | 779 | ARG  | NE-CZ-NH1  | 6.02  | 123.31      | 120.30   |
| 2   | B     | 129 | THR  | CA-CB-CG2  | 6.02  | 120.82      | 112.40   |
| 1   | D     | 378 | ASP  | CB-CG-OD1  | -6.01 | 112.89      | 118.30   |
| 4   | 6     | 335 | ARG  | NE-CZ-NH2  | -6.01 | 117.29      | 120.30   |
| 4   | X     | 349 | LEU  | CA-C-N     | -6.01 | 103.97      | 117.20   |
| 1   | A     | 625 | THR  | CA-CB-OG1  | 6.01  | 121.62      | 109.00   |
| 1   | D     | 192 | VAL  | CA-CB-CG1  | -6.01 | 101.89      | 110.90   |
| 1   | D     | 447 | GLN  | N-CA-CB    | 6.01  | 121.42      | 110.60   |
| 1   | D     | 682 | THR  | CA-CB-CG2  | -6.01 | 103.99      | 112.40   |
| 4   | V     | 349 | LEU  | CA-C-N     | -6.01 | 103.98      | 117.20   |
| 1   | A     | 810 | ARG  | NE-CZ-NH1  | 6.01  | 123.30      | 120.30   |
| 1   | A     | 447 | GLN  | N-CA-CB    | 6.00  | 121.41      | 110.60   |
| 1   | G     | 447 | GLN  | N-CA-CB    | 6.00  | 121.41      | 110.60   |
| 1   | D     | 625 | THR  | CA-CB-OG1  | 6.00  | 121.59      | 109.00   |
| 1   | G     | 192 | VAL  | CA-CB-CG1  | -5.99 | 101.91      | 110.90   |
| 1   | J     | 447 | GLN  | N-CA-CB    | 5.99  | 121.38      | 110.60   |
| 4   | Z     | 116 | ARG  | NE-CZ-NH1  | 5.99  | 123.30      | 120.30   |
| 4   | 6     | 116 | ARG  | NE-CZ-NH1  | 5.99  | 123.29      | 120.30   |
| 4   | 1     | 79  | TRP  | CG-CD2-CE3 | 5.98  | 139.28      | 133.90   |
| 1   | D     | 450 | ASP  | CB-CG-OD1  | -5.98 | 112.92      | 118.30   |
| 1   | D     | 780 | ASP  | CB-CG-OD2  | 5.97  | 123.67      | 118.30   |
| 1   | G     | 780 | ASP  | CB-CG-OD2  | 5.96  | 123.67      | 118.30   |
| 1   | D     | 754 | ASP  | CB-CG-OD2  | -5.96 | 112.94      | 118.30   |
| 1   | G     | 752 | ASP  | CB-CG-OD2  | 5.96  | 123.66      | 118.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | V     | 116 | ARG  | NE-CZ-NH1  | 5.96  | 123.28      | 120.30   |
| 4   | X     | 79  | TRP  | CG-CD2-CE3 | 5.95  | 139.26      | 133.90   |
| 1   | G     | 378 | ASP  | CB-CG-OD1  | -5.95 | 112.94      | 118.30   |
| 4   | Z     | 335 | ARG  | NE-CZ-NH2  | -5.95 | 117.33      | 120.30   |
| 4   | 3     | 335 | ARG  | NE-CZ-NH2  | -5.94 | 117.33      | 120.30   |
| 1   | A     | 665 | ARG  | NE-CZ-NH2  | -5.94 | 117.33      | 120.30   |
| 1   | J     | 378 | ASP  | CB-CG-OD1  | -5.94 | 112.95      | 118.30   |
| 1   | G     | 754 | ASP  | CB-CG-OD2  | -5.94 | 112.96      | 118.30   |
| 4   | Y     | 335 | ARG  | NE-CZ-NH2  | -5.93 | 117.33      | 120.30   |
| 1   | A     | 192 | VAL  | CA-CB-CG1  | -5.93 | 102.00      | 110.90   |
| 4   | 3     | 116 | ARG  | NE-CZ-NH1  | 5.93  | 123.27      | 120.30   |
| 4   | 4     | 335 | ARG  | NE-CZ-NH2  | -5.93 | 117.33      | 120.30   |
| 1   | D     | 556 | ASP  | CB-CG-OD1  | -5.93 | 112.97      | 118.30   |
| 4   | 8     | 79  | TRP  | CG-CD2-CE3 | 5.92  | 139.23      | 133.90   |
| 1   | A     | 815 | CYS  | CA-CB-SG   | -5.92 | 103.34      | 114.00   |
| 1   | A     | 104 | TYR  | CB-CG-CD1  | -5.92 | 117.45      | 121.00   |
| 1   | D     | 665 | ARG  | NE-CZ-NH2  | -5.92 | 117.34      | 120.30   |
| 1   | G     | 450 | ASP  | CB-CG-OD1  | -5.91 | 112.98      | 118.30   |
| 1   | J     | 780 | ASP  | CB-CG-OD2  | 5.91  | 123.62      | 118.30   |
| 4   | V     | 335 | ARG  | NE-CZ-NH2  | -5.91 | 117.35      | 120.30   |
| 4   | W     | 335 | ARG  | NE-CZ-NH2  | -5.91 | 117.34      | 120.30   |
| 1   | D     | 339 | ASP  | CB-CG-OD2  | 5.90  | 123.61      | 118.30   |
| 1   | G     | 665 | ARG  | NE-CZ-NH2  | -5.90 | 117.35      | 120.30   |
| 4   | 5     | 254 | ARG  | NE-CZ-NH1  | 5.90  | 123.25      | 120.30   |
| 4   | 5     | 116 | ARG  | NE-CZ-NH1  | 5.90  | 123.25      | 120.30   |
| 1   | D     | 471 | ASP  | CB-CG-OD1  | -5.89 | 113.00      | 118.30   |
| 4   | X     | 335 | ARG  | NE-CZ-NH2  | -5.89 | 117.36      | 120.30   |
| 1   | G     | 339 | ASP  | CB-CG-OD2  | 5.89  | 123.60      | 118.30   |
| 1   | J     | 754 | ASP  | CB-CG-OD2  | -5.88 | 113.00      | 118.30   |
| 4   | 1     | 200 | PHE  | CA-C-N     | -5.88 | 104.25      | 117.20   |
| 4   | 5     | 200 | PHE  | CA-C-N     | -5.88 | 104.26      | 117.20   |
| 1   | D     | 779 | ARG  | NE-CZ-NH1  | 5.88  | 123.24      | 120.30   |
| 4   | 4     | 200 | PHE  | CA-C-N     | -5.88 | 104.26      | 117.20   |
| 4   | 7     | 200 | PHE  | CA-C-N     | -5.88 | 104.26      | 117.20   |
| 4   | X     | 200 | PHE  | CA-C-N     | -5.88 | 104.26      | 117.20   |
| 4   | 5     | 79  | TRP  | CG-CD2-CE3 | 5.88  | 139.19      | 133.90   |
| 4   | W     | 116 | ARG  | NE-CZ-NH1  | 5.88  | 123.24      | 120.30   |
| 4   | 6     | 200 | PHE  | CA-C-N     | -5.88 | 104.28      | 117.20   |
| 4   | W     | 200 | PHE  | CA-C-N     | -5.88 | 104.28      | 117.20   |
| 1   | A     | 450 | ASP  | CB-CG-OD1  | -5.87 | 113.02      | 118.30   |
| 1   | A     | 752 | ASP  | CB-CG-OD2  | 5.87  | 123.58      | 118.30   |
| 4   | Y     | 200 | PHE  | CA-C-N     | -5.87 | 104.29      | 117.20   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 738 | MET  | CG-SD-CE   | 5.86  | 109.58      | 100.20   |
| 1   | J     | 471 | ASP  | CB-CG-OD1  | -5.86 | 113.02      | 118.30   |
| 4   | 8     | 116 | ARG  | NE-CZ-NH1  | 5.86  | 123.23      | 120.30   |
| 1   | A     | 754 | ASP  | CB-CG-OD2  | -5.86 | 113.03      | 118.30   |
| 1   | G     | 738 | MET  | CG-SD-CE   | 5.86  | 109.58      | 100.20   |
| 4   | 0     | 79  | TRP  | CG-CD2-CE3 | 5.86  | 139.17      | 133.90   |
| 4   | 3     | 200 | PHE  | CA-C-N     | -5.86 | 104.31      | 117.20   |
| 1   | G     | 809 | ARG  | NE-CZ-NH2  | -5.86 | 117.37      | 120.30   |
| 4   | 8     | 254 | ARG  | NE-CZ-NH1  | 5.86  | 123.23      | 120.30   |
| 4   | 2     | 335 | ARG  | NE-CZ-NH2  | -5.86 | 117.37      | 120.30   |
| 1   | D     | 738 | MET  | CG-SD-CE   | 5.86  | 109.57      | 100.20   |
| 1   | J     | 738 | MET  | CG-SD-CE   | 5.86  | 109.57      | 100.20   |
| 4   | 2     | 200 | PHE  | CA-C-N     | -5.85 | 104.32      | 117.20   |
| 1   | A     | 378 | ASP  | CB-CG-OD1  | -5.85 | 113.03      | 118.30   |
| 4   | 0     | 200 | PHE  | CA-C-N     | -5.85 | 104.33      | 117.20   |
| 4   | V     | 200 | PHE  | CA-C-N     | -5.85 | 104.33      | 117.20   |
| 4   | Z     | 200 | PHE  | CA-C-N     | -5.85 | 104.33      | 117.20   |
| 1   | J     | 346 | ASP  | CB-CG-OD1  | 5.85  | 123.56      | 118.30   |
| 4   | 2     | 116 | ARG  | NE-CZ-NH1  | 5.84  | 123.22      | 120.30   |
| 1   | G     | 780 | ASP  | CB-CG-OD1  | -5.84 | 113.04      | 118.30   |
| 1   | D     | 752 | ASP  | CB-CG-OD2  | 5.84  | 123.56      | 118.30   |
| 1   | J     | 556 | ASP  | CB-CG-OD1  | -5.84 | 113.04      | 118.30   |
| 4   | 8     | 200 | PHE  | CA-C-N     | -5.84 | 104.36      | 117.20   |
| 4   | 4     | 79  | TRP  | CG-CD2-CE3 | 5.83  | 139.15      | 133.90   |
| 4   | V     | 254 | ARG  | NE-CZ-NH1  | 5.83  | 123.21      | 120.30   |
| 1   | J     | 815 | CYS  | CA-CB-SG   | -5.83 | 103.51      | 114.00   |
| 4   | 2     | 79  | TRP  | CG-CD2-CE3 | 5.82  | 139.14      | 133.90   |
| 4   | Y     | 116 | ARG  | NE-CZ-NH1  | 5.82  | 123.21      | 120.30   |
| 4   | Y     | 254 | ARG  | NE-CZ-NH1  | 5.82  | 123.21      | 120.30   |
| 4   | 8     | 95  | ARG  | CA-CB-CG   | 5.82  | 126.20      | 113.40   |
| 1   | D     | 809 | ARG  | NE-CZ-NH2  | -5.82 | 117.39      | 120.30   |
| 4   | 6     | 79  | TRP  | CG-CD2-CE3 | 5.82  | 139.13      | 133.90   |
| 4   | Z     | 79  | TRP  | CG-CD2-CE3 | 5.82  | 139.13      | 133.90   |
| 4   | 1     | 335 | ARG  | NE-CZ-NH2  | -5.82 | 117.39      | 120.30   |
| 1   | G     | 471 | ASP  | CB-CG-OD1  | -5.81 | 113.07      | 118.30   |
| 4   | 1     | 95  | ARG  | CA-CB-CG   | 5.81  | 126.19      | 113.40   |
| 1   | A     | 780 | ASP  | CB-CG-OD1  | -5.81 | 113.07      | 118.30   |
| 4   | V     | 95  | ARG  | CA-CB-CG   | 5.81  | 126.18      | 113.40   |
| 4   | Z     | 95  | ARG  | CA-CB-CG   | 5.81  | 126.17      | 113.40   |
| 4   | 3     | 79  | TRP  | CG-CD2-CE3 | 5.80  | 139.12      | 133.90   |
| 4   | 7     | 95  | ARG  | CA-CB-CG   | 5.80  | 126.16      | 113.40   |
| 4   | X     | 95  | ARG  | CA-CB-CG   | 5.80  | 126.16      | 113.40   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | Y     | 79  | TRP  | CG-CD2-CE3 | 5.80  | 139.12      | 133.90   |
| 4   | 4     | 254 | ARG  | NE-CZ-NH1  | 5.80  | 123.20      | 120.30   |
| 1   | D     | 815 | CYS  | CA-CB-SG   | -5.79 | 103.57      | 114.00   |
| 4   | 1     | 254 | ARG  | NE-CZ-NH1  | 5.79  | 123.20      | 120.30   |
| 4   | W     | 79  | TRP  | CG-CD2-CE3 | 5.79  | 139.11      | 133.90   |
| 4   | 8     | 335 | ARG  | NE-CZ-NH2  | -5.79 | 117.41      | 120.30   |
| 1   | A     | 346 | ASP  | CB-CG-OD1  | 5.79  | 123.51      | 118.30   |
| 4   | 7     | 79  | TRP  | CG-CD2-CE3 | 5.79  | 139.11      | 133.90   |
| 1   | G     | 556 | ASP  | CB-CG-OD1  | -5.78 | 113.09      | 118.30   |
| 4   | 4     | 95  | ARG  | CA-CB-CG   | 5.78  | 126.12      | 113.40   |
| 4   | 6     | 95  | ARG  | CA-CB-CG   | 5.78  | 126.12      | 113.40   |
| 4   | Y     | 95  | ARG  | CA-CB-CG   | 5.78  | 126.12      | 113.40   |
| 1   | A     | 4   | ASP  | CB-CG-OD2  | 5.78  | 123.50      | 118.30   |
| 1   | J     | 339 | ASP  | CB-CG-OD2  | 5.78  | 123.50      | 118.30   |
| 1   | J     | 809 | ARG  | NE-CZ-NH2  | -5.78 | 117.41      | 120.30   |
| 4   | 0     | 95  | ARG  | CA-CB-CG   | 5.78  | 126.11      | 113.40   |
| 1   | A     | 556 | ASP  | CB-CG-OD1  | -5.77 | 113.10      | 118.30   |
| 1   | A     | 471 | ASP  | CB-CG-OD1  | -5.77 | 113.11      | 118.30   |
| 4   | 0     | 254 | ARG  | NE-CZ-NH1  | 5.77  | 123.19      | 120.30   |
| 4   | 0     | 335 | ARG  | NE-CZ-NH2  | -5.77 | 117.42      | 120.30   |
| 4   | 2     | 95  | ARG  | CA-CB-CG   | 5.77  | 126.09      | 113.40   |
| 4   | W     | 95  | ARG  | CA-CB-CG   | 5.77  | 126.09      | 113.40   |
| 4   | 7     | 335 | ARG  | NE-CZ-NH2  | -5.76 | 117.42      | 120.30   |
| 4   | V     | 79  | TRP  | CG-CD2-CE3 | 5.76  | 139.09      | 133.90   |
| 4   | Z     | 254 | ARG  | NE-CZ-NH1  | 5.76  | 123.18      | 120.30   |
| 4   | 0     | 116 | ARG  | NE-CZ-NH1  | 5.76  | 123.18      | 120.30   |
| 4   | 5     | 95  | ARG  | CA-CB-CG   | 5.76  | 126.07      | 113.40   |
| 4   | 1     | 116 | ARG  | NE-CZ-NH1  | 5.76  | 123.18      | 120.30   |
| 4   | 3     | 95  | ARG  | CA-CB-CG   | 5.75  | 126.06      | 113.40   |
| 1   | D     | 352 | TYR  | N-CA-CB    | 5.75  | 120.94      | 110.60   |
| 1   | A     | 809 | ARG  | NE-CZ-NH2  | -5.74 | 117.43      | 120.30   |
| 1   | D     | 781 | ASP  | CB-CG-OD2  | 5.74  | 123.47      | 118.30   |
| 2   | B     | 149 | ASP  | N-CA-CB    | 5.74  | 120.93      | 110.60   |
| 1   | D     | 4   | ASP  | CB-CG-OD2  | 5.74  | 123.46      | 118.30   |
| 1   | A     | 339 | ASP  | CB-CG-OD2  | 5.73  | 123.46      | 118.30   |
| 2   | H     | 149 | ASP  | N-CA-CB    | 5.73  | 120.91      | 110.60   |
| 1   | J     | 165 | PHE  | N-CA-CB    | -5.73 | 100.29      | 110.60   |
| 4   | W     | 254 | ARG  | NE-CZ-NH1  | 5.73  | 123.16      | 120.30   |
| 2   | K     | 149 | ASP  | N-CA-CB    | 5.72  | 120.90      | 110.60   |
| 4   | 0     | 335 | ARG  | CA-CB-CG   | 5.72  | 125.99      | 113.40   |
| 4   | X     | 254 | ARG  | NE-CZ-NH1  | 5.72  | 123.16      | 120.30   |
| 1   | A     | 165 | PHE  | N-CA-CB    | -5.72 | 100.31      | 110.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | 6     | 254 | ARG  | NE-CZ-NH1  | 5.72  | 123.16      | 120.30   |
| 1   | G     | 815 | CYS  | CA-CB-SG   | -5.72 | 103.71      | 114.00   |
| 4   | 7     | 335 | ARG  | CA-CB-CG   | 5.72  | 125.98      | 113.40   |
| 4   | V     | 335 | ARG  | CA-CB-CG   | 5.72  | 125.98      | 113.40   |
| 1   | J     | 4   | ASP  | CB-CG-OD2  | 5.71  | 123.44      | 118.30   |
| 4   | 1     | 335 | ARG  | CA-CB-CG   | 5.71  | 125.96      | 113.40   |
| 4   | 2     | 335 | ARG  | CA-CB-CG   | 5.71  | 125.96      | 113.40   |
| 1   | G     | 4   | ASP  | CB-CG-OD2  | 5.71  | 123.44      | 118.30   |
| 4   | 5     | 335 | ARG  | CA-CB-CG   | 5.71  | 125.95      | 113.40   |
| 4   | 7     | 254 | ARG  | NE-CZ-NH1  | 5.71  | 123.15      | 120.30   |
| 4   | 3     | 335 | ARG  | CA-CB-CG   | 5.71  | 125.95      | 113.40   |
| 4   | 4     | 335 | ARG  | CA-CB-CG   | 5.70  | 125.94      | 113.40   |
| 4   | X     | 335 | ARG  | CA-CB-CG   | 5.70  | 125.94      | 113.40   |
| 1   | G     | 165 | PHE  | N-CA-CB    | -5.70 | 100.35      | 110.60   |
| 4   | 6     | 335 | ARG  | CA-CB-CG   | 5.70  | 125.93      | 113.40   |
| 4   | 8     | 335 | ARG  | CA-CB-CG   | 5.70  | 125.93      | 113.40   |
| 4   | W     | 335 | ARG  | CA-CB-CG   | 5.69  | 125.92      | 113.40   |
| 4   | 4     | 116 | ARG  | NE-CZ-NH1  | 5.68  | 123.14      | 120.30   |
| 4   | Z     | 335 | ARG  | CA-CB-CG   | 5.68  | 125.90      | 113.40   |
| 4   | Y     | 335 | ARG  | CA-CB-CG   | 5.68  | 125.89      | 113.40   |
| 4   | 2     | 254 | ARG  | NE-CZ-NH1  | 5.67  | 123.14      | 120.30   |
| 1   | D     | 780 | ASP  | CB-CG-OD1  | -5.67 | 113.20      | 118.30   |
| 1   | G     | 352 | TYR  | N-CA-CB    | 5.66  | 120.79      | 110.60   |
| 1   | D     | 165 | PHE  | N-CA-CB    | -5.66 | 100.42      | 110.60   |
| 2   | E     | 149 | ASP  | N-CA-CB    | 5.65  | 120.77      | 110.60   |
| 1   | G     | 693 | HIS  | CA-CB-CG   | -5.63 | 104.02      | 113.60   |
| 4   | 7     | 116 | ARG  | NE-CZ-NH1  | 5.63  | 123.11      | 120.30   |
| 4   | Z     | 294 | TYR  | CB-CG-CD2  | -5.63 | 117.62      | 121.00   |
| 4   | X     | 294 | TYR  | CB-CG-CD2  | -5.62 | 117.63      | 121.00   |
| 4   | X     | 116 | ARG  | NE-CZ-NH1  | 5.62  | 123.11      | 120.30   |
| 1   | J     | 693 | HIS  | CA-CB-CG   | -5.62 | 104.05      | 113.60   |
| 4   | 3     | 113 | LYS  | CA-CB-CG   | 5.62  | 125.76      | 113.40   |
| 1   | G     | 785 | GLU  | O-C-N      | 5.62  | 131.69      | 122.70   |
| 1   | J     | 780 | ASP  | CB-CG-OD1  | -5.61 | 113.25      | 118.30   |
| 1   | A     | 781 | ASP  | CB-CG-OD2  | 5.61  | 123.35      | 118.30   |
| 1   | J     | 352 | TYR  | N-CA-CB    | 5.61  | 120.69      | 110.60   |
| 4   | 0     | 113 | LYS  | CA-CB-CG   | 5.61  | 125.74      | 113.40   |
| 4   | 3     | 356 | TRP  | CG-CD2-CE3 | 5.61  | 138.95      | 133.90   |
| 4   | 8     | 356 | TRP  | CG-CD2-CE3 | 5.61  | 138.94      | 133.90   |
| 1   | A     | 352 | TYR  | N-CA-CB    | 5.60  | 120.68      | 110.60   |
| 1   | D     | 693 | HIS  | CA-CB-CG   | -5.60 | 104.08      | 113.60   |
| 4   | 5     | 113 | LYS  | CA-CB-CG   | 5.59  | 125.71      | 113.40   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | 2     | 113 | LYS  | CA-CB-CG   | 5.59  | 125.70      | 113.40   |
| 4   | 5     | 356 | TRP  | CG-CD2-CE3 | 5.59  | 138.93      | 133.90   |
| 4   | 5     | 294 | TYR  | CB-CG-CD2  | -5.59 | 117.65      | 121.00   |
| 4   | V     | 113 | LYS  | CA-CB-CG   | 5.59  | 125.69      | 113.40   |
| 4   | 2     | 356 | TRP  | CG-CD2-CE3 | 5.59  | 138.93      | 133.90   |
| 4   | 8     | 113 | LYS  | CA-CB-CG   | 5.58  | 125.69      | 113.40   |
| 4   | X     | 113 | LYS  | CA-CB-CG   | 5.58  | 125.68      | 113.40   |
| 4   | 1     | 113 | LYS  | CA-CB-CG   | 5.58  | 125.68      | 113.40   |
| 4   | 6     | 294 | TYR  | CB-CG-CD2  | -5.58 | 117.65      | 121.00   |
| 1   | G     | 320 | ILE  | CB-CA-C    | -5.57 | 100.45      | 111.60   |
| 4   | Y     | 294 | TYR  | CB-CG-CD2  | -5.57 | 117.66      | 121.00   |
| 4   | Z     | 113 | LYS  | CA-CB-CG   | 5.57  | 125.66      | 113.40   |
| 4   | Y     | 356 | TRP  | CG-CD2-CE3 | 5.57  | 138.91      | 133.90   |
| 4   | 1     | 279 | TYR  | CB-CG-CD2  | -5.57 | 117.66      | 121.00   |
| 4   | W     | 356 | TRP  | CG-CD2-CE3 | 5.57  | 138.91      | 133.90   |
| 4   | 7     | 294 | TYR  | CB-CG-CD2  | -5.57 | 117.66      | 121.00   |
| 4   | 8     | 279 | TYR  | CB-CG-CD2  | -5.57 | 117.66      | 121.00   |
| 4   | W     | 113 | LYS  | CA-CB-CG   | 5.57  | 125.65      | 113.40   |
| 1   | J     | 33  | ASP  | CB-CG-OD2  | 5.57  | 123.31      | 118.30   |
| 1   | G     | 781 | ASP  | CB-CG-OD2  | 5.56  | 123.31      | 118.30   |
| 4   | 0     | 11  | ASP  | CB-CG-OD1  | 5.56  | 123.31      | 118.30   |
| 4   | 4     | 294 | TYR  | CB-CG-CD2  | -5.56 | 117.66      | 121.00   |
| 4   | 6     | 113 | LYS  | CA-CB-CG   | 5.56  | 125.63      | 113.40   |
| 4   | 7     | 113 | LYS  | CA-CB-CG   | 5.56  | 125.63      | 113.40   |
| 4   | Y     | 113 | LYS  | CA-CB-CG   | 5.56  | 125.63      | 113.40   |
| 4   | W     | 294 | TYR  | CB-CG-CD2  | -5.55 | 117.67      | 121.00   |
| 1   | J     | 686 | MET  | N-CA-CB    | -5.55 | 100.61      | 110.60   |
| 1   | J     | 384 | ASP  | CB-CG-OD1  | -5.55 | 113.30      | 118.30   |
| 4   | 0     | 254 | ARG  | N-CA-CB    | -5.55 | 100.61      | 110.60   |
| 4   | 6     | 356 | TRP  | CG-CD2-CE3 | 5.55  | 138.89      | 133.90   |
| 4   | 4     | 113 | LYS  | CA-CB-CG   | 5.55  | 125.61      | 113.40   |
| 4   | 7     | 254 | ARG  | N-CA-CB    | -5.55 | 100.61      | 110.60   |
| 1   | J     | 781 | ASP  | CB-CG-OD2  | 5.55  | 123.29      | 118.30   |
| 4   | 3     | 254 | ARG  | N-CA-CB    | -5.55 | 100.62      | 110.60   |
| 1   | D     | 384 | ASP  | CB-CG-OD1  | -5.54 | 113.31      | 118.30   |
| 1   | G     | 686 | MET  | N-CA-CB    | -5.54 | 100.62      | 110.60   |
| 4   | 0     | 356 | TRP  | CG-CD2-CE3 | 5.54  | 138.89      | 133.90   |
| 4   | Y     | 279 | TYR  | CB-CG-CD2  | -5.54 | 117.67      | 121.00   |
| 4   | Z     | 254 | ARG  | N-CA-CB    | -5.54 | 100.62      | 110.60   |
| 1   | D     | 686 | MET  | N-CA-CB    | -5.54 | 100.63      | 110.60   |
| 1   | A     | 693 | HIS  | CA-CB-CG   | -5.54 | 104.19      | 113.60   |
| 4   | 3     | 279 | TYR  | CB-CG-CD2  | -5.54 | 117.68      | 121.00   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | 0     | 294 | TYR  | CB-CG-CD2  | -5.54 | 117.68      | 121.00   |
| 1   | D     | 752 | ASP  | CB-CA-C    | 5.54  | 121.47      | 110.40   |
| 4   | V     | 294 | TYR  | CB-CG-CD2  | -5.54 | 117.68      | 121.00   |
| 4   | W     | 254 | ARG  | N-CA-CB    | -5.54 | 100.64      | 110.60   |
| 4   | 7     | 279 | TYR  | CB-CG-CD2  | -5.53 | 117.68      | 121.00   |
| 4   | 6     | 254 | ARG  | N-CA-CB    | -5.53 | 100.65      | 110.60   |
| 1   | D     | 306 | THR  | CA-CB-CG2  | -5.53 | 104.66      | 112.40   |
| 4   | 4     | 254 | ARG  | N-CA-CB    | -5.53 | 100.65      | 110.60   |
| 1   | G     | 306 | THR  | CA-CB-CG2  | -5.53 | 104.67      | 112.40   |
| 4   | 3     | 294 | TYR  | CB-CG-CD2  | -5.53 | 117.69      | 121.00   |
| 4   | 5     | 254 | ARG  | N-CA-CB    | -5.53 | 100.66      | 110.60   |
| 4   | 8     | 254 | ARG  | N-CA-CB    | -5.52 | 100.66      | 110.60   |
| 4   | 8     | 11  | ASP  | CB-CG-OD1  | 5.52  | 123.27      | 118.30   |
| 4   | 4     | 279 | TYR  | CB-CG-CD2  | -5.52 | 117.69      | 121.00   |
| 4   | 1     | 294 | TYR  | CB-CG-CD2  | -5.52 | 117.69      | 121.00   |
| 4   | X     | 254 | ARG  | N-CA-CB    | -5.52 | 100.66      | 110.60   |
| 4   | 1     | 254 | ARG  | N-CA-CB    | -5.52 | 100.67      | 110.60   |
| 4   | Y     | 254 | ARG  | N-CA-CB    | -5.52 | 100.67      | 110.60   |
| 4   | 2     | 254 | ARG  | N-CA-CB    | -5.51 | 100.67      | 110.60   |
| 4   | V     | 254 | ARG  | N-CA-CB    | -5.51 | 100.67      | 110.60   |
| 1   | J     | 343 | PHE  | CB-CG-CD2  | -5.51 | 116.94      | 120.80   |
| 1   | J     | 752 | ASP  | CB-CA-C    | 5.51  | 121.42      | 110.40   |
| 1   | A     | 752 | ASP  | CB-CA-C    | 5.51  | 121.41      | 110.40   |
| 4   | 7     | 356 | TRP  | CG-CD2-CE3 | 5.51  | 138.86      | 133.90   |
| 1   | A     | 686 | MET  | N-CA-CB    | -5.50 | 100.69      | 110.60   |
| 4   | 4     | 11  | ASP  | CB-CG-OD1  | 5.50  | 123.25      | 118.30   |
| 1   | G     | 752 | ASP  | CB-CA-C    | 5.50  | 121.40      | 110.40   |
| 4   | 2     | 294 | TYR  | CB-CG-CD2  | -5.50 | 117.70      | 121.00   |
| 4   | V     | 11  | ASP  | CB-CG-OD1  | 5.49  | 123.24      | 118.30   |
| 4   | 4     | 356 | TRP  | CG-CD2-CE3 | 5.49  | 138.84      | 133.90   |
| 4   | 6     | 147 | ARG  | NE-CZ-NH2  | -5.49 | 117.56      | 120.30   |
| 4   | 6     | 279 | TYR  | CB-CG-CD2  | -5.49 | 117.71      | 121.00   |
| 4   | Z     | 279 | TYR  | CB-CG-CD2  | -5.49 | 117.71      | 121.00   |
| 4   | 3     | 254 | ARG  | NE-CZ-NH1  | 5.49  | 123.04      | 120.30   |
| 1   | J     | 320 | ILE  | CB-CA-C    | -5.48 | 100.63      | 111.60   |
| 1   | D     | 723 | ARG  | NE-CZ-NH1  | 5.48  | 123.04      | 120.30   |
| 4   | 0     | 279 | TYR  | CB-CG-CD2  | -5.48 | 117.71      | 121.00   |
| 4   | 1     | 356 | TRP  | CG-CD2-CE3 | 5.48  | 138.83      | 133.90   |
| 4   | 2     | 79  | TRP  | CB-CG-CD1  | -5.48 | 119.88      | 127.00   |
| 4   | 3     | 11  | ASP  | CB-CG-OD1  | 5.48  | 123.23      | 118.30   |
| 4   | 8     | 294 | TYR  | CB-CG-CD2  | -5.48 | 117.71      | 121.00   |
| 4   | Z     | 11  | ASP  | CB-CG-OD1  | 5.48  | 123.23      | 118.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | D     | 33  | ASP  | CB-CG-OD2  | 5.48  | 123.23      | 118.30   |
| 1   | A     | 33  | ASP  | CB-CG-OD2  | 5.47  | 123.22      | 118.30   |
| 4   | X     | 279 | TYR  | CB-CG-CD2  | -5.47 | 117.72      | 121.00   |
| 1   | A     | 241 | ASP  | CB-CG-OD2  | 5.47  | 123.22      | 118.30   |
| 4   | 5     | 11  | ASP  | CB-CG-OD1  | 5.47  | 123.22      | 118.30   |
| 4   | Y     | 11  | ASP  | CB-CG-OD1  | 5.47  | 123.22      | 118.30   |
| 4   | W     | 11  | ASP  | CB-CG-OD1  | 5.47  | 123.22      | 118.30   |
| 4   | X     | 356 | TRP  | CG-CD2-CE3 | 5.47  | 138.82      | 133.90   |
| 4   | Z     | 356 | TRP  | CG-CD2-CE3 | 5.47  | 138.82      | 133.90   |
| 1   | D     | 320 | ILE  | CB-CA-C    | -5.46 | 100.68      | 111.60   |
| 4   | V     | 279 | TYR  | CB-CG-CD2  | -5.46 | 117.72      | 121.00   |
| 4   | 2     | 279 | TYR  | CB-CG-CD2  | -5.46 | 117.73      | 121.00   |
| 4   | W     | 356 | TRP  | CB-CG-CD1  | -5.46 | 119.91      | 127.00   |
| 1   | A     | 306 | THR  | CA-CB-CG2  | -5.45 | 104.77      | 112.40   |
| 4   | V     | 356 | TRP  | CG-CD2-CE3 | 5.45  | 138.81      | 133.90   |
| 1   | A     | 320 | ILE  | CB-CA-C    | -5.45 | 100.70      | 111.60   |
| 4   | 7     | 79  | TRP  | CB-CG-CD1  | -5.45 | 119.92      | 127.00   |
| 1   | J     | 547 | ASP  | CB-CG-OD2  | 5.45  | 123.20      | 118.30   |
| 4   | 2     | 147 | ARG  | NE-CZ-NH2  | -5.44 | 117.58      | 120.30   |
| 1   | D     | 326 | ASP  | CB-CG-OD2  | 5.44  | 123.20      | 118.30   |
| 4   | 2     | 11  | ASP  | CB-CG-OD1  | 5.44  | 123.20      | 118.30   |
| 4   | 4     | 356 | TRP  | CB-CG-CD1  | -5.44 | 119.93      | 127.00   |
| 4   | 5     | 279 | TYR  | CB-CG-CD2  | -5.44 | 117.74      | 121.00   |
| 4   | W     | 279 | TYR  | CB-CG-CD2  | -5.44 | 117.74      | 121.00   |
| 1   | J     | 326 | ASP  | CB-CG-OD2  | 5.43  | 123.19      | 118.30   |
| 4   | X     | 335 | ARG  | NE-CZ-NH1  | 5.43  | 123.02      | 120.30   |
| 1   | D     | 547 | ASP  | CB-CG-OD2  | 5.43  | 123.19      | 118.30   |
| 1   | J     | 306 | THR  | CA-CB-CG2  | -5.43 | 104.80      | 112.40   |
| 4   | 4     | 356 | TRP  | CG-CD1-NE1 | -5.43 | 104.67      | 110.10   |
| 1   | A     | 343 | PHE  | CB-CG-CD2  | -5.43 | 117.00      | 120.80   |
| 4   | 1     | 79  | TRP  | CB-CG-CD1  | -5.43 | 119.94      | 127.00   |
| 4   | 3     | 79  | TRP  | CB-CG-CD1  | -5.43 | 119.94      | 127.00   |
| 1   | J     | 218 | LEU  | O-C-N      | 5.43  | 131.38      | 122.70   |
| 4   | 6     | 356 | TRP  | CB-CG-CD1  | -5.43 | 119.95      | 127.00   |
| 4   | W     | 356 | TRP  | CG-CD1-NE1 | -5.43 | 104.67      | 110.10   |
| 4   | W     | 147 | ARG  | NE-CZ-NH2  | -5.42 | 117.59      | 120.30   |
| 4   | 7     | 11  | ASP  | CB-CG-OD1  | 5.42  | 123.18      | 118.30   |
| 4   | 1     | 11  | ASP  | CB-CG-OD1  | 5.42  | 123.18      | 118.30   |
| 4   | 3     | 356 | TRP  | CB-CG-CD1  | -5.42 | 119.95      | 127.00   |
| 1   | A     | 723 | ARG  | NE-CZ-NH1  | 5.42  | 123.01      | 120.30   |
| 4   | 2     | 356 | TRP  | CB-CG-CD1  | -5.42 | 119.96      | 127.00   |
| 4   | 7     | 356 | TRP  | CB-CG-CD1  | -5.42 | 119.96      | 127.00   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | 2     | 356 | TRP  | CG-CD1-NE1 | -5.42 | 104.69      | 110.10   |
| 4   | Z     | 356 | TRP  | CB-CG-CD1  | -5.42 | 119.96      | 127.00   |
| 4   | 8     | 356 | TRP  | CG-CD1-NE1 | -5.41 | 104.69      | 110.10   |
| 4   | Z     | 79  | TRP  | CB-CG-CD1  | -5.41 | 119.96      | 127.00   |
| 4   | 4     | 79  | TRP  | CB-CG-CD1  | -5.41 | 119.97      | 127.00   |
| 4   | 5     | 79  | TRP  | CB-CG-CD1  | -5.41 | 119.97      | 127.00   |
| 4   | 6     | 356 | TRP  | CG-CD1-NE1 | -5.41 | 104.69      | 110.10   |
| 4   | V     | 79  | TRP  | CB-CG-CD1  | -5.41 | 119.97      | 127.00   |
| 4   | Y     | 356 | TRP  | CG-CD1-NE1 | -5.41 | 104.69      | 110.10   |
| 4   | W     | 79  | TRP  | CB-CG-CD1  | -5.41 | 119.97      | 127.00   |
| 4   | Y     | 356 | TRP  | CB-CG-CD1  | -5.41 | 119.97      | 127.00   |
| 1   | A     | 326 | ASP  | CB-CG-OD2  | 5.40  | 123.16      | 118.30   |
| 4   | 6     | 11  | ASP  | CB-CG-OD1  | 5.40  | 123.16      | 118.30   |
| 4   | V     | 356 | TRP  | CB-CG-CD1  | -5.40 | 119.98      | 127.00   |
| 4   | X     | 11  | ASP  | CB-CG-OD1  | 5.40  | 123.16      | 118.30   |
| 4   | X     | 79  | TRP  | CB-CG-CD1  | -5.40 | 119.98      | 127.00   |
| 4   | 1     | 356 | TRP  | CB-CG-CD1  | -5.40 | 119.98      | 127.00   |
| 4   | Y     | 79  | TRP  | CB-CG-CD1  | -5.40 | 119.98      | 127.00   |
| 1   | A     | 601 | ASP  | CB-CG-OD2  | 5.39  | 123.16      | 118.30   |
| 4   | 6     | 79  | TRP  | CB-CG-CD1  | -5.39 | 119.99      | 127.00   |
| 4   | 6     | 335 | ARG  | NE-CZ-NH1  | 5.39  | 123.00      | 120.30   |
| 4   | X     | 356 | TRP  | CB-CG-CD1  | -5.39 | 120.00      | 127.00   |
| 1   | G     | 33  | ASP  | CB-CG-OD2  | 5.39  | 123.15      | 118.30   |
| 4   | 0     | 79  | TRP  | CB-CG-CD1  | -5.39 | 120.00      | 127.00   |
| 4   | 5     | 335 | ARG  | NE-CZ-NH1  | 5.39  | 122.99      | 120.30   |
| 1   | A     | 384 | ASP  | CB-CG-OD1  | -5.38 | 113.45      | 118.30   |
| 4   | 0     | 356 | TRP  | CB-CG-CD1  | -5.38 | 120.00      | 127.00   |
| 4   | 5     | 356 | TRP  | CB-CG-CD1  | -5.38 | 120.00      | 127.00   |
| 4   | 8     | 356 | TRP  | CB-CG-CD1  | -5.38 | 120.00      | 127.00   |
| 1   | A     | 686 | MET  | CG-SD-CE   | -5.38 | 91.60       | 100.20   |
| 4   | 1     | 356 | TRP  | CG-CD1-NE1 | -5.38 | 104.72      | 110.10   |
| 4   | 5     | 356 | TRP  | CG-CD1-NE1 | -5.38 | 104.72      | 110.10   |
| 4   | 5     | 251 | GLY  | CA-C-N     | -5.38 | 105.38      | 117.20   |
| 1   | J     | 241 | ASP  | CB-CG-OD2  | 5.37  | 123.14      | 118.30   |
| 4   | V     | 251 | GLY  | CA-C-N     | -5.37 | 105.38      | 117.20   |
| 4   | Z     | 356 | TRP  | CG-CD1-NE1 | -5.37 | 104.73      | 110.10   |
| 4   | X     | 251 | GLY  | CA-C-N     | -5.37 | 105.40      | 117.20   |
| 1   | G     | 686 | MET  | CG-SD-CE   | -5.36 | 91.62       | 100.20   |
| 1   | G     | 218 | LEU  | O-C-N      | 5.36  | 131.28      | 122.70   |
| 4   | Z     | 147 | ARG  | NE-CZ-NH2  | -5.36 | 117.62      | 120.30   |
| 1   | J     | 686 | MET  | CG-SD-CE   | -5.36 | 91.63       | 100.20   |
| 4   | 8     | 79  | TRP  | CB-CG-CD1  | -5.36 | 120.04      | 127.00   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | 0     | 356 | TRP  | CG-CD1-NE1 | -5.35 | 104.75      | 110.10   |
| 4   | 7     | 356 | TRP  | CG-CD1-NE1 | -5.35 | 104.75      | 110.10   |
| 4   | V     | 147 | ARG  | NE-CZ-NH2  | -5.35 | 117.62      | 120.30   |
| 4   | 4     | 251 | GLY  | CA-C-N     | -5.35 | 105.43      | 117.20   |
| 1   | G     | 326 | ASP  | CB-CG-OD2  | 5.35  | 123.11      | 118.30   |
| 2   | K     | 136 | MET  | CG-SD-CE   | 5.35  | 108.76      | 100.20   |
| 4   | 0     | 251 | GLY  | CA-C-N     | -5.35 | 105.43      | 117.20   |
| 4   | 2     | 251 | GLY  | CA-C-N     | -5.35 | 105.43      | 117.20   |
| 4   | X     | 356 | TRP  | CG-CD1-NE1 | -5.35 | 104.75      | 110.10   |
| 4   | 3     | 251 | GLY  | CA-C-N     | -5.35 | 105.44      | 117.20   |
| 4   | 7     | 251 | GLY  | CA-C-N     | -5.35 | 105.44      | 117.20   |
| 1   | G     | 800 | ARG  | NH1-CZ-NH2 | 5.34  | 125.28      | 119.40   |
| 2   | B     | 136 | MET  | CG-SD-CE   | 5.34  | 108.75      | 100.20   |
| 1   | D     | 601 | ASP  | CB-CG-OD2  | 5.34  | 123.11      | 118.30   |
| 4   | 5     | 147 | ARG  | NE-CZ-NH2  | -5.34 | 117.63      | 120.30   |
| 4   | W     | 251 | GLY  | CA-C-N     | -5.34 | 105.46      | 117.20   |
| 4   | 4     | 335 | ARG  | NE-CZ-NH1  | 5.34  | 122.97      | 120.30   |
| 4   | 7     | 147 | ARG  | NE-CZ-NH2  | -5.34 | 117.63      | 120.30   |
| 4   | 8     | 251 | GLY  | CA-C-N     | -5.34 | 105.46      | 117.20   |
| 1   | D     | 241 | ASP  | CB-CG-OD2  | 5.33  | 123.10      | 118.30   |
| 1   | D     | 800 | ARG  | NH1-CZ-NH2 | 5.33  | 125.27      | 119.40   |
| 4   | 6     | 251 | GLY  | CA-C-N     | -5.33 | 105.47      | 117.20   |
| 4   | 1     | 251 | GLY  | CA-C-N     | -5.33 | 105.47      | 117.20   |
| 1   | J     | 601 | ASP  | CB-CG-OD2  | 5.33  | 123.09      | 118.30   |
| 1   | J     | 723 | ARG  | NE-CZ-NH1  | 5.33  | 122.96      | 120.30   |
| 4   | W     | 176 | MET  | CG-SD-CE   | 5.33  | 108.72      | 100.20   |
| 4   | Z     | 251 | GLY  | CA-C-N     | -5.33 | 105.48      | 117.20   |
| 1   | G     | 241 | ASP  | CB-CG-OD2  | 5.32  | 123.09      | 118.30   |
| 4   | Y     | 251 | GLY  | CA-C-N     | -5.32 | 105.49      | 117.20   |
| 1   | A     | 125 | THR  | CA-CB-CG2  | -5.32 | 104.95      | 112.40   |
| 1   | G     | 125 | THR  | CA-CB-CG2  | -5.32 | 104.95      | 112.40   |
| 1   | G     | 601 | ASP  | CB-CG-OD2  | 5.32  | 123.09      | 118.30   |
| 4   | 6     | 176 | MET  | CG-SD-CE   | 5.32  | 108.71      | 100.20   |
| 4   | 6     | 337 | TYR  | CB-CG-CD1  | -5.32 | 117.81      | 121.00   |
| 4   | Y     | 147 | ARG  | NE-CZ-NH2  | -5.32 | 117.64      | 120.30   |
| 4   | V     | 356 | TRP  | CG-CD1-NE1 | -5.31 | 104.79      | 110.10   |
| 4   | Z     | 176 | MET  | CG-SD-CE   | 5.31  | 108.70      | 100.20   |
| 4   | 4     | 176 | MET  | CG-SD-CE   | 5.31  | 108.70      | 100.20   |
| 1   | D     | 343 | PHE  | CB-CG-CD2  | -5.31 | 117.08      | 120.80   |
| 4   | V     | 176 | MET  | CG-SD-CE   | 5.31  | 108.69      | 100.20   |
| 4   | X     | 176 | MET  | CG-SD-CE   | 5.31  | 108.69      | 100.20   |
| 1   | D     | 354 | LEU  | CB-CG-CD2  | -5.30 | 101.98      | 111.00   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | G     | 660 | LEU  | CB-CG-CD2  | 5.30  | 120.02      | 111.00   |
| 4   | 3     | 356 | TRP  | CG-CD1-NE1 | -5.30 | 104.80      | 110.10   |
| 4   | 3     | 147 | ARG  | NE-CZ-NH2  | -5.30 | 117.65      | 120.30   |
| 1   | A     | 660 | LEU  | CB-CG-CD2  | 5.30  | 120.01      | 111.00   |
| 1   | G     | 723 | ARG  | NE-CZ-NH1  | 5.30  | 122.95      | 120.30   |
| 4   | 2     | 176 | MET  | CG-SD-CE   | 5.30  | 108.67      | 100.20   |
| 4   | 7     | 176 | MET  | CG-SD-CE   | 5.30  | 108.67      | 100.20   |
| 1   | D     | 760 | PHE  | CB-CG-CD1  | 5.29  | 124.50      | 120.80   |
| 4   | 3     | 176 | MET  | CG-SD-CE   | 5.29  | 108.67      | 100.20   |
| 4   | 4     | 147 | ARG  | NE-CZ-NH2  | -5.29 | 117.65      | 120.30   |
| 1   | G     | 384 | ASP  | CB-CG-OD1  | -5.29 | 113.54      | 118.30   |
| 4   | Y     | 176 | MET  | CG-SD-CE   | 5.29  | 108.66      | 100.20   |
| 4   | 1     | 176 | MET  | CG-SD-CE   | 5.29  | 108.66      | 100.20   |
| 2   | E     | 136 | MET  | CG-SD-CE   | 5.29  | 108.66      | 100.20   |
| 1   | J     | 170 | ARG  | NE-CZ-NH1  | 5.29  | 122.94      | 120.30   |
| 4   | 0     | 176 | MET  | CG-SD-CE   | 5.28  | 108.65      | 100.20   |
| 4   | X     | 147 | ARG  | NE-CZ-NH2  | -5.28 | 117.66      | 120.30   |
| 1   | D     | 125 | THR  | CA-CB-CG2  | -5.28 | 105.01      | 112.40   |
| 1   | D     | 660 | LEU  | CB-CG-CD2  | 5.28  | 119.97      | 111.00   |
| 2   | H     | 136 | MET  | CG-SD-CE   | 5.28  | 108.65      | 100.20   |
| 1   | J     | 125 | THR  | CA-CB-CG2  | -5.28 | 105.01      | 112.40   |
| 1   | A     | 354 | LEU  | CB-CG-CD2  | -5.28 | 102.03      | 111.00   |
| 1   | J     | 800 | ARG  | NH1-CZ-NH2 | 5.28  | 125.20      | 119.40   |
| 4   | 0     | 147 | ARG  | NE-CZ-NH2  | -5.27 | 117.66      | 120.30   |
| 1   | D     | 686 | MET  | CG-SD-CE   | -5.27 | 91.76       | 100.20   |
| 4   | Z     | 62  | ARG  | NE-CZ-NH1  | 5.27  | 122.94      | 120.30   |
| 4   | 1     | 335 | ARG  | NE-CZ-NH1  | 5.27  | 122.94      | 120.30   |
| 1   | A     | 800 | ARG  | NH1-CZ-NH2 | 5.26  | 125.19      | 119.40   |
| 4   | 8     | 62  | ARG  | NE-CZ-NH1  | 5.26  | 122.93      | 120.30   |
| 4   | 8     | 176 | MET  | CG-SD-CE   | 5.26  | 108.62      | 100.20   |
| 1   | G     | 354 | LEU  | CB-CG-CD2  | -5.26 | 102.06      | 111.00   |
| 4   | 5     | 176 | MET  | CG-SD-CE   | 5.25  | 108.60      | 100.20   |
| 1   | J     | 660 | LEU  | CB-CG-CD2  | 5.25  | 119.93      | 111.00   |
| 4   | Z     | 335 | ARG  | NE-CZ-NH1  | 5.24  | 122.92      | 120.30   |
| 1   | A     | 346 | ASP  | N-CA-CB    | -5.24 | 101.17      | 110.60   |
| 1   | G     | 547 | ASP  | CB-CG-OD2  | 5.23  | 123.00      | 118.30   |
| 1   | G     | 555 | TYR  | CB-CG-CD1  | 5.22  | 124.14      | 121.00   |
| 4   | V     | 62  | ARG  | NE-CZ-NH1  | 5.22  | 122.91      | 120.30   |
| 1   | A     | 218 | LEU  | O-C-N      | 5.22  | 131.06      | 122.70   |
| 1   | D     | 218 | LEU  | O-C-N      | 5.22  | 131.05      | 122.70   |
| 4   | 1     | 62  | ARG  | NE-CZ-NH1  | 5.22  | 122.91      | 120.30   |
| 4   | 8     | 147 | ARG  | NE-CZ-NH2  | -5.22 | 117.69      | 120.30   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 4   | W     | 335 | ARG  | NE-CZ-NH1 | 5.22  | 122.91      | 120.30   |
| 1   | A     | 760 | PHE  | CB-CG-CD1 | 5.21  | 124.45      | 120.80   |
| 1   | J     | 346 | ASP  | N-CA-CB   | -5.21 | 101.22      | 110.60   |
| 1   | D     | 346 | ASP  | N-CA-CB   | -5.21 | 101.22      | 110.60   |
| 1   | J     | 354 | LEU  | CB-CG-CD2 | -5.21 | 102.14      | 111.00   |
| 4   | 3     | 337 | TYR  | CB-CG-CD1 | -5.21 | 117.87      | 121.00   |
| 1   | A     | 547 | ASP  | CB-CG-OD2 | 5.21  | 122.99      | 118.30   |
| 1   | G     | 343 | PHE  | CB-CG-CD2 | -5.20 | 117.16      | 120.80   |
| 1   | J     | 760 | PHE  | CB-CG-CD1 | 5.20  | 124.44      | 120.80   |
| 4   | 3     | 62  | ARG  | NE-CZ-NH1 | 5.20  | 122.90      | 120.30   |
| 1   | D     | 4   | ASP  | CB-CG-OD1 | -5.20 | 113.62      | 118.30   |
| 1   | J     | 4   | ASP  | CB-CG-OD1 | -5.19 | 113.63      | 118.30   |
| 1   | A     | 90  | ASP  | CB-CG-OD1 | -5.19 | 113.63      | 118.30   |
| 4   | 8     | 335 | ARG  | NE-CZ-NH1 | 5.19  | 122.90      | 120.30   |
| 1   | G     | 4   | ASP  | CB-CG-OD1 | -5.19 | 113.63      | 118.30   |
| 4   | 0     | 337 | TYR  | CB-CG-CD1 | -5.19 | 117.89      | 121.00   |
| 4   | 0     | 62  | ARG  | NE-CZ-NH1 | 5.18  | 122.89      | 120.30   |
| 4   | V     | 290 | ARG  | CA-C-N    | 5.17  | 128.59      | 117.20   |
| 4   | 1     | 147 | ARG  | NE-CZ-NH2 | -5.17 | 117.72      | 120.30   |
| 4   | V     | 335 | ARG  | NE-CZ-NH1 | 5.17  | 122.89      | 120.30   |
| 4   | X     | 337 | TYR  | CB-CG-CD1 | -5.17 | 117.90      | 121.00   |
| 4   | 4     | 290 | ARG  | CA-C-N    | 5.17  | 128.56      | 117.20   |
| 4   | 5     | 290 | ARG  | CA-C-N    | 5.17  | 128.56      | 117.20   |
| 4   | 6     | 290 | ARG  | CA-C-N    | 5.16  | 128.56      | 117.20   |
| 4   | X     | 290 | ARG  | CA-C-N    | 5.16  | 128.56      | 117.20   |
| 4   | Y     | 290 | ARG  | CA-C-N    | 5.16  | 128.56      | 117.20   |
| 4   | 2     | 62  | ARG  | NE-CZ-NH1 | 5.16  | 122.88      | 120.30   |
| 4   | 7     | 335 | ARG  | NE-CZ-NH1 | 5.16  | 122.88      | 120.30   |
| 4   | 0     | 290 | ARG  | CA-C-N    | 5.16  | 128.55      | 117.20   |
| 4   | 8     | 290 | ARG  | CA-C-N    | 5.16  | 128.55      | 117.20   |
| 4   | 3     | 290 | ARG  | CA-C-N    | 5.16  | 128.54      | 117.20   |
| 4   | 2     | 290 | ARG  | CA-C-N    | 5.16  | 128.54      | 117.20   |
| 4   | 3     | 335 | ARG  | NE-CZ-NH1 | 5.16  | 122.88      | 120.30   |
| 4   | 1     | 290 | ARG  | CA-C-N    | 5.15  | 128.54      | 117.20   |
| 4   | V     | 53  | TYR  | CB-CG-CD1 | -5.15 | 117.91      | 121.00   |
| 4   | Z     | 290 | ARG  | CA-C-N    | 5.15  | 128.54      | 117.20   |
| 1   | A     | 4   | ASP  | CB-CG-OD1 | -5.15 | 113.67      | 118.30   |
| 4   | 2     | 337 | TYR  | CB-CG-CD1 | -5.15 | 117.91      | 121.00   |
| 4   | 6     | 53  | TYR  | CB-CG-CD1 | -5.15 | 117.91      | 121.00   |
| 4   | 7     | 290 | ARG  | CA-C-N    | 5.15  | 128.53      | 117.20   |
| 4   | W     | 290 | ARG  | CA-C-N    | 5.15  | 128.52      | 117.20   |
| 4   | 6     | 62  | ARG  | NE-CZ-NH1 | 5.14  | 122.87      | 120.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | Y     | 335 | ARG  | NE-CZ-NH1  | 5.14  | 122.87      | 120.30   |
| 4   | W     | 91  | TYR  | CB-CG-CD2  | -5.14 | 117.92      | 121.00   |
| 4   | Z     | 53  | TYR  | CB-CG-CD1  | -5.14 | 117.92      | 121.00   |
| 4   | 0     | 335 | ARG  | NE-CZ-NH1  | 5.14  | 122.87      | 120.30   |
| 4   | W     | 337 | TYR  | CB-CG-CD1  | -5.13 | 117.92      | 121.00   |
| 4   | Y     | 62  | ARG  | NE-CZ-NH1  | 5.13  | 122.87      | 120.30   |
| 1   | G     | 346 | ASP  | N-CA-CB    | -5.13 | 101.36      | 110.60   |
| 4   | 1     | 91  | TYR  | CB-CG-CD2  | -5.13 | 117.92      | 121.00   |
| 4   | 7     | 62  | ARG  | NE-CZ-NH1  | 5.13  | 122.86      | 120.30   |
| 4   | 8     | 91  | TYR  | CB-CG-CD2  | -5.12 | 117.92      | 121.00   |
| 4   | Y     | 86  | TRP  | CG-CD1-NE1 | -5.12 | 104.97      | 110.10   |
| 1   | A     | 160 | ASP  | CB-CG-OD2  | -5.12 | 113.69      | 118.30   |
| 1   | D     | 576 | GLU  | CA-CB-CG   | -5.12 | 102.13      | 113.40   |
| 1   | J     | 576 | GLU  | CA-CB-CG   | -5.12 | 102.13      | 113.40   |
| 4   | 2     | 335 | ARG  | NE-CZ-NH1  | 5.12  | 122.86      | 120.30   |
| 1   | A     | 576 | GLU  | CA-CB-CG   | -5.12 | 102.14      | 113.40   |
| 4   | Z     | 62  | ARG  | CA-CB-CG   | 5.12  | 124.66      | 113.40   |
| 1   | G     | 760 | PHE  | CB-CG-CD1  | 5.11  | 124.38      | 120.80   |
| 1   | G     | 160 | ASP  | CB-CG-OD2  | -5.11 | 113.70      | 118.30   |
| 1   | G     | 576 | GLU  | CA-CB-CG   | -5.11 | 102.16      | 113.40   |
| 4   | 0     | 53  | TYR  | CB-CG-CD1  | -5.11 | 117.93      | 121.00   |
| 4   | 5     | 337 | TYR  | CB-CG-CD1  | -5.11 | 117.93      | 121.00   |
| 4   | 7     | 86  | TRP  | CG-CD1-NE1 | -5.11 | 104.99      | 110.10   |
| 4   | Y     | 337 | TYR  | CB-CG-CD1  | -5.11 | 117.93      | 121.00   |
| 1   | J     | 628 | GLY  | O-C-N      | -5.11 | 114.53      | 122.70   |
| 1   | D     | 628 | GLY  | O-C-N      | -5.11 | 114.53      | 122.70   |
| 1   | J     | 301 | ASP  | CB-CG-OD2  | 5.11  | 122.90      | 118.30   |
| 4   | 5     | 62  | ARG  | CA-CB-CG   | 5.11  | 124.64      | 113.40   |
| 4   | 8     | 62  | ARG  | CA-CB-CG   | 5.11  | 124.63      | 113.40   |
| 4   | Z     | 86  | TRP  | CG-CD1-NE1 | -5.10 | 105.00      | 110.10   |
| 4   | 7     | 53  | TYR  | CB-CG-CD1  | -5.10 | 117.94      | 121.00   |
| 4   | 1     | 53  | TYR  | CB-CG-CD1  | -5.10 | 117.94      | 121.00   |
| 4   | 8     | 337 | TYR  | CB-CG-CD1  | -5.10 | 117.94      | 121.00   |
| 1   | G     | 90  | ASP  | CB-CG-OD1  | -5.10 | 113.71      | 118.30   |
| 4   | 6     | 62  | ARG  | CA-CB-CG   | 5.10  | 124.62      | 113.40   |
| 4   | W     | 62  | ARG  | CA-CB-CG   | 5.10  | 124.61      | 113.40   |
| 4   | 7     | 337 | TYR  | CB-CG-CD1  | -5.10 | 117.94      | 121.00   |
| 4   | 5     | 86  | TRP  | CG-CD1-NE1 | -5.09 | 105.00      | 110.10   |
| 1   | A     | 218 | LEU  | CA-CB-CG   | 5.09  | 127.01      | 115.30   |
| 4   | W     | 62  | ARG  | NE-CZ-NH1  | 5.09  | 122.85      | 120.30   |
| 4   | 4     | 62  | ARG  | CA-CB-CG   | 5.09  | 124.59      | 113.40   |
| 4   | 8     | 53  | TYR  | CB-CG-CD1  | -5.09 | 117.95      | 121.00   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | Z     | 337 | TYR  | CB-CG-CD1  | -5.09 | 117.95      | 121.00   |
| 4   | 1     | 62  | ARG  | CA-CB-CG   | 5.09  | 124.59      | 113.40   |
| 4   | 2     | 62  | ARG  | CA-CB-CG   | 5.09  | 124.59      | 113.40   |
| 4   | Y     | 62  | ARG  | CA-CB-CG   | 5.08  | 124.59      | 113.40   |
| 1   | D     | 82  | PRO  | N-CA-CB    | 5.08  | 109.40      | 103.30   |
| 1   | D     | 218 | LEU  | CA-CB-CG   | 5.08  | 126.99      | 115.30   |
| 4   | 7     | 62  | ARG  | CA-CB-CG   | 5.08  | 124.58      | 113.40   |
| 1   | D     | 621 | LEU  | CA-CB-CG   | -5.08 | 103.61      | 115.30   |
| 1   | J     | 555 | TYR  | CB-CG-CD1  | 5.08  | 124.05      | 121.00   |
| 4   | 4     | 337 | TYR  | CB-CG-CD1  | -5.08 | 117.95      | 121.00   |
| 4   | X     | 62  | ARG  | CA-CB-CG   | 5.08  | 124.58      | 113.40   |
| 4   | X     | 91  | TYR  | CB-CG-CD2  | -5.08 | 117.95      | 121.00   |
| 4   | 4     | 191 | LYS  | CA-C-N     | 5.08  | 128.38      | 117.20   |
| 4   | V     | 62  | ARG  | CA-CB-CG   | 5.08  | 124.58      | 113.40   |
| 4   | V     | 91  | TYR  | CB-CG-CD2  | -5.08 | 117.95      | 121.00   |
| 4   | 0     | 91  | TYR  | CB-CG-CD2  | -5.08 | 117.95      | 121.00   |
| 4   | 3     | 53  | TYR  | CB-CG-CD1  | -5.08 | 117.95      | 121.00   |
| 4   | 5     | 191 | LYS  | CA-C-N     | 5.08  | 128.37      | 117.20   |
| 4   | Y     | 191 | LYS  | CA-C-N     | 5.08  | 128.37      | 117.20   |
| 1   | G     | 621 | LEU  | CA-CB-CG   | -5.08 | 103.62      | 115.30   |
| 4   | 0     | 62  | ARG  | CA-CB-CG   | 5.08  | 124.57      | 113.40   |
| 4   | 3     | 62  | ARG  | CA-CB-CG   | 5.07  | 124.56      | 113.40   |
| 1   | G     | 170 | ARG  | NE-CZ-NH1  | 5.07  | 122.84      | 120.30   |
| 4   | 5     | 91  | TYR  | CB-CG-CD2  | -5.07 | 117.96      | 121.00   |
| 4   | W     | 191 | LYS  | CA-C-N     | 5.07  | 128.35      | 117.20   |
| 4   | X     | 191 | LYS  | CA-C-N     | 5.07  | 128.35      | 117.20   |
| 1   | J     | 160 | ASP  | CB-CG-OD2  | -5.07 | 113.74      | 118.30   |
| 4   | X     | 86  | TRP  | CG-CD1-NE1 | -5.07 | 105.03      | 110.10   |
| 1   | A     | 621 | LEU  | CA-CB-CG   | -5.06 | 103.66      | 115.30   |
| 4   | 0     | 191 | LYS  | CA-C-N     | 5.06  | 128.34      | 117.20   |
| 4   | X     | 62  | ARG  | NE-CZ-NH1  | 5.06  | 122.83      | 120.30   |
| 4   | 3     | 191 | LYS  | CA-C-N     | 5.06  | 128.33      | 117.20   |
| 4   | 6     | 86  | TRP  | CG-CD1-NE1 | -5.06 | 105.04      | 110.10   |
| 1   | J     | 621 | LEU  | CA-CB-CG   | -5.06 | 103.67      | 115.30   |
| 4   | 8     | 191 | LYS  | CA-C-N     | 5.06  | 128.33      | 117.20   |
| 4   | 4     | 86  | TRP  | CG-CD1-NE1 | -5.05 | 105.05      | 110.10   |
| 4   | V     | 337 | TYR  | CB-CG-CD1  | -5.05 | 117.97      | 121.00   |
| 4   | Y     | 53  | TYR  | CB-CG-CD1  | -5.05 | 117.97      | 121.00   |
| 1   | A     | 628 | GLY  | O-C-N      | -5.05 | 114.62      | 122.70   |
| 1   | D     | 160 | ASP  | CB-CG-OD2  | -5.05 | 113.75      | 118.30   |
| 1   | J     | 218 | LEU  | CA-CB-CG   | 5.05  | 126.92      | 115.30   |
| 1   | A     | 739 | ASP  | CA-CB-CG   | -5.05 | 102.29      | 113.40   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 82  | PRO  | N-CA-CB    | 5.05  | 109.36      | 103.30   |
| 4   | 4     | 91  | TYR  | CB-CG-CD2  | -5.05 | 117.97      | 121.00   |
| 4   | Z     | 191 | LYS  | CA-C-N     | 5.05  | 128.30      | 117.20   |
| 4   | 2     | 86  | TRP  | CG-CD1-NE1 | -5.04 | 105.06      | 110.10   |
| 4   | 1     | 191 | LYS  | CA-C-N     | 5.04  | 128.29      | 117.20   |
| 4   | 4     | 53  | TYR  | CB-CG-CD1  | -5.04 | 117.97      | 121.00   |
| 4   | 6     | 91  | TYR  | CB-CG-CD2  | -5.04 | 117.97      | 121.00   |
| 4   | 7     | 191 | LYS  | CA-C-N     | 5.04  | 128.29      | 117.20   |
| 1   | J     | 82  | PRO  | N-CA-CB    | 5.04  | 109.35      | 103.30   |
| 4   | 2     | 191 | LYS  | CA-C-N     | 5.04  | 128.28      | 117.20   |
| 1   | A     | 235 | ALA  | N-CA-CB    | -5.04 | 103.05      | 110.10   |
| 4   | 2     | 91  | TYR  | CB-CG-CD2  | -5.04 | 117.98      | 121.00   |
| 4   | 5     | 62  | ARG  | NE-CZ-NH1  | 5.04  | 122.82      | 120.30   |
| 4   | W     | 53  | TYR  | CB-CG-CD1  | -5.03 | 117.98      | 121.00   |
| 1   | G     | 218 | LEU  | CA-CB-CG   | 5.03  | 126.87      | 115.30   |
| 4   | 2     | 53  | TYR  | CB-CG-CD1  | -5.03 | 117.98      | 121.00   |
| 1   | J     | 739 | ASP  | N-CA-CB    | 5.03  | 119.65      | 110.60   |
| 1   | G     | 739 | ASP  | N-CA-CB    | 5.03  | 119.64      | 110.60   |
| 1   | D     | 739 | ASP  | N-CA-CB    | 5.02  | 119.64      | 110.60   |
| 1   | G     | 628 | GLY  | O-C-N      | -5.02 | 114.66      | 122.70   |
| 4   | 7     | 91  | TYR  | CB-CG-CD2  | -5.02 | 117.99      | 121.00   |
| 1   | D     | 90  | ASP  | CB-CG-OD1  | -5.02 | 113.78      | 118.30   |
| 4   | V     | 191 | LYS  | CA-C-N     | 5.02  | 128.25      | 117.20   |
| 4   | 6     | 191 | LYS  | CA-C-N     | 5.02  | 128.24      | 117.20   |
| 4   | V     | 86  | TRP  | CG-CD1-NE1 | -5.02 | 105.08      | 110.10   |
| 4   | 0     | 86  | TRP  | CG-CD1-NE1 | -5.01 | 105.09      | 110.10   |
| 4   | 3     | 91  | TYR  | CB-CG-CD2  | -5.01 | 117.99      | 121.00   |
| 4   | Z     | 91  | TYR  | CB-CG-CD2  | -5.01 | 117.99      | 121.00   |
| 1   | G     | 82  | PRO  | N-CA-CB    | 5.01  | 109.32      | 103.30   |
| 1   | D     | 235 | ALA  | N-CA-CB    | -5.01 | 103.09      | 110.10   |

All (5) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 1   | A     | 648 | THR  | CB   |
| 1   | D     | 648 | THR  | CB   |
| 1   | G     | 75  | ASP  | CA   |
| 1   | G     | 648 | THR  | CB   |
| 1   | J     | 648 | THR  | CB   |

All (52) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 4   | 0     | 62  | ARG  | Sidechain         |
| 4   | 1     | 62  | ARG  | Sidechain         |
| 4   | 2     | 62  | ARG  | Sidechain         |
| 4   | 3     | 62  | ARG  | Sidechain         |
| 4   | 4     | 62  | ARG  | Sidechain         |
| 4   | 5     | 62  | ARG  | Sidechain         |
| 4   | 6     | 62  | ARG  | Sidechain         |
| 4   | 7     | 62  | ARG  | Sidechain         |
| 4   | 8     | 62  | ARG  | Sidechain         |
| 1   | A     | 623 | PHE  | Sidechain         |
| 1   | A     | 637 | LYS  | Mainchain         |
| 1   | A     | 649 | VAL  | Mainchain         |
| 1   | A     | 98  | HIS  | Mainchain         |
| 2   | B     | 150 | TYR  | Sidechain         |
| 2   | B     | 155 | TYR  | Mainchain         |
| 2   | B     | 22  | THR  | Mainchain         |
| 3   | C     | 75  | ALA  | Mainchain         |
| 3   | C     | 85  | GLU  | Mainchain         |
| 1   | D     | 623 | PHE  | Sidechain         |
| 1   | D     | 637 | LYS  | Mainchain         |
| 1   | D     | 649 | VAL  | Mainchain         |
| 1   | D     | 98  | HIS  | Mainchain         |
| 2   | E     | 150 | TYR  | Sidechain         |
| 2   | E     | 155 | TYR  | Mainchain         |
| 2   | E     | 22  | THR  | Mainchain         |
| 3   | F     | 75  | ALA  | Mainchain         |
| 3   | F     | 85  | GLU  | Mainchain         |
| 1   | G     | 623 | PHE  | Sidechain         |
| 1   | G     | 637 | LYS  | Mainchain         |
| 1   | G     | 649 | VAL  | Mainchain         |
| 1   | G     | 98  | HIS  | Mainchain         |
| 2   | H     | 150 | TYR  | Sidechain         |
| 2   | H     | 155 | TYR  | Mainchain         |
| 2   | H     | 22  | THR  | Mainchain         |
| 3   | I     | 75  | ALA  | Mainchain         |
| 3   | I     | 85  | GLU  | Mainchain         |
| 1   | J     | 623 | PHE  | Sidechain         |
| 1   | J     | 637 | LYS  | Mainchain         |
| 1   | J     | 649 | VAL  | Mainchain         |
| 1   | J     | 709 | LYS  | Mainchain,Peptide |
| 1   | J     | 98  | HIS  | Mainchain         |
| 2   | K     | 150 | TYR  | Sidechain         |
| 2   | K     | 155 | TYR  | Mainchain         |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 2   | K     | 22  | THR  | Mainchain |
| 3   | L     | 75  | ALA  | Mainchain |
| 3   | L     | 85  | GLU  | Mainchain |
| 4   | V     | 62  | ARG  | Sidechain |
| 4   | W     | 62  | ARG  | Sidechain |
| 4   | X     | 62  | ARG  | Sidechain |
| 4   | Y     | 62  | ARG  | Sidechain |
| 4   | Z     | 62  | ARG  | Sidechain |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 6797  | 0        | 6752     | 1414    | 0            |
| 1   | D     | 6797  | 0        | 6761     | 1431    | 0            |
| 1   | G     | 6797  | 0        | 6754     | 1380    | 0            |
| 1   | J     | 6797  | 0        | 6760     | 1429    | 0            |
| 2   | B     | 1127  | 0        | 1086     | 252     | 0            |
| 2   | E     | 1127  | 0        | 1087     | 320     | 0            |
| 2   | H     | 1127  | 0        | 1087     | 228     | 0            |
| 2   | K     | 1127  | 0        | 1087     | 227     | 0            |
| 3   | C     | 1123  | 0        | 1084     | 181     | 0            |
| 3   | F     | 1123  | 0        | 1082     | 139     | 0            |
| 3   | I     | 1123  | 0        | 1084     | 169     | 0            |
| 3   | L     | 1123  | 0        | 1084     | 165     | 0            |
| 4   | 0     | 2906  | 0        | 2866     | 75      | 3476         |
| 4   | 1     | 2906  | 0        | 2866     | 77      | 3458         |
| 4   | 2     | 2906  | 0        | 2864     | 102     | 3464         |
| 4   | 3     | 2906  | 0        | 2864     | 100     | 410          |
| 4   | 4     | 2906  | 0        | 2855     | 345     | 94           |
| 4   | 5     | 2906  | 0        | 2855     | 340     | 0            |
| 4   | 6     | 2906  | 0        | 2852     | 382     | 0            |
| 4   | 7     | 2906  | 0        | 2852     | 377     | 0            |
| 4   | 8     | 2906  | 0        | 2861     | 150     | 0            |
| 4   | V     | 2906  | 0        | 2861     | 142     | 95           |
| 4   | W     | 2906  | 0        | 2864     | 107     | 400          |
| 4   | X     | 2906  | 0        | 2864     | 105     | 3474         |
| 4   | Y     | 2906  | 0        | 2865     | 78      | 3456         |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | Z     | 2906  | 0        | 2865     | 78      | 3477         |
| All | All   | 76872 | 0        | 75762    | 7444    | 10902        |

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 49.

All (7444) 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:G:797:PHE:CD1  | 3:I:149:VAL:HG11 | 1.20                     | 1.68              |
| 2:E:144:VAL:HG13 | 2:E:153:ILE:CD1  | 1.22                     | 1.66              |
| 1:G:798:LEU:CD1  | 3:I:126:LEU:HD21 | 1.20                     | 1.65              |
| 1:A:725:ARG:HE   | 1:A:733:PRO:CB   | 1.09                     | 1.64              |
| 1:D:725:ARG:HE   | 1:D:733:PRO:CB   | 1.09                     | 1.64              |
| 1:A:757:GLN:CB   | 1:A:771:LEU:HD11 | 1.19                     | 1.64              |
| 1:J:831:TRP:CZ3  | 2:K:34:ILE:HD13  | 1.21                     | 1.64              |
| 2:B:144:VAL:HG13 | 2:B:153:ILE:CG1  | 1.17                     | 1.64              |
| 2:H:144:VAL:HG13 | 2:H:153:ILE:CD1  | 1.22                     | 1.62              |
| 2:K:144:VAL:HG13 | 2:K:153:ILE:CG1  | 1.17                     | 1.62              |
| 1:D:831:TRP:HZ2  | 2:E:47:LEU:CA    | 1.09                     | 1.61              |
| 1:J:510:TRP:CH2  | 1:J:768:MLY:HH11 | 1.34                     | 1.61              |
| 1:A:206:LYS:CD   | 1:A:217:THR:HG23 | 1.28                     | 1.61              |
| 1:A:757:GLN:HB3  | 1:A:771:LEU:CD1  | 1.26                     | 1.61              |
| 1:G:831:TRP:HH2  | 2:H:47:LEU:CD2   | 1.06                     | 1.59              |
| 2:E:144:VAL:HG13 | 2:E:153:ILE:CG1  | 1.17                     | 1.59              |
| 1:G:838:ILE:HD11 | 2:H:54:MET:CE    | 1.26                     | 1.59              |
| 1:G:206:LYS:CD   | 1:G:217:THR:HG23 | 1.28                     | 1.59              |
| 1:J:538:GLU:CA   | 4:7:349:LEU:CD1  | 1.79                     | 1.59              |
| 1:J:206:LYS:CD   | 1:J:217:THR:HG23 | 1.28                     | 1.59              |
| 1:J:84:MLY:CH1   | 1:J:715:VAL:HG13 | 1.22                     | 1.59              |
| 2:B:144:VAL:HG13 | 2:B:153:ILE:CD1  | 1.22                     | 1.59              |
| 2:K:144:VAL:HG13 | 2:K:153:ILE:CD1  | 1.22                     | 1.58              |
| 1:G:769:ALA:CB   | 1:G:770:GLY:HA2  | 1.20                     | 1.58              |
| 1:G:725:ARG:HE   | 1:G:733:PRO:CB   | 1.09                     | 1.58              |
| 1:A:799:MET:SD   | 3:C:32:ASP:HB3   | 1.43                     | 1.58              |
| 1:J:725:ARG:HE   | 1:J:733:PRO:CB   | 1.09                     | 1.58              |
| 1:D:831:TRP:CZ2  | 2:E:47:LEU:HA    | 1.11                     | 1.58              |
| 1:D:538:GLU:CA   | 4:5:349:LEU:CD1  | 1.78                     | 1.58              |
| 1:G:93:MET:CE    | 1:G:763:THR:HB   | 1.22                     | 1.57              |
| 2:H:144:VAL:HG13 | 2:H:153:ILE:CG1  | 1.17                     | 1.57              |
| 1:G:538:GLU:CA   | 4:6:349:LEU:CD1  | 1.79                     | 1.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:797:PHE:HD1  | 3:I:149:VAL:CG1  | 1.17                     | 1.57              |
| 1:A:798:LEU:CD1  | 3:C:126:LEU:HD21 | 1.27                     | 1.56              |
| 1:J:530:MET:HG2  | 4:7:354:GLN:CB   | 1.36                     | 1.56              |
| 1:D:206:LYS:CD   | 1:D:217:THR:HG23 | 1.28                     | 1.56              |
| 1:A:736:GLN:HA   | 1:A:743:ALA:CB   | 1.35                     | 1.55              |
| 1:G:831:TRP:CH2  | 2:H:47:LEU:HD22  | 1.39                     | 1.55              |
| 1:A:530:MET:HG2  | 4:4:354:GLN:CB   | 1.35                     | 1.55              |
| 1:D:830:PRO:CG   | 2:E:67:MET:CE    | 1.82                     | 1.55              |
| 1:G:530:MET:HG2  | 4:6:354:GLN:CB   | 1.35                     | 1.54              |
| 1:A:836:PHE:CZ   | 2:B:160:GLY:N    | 1.71                     | 1.54              |
| 1:A:538:GLU:CA   | 4:4:349:LEU:CD1  | 1.78                     | 1.54              |
| 1:D:530:MET:HG2  | 4:5:354:GLN:CB   | 1.35                     | 1.54              |
| 1:D:641:LYS:HG3  | 1:D:647:GLN:CG   | 1.36                     | 1.53              |
| 1:J:768:MLY:CH2  | 1:J:772:LEU:HD22 | 1.37                     | 1.53              |
| 1:J:641:LYS:HG3  | 1:J:647:GLN:CG   | 1.37                     | 1.53              |
| 1:J:800:ARG:CD   | 3:L:149:VAL:CG2  | 1.81                     | 1.53              |
| 1:J:829:TRP:HZ3  | 2:K:84:PHE:CZ    | 1.27                     | 1.52              |
| 1:D:736:GLN:HA   | 1:D:743:ALA:CB   | 1.35                     | 1.52              |
| 1:J:829:TRP:CZ3  | 2:K:84:PHE:CZ    | 1.96                     | 1.52              |
| 1:A:641:LYS:HG3  | 1:A:647:GLN:CG   | 1.37                     | 1.52              |
| 1:D:799:MET:SD   | 3:F:32:ASP:HB3   | 1.48                     | 1.52              |
| 1:G:206:LYS:HD3  | 1:G:217:THR:CG2  | 1.40                     | 1.51              |
| 1:J:84:MLY:CE    | 1:J:719:ASP:HB3  | 1.08                     | 1.51              |
| 1:D:834:LEU:CG   | 2:E:54:MET:HG3   | 1.38                     | 1.51              |
| 1:J:757:GLN:CG   | 1:J:776:GLU:HG3  | 1.34                     | 1.51              |
| 1:G:736:GLN:HA   | 1:G:743:ALA:CB   | 1.35                     | 1.51              |
| 1:J:736:GLN:HA   | 1:J:743:ALA:CB   | 1.35                     | 1.51              |
| 1:G:641:LYS:HG3  | 1:G:647:GLN:CG   | 1.37                     | 1.51              |
| 1:G:93:MET:HE1   | 1:G:763:THR:CB   | 1.38                     | 1.50              |
| 2:K:117:LEU:HD12 | 2:K:147:ASN:CB   | 1.41                     | 1.50              |
| 1:J:800:ARG:CD   | 3:L:149:VAL:HG22 | 1.39                     | 1.49              |
| 1:D:831:TRP:CH2  | 2:E:47:LEU:HA    | 1.41                     | 1.49              |
| 1:J:768:MLY:HH12 | 1:J:772:LEU:CD2  | 1.41                     | 1.49              |
| 1:D:206:LYS:HD3  | 1:D:217:THR:CG2  | 1.40                     | 1.49              |
| 1:A:813:ILE:CG2  | 2:B:127:ARG:HD2  | 1.39                     | 1.49              |
| 1:G:84:MLY:CH1   | 1:G:715:VAL:HG13 | 1.35                     | 1.49              |
| 2:E:117:LEU:HD12 | 2:E:147:ASN:CB   | 1.41                     | 1.48              |
| 1:J:206:LYS:HD3  | 1:J:217:THR:CG2  | 1.40                     | 1.48              |
| 2:E:111:SER:HB2  | 2:E:148:VAL:C    | 1.23                     | 1.48              |
| 2:K:111:SER:HB2  | 2:K:148:VAL:C    | 1.23                     | 1.48              |
| 2:B:117:LEU:HD12 | 2:B:147:ASN:CB   | 1.42                     | 1.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:508:ILE:HD11 | 1:J:759:ALA:CB   | 1.41                     | 1.48              |
| 1:D:831:TRP:CZ2  | 2:E:47:LEU:CA    | 1.82                     | 1.48              |
| 1:A:206:LYS:HD3  | 1:A:217:THR:CG2  | 1.40                     | 1.47              |
| 2:E:117:LEU:HD12 | 2:E:147:ASN:CG   | 1.30                     | 1.47              |
| 2:B:111:SER:HB2  | 2:B:148:VAL:C    | 1.23                     | 1.47              |
| 1:D:830:PRO:CG   | 2:E:67:MET:HE3   | 1.38                     | 1.47              |
| 1:J:795:ARG:CD   | 3:L:35:ARG:HH22  | 1.28                     | 1.47              |
| 1:J:768:MLY:HH23 | 1:J:772:LEU:CD2  | 1.44                     | 1.47              |
| 1:G:641:LYS:CG   | 1:G:647:GLN:NE2  | 1.76                     | 1.47              |
| 1:D:831:TRP:CZ3  | 2:E:34:ILE:HG23  | 1.48                     | 1.47              |
| 2:K:117:LEU:HD12 | 2:K:147:ASN:CG   | 1.29                     | 1.47              |
| 1:J:800:ARG:HD2  | 3:L:149:VAL:CG2  | 1.03                     | 1.46              |
| 2:H:117:LEU:HD12 | 2:H:147:ASN:CB   | 1.42                     | 1.46              |
| 1:J:795:ARG:HD2  | 3:L:35:ARG:NH2   | 1.23                     | 1.46              |
| 1:A:641:LYS:CG   | 1:A:647:GLN:NE2  | 1.76                     | 1.46              |
| 1:J:538:GLU:C    | 4:7:349:LEU:CD1  | 1.84                     | 1.46              |
| 1:J:641:LYS:CG   | 1:J:647:GLN:NE2  | 1.77                     | 1.46              |
| 1:G:538:GLU:C    | 4:6:349:LEU:CD1  | 1.84                     | 1.46              |
| 2:H:111:SER:HB2  | 2:H:148:VAL:C    | 1.23                     | 1.46              |
| 1:A:641:LYS:CD   | 1:A:647:GLN:CD   | 1.85                     | 1.45              |
| 2:B:117:LEU:HD12 | 2:B:147:ASN:CG   | 1.30                     | 1.45              |
| 1:J:641:LYS:CD   | 1:J:647:GLN:CD   | 1.85                     | 1.45              |
| 1:D:830:PRO:HG2  | 2:E:67:MET:CE    | 0.99                     | 1.45              |
| 1:A:800:ARG:HB3  | 3:C:149:VAL:CG2  | 1.44                     | 1.45              |
| 1:D:538:GLU:C    | 4:5:349:LEU:CD1  | 1.84                     | 1.45              |
| 1:G:641:LYS:CD   | 1:G:647:GLN:CD   | 1.85                     | 1.45              |
| 1:A:836:PHE:CE1  | 2:B:160:GLY:N    | 1.82                     | 1.45              |
| 1:G:798:LEU:CD1  | 3:I:126:LEU:CD2  | 1.93                     | 1.45              |
| 1:J:769:ALA:HB3  | 1:J:770:GLY:CA   | 1.45                     | 1.45              |
| 2:H:117:LEU:HD12 | 2:H:147:ASN:CG   | 1.30                     | 1.44              |
| 1:D:641:LYS:CG   | 1:D:647:GLN:NE2  | 1.76                     | 1.44              |
| 1:J:93:MET:CG    | 1:J:764:MLY:HD3  | 1.43                     | 1.44              |
| 1:A:538:GLU:C    | 4:4:349:LEU:CD1  | 1.84                     | 1.44              |
| 1:D:814:PHE:CD1  | 2:E:127:ARG:NH2  | 1.78                     | 1.44              |
| 1:J:721:LYS:HG3  | 1:J:736:GLN:CG   | 1.15                     | 1.43              |
| 1:D:641:LYS:CD   | 1:D:647:GLN:CD   | 1.85                     | 1.42              |
| 1:D:768:MLY:C    | 1:D:771:LEU:HD13 | 1.34                     | 1.42              |
| 1:G:93:MET:CE    | 1:G:763:THR:CB   | 1.89                     | 1.42              |
| 1:G:721:LYS:HG3  | 1:G:736:GLN:CG   | 1.15                     | 1.42              |
| 1:G:800:ARG:NH1  | 3:I:149:VAL:HG22 | 1.33                     | 1.42              |
| 1:D:736:GLN:N    | 1:D:743:ALA:HB1  | 1.34                     | 1.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:733:PRO:O    | 1:A:737:PHE:CD1  | 1.73                     | 1.42              |
| 1:G:733:PRO:O    | 1:G:737:PHE:CD1  | 1.74                     | 1.41              |
| 1:G:736:GLN:N    | 1:G:743:ALA:HB1  | 1.34                     | 1.41              |
| 2:H:144:VAL:CG1  | 2:H:153:ILE:CD1  | 1.99                     | 1.41              |
| 1:A:530:MET:CG   | 4:4:354:GLN:HB2  | 1.50                     | 1.41              |
| 2:B:144:VAL:CG1  | 2:B:153:ILE:CD1  | 1.99                     | 1.41              |
| 1:D:530:MET:CG   | 4:5:354:GLN:HB2  | 1.50                     | 1.41              |
| 1:J:202:SER:HA   | 1:J:207:LYS:CE   | 1.51                     | 1.40              |
| 1:J:218:LEU:CB   | 1:J:221:GLN:HG3  | 1.52                     | 1.40              |
| 1:G:730:SER:OG   | 3:I:109:HIS:CD2  | 1.72                     | 1.40              |
| 1:J:768:MLY:HH23 | 1:J:772:LEU:CG   | 1.51                     | 1.40              |
| 1:A:202:SER:HA   | 1:A:207:LYS:CE   | 1.51                     | 1.40              |
| 1:D:218:LEU:CB   | 1:D:221:GLN:HG3  | 1.52                     | 1.40              |
| 1:D:736:GLN:CA   | 1:D:743:ALA:CB   | 2.00                     | 1.39              |
| 1:A:149:GLN:CB   | 1:A:719:ASP:OD1  | 1.71                     | 1.39              |
| 1:A:537:GLU:O    | 4:4:349:LEU:CD1  | 1.70                     | 1.39              |
| 1:D:537:GLU:O    | 4:5:349:LEU:CD1  | 1.70                     | 1.39              |
| 2:E:144:VAL:CG1  | 2:E:153:ILE:CD1  | 1.99                     | 1.39              |
| 1:J:733:PRO:O    | 1:J:737:PHE:CD1  | 1.73                     | 1.39              |
| 1:G:202:SER:HA   | 1:G:207:LYS:CE   | 1.51                     | 1.39              |
| 1:G:821:ARG:NH2  | 2:H:127:ARG:HG2  | 1.07                     | 1.39              |
| 1:D:202:SER:HA   | 1:D:207:LYS:CE   | 1.51                     | 1.39              |
| 2:K:144:VAL:CG1  | 2:K:153:ILE:CD1  | 1.99                     | 1.39              |
| 1:D:733:PRO:O    | 1:D:737:PHE:CD1  | 1.74                     | 1.39              |
| 1:J:530:MET:CG   | 4:7:354:GLN:HB2  | 1.51                     | 1.38              |
| 1:G:819:ASN:CA   | 2:H:90:GLY:O     | 1.67                     | 1.38              |
| 1:A:800:ARG:CD   | 3:C:149:VAL:HG22 | 1.53                     | 1.38              |
| 1:D:831:TRP:HZ2  | 2:E:47:LEU:CB    | 1.36                     | 1.38              |
| 1:A:831:TRP:NE1  | 2:B:51:PHE:CZ    | 1.91                     | 1.38              |
| 1:J:736:GLN:CA   | 1:J:743:ALA:CB   | 2.00                     | 1.38              |
| 1:A:218:LEU:CB   | 1:A:221:GLN:HG3  | 1.52                     | 1.38              |
| 1:G:831:TRP:CH2  | 2:H:47:LEU:CD2   | 1.98                     | 1.38              |
| 1:G:795:ARG:CD   | 3:I:35:ARG:HH22  | 1.34                     | 1.38              |
| 1:J:537:GLU:O    | 4:7:349:LEU:CD1  | 1.70                     | 1.38              |
| 1:D:736:GLN:CA   | 1:D:743:ALA:HB1  | 1.53                     | 1.38              |
| 1:A:736:GLN:CA   | 1:A:743:ALA:CB   | 2.00                     | 1.37              |
| 2:E:144:VAL:CG1  | 2:E:153:ILE:HG12 | 1.54                     | 1.37              |
| 1:G:534:SER:O    | 4:6:351:THR:CG2  | 1.64                     | 1.37              |
| 1:J:768:MLY:CH1  | 1:J:772:LEU:HD22 | 1.52                     | 1.37              |
| 1:G:218:LEU:CB   | 1:G:221:GLN:HG3  | 1.52                     | 1.37              |
| 1:A:736:GLN:N    | 1:A:743:ALA:HB1  | 1.35                     | 1.37              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:736:GLN:CA   | 1:A:743:ALA:HB1  | 1.53                     | 1.37              |
| 1:D:721:LYS:CG   | 1:D:736:GLN:CG   | 1.97                     | 1.37              |
| 1:D:641:LYS:CG   | 1:D:647:GLN:CD   | 1.93                     | 1.37              |
| 1:D:642:LYS:HG3  | 4:5:23:GLY:N     | 1.40                     | 1.37              |
| 2:H:144:VAL:CG1  | 2:H:153:ILE:HG12 | 1.54                     | 1.37              |
| 1:J:736:GLN:CA   | 1:J:743:ALA:HB1  | 1.53                     | 1.37              |
| 2:K:144:VAL:CG1  | 2:K:153:ILE:CG1  | 2.03                     | 1.37              |
| 2:B:117:LEU:HB2  | 2:B:147:ASN:ND2  | 1.39                     | 1.36              |
| 1:A:641:LYS:HG3  | 1:A:647:GLN:CD   | 1.46                     | 1.36              |
| 1:A:721:LYS:HG3  | 1:A:736:GLN:CG   | 1.15                     | 1.36              |
| 1:G:537:GLU:O    | 4:6:349:LEU:CD1  | 1.71                     | 1.36              |
| 2:H:117:LEU:HB2  | 2:H:147:ASN:ND2  | 1.40                     | 1.36              |
| 1:G:530:MET:CG   | 4:6:354:GLN:HB2  | 1.51                     | 1.36              |
| 1:A:649:VAL:CG1  | 1:A:649:VAL:O    | 1.74                     | 1.36              |
| 2:B:144:VAL:CG1  | 2:B:153:ILE:HG12 | 1.54                     | 1.36              |
| 1:J:642:LYS:HG3  | 4:7:23:GLY:N     | 1.40                     | 1.36              |
| 1:J:641:LYS:CG   | 1:J:647:GLN:CD   | 1.93                     | 1.36              |
| 2:K:144:VAL:CG1  | 2:K:153:ILE:HG12 | 1.54                     | 1.36              |
| 1:J:831:TRP:HZ3  | 2:K:34:ILE:CD1   | 1.36                     | 1.36              |
| 1:G:649:VAL:CG1  | 1:G:649:VAL:O    | 1.74                     | 1.36              |
| 1:D:800:ARG:HB3  | 3:F:149:VAL:CG2  | 1.56                     | 1.35              |
| 1:G:538:GLU:CA   | 4:6:349:LEU:HD12 | 0.88                     | 1.35              |
| 2:B:117:LEU:CD1  | 2:B:147:ASN:OD1  | 1.74                     | 1.35              |
| 1:D:831:TRP:CE2  | 2:E:47:LEU:HD22  | 1.61                     | 1.35              |
| 1:G:642:LYS:HG3  | 4:6:23:GLY:N     | 1.39                     | 1.35              |
| 1:J:736:GLN:N    | 1:J:743:ALA:HB1  | 1.35                     | 1.35              |
| 1:G:736:GLN:CA   | 1:G:743:ALA:CB   | 2.00                     | 1.35              |
| 2:K:117:LEU:HB2  | 2:K:147:ASN:ND2  | 1.39                     | 1.35              |
| 2:B:144:VAL:CG1  | 2:B:153:ILE:CG1  | 2.03                     | 1.35              |
| 1:G:736:GLN:CA   | 1:G:743:ALA:HB1  | 1.53                     | 1.35              |
| 1:D:721:LYS:HG3  | 1:D:736:GLN:CG   | 1.15                     | 1.35              |
| 1:A:530:MET:HA   | 4:4:354:GLN:CG   | 1.56                     | 1.35              |
| 1:A:534:SER:O    | 4:4:351:THR:CG2  | 1.64                     | 1.35              |
| 1:G:721:LYS:CG   | 1:G:736:GLN:CG   | 1.97                     | 1.35              |
| 2:H:144:VAL:CG1  | 2:H:153:ILE:CG1  | 2.03                     | 1.35              |
| 1:J:538:GLU:CA   | 4:7:349:LEU:HD12 | 0.88                     | 1.34              |
| 1:D:534:SER:O    | 4:5:351:THR:CG2  | 1.64                     | 1.34              |
| 1:G:641:LYS:CG   | 1:G:647:GLN:CD   | 1.93                     | 1.34              |
| 1:G:834:LEU:HD13 | 2:H:51:PHE:CE1   | 1.61                     | 1.34              |
| 2:K:117:LEU:CD1  | 2:K:147:ASN:OD1  | 1.74                     | 1.34              |
| 1:D:649:VAL:O    | 1:D:649:VAL:CG1  | 1.73                     | 1.34              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:144:VAL:CG1  | 2:E:153:ILE:CG1  | 2.03                     | 1.34              |
| 1:A:642:LYS:HG3  | 4:4:23:GLY:N     | 1.40                     | 1.34              |
| 1:A:538:GLU:CA   | 4:4:349:LEU:HD12 | 0.87                     | 1.34              |
| 1:A:641:LYS:CG   | 1:A:647:GLN:CD   | 1.93                     | 1.34              |
| 2:E:117:LEU:CD1  | 2:E:147:ASN:OD1  | 1.74                     | 1.33              |
| 2:H:117:LEU:CD1  | 2:H:147:ASN:OD1  | 1.74                     | 1.33              |
| 2:H:114:LYS:CA   | 2:H:146:GLY:O    | 1.76                     | 1.33              |
| 1:D:538:GLU:CA   | 4:5:349:LEU:HD12 | 0.87                     | 1.33              |
| 1:J:629:GLU:HA   | 1:J:643:GLY:O    | 1.17                     | 1.33              |
| 1:J:821:ARG:NH2  | 2:K:127:ARG:HG2  | 1.42                     | 1.33              |
| 1:J:641:LYS:HG3  | 1:J:647:GLN:CD   | 1.46                     | 1.33              |
| 1:J:795:ARG:HD2  | 3:L:35:ARG:CZ    | 1.57                     | 1.33              |
| 2:E:117:LEU:HB2  | 2:E:147:ASN:ND2  | 1.40                     | 1.33              |
| 1:D:635:GLY:CA   | 4:5:334:GLU:HG2  | 1.59                     | 1.33              |
| 1:J:530:MET:HA   | 4:7:354:GLN:CG   | 1.56                     | 1.33              |
| 1:D:530:MET:HA   | 4:5:354:GLN:CG   | 1.56                     | 1.33              |
| 1:J:649:VAL:O    | 1:J:649:VAL:CG1  | 1.74                     | 1.33              |
| 1:A:813:ILE:CG2  | 2:B:127:ARG:CD   | 2.07                     | 1.33              |
| 1:G:831:TRP:HE1  | 2:H:67:MET:CG    | 1.41                     | 1.33              |
| 1:J:635:GLY:CA   | 4:7:334:GLU:HG2  | 1.59                     | 1.33              |
| 1:J:735:GLY:O    | 1:J:743:ALA:HB2  | 1.29                     | 1.33              |
| 1:J:534:SER:O    | 4:7:351:THR:CG2  | 1.64                     | 1.32              |
| 1:D:629:GLU:HA   | 1:D:643:GLY:O    | 1.17                     | 1.32              |
| 1:G:530:MET:HA   | 4:6:354:GLN:CG   | 1.57                     | 1.32              |
| 1:J:792:ALA:CB   | 3:L:40:ASN:HB3   | 1.59                     | 1.32              |
| 1:D:831:TRP:CZ2  | 2:E:47:LEU:HD23  | 1.64                     | 1.32              |
| 1:D:799:MET:SD   | 3:F:32:ASP:CB    | 2.18                     | 1.32              |
| 1:J:721:LYS:CG   | 1:J:736:GLN:CD   | 1.98                     | 1.32              |
| 1:A:725:ARG:NE   | 1:A:733:PRO:HB3  | 0.99                     | 1.32              |
| 1:G:769:ALA:CB   | 1:G:770:GLY:CA   | 2.07                     | 1.32              |
| 2:E:114:LYS:CA   | 2:E:146:GLY:O    | 1.76                     | 1.32              |
| 1:D:831:TRP:NE1  | 2:E:47:LEU:HD22  | 1.44                     | 1.32              |
| 1:G:757:GLN:OE1  | 1:G:772:LEU:HB3  | 1.30                     | 1.32              |
| 2:K:114:LYS:CA   | 2:K:146:GLY:O    | 1.76                     | 1.31              |
| 1:A:538:GLU:O    | 4:4:349:LEU:CD1  | 1.78                     | 1.31              |
| 1:A:813:ILE:HG22 | 2:B:127:ARG:CD   | 1.58                     | 1.31              |
| 1:J:831:TRP:CZ3  | 2:K:34:ILE:CD1   | 2.11                     | 1.31              |
| 2:K:121:LEU:O    | 2:K:128:PHE:CB   | 1.78                     | 1.31              |
| 1:A:629:GLU:HA   | 1:A:643:GLY:O    | 1.17                     | 1.31              |
| 1:G:629:GLU:HA   | 1:G:643:GLY:O    | 1.17                     | 1.31              |
| 2:B:114:LYS:CA   | 2:B:146:GLY:O    | 1.76                     | 1.31              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:721:LYS:HG2  | 1:D:736:GLN:OE1  | 1.28                     | 1.31              |
| 1:D:831:TRP:CE2  | 2:E:47:LEU:CD2   | 2.13                     | 1.31              |
| 1:J:725:ARG:NE   | 1:J:733:PRO:HB3  | 1.00                     | 1.31              |
| 1:A:721:LYS:CG   | 1:A:736:GLN:CD   | 1.98                     | 1.31              |
| 1:G:635:GLY:CA   | 4:6:334:GLU:HG2  | 1.59                     | 1.31              |
| 1:G:798:LEU:HD11 | 3:I:126:LEU:CD2  | 1.55                     | 1.31              |
| 1:A:635:GLY:CA   | 4:4:334:GLU:HG2  | 1.59                     | 1.30              |
| 1:D:599:ASN:HA   | 1:D:649:VAL:CB   | 1.60                     | 1.30              |
| 1:D:839:MLY:CH1  | 2:E:159:HIS:CD2  | 2.15                     | 1.30              |
| 1:D:725:ARG:NE   | 1:D:733:PRO:HB3  | 1.00                     | 1.30              |
| 1:D:721:LYS:CG   | 1:D:736:GLN:CD   | 1.98                     | 1.30              |
| 1:G:641:LYS:HG3  | 1:G:647:GLN:CD   | 1.45                     | 1.30              |
| 1:A:819:ASN:OD1  | 2:B:91:ALA:CA    | 1.79                     | 1.30              |
| 1:A:834:LEU:HD11 | 2:B:54:MET:CB    | 1.60                     | 1.30              |
| 2:E:121:LEU:O    | 2:E:128:PHE:CB   | 1.79                     | 1.30              |
| 1:G:789:ALA:HB2  | 3:I:81:GLN:NE2   | 1.43                     | 1.30              |
| 1:J:599:ASN:HA   | 1:J:649:VAL:CB   | 1.60                     | 1.30              |
| 1:G:538:GLU:O    | 4:6:349:LEU:CD1  | 1.78                     | 1.30              |
| 1:G:725:ARG:NE   | 1:G:733:PRO:HB3  | 0.99                     | 1.30              |
| 1:A:831:TRP:CE2  | 2:B:51:PHE:CZ    | 2.20                     | 1.30              |
| 1:G:721:LYS:CG   | 1:G:736:GLN:CD   | 1.98                     | 1.30              |
| 1:D:723:ARG:O    | 1:D:782:MLY:HD3  | 1.30                     | 1.29              |
| 1:D:735:GLY:C    | 1:D:743:ALA:CB   | 2.01                     | 1.29              |
| 1:G:800:ARG:HH11 | 3:I:149:VAL:CG2  | 1.42                     | 1.29              |
| 1:A:735:GLY:O    | 1:A:743:ALA:HB2  | 1.29                     | 1.29              |
| 1:G:735:GLY:C    | 1:G:743:ALA:CB   | 2.01                     | 1.29              |
| 2:B:121:LEU:O    | 2:B:128:PHE:CB   | 1.79                     | 1.29              |
| 1:A:599:ASN:HA   | 1:A:649:VAL:CB   | 1.60                     | 1.29              |
| 1:D:641:LYS:HG3  | 1:D:647:GLN:CD   | 1.45                     | 1.29              |
| 1:G:599:ASN:HA   | 1:G:649:VAL:CB   | 1.60                     | 1.29              |
| 1:D:215:GLN:N    | 1:D:340:ILE:HG12 | 1.20                     | 1.29              |
| 1:J:768:MLY:CH1  | 1:J:772:LEU:CD2  | 2.10                     | 1.29              |
| 1:J:537:GLU:C    | 4:7:349:LEU:HD13 | 1.52                     | 1.29              |
| 1:J:735:GLY:C    | 1:J:743:ALA:CB   | 2.01                     | 1.29              |
| 1:G:537:GLU:C    | 4:6:349:LEU:HD13 | 1.53                     | 1.28              |
| 1:J:800:ARG:CB   | 3:L:149:VAL:HG21 | 1.62                     | 1.28              |
| 1:A:836:PHE:HB2  | 2:B:161:GLU:OE1  | 1.32                     | 1.28              |
| 1:J:215:GLN:N    | 1:J:340:ILE:HG12 | 1.19                     | 1.28              |
| 1:G:795:ARG:HD2  | 3:I:35:ARG:NH2   | 1.47                     | 1.28              |
| 1:J:721:LYS:HG2  | 1:J:736:GLN:OE1  | 1.29                     | 1.28              |
| 1:G:721:LYS:HG2  | 1:G:736:GLN:OE1  | 1.29                     | 1.28              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:819:ASN:HA   | 2:K:90:GLY:O     | 1.19                     | 1.28              |
| 1:G:752:ASP:O    | 1:G:779:ARG:NH1  | 1.66                     | 1.28              |
| 2:H:121:LEU:O    | 2:H:128:PHE:CB   | 1.78                     | 1.28              |
| 1:D:831:TRP:CZ2  | 2:E:47:LEU:CD2   | 2.17                     | 1.27              |
| 1:G:836:PHE:CE1  | 2:H:159:HIS:HA   | 1.67                     | 1.27              |
| 1:A:537:GLU:C    | 4:4:349:LEU:HD13 | 1.52                     | 1.27              |
| 1:A:735:GLY:C    | 1:A:743:ALA:CB   | 2.01                     | 1.27              |
| 1:J:538:GLU:O    | 4:7:349:LEU:CD1  | 1.78                     | 1.27              |
| 1:A:534:SER:O    | 4:4:351:THR:CA   | 1.81                     | 1.27              |
| 1:D:721:LYS:CG   | 1:D:736:GLN:OE1  | 1.82                     | 1.27              |
| 1:J:733:PRO:O    | 1:J:737:PHE:HD1  | 0.93                     | 1.26              |
| 1:D:534:SER:O    | 4:5:351:THR:CA   | 1.82                     | 1.26              |
| 1:J:534:SER:O    | 4:7:351:THR:CA   | 1.82                     | 1.26              |
| 1:D:735:GLY:O    | 1:D:743:ALA:HB2  | 1.29                     | 1.26              |
| 1:G:721:LYS:CG   | 1:G:736:GLN:OE1  | 1.83                     | 1.26              |
| 1:J:768:MLY:HH23 | 1:J:772:LEU:CB   | 1.65                     | 1.26              |
| 1:A:836:PHE:CB   | 2:B:161:GLU:OE1  | 1.81                     | 1.26              |
| 1:D:537:GLU:C    | 4:5:349:LEU:HD13 | 1.52                     | 1.26              |
| 1:A:813:ILE:HG22 | 2:B:127:ARG:NE   | 1.45                     | 1.26              |
| 1:D:721:LYS:HG3  | 1:D:736:GLN:CD   | 1.53                     | 1.26              |
| 1:G:790:THR:OG1  | 3:I:87:PHE:CE2   | 1.89                     | 1.26              |
| 1:A:149:GLN:HB3  | 1:A:719:ASP:OD1  | 1.12                     | 1.26              |
| 1:D:538:GLU:O    | 4:5:349:LEU:CD1  | 1.78                     | 1.25              |
| 1:A:733:PRO:O    | 1:A:737:PHE:HD1  | 0.92                     | 1.25              |
| 1:G:508:ILE:HD11 | 1:G:759:ALA:CB   | 1.62                     | 1.25              |
| 1:G:821:ARG:NH2  | 2:H:127:ARG:CG   | 1.99                     | 1.25              |
| 1:J:768:MLY:CH2  | 1:J:772:LEU:HB2  | 1.66                     | 1.25              |
| 1:G:735:GLY:O    | 1:G:743:ALA:HB2  | 1.29                     | 1.25              |
| 1:A:797:PHE:CD1  | 3:C:149:VAL:HG11 | 1.71                     | 1.25              |
| 1:J:630:ALA:O    | 4:7:25:ASP:OD2   | 1.52                     | 1.25              |
| 1:G:721:LYS:HG3  | 1:G:736:GLN:CD   | 1.53                     | 1.25              |
| 1:J:508:ILE:CD1  | 1:J:759:ALA:HB2  | 1.63                     | 1.25              |
| 1:G:534:SER:O    | 4:6:351:THR:CA   | 1.83                     | 1.24              |
| 1:D:641:LYS:CG   | 1:D:647:GLN:CG   | 2.15                     | 1.24              |
| 4:5:322:PRO:CB   | 4:7:244:ASP:OD2  | 1.86                     | 1.24              |
| 1:G:93:MET:SD    | 1:G:716:LEU:HD12 | 1.75                     | 1.24              |
| 1:J:641:LYS:CD   | 1:J:647:GLN:NE2  | 1.99                     | 1.24              |
| 1:A:721:LYS:CG   | 1:A:736:GLN:CG   | 1.97                     | 1.24              |
| 1:G:646:PHE:CE2  | 1:G:652:LEU:HD11 | 1.73                     | 1.24              |
| 1:J:792:ALA:HB1  | 3:L:40:ASN:CB    | 1.67                     | 1.24              |
| 2:K:117:LEU:CD1  | 2:K:147:ASN:CG   | 2.05                     | 1.24              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:7:322:PRO:CB   | 4:V:244:ASP:OD2  | 1.86                     | 1.24              |
| 1:G:733:PRO:O    | 1:G:737:PHE:HD1  | 0.93                     | 1.24              |
| 1:G:508:ILE:CD1  | 1:G:759:ALA:HB2  | 1.67                     | 1.24              |
| 1:J:721:LYS:HG3  | 1:J:736:GLN:CD   | 1.54                     | 1.24              |
| 1:A:795:ARG:HD2  | 3:C:35:ARG:NH1   | 1.49                     | 1.24              |
| 1:D:646:PHE:CE2  | 1:D:652:LEU:HD11 | 1.73                     | 1.24              |
| 1:A:646:PHE:CE2  | 1:A:652:LEU:HD11 | 1.73                     | 1.24              |
| 1:J:641:LYS:CG   | 1:J:647:GLN:CG   | 2.16                     | 1.24              |
| 1:A:834:LEU:HD11 | 2:B:54:MET:CG    | 1.67                     | 1.24              |
| 1:D:836:PHE:HB3  | 2:E:161:GLU:OE1  | 1.35                     | 1.24              |
| 4:3:322:PRO:CB   | 4:5:244:ASP:OD2  | 1.86                     | 1.23              |
| 1:A:721:LYS:HG2  | 1:A:736:GLN:OE1  | 1.29                     | 1.23              |
| 1:J:721:LYS:CG   | 1:J:736:GLN:OE1  | 1.83                     | 1.23              |
| 1:J:795:ARG:CD   | 3:L:35:ARG:NH2   | 1.90                     | 1.23              |
| 2:K:117:LEU:HD12 | 2:K:147:ASN:OD1  | 1.32                     | 1.23              |
| 4:8:322:PRO:CB   | 4:W:244:ASP:OD2  | 1.86                     | 1.23              |
| 4:4:322:PRO:CB   | 4:6:244:ASP:OD2  | 1.86                     | 1.23              |
| 2:B:117:LEU:CD1  | 2:B:147:ASN:CG   | 2.05                     | 1.23              |
| 1:D:795:ARG:NH2  | 3:F:116:GLU:OE2  | 1.67                     | 1.23              |
| 2:E:121:LEU:C    | 2:E:128:PHE:CB   | 2.07                     | 1.23              |
| 4:V:322:PRO:CB   | 4:X:244:ASP:OD2  | 1.86                     | 1.23              |
| 1:A:538:GLU:O    | 4:4:349:LEU:HD11 | 1.35                     | 1.23              |
| 1:A:630:ALA:O    | 4:4:25:ASP:OD2   | 1.53                     | 1.23              |
| 1:A:800:ARG:HD2  | 3:C:149:VAL:CG2  | 1.68                     | 1.23              |
| 1:A:800:ARG:CB   | 3:C:149:VAL:CG2  | 2.17                     | 1.23              |
| 1:A:795:ARG:NH2  | 3:C:116:GLU:OE2  | 1.69                     | 1.23              |
| 1:D:834:LEU:HD11 | 2:E:54:MET:CG    | 1.66                     | 1.23              |
| 1:J:646:PHE:CE2  | 1:J:652:LEU:HD11 | 1.73                     | 1.23              |
| 1:A:629:GLU:CA   | 1:A:643:GLY:O    | 1.87                     | 1.23              |
| 1:A:721:LYS:CG   | 1:A:736:GLN:OE1  | 1.82                     | 1.23              |
| 4:2:322:PRO:CB   | 4:4:244:ASP:OD2  | 1.86                     | 1.23              |
| 1:A:506:GLU:OE2  | 1:A:717:TYR:OH   | 1.57                     | 1.23              |
| 1:G:783:LEU:O    | 1:G:787:ILE:N    | 1.71                     | 1.23              |
| 4:W:322:PRO:CB   | 4:Y:244:ASP:OD2  | 1.86                     | 1.23              |
| 4:0:322:PRO:CB   | 4:2:244:ASP:OD2  | 1.86                     | 1.22              |
| 1:G:538:GLU:C    | 4:6:349:LEU:HD12 | 1.48                     | 1.22              |
| 1:G:838:ILE:CD1  | 2:H:54:MET:HE3   | 1.69                     | 1.22              |
| 1:D:538:GLU:C    | 4:5:349:LEU:HD12 | 1.48                     | 1.22              |
| 4:X:322:PRO:CB   | 4:Z:244:ASP:OD2  | 1.86                     | 1.22              |
| 1:A:534:SER:O    | 4:4:351:THR:CB   | 1.87                     | 1.22              |
| 1:A:215:GLN:N    | 1:A:340:ILE:CG1  | 2.02                     | 1.22              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:G:641:LYS:CD  | 1:G:647:GLN:NE2  | 1.99                     | 1.22              |
| 1:A:641:LYS:CG  | 1:A:647:GLN:CG   | 2.16                     | 1.22              |
| 1:A:836:PHE:CZ  | 2:B:160:GLY:CA   | 2.20                     | 1.22              |
| 2:B:121:LEU:C   | 2:B:128:PHE:CB   | 2.07                     | 1.22              |
| 1:D:641:LYS:CD  | 1:D:647:GLN:NE2  | 1.99                     | 1.22              |
| 1:D:733:PRO:O   | 1:D:737:PHE:HD1  | 0.93                     | 1.22              |
| 1:G:757:GLN:OE1 | 1:G:772:LEU:CB   | 1.86                     | 1.22              |
| 4:1:322:PRO:CB  | 4:3:244:ASP:OD2  | 1.86                     | 1.22              |
| 1:D:630:ALA:O   | 4:5:25:ASP:OD2   | 1.52                     | 1.22              |
| 1:G:553:MLY:CE  | 4:8:45:VAL:HA    | 1.52                     | 1.22              |
| 1:J:215:GLN:N   | 1:J:340:ILE:CG1  | 2.02                     | 1.22              |
| 1:D:799:MET:SD  | 3:F:32:ASP:O     | 1.97                     | 1.22              |
| 2:E:117:LEU:CD1 | 2:E:147:ASN:CG   | 2.05                     | 1.22              |
| 1:G:215:GLN:N   | 1:G:340:ILE:CG1  | 2.02                     | 1.22              |
| 2:H:144:VAL:CG1 | 2:H:153:ILE:HD11 | 1.64                     | 1.22              |
| 1:G:538:GLU:O   | 4:6:349:LEU:HD11 | 1.34                     | 1.21              |
| 1:A:798:LEU:CD1 | 3:C:126:LEU:CD2  | 2.16                     | 1.21              |
| 1:D:799:MET:SD  | 3:F:32:ASP:C     | 2.18                     | 1.21              |
| 1:G:707:CYS:HB3 | 1:G:714:ARG:NH1  | 1.54                     | 1.21              |
| 1:J:534:SER:O   | 4:7:351:THR:CB   | 1.87                     | 1.21              |
| 1:D:534:SER:O   | 4:5:351:THR:CB   | 1.87                     | 1.21              |
| 1:A:641:LYS:CG  | 1:A:647:GLN:HG3  | 1.71                     | 1.21              |
| 4:6:322:PRO:CB  | 4:8:244:ASP:OD2  | 1.86                     | 1.21              |
| 1:G:629:GLU:CA  | 1:G:643:GLY:O    | 1.87                     | 1.21              |
| 2:B:144:VAL:CG1 | 2:B:153:ILE:HD11 | 1.65                     | 1.21              |
| 1:D:629:GLU:CA  | 1:D:643:GLY:O    | 1.87                     | 1.21              |
| 2:H:121:LEU:C   | 2:H:128:PHE:CB   | 2.07                     | 1.21              |
| 1:J:629:GLU:CA  | 1:J:643:GLY:O    | 1.87                     | 1.21              |
| 2:K:121:LEU:C   | 2:K:128:PHE:CB   | 2.07                     | 1.21              |
| 1:A:641:LYS:CD  | 1:A:647:GLN:NE2  | 1.99                     | 1.21              |
| 1:D:215:GLN:N   | 1:D:340:ILE:CG1  | 2.02                     | 1.21              |
| 1:D:822:SER:OG  | 2:E:88:LEU:HD23  | 1.06                     | 1.21              |
| 1:D:641:LYS:CG  | 1:D:647:GLN:HG3  | 1.71                     | 1.21              |
| 2:E:144:VAL:CG1 | 2:E:153:ILE:HD11 | 1.65                     | 1.21              |
| 1:A:795:ARG:HB3 | 3:C:35:ARG:NH2   | 1.56                     | 1.20              |
| 1:G:641:LYS:CG  | 1:G:647:GLN:HG3  | 1.71                     | 1.20              |
| 2:B:117:LEU:CD1 | 2:B:147:ASN:CB   | 2.19                     | 1.20              |
| 2:H:117:LEU:CD1 | 2:H:147:ASN:CB   | 2.19                     | 1.20              |
| 1:G:215:GLN:N   | 1:G:340:ILE:HG12 | 1.19                     | 1.20              |
| 1:J:93:MET:SD   | 1:J:716:LEU:HD12 | 1.82                     | 1.20              |
| 4:0:322:PRO:HB2 | 4:2:244:ASP:OD2  | 1.39                     | 1.20              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:797:PHE:HD1  | 3:C:149:VAL:CG1  | 1.54                     | 1.20              |
| 1:J:826:VAL:HG21 | 2:K:88:LEU:HD21  | 1.21                     | 1.20              |
| 1:A:757:GLN:CG   | 1:A:771:LEU:HD11 | 1.71                     | 1.20              |
| 1:D:553:MLY:CE   | 4:7:45:VAL:HA    | 1.52                     | 1.20              |
| 4:5:322:PRO:HB2  | 4:7:244:ASP:OD2  | 1.39                     | 1.20              |
| 4:2:322:PRO:HB2  | 4:4:244:ASP:OD2  | 1.39                     | 1.19              |
| 1:G:534:SER:O    | 4:6:351:THR:CB   | 1.88                     | 1.19              |
| 1:A:721:LYS:HG3  | 1:A:736:GLN:CD   | 1.53                     | 1.19              |
| 1:G:538:GLU:OE2  | 4:6:355:MET:CE   | 1.90                     | 1.19              |
| 1:A:538:GLU:OE2  | 4:4:355:MET:CE   | 1.91                     | 1.19              |
| 1:G:769:ALA:HB3  | 1:G:770:GLY:CA   | 1.65                     | 1.19              |
| 2:H:117:LEU:CD1  | 2:H:147:ASN:CG   | 2.05                     | 1.19              |
| 1:J:538:GLU:OE2  | 4:7:355:MET:CE   | 1.90                     | 1.19              |
| 1:A:822:SER:OG   | 2:B:88:LEU:HD23  | 1.04                     | 1.19              |
| 1:J:557:GLU:H    | 4:V:48:GLY:CA    | 1.56                     | 1.19              |
| 1:G:834:LEU:CD1  | 2:H:51:PHE:HE1   | 1.56                     | 1.19              |
| 1:G:838:ILE:CD1  | 2:H:54:MET:CE    | 2.20                     | 1.19              |
| 4:1:322:PRO:HB2  | 4:3:244:ASP:OD2  | 1.39                     | 1.19              |
| 1:A:538:GLU:C    | 4:4:349:LEU:HD11 | 1.54                     | 1.19              |
| 1:A:538:GLU:C    | 4:4:349:LEU:HD12 | 1.48                     | 1.19              |
| 1:D:538:GLU:OE2  | 4:5:355:MET:CE   | 1.90                     | 1.19              |
| 1:J:800:ARG:CD   | 3:L:149:VAL:HG23 | 1.57                     | 1.19              |
| 1:D:735:GLY:O    | 1:D:743:ALA:CB   | 1.91                     | 1.19              |
| 1:J:90:ASP:CG    | 1:J:764:MLY:HH11 | 1.61                     | 1.19              |
| 1:A:557:GLU:H    | 4:6:48:GLY:CA    | 1.56                     | 1.18              |
| 4:4:322:PRO:HB2  | 4:6:244:ASP:OD2  | 1.39                     | 1.18              |
| 1:D:834:LEU:HG   | 2:E:54:MET:HG3   | 1.21                     | 1.18              |
| 1:G:510:TRP:CZ3  | 1:G:768:MLY:HH11 | 1.77                     | 1.18              |
| 1:G:641:LYS:CB   | 1:G:647:GLN:NE2  | 2.07                     | 1.18              |
| 1:D:557:GLU:H    | 4:7:48:GLY:CA    | 1.56                     | 1.18              |
| 2:K:117:LEU:CD1  | 2:K:147:ASN:CB   | 2.19                     | 1.18              |
| 1:J:641:LYS:CG   | 1:J:647:GLN:HG3  | 1.71                     | 1.18              |
| 1:G:795:ARG:CB   | 3:I:35:ARG:NH2   | 2.07                     | 1.18              |
| 1:J:721:LYS:HG3  | 1:J:736:GLN:HG2  | 1.25                     | 1.18              |
| 1:J:817:GLN:CD   | 2:K:127:ARG:HD2  | 1.64                     | 1.18              |
| 1:A:735:GLY:O    | 1:A:743:ALA:CB   | 1.91                     | 1.18              |
| 1:G:721:LYS:HA   | 1:G:736:GLN:NE2  | 1.58                     | 1.18              |
| 1:J:641:LYS:CB   | 1:J:647:GLN:NE2  | 2.07                     | 1.18              |
| 1:J:538:GLU:C    | 4:7:349:LEU:HD12 | 1.48                     | 1.18              |
| 4:7:322:PRO:HB2  | 4:V:244:ASP:OD2  | 1.39                     | 1.18              |
| 1:G:557:GLU:H    | 4:8:48:GLY:CA    | 1.56                     | 1.17              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:J:538:GLU:HA  | 4:7:349:LEU:CD1  | 1.55                     | 1.17              |
| 1:J:768:MLY:HD3 | 1:J:772:LEU:CB   | 1.72                     | 1.17              |
| 1:J:829:TRP:HZ3 | 2:K:84:PHE:CE2   | 1.62                     | 1.17              |
| 2:E:117:LEU:CD1 | 2:E:147:ASN:CB   | 2.19                     | 1.17              |
| 1:J:798:LEU:CD2 | 3:L:126:LEU:HD11 | 1.73                     | 1.17              |
| 4:X:322:PRO:HB2 | 4:Z:244:ASP:OD2  | 1.39                     | 1.17              |
| 1:A:721:LYS:HA  | 1:A:736:GLN:NE2  | 1.58                     | 1.17              |
| 1:D:769:ALA:HA  | 1:D:771:LEU:CA   | 1.73                     | 1.17              |
| 1:G:754:ASP:HB2 | 1:G:776:GLU:OE2  | 1.41                     | 1.17              |
| 1:G:817:GLN:CG  | 2:H:127:ARG:HD2  | 1.72                     | 1.17              |
| 4:W:290:ARG:NH2 | 4:Y:202:THR:HG23 | 1.59                     | 1.17              |
| 1:A:215:GLN:N   | 1:A:340:ILE:HG12 | 1.20                     | 1.17              |
| 1:A:502:GLU:HG3 | 1:A:761:GLY:CA   | 1.75                     | 1.17              |
| 1:D:725:ARG:N   | 1:D:782:MLY:HH21 | 1.57                     | 1.17              |
| 4:4:290:ARG:NH2 | 4:6:202:THR:HG23 | 1.59                     | 1.17              |
| 1:D:829:TRP:NE1 | 2:E:67:MET:HG2   | 1.56                     | 1.17              |
| 1:G:201:ALA:O   | 1:G:202:SER:HB3  | 1.35                     | 1.17              |
| 1:J:530:MET:HE2 | 4:7:354:GLN:HG2  | 1.24                     | 1.17              |
| 4:3:322:PRO:HB2 | 4:5:244:ASP:OD2  | 1.39                     | 1.17              |
| 4:8:322:PRO:HB2 | 4:W:244:ASP:OD2  | 1.39                     | 1.17              |
| 1:J:829:TRP:CH2 | 2:K:84:PHE:CE1   | 2.33                     | 1.17              |
| 1:J:800:ARG:CB  | 3:L:149:VAL:CG2  | 2.20                     | 1.17              |
| 1:G:735:GLY:O   | 1:G:743:ALA:CB   | 1.91                     | 1.17              |
| 1:J:735:GLY:O   | 1:J:743:ALA:CB   | 1.91                     | 1.17              |
| 1:J:829:TRP:HH2 | 2:K:84:PHE:CE1   | 1.60                     | 1.17              |
| 1:J:641:LYS:CE  | 4:7:348:SER:O    | 1.93                     | 1.17              |
| 1:D:538:GLU:HA  | 4:5:349:LEU:CD1  | 1.55                     | 1.17              |
| 1:D:641:LYS:CE  | 4:5:348:SER:O    | 1.93                     | 1.17              |
| 2:E:117:LEU:CD1 | 2:E:147:ASN:HB3  | 1.75                     | 1.17              |
| 4:6:290:ARG:NH2 | 4:8:202:THR:HG23 | 1.59                     | 1.17              |
| 1:D:641:LYS:CB  | 1:D:647:GLN:NE2  | 2.07                     | 1.17              |
| 1:D:830:PRO:HB2 | 2:E:51:PHE:CZ    | 1.78                     | 1.17              |
| 4:7:290:ARG:NH2 | 4:V:202:THR:HG23 | 1.59                     | 1.17              |
| 1:A:553:MLY:CE  | 4:6:45:VAL:HA    | 1.52                     | 1.16              |
| 1:A:641:LYS:CB  | 1:A:647:GLN:NE2  | 2.07                     | 1.16              |
| 1:G:201:ALA:O   | 1:G:202:SER:CB   | 1.92                     | 1.16              |
| 4:5:290:ARG:NH2 | 4:7:202:THR:HG23 | 1.59                     | 1.16              |
| 1:A:831:TRP:CD1 | 2:B:51:PHE:HZ    | 1.62                     | 1.16              |
| 1:D:538:GLU:OE2 | 4:5:355:MET:HE1  | 1.44                     | 1.16              |
| 4:8:290:ARG:NH2 | 4:W:202:THR:HG23 | 1.59                     | 1.16              |
| 1:J:721:LYS:CG  | 1:J:736:GLN:CG   | 1.97                     | 1.16              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:V:290:ARG:NH2  | 4:X:202:THR:HG23 | 1.59                     | 1.16              |
| 1:A:201:ALA:O    | 1:A:202:SER:HB3  | 1.35                     | 1.16              |
| 1:D:822:SER:OG   | 2:E:88:LEU:CD2   | 1.92                     | 1.16              |
| 1:G:739:ASP:HB3  | 1:G:742:LYS:HB3  | 1.21                     | 1.16              |
| 1:J:510:TRP:CH2  | 1:J:768:MLY:CH1  | 2.28                     | 1.16              |
| 1:D:726:VAL:HB   | 1:D:782:MLY:CH1  | 1.75                     | 1.16              |
| 1:G:215:GLN:HA   | 1:G:340:ILE:CG2  | 1.75                     | 1.16              |
| 1:J:215:GLN:HA   | 1:J:340:ILE:CG2  | 1.75                     | 1.16              |
| 1:J:800:ARG:NH1  | 3:L:149:VAL:HG13 | 1.59                     | 1.16              |
| 1:G:642:LYS:CG   | 4:6:23:GLY:N     | 2.08                     | 1.16              |
| 1:D:769:ALA:HB1  | 1:D:770:GLY:CA   | 1.74                     | 1.16              |
| 1:J:641:LYS:HD2  | 1:J:647:GLN:NE2  | 1.58                     | 1.16              |
| 2:K:144:VAL:CG1  | 2:K:153:ILE:HD11 | 1.65                     | 1.16              |
| 4:W:322:PRO:HB2  | 4:Y:244:ASP:OD2  | 1.39                     | 1.16              |
| 4:3:290:ARG:NH2  | 4:5:202:THR:HG23 | 1.59                     | 1.16              |
| 1:A:639:GLY:CA   | 4:4:345:ILE:HA   | 1.74                     | 1.16              |
| 1:J:201:ALA:O    | 1:J:202:SER:CB   | 1.92                     | 1.16              |
| 1:J:538:GLU:C    | 4:7:349:LEU:HD11 | 1.54                     | 1.16              |
| 1:J:510:TRP:CZ2  | 1:J:768:MLY:HH11 | 1.80                     | 1.16              |
| 2:K:117:LEU:CD1  | 2:K:147:ASN:HB3  | 1.76                     | 1.16              |
| 1:A:553:MLY:HB3  | 4:6:46:GLY:CA    | 1.51                     | 1.15              |
| 1:A:641:LYS:HD2  | 1:A:647:GLN:NE2  | 1.59                     | 1.15              |
| 1:G:93:MET:HE1   | 1:G:763:THR:CA   | 1.76                     | 1.15              |
| 1:A:641:LYS:CE   | 4:4:348:SER:O    | 1.93                     | 1.15              |
| 1:J:538:GLU:OE2  | 4:7:355:MET:HE1  | 1.44                     | 1.15              |
| 1:G:553:MLY:HB3  | 4:8:46:GLY:CA    | 1.51                     | 1.15              |
| 1:G:640:LYS:HB3  | 1:G:645:SER:OG   | 1.46                     | 1.15              |
| 1:G:93:MET:CE    | 1:G:763:THR:CG2  | 2.25                     | 1.15              |
| 2:H:117:LEU:CD1  | 2:H:147:ASN:HB3  | 1.75                     | 1.15              |
| 1:D:839:MLY:HH11 | 2:E:159:HIS:CD2  | 1.79                     | 1.15              |
| 1:J:640:LYS:HB3  | 1:J:645:SER:OG   | 1.45                     | 1.15              |
| 4:1:290:ARG:NH2  | 4:3:202:THR:HG23 | 1.59                     | 1.15              |
| 1:D:649:VAL:HA   | 1:D:649:VAL:CG2  | 1.76                     | 1.15              |
| 2:H:111:SER:CA   | 2:H:148:VAL:O    | 1.95                     | 1.15              |
| 4:X:290:ARG:NH2  | 4:Z:202:THR:HG23 | 1.59                     | 1.15              |
| 4:0:290:ARG:NH2  | 4:2:202:THR:HG23 | 1.59                     | 1.15              |
| 4:2:290:ARG:NH2  | 4:4:202:THR:HG23 | 1.59                     | 1.15              |
| 1:J:749:GLY:O    | 3:L:114:LEU:HD21 | 1.45                     | 1.15              |
| 1:J:635:GLY:HA2  | 4:7:334:GLU:HG2  | 1.16                     | 1.15              |
| 1:D:641:LYS:HD2  | 1:D:647:GLN:NE2  | 1.59                     | 1.15              |
| 1:G:641:LYS:HD2  | 1:G:647:GLN:NE2  | 1.59                     | 1.15              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:639:GLY:HA3  | 4:4:344:SER:O    | 1.47                     | 1.15              |
| 1:D:215:GLN:HA   | 1:D:340:ILE:CG2  | 1.75                     | 1.15              |
| 1:D:538:GLU:C    | 4:5:349:LEU:HD11 | 1.54                     | 1.15              |
| 1:D:542:PHE:HA   | 4:5:143:TYR:CE1  | 1.82                     | 1.15              |
| 1:D:721:LYS:HA   | 1:D:736:GLN:NE2  | 1.58                     | 1.15              |
| 1:J:642:LYS:CG   | 4:7:23:GLY:N     | 2.08                     | 1.15              |
| 1:J:721:LYS:HA   | 1:J:736:GLN:NE2  | 1.58                     | 1.15              |
| 1:D:642:LYS:CG   | 4:5:23:GLY:N     | 2.08                     | 1.15              |
| 1:J:542:PHE:HA   | 4:7:143:TYR:CE1  | 1.82                     | 1.15              |
| 2:E:111:SER:CB   | 2:E:148:VAL:C    | 1.93                     | 1.15              |
| 2:H:121:LEU:CA   | 2:H:128:PHE:HB3  | 1.77                     | 1.15              |
| 1:A:215:GLN:HA   | 1:A:340:ILE:CG2  | 1.76                     | 1.15              |
| 1:A:542:PHE:HA   | 4:4:143:TYR:CE1  | 1.82                     | 1.15              |
| 4:1:287:ILE:HG21 | 4:3:205:GLU:HG2  | 1.17                     | 1.14              |
| 1:G:639:GLY:HA3  | 4:6:344:SER:O    | 1.46                     | 1.14              |
| 1:G:639:GLY:HA2  | 4:6:345:ILE:HA   | 1.26                     | 1.14              |
| 1:A:642:LYS:CG   | 4:4:23:GLY:N     | 2.09                     | 1.14              |
| 1:A:649:VAL:HG13 | 1:A:649:VAL:HG22 | 1.21                     | 1.14              |
| 1:D:639:GLY:CA   | 4:5:345:ILE:HA   | 1.73                     | 1.14              |
| 1:J:739:ASP:HB3  | 1:J:742:LYS:HB3  | 1.21                     | 1.14              |
| 1:J:757:GLN:CG   | 1:J:776:GLU:CG   | 2.23                     | 1.14              |
| 4:3:287:ILE:HG21 | 4:5:205:GLU:HG2  | 1.17                     | 1.14              |
| 2:B:117:LEU:CD1  | 2:B:147:ASN:HB3  | 1.76                     | 1.14              |
| 1:D:640:LYS:HB3  | 1:D:645:SER:OG   | 1.46                     | 1.14              |
| 1:J:649:VAL:CG2  | 1:J:649:VAL:HA   | 1.76                     | 1.14              |
| 1:G:542:PHE:HA   | 4:6:143:TYR:CE1  | 1.82                     | 1.14              |
| 1:A:813:ILE:HG22 | 2:B:127:ARG:CZ   | 1.77                     | 1.14              |
| 1:D:726:VAL:HG23 | 1:D:782:MLY:HH22 | 1.16                     | 1.14              |
| 2:E:111:SER:CA   | 2:E:148:VAL:O    | 1.95                     | 1.14              |
| 1:D:641:LYS:NZ   | 4:5:348:SER:O    | 1.80                     | 1.14              |
| 1:J:639:GLY:HA3  | 4:7:344:SER:O    | 1.46                     | 1.14              |
| 2:E:121:LEU:CA   | 2:E:128:PHE:HB3  | 1.77                     | 1.14              |
| 1:G:649:VAL:HA   | 1:G:649:VAL:CG2  | 1.76                     | 1.14              |
| 2:K:121:LEU:C    | 2:K:128:PHE:HB2  | 1.67                     | 1.14              |
| 1:A:149:GLN:CG   | 1:A:719:ASP:OD1  | 1.96                     | 1.14              |
| 1:A:836:PHE:CE2  | 2:B:160:GLY:HA3  | 1.81                     | 1.14              |
| 1:A:795:ARG:HE   | 3:C:118:MET:HE1  | 1.04                     | 1.14              |
| 1:D:201:ALA:O    | 1:D:202:SER:HB3  | 1.36                     | 1.14              |
| 1:D:839:MLY:HH13 | 2:E:159:HIS:CD2  | 1.82                     | 1.14              |
| 1:J:768:MLY:NZ   | 1:J:772:LEU:HD22 | 1.62                     | 1.14              |
| 2:K:111:SER:CA   | 2:K:148:VAL:O    | 1.95                     | 1.14              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:797:PHE:HD1  | 3:L:149:VAL:CG1  | 1.59                     | 1.14              |
| 4:6:322:PRO:HB2  | 4:8:244:ASP:OD2  | 1.39                     | 1.14              |
| 1:A:501:GLU:HG2  | 1:A:762:HIS:ND1  | 1.62                     | 1.14              |
| 1:A:640:LYS:HB3  | 1:A:645:SER:OG   | 1.46                     | 1.14              |
| 2:B:121:LEU:CA   | 2:B:128:PHE:HB3  | 1.78                     | 1.14              |
| 1:G:641:LYS:CE   | 4:6:348:SER:O    | 1.93                     | 1.14              |
| 2:K:121:LEU:CA   | 2:K:128:PHE:HB3  | 1.77                     | 1.14              |
| 1:D:635:GLY:HA2  | 4:5:334:GLU:HG2  | 1.16                     | 1.14              |
| 2:B:111:SER:CA   | 2:B:148:VAL:O    | 1.95                     | 1.14              |
| 1:D:736:GLN:N    | 1:D:743:ALA:CB   | 2.05                     | 1.14              |
| 2:E:117:LEU:HD12 | 2:E:147:ASN:OD1  | 1.32                     | 1.14              |
| 1:A:649:VAL:CG2  | 1:A:649:VAL:HA   | 1.76                     | 1.14              |
| 2:B:117:LEU:HD12 | 2:B:147:ASN:OD1  | 1.32                     | 1.14              |
| 1:G:831:TRP:NE1  | 2:H:67:MET:HG2   | 1.63                     | 1.14              |
| 4:5:287:ILE:HG21 | 4:7:205:GLU:HG2  | 1.17                     | 1.14              |
| 1:G:599:ASN:OD1  | 1:G:649:VAL:CB   | 1.96                     | 1.14              |
| 1:J:757:GLN:HG2  | 1:J:776:GLU:CG   | 1.76                     | 1.14              |
| 2:K:112:ILE:O    | 2:K:147:ASN:O    | 1.65                     | 1.13              |
| 1:D:641:LYS:HG3  | 1:D:647:GLN:HG3  | 1.20                     | 1.13              |
| 1:D:739:ASP:HB3  | 1:D:742:LYS:HB3  | 1.21                     | 1.13              |
| 1:G:649:VAL:HG22 | 1:G:649:VAL:HG13 | 1.21                     | 1.13              |
| 2:H:117:LEU:HD12 | 2:H:147:ASN:OD1  | 1.32                     | 1.13              |
| 1:G:93:MET:HE1   | 1:G:763:THR:C    | 1.67                     | 1.13              |
| 1:G:768:MLY:HD3  | 1:G:772:LEU:HD22 | 1.19                     | 1.13              |
| 1:J:541:MET:C    | 4:7:143:TYR:OH   | 1.87                     | 1.13              |
| 2:B:121:LEU:C    | 2:B:128:PHE:HB2  | 1.67                     | 1.13              |
| 1:D:639:GLY:HA3  | 4:5:344:SER:O    | 1.46                     | 1.13              |
| 1:D:830:PRO:CG   | 2:E:67:MET:HE1   | 1.77                     | 1.13              |
| 1:G:84:MLY:HH11  | 1:G:715:VAL:CG1  | 1.76                     | 1.13              |
| 1:A:599:ASN:OD1  | 1:A:649:VAL:CB   | 1.96                     | 1.13              |
| 1:A:641:LYS:CE   | 1:A:647:GLN:OE1  | 1.97                     | 1.13              |
| 1:G:538:GLU:C    | 4:6:349:LEU:HD11 | 1.54                     | 1.13              |
| 2:H:112:ILE:O    | 2:H:147:ASN:O    | 1.65                     | 1.13              |
| 1:D:599:ASN:OD1  | 1:D:649:VAL:CB   | 1.96                     | 1.13              |
| 1:D:834:LEU:CD1  | 2:E:54:MET:HG3   | 1.78                     | 1.13              |
| 1:A:768:MLY:HB3  | 1:A:771:LEU:HD13 | 1.31                     | 1.13              |
| 1:A:795:ARG:HH21 | 3:C:116:GLU:HB3  | 1.01                     | 1.13              |
| 1:G:768:MLY:HD3  | 1:G:772:LEU:CD2  | 1.79                     | 1.13              |
| 1:J:641:LYS:CE   | 1:J:647:GLN:OE1  | 1.97                     | 1.13              |
| 1:J:599:ASN:OD1  | 1:J:649:VAL:CB   | 1.96                     | 1.13              |
| 1:J:831:TRP:HZ2  | 2:K:47:LEU:HD22  | 1.08                     | 1.13              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:831:TRP:NE1  | 2:B:51:PHE:HZ    | 1.32                     | 1.13              |
| 1:A:800:ARG:NH1  | 3:C:149:VAL:HG13 | 1.61                     | 1.13              |
| 1:D:726:VAL:CB   | 1:D:782:MLY:HH13 | 1.77                     | 1.13              |
| 1:D:541:MET:C    | 4:5:143:TYR:OH   | 1.87                     | 1.12              |
| 1:G:639:GLY:CA   | 4:6:345:ILE:HA   | 1.73                     | 1.12              |
| 1:D:201:ALA:O    | 1:D:202:SER:CB   | 1.92                     | 1.12              |
| 1:G:541:MET:C    | 4:6:143:TYR:OH   | 1.87                     | 1.12              |
| 1:J:510:TRP:CZ3  | 1:J:768:MLY:HH11 | 1.83                     | 1.12              |
| 1:A:541:MET:C    | 4:4:143:TYR:OH   | 1.87                     | 1.12              |
| 4:W:287:ILE:HG21 | 4:Y:205:GLU:HG2  | 1.17                     | 1.12              |
| 1:D:724:TYR:CE1  | 1:D:778:MET:HB3  | 1.85                     | 1.12              |
| 1:G:641:LYS:NZ   | 4:6:348:SER:O    | 1.80                     | 1.12              |
| 1:A:641:LYS:NZ   | 4:4:348:SER:O    | 1.80                     | 1.12              |
| 1:A:839:MLY:HH21 | 2:B:158:THR:HG22 | 1.30                     | 1.12              |
| 2:B:112:ILE:O    | 2:B:147:ASN:O    | 1.65                     | 1.12              |
| 1:D:641:LYS:CE   | 1:D:647:GLN:OE1  | 1.97                     | 1.12              |
| 1:D:831:TRP:CZ3  | 2:E:34:ILE:CG2   | 2.32                     | 1.12              |
| 1:G:834:LEU:CD1  | 2:H:51:PHE:CE1   | 2.30                     | 1.12              |
| 1:A:201:ALA:O    | 1:A:202:SER:CB   | 1.92                     | 1.12              |
| 1:D:507:GLY:O    | 1:D:761:GLY:CA   | 1.97                     | 1.12              |
| 1:G:819:ASN:CG   | 2:H:92:ASP:HB2   | 1.62                     | 1.12              |
| 1:D:538:GLU:O    | 4:5:349:LEU:HD11 | 1.35                     | 1.12              |
| 4:7:287:ILE:HG21 | 4:V:205:GLU:HG2  | 1.17                     | 1.12              |
| 1:G:641:LYS:CE   | 1:G:647:GLN:OE1  | 1.97                     | 1.12              |
| 2:K:111:SER:HB3  | 2:K:148:VAL:O    | 1.50                     | 1.12              |
| 1:A:707:CYS:HA   | 1:A:714:ARG:HH12 | 1.11                     | 1.12              |
| 1:J:623:PHE:CG   | 1:J:623:PHE:CB   | 2.33                     | 1.12              |
| 1:J:92:ALA:O     | 1:J:714:ARG:HD2  | 1.49                     | 1.12              |
| 2:B:121:LEU:O    | 2:B:128:PHE:HB2  | 0.94                     | 1.12              |
| 1:J:821:ARG:NH2  | 2:K:127:ARG:CG   | 2.13                     | 1.12              |
| 1:J:829:TRP:CH2  | 2:K:84:PHE:CZ    | 2.38                     | 1.12              |
| 1:G:538:GLU:OE2  | 4:6:355:MET:HE1  | 1.50                     | 1.12              |
| 3:C:48:LYS:C     | 3:C:52:ASN:ND2   | 2.03                     | 1.12              |
| 1:A:530:MET:HE2  | 4:4:354:GLN:HG2  | 1.30                     | 1.12              |
| 1:A:707:CYS:HA   | 1:A:714:ARG:NH1  | 1.64                     | 1.12              |
| 2:E:112:ILE:O    | 2:E:147:ASN:O    | 1.65                     | 1.12              |
| 1:J:795:ARG:NH2  | 3:L:116:GLU:OE2  | 1.83                     | 1.12              |
| 3:I:48:LYS:C     | 3:I:52:ASN:ND2   | 2.03                     | 1.11              |
| 1:G:649:VAL:HG12 | 1:G:649:VAL:O    | 0.94                     | 1.11              |
| 1:G:788:THR:C    | 3:I:42:THR:HG22  | 1.56                     | 1.11              |
| 1:J:641:LYS:NZ   | 4:7:348:SER:O    | 1.80                     | 1.11              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:8:287:ILE:HG21 | 4:W:205:GLU:HG2  | 1.17                     | 1.11              |
| 4:8:290:ARG:CZ   | 4:W:202:THR:HG21 | 1.81                     | 1.11              |
| 4:V:322:PRO:HB2  | 4:X:244:ASP:OD2  | 1.39                     | 1.11              |
| 4:5:290:ARG:CZ   | 4:7:202:THR:HG21 | 1.81                     | 1.11              |
| 4:7:290:ARG:CZ   | 4:V:202:THR:HG21 | 1.81                     | 1.11              |
| 2:B:117:LEU:HB2  | 2:B:147:ASN:CG   | 1.70                     | 1.11              |
| 1:A:798:LEU:HD11 | 3:C:126:LEU:HD21 | 1.29                     | 1.11              |
| 1:G:819:ASN:CG   | 2:H:90:GLY:O     | 1.88                     | 1.11              |
| 3:L:24:LYS:CB    | 3:L:63:ILE:O     | 1.99                     | 1.11              |
| 4:0:290:ARG:CZ   | 4:2:202:THR:HG21 | 1.81                     | 1.11              |
| 3:C:24:LYS:CB    | 3:C:63:ILE:O     | 1.99                     | 1.11              |
| 1:D:623:PHE:CG   | 1:D:623:PHE:CB   | 2.33                     | 1.11              |
| 1:D:641:LYS:CE   | 1:D:647:GLN:CD   | 2.18                     | 1.11              |
| 2:H:117:LEU:HB2  | 2:H:147:ASN:CG   | 1.70                     | 1.11              |
| 1:A:649:VAL:O    | 1:A:649:VAL:HG12 | 0.94                     | 1.11              |
| 1:A:814:PHE:CD1  | 2:B:127:ARG:NH2  | 2.16                     | 1.11              |
| 1:G:736:GLN:N    | 1:G:743:ALA:CB   | 2.04                     | 1.11              |
| 2:H:111:SER:CB   | 2:H:148:VAL:C    | 1.93                     | 1.11              |
| 1:A:623:PHE:CG   | 1:A:623:PHE:CB   | 2.33                     | 1.11              |
| 1:D:834:LEU:CD1  | 2:E:54:MET:CG    | 2.28                     | 1.11              |
| 1:G:798:LEU:HD13 | 3:I:126:LEU:CD2  | 1.67                     | 1.11              |
| 1:G:817:GLN:CD   | 2:H:127:ARG:HD2  | 1.68                     | 1.11              |
| 1:J:641:LYS:CE   | 1:J:647:GLN:CD   | 2.18                     | 1.11              |
| 1:J:798:LEU:HD22 | 3:L:126:LEU:CD1  | 1.79                     | 1.11              |
| 4:6:290:ARG:CZ   | 4:8:202:THR:HG21 | 1.81                     | 1.11              |
| 3:F:48:LYS:C     | 3:F:52:ASN:ND2   | 2.03                     | 1.11              |
| 1:D:530:MET:CE   | 4:5:354:GLN:HG2  | 1.80                     | 1.10              |
| 1:D:530:MET:HE2  | 4:5:354:GLN:HG2  | 1.22                     | 1.10              |
| 1:D:799:MET:SD   | 3:F:32:ASP:CA    | 2.38                     | 1.10              |
| 1:G:93:MET:SD    | 1:G:716:LEU:CD1  | 2.39                     | 1.10              |
| 1:D:798:LEU:HD11 | 3:F:126:LEU:HD21 | 1.27                     | 1.10              |
| 1:G:623:PHE:CG   | 1:G:623:PHE:CB   | 2.33                     | 1.10              |
| 1:G:641:LYS:HG3  | 1:G:647:GLN:HG3  | 1.21                     | 1.10              |
| 1:J:84:MLY:HH11  | 1:J:715:VAL:CG1  | 1.70                     | 1.10              |
| 1:J:538:GLU:O    | 4:7:349:LEU:HD11 | 1.35                     | 1.10              |
| 1:J:530:MET:CE   | 4:7:354:GLN:HG2  | 1.80                     | 1.10              |
| 2:E:117:LEU:HB2  | 2:E:147:ASN:CG   | 1.70                     | 1.10              |
| 2:E:121:LEU:O    | 2:E:128:PHE:HB2  | 0.94                     | 1.10              |
| 1:G:641:LYS:CE   | 1:G:647:GLN:CD   | 2.18                     | 1.10              |
| 4:W:290:ARG:CZ   | 4:Y:202:THR:HG21 | 1.81                     | 1.10              |
| 1:A:641:LYS:CE   | 1:A:647:GLN:CD   | 2.18                     | 1.10              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:730:SER:OG   | 3:I:109:HIS:CG   | 2.05                     | 1.10              |
| 1:G:838:ILE:HD11 | 2:H:54:MET:HE1   | 1.19                     | 1.10              |
| 3:L:48:LYS:C     | 3:L:52:ASN:ND2   | 2.03                     | 1.10              |
| 4:V:287:ILE:HG21 | 4:X:205:GLU:HG2  | 1.17                     | 1.10              |
| 4:2:290:ARG:CZ   | 4:4:202:THR:HG21 | 1.81                     | 1.10              |
| 1:D:649:VAL:HG13 | 1:D:649:VAL:HG22 | 1.21                     | 1.10              |
| 1:J:218:LEU:HB2  | 1:J:221:GLN:HG3  | 1.17                     | 1.10              |
| 4:V:290:ARG:CZ   | 4:X:202:THR:HG21 | 1.81                     | 1.10              |
| 2:H:121:LEU:O    | 2:H:128:PHE:HB2  | 0.94                     | 1.10              |
| 4:3:290:ARG:CZ   | 4:5:202:THR:HG21 | 1.81                     | 1.10              |
| 1:A:202:SER:CA   | 1:A:207:LYS:HE2  | 1.82                     | 1.10              |
| 1:A:218:LEU:HB2  | 1:A:221:GLN:HG3  | 1.17                     | 1.10              |
| 1:J:797:PHE:CD1  | 3:L:149:VAL:CG1  | 2.34                     | 1.10              |
| 1:J:800:ARG:NE   | 3:L:149:VAL:HG22 | 1.65                     | 1.10              |
| 1:J:553:MLY:CE   | 4:V:45:VAL:HA    | 1.52                     | 1.10              |
| 1:D:822:SER:CB   | 2:E:88:LEU:HD23  | 1.82                     | 1.10              |
| 1:D:831:TRP:CD1  | 2:E:67:MET:SD    | 2.45                     | 1.10              |
| 1:D:817:GLN:CD   | 2:E:127:ARG:NE   | 2.04                     | 1.10              |
| 1:J:641:LYS:HE3  | 1:J:647:GLN:OE1  | 1.50                     | 1.10              |
| 1:A:641:LYS:HE3  | 1:A:647:GLN:OE1  | 1.50                     | 1.10              |
| 1:A:822:SER:OG   | 2:B:88:LEU:CD2   | 2.00                     | 1.10              |
| 1:D:831:TRP:CZ2  | 2:E:47:LEU:CB    | 2.23                     | 1.10              |
| 1:G:202:SER:CA   | 1:G:207:LYS:HE2  | 1.82                     | 1.10              |
| 4:6:287:ILE:HG21 | 4:8:205:GLU:HG2  | 1.17                     | 1.09              |
| 1:A:739:ASP:HB3  | 1:A:742:LYS:HB3  | 1.21                     | 1.09              |
| 1:D:734:GLU:O    | 1:D:738:MET:HG2  | 1.51                     | 1.09              |
| 1:A:721:LYS:HA   | 1:A:736:GLN:CD   | 1.73                     | 1.09              |
| 1:A:799:MET:SD   | 3:C:32:ASP:CB    | 2.38                     | 1.09              |
| 1:D:639:GLY:HA2  | 4:5:345:ILE:HA   | 1.26                     | 1.09              |
| 1:D:817:GLN:HE21 | 2:E:127:ARG:HG2  | 1.12                     | 1.09              |
| 3:I:24:LYS:CB    | 3:I:63:ILE:O     | 1.99                     | 1.09              |
| 1:J:641:LYS:HD2  | 1:J:647:GLN:CD   | 1.70                     | 1.09              |
| 1:J:768:MLY:HD3  | 1:J:772:LEU:HB3  | 1.30                     | 1.09              |
| 4:4:290:ARG:CZ   | 4:6:202:THR:HG21 | 1.81                     | 1.09              |
| 1:A:538:GLU:HA   | 4:4:349:LEU:CD1  | 1.54                     | 1.09              |
| 1:A:530:MET:CE   | 4:4:354:GLN:HG2  | 1.80                     | 1.09              |
| 1:D:768:MLY:O    | 1:D:771:LEU:HD11 | 1.29                     | 1.09              |
| 2:E:121:LEU:C    | 2:E:128:PHE:HB2  | 1.67                     | 1.09              |
| 1:J:649:VAL:O    | 1:J:649:VAL:HG12 | 0.94                     | 1.09              |
| 1:G:530:MET:CE   | 4:6:354:GLN:HG2  | 1.80                     | 1.09              |
| 1:D:218:LEU:HB2  | 1:D:221:GLN:HG3  | 1.17                     | 1.09              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:571:ALA:O    | 1:J:572:LYS:HG3  | 1.52                     | 1.09              |
| 3:F:24:LYS:CB    | 3:F:63:ILE:O     | 1.99                     | 1.09              |
| 1:J:754:ASP:OD2  | 1:J:776:GLU:CA   | 1.99                     | 1.09              |
| 2:K:121:LEU:O    | 2:K:128:PHE:HB2  | 0.94                     | 1.09              |
| 4:X:290:ARG:CZ   | 4:Z:202:THR:HG21 | 1.81                     | 1.09              |
| 1:D:571:ALA:O    | 1:D:572:LYS:HG3  | 1.52                     | 1.09              |
| 1:G:218:LEU:HB2  | 1:G:221:GLN:HG3  | 1.17                     | 1.09              |
| 1:J:641:LYS:HG3  | 1:J:647:GLN:HG3  | 1.20                     | 1.09              |
| 1:J:721:LYS:HA   | 1:J:736:GLN:CD   | 1.73                     | 1.09              |
| 1:J:93:MET:O     | 1:J:714:ARG:O    | 1.71                     | 1.09              |
| 4:1:290:ARG:CZ   | 4:3:202:THR:HG21 | 1.81                     | 1.09              |
| 1:D:649:VAL:O    | 1:D:649:VAL:HG12 | 0.94                     | 1.09              |
| 1:D:809:ARG:NH1  | 2:E:124:GLY:HA2  | 1.68                     | 1.09              |
| 1:G:831:TRP:NE1  | 2:H:67:MET:CG    | 2.13                     | 1.09              |
| 1:G:831:TRP:HE1  | 2:H:67:MET:HG2   | 0.92                     | 1.09              |
| 1:J:201:ALA:O    | 1:J:202:SER:HB3  | 1.36                     | 1.09              |
| 1:J:734:GLU:O    | 1:J:738:MET:HG2  | 1.51                     | 1.09              |
| 4:0:287:ILE:HG21 | 4:2:205:GLU:HG2  | 1.17                     | 1.09              |
| 1:D:641:LYS:HE3  | 1:D:647:GLN:OE1  | 1.50                     | 1.09              |
| 1:G:707:CYS:CB   | 1:G:714:ARG:HH12 | 1.65                     | 1.09              |
| 1:G:84:MLY:HH12  | 1:G:715:VAL:HG13 | 1.32                     | 1.09              |
| 2:H:121:LEU:C    | 2:H:128:PHE:HB2  | 1.67                     | 1.09              |
| 1:J:649:VAL:HG22 | 1:J:649:VAL:HG13 | 1.21                     | 1.09              |
| 2:K:121:LEU:C    | 2:K:128:PHE:HB3  | 1.71                     | 1.09              |
| 1:D:202:SER:CA   | 1:D:207:LYS:HE2  | 1.82                     | 1.09              |
| 2:H:111:SER:OG   | 2:H:148:VAL:O    | 1.71                     | 1.09              |
| 1:G:791:GLN:OE1  | 3:I:116:GLU:HB2  | 1.52                     | 1.09              |
| 1:A:734:GLU:O    | 1:A:738:MET:HG2  | 1.51                     | 1.09              |
| 1:G:821:ARG:HH22 | 2:H:127:ARG:CG   | 1.63                     | 1.09              |
| 1:G:84:MLY:HH13  | 1:G:715:VAL:HG13 | 1.17                     | 1.09              |
| 1:J:643:GLY:O    | 1:J:644:SER:OG   | 1.70                     | 1.09              |
| 2:K:117:LEU:HB2  | 2:K:147:ASN:CG   | 1.70                     | 1.09              |
| 1:A:798:LEU:HD13 | 3:C:126:LEU:HD21 | 1.09                     | 1.08              |
| 1:G:538:GLU:HA   | 4:6:349:LEU:CD1  | 1.55                     | 1.08              |
| 2:K:111:SER:OG   | 2:K:148:VAL:O    | 1.71                     | 1.08              |
| 1:D:530:MET:HE2  | 4:5:354:GLN:CG   | 1.82                     | 1.08              |
| 1:D:721:LYS:HA   | 1:D:736:GLN:CD   | 1.73                     | 1.08              |
| 1:D:829:TRP:HE1  | 2:E:67:MET:CG    | 1.64                     | 1.08              |
| 4:X:287:ILE:HG21 | 4:Z:205:GLU:HG2  | 1.17                     | 1.08              |
| 2:B:111:SER:CB   | 2:B:148:VAL:C    | 1.93                     | 1.08              |
| 1:D:721:LYS:HG3  | 1:D:736:GLN:HG2  | 1.25                     | 1.08              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:769:ALA:CB   | 1:J:770:GLY:CA   | 2.31                     | 1.08              |
| 1:J:95:THR:OG1   | 1:J:713:SER:HB3  | 1.50                     | 1.08              |
| 1:D:800:ARG:CB   | 3:F:149:VAL:HG22 | 1.83                     | 1.08              |
| 4:4:287:ILE:HG21 | 4:6:205:GLU:HG2  | 1.17                     | 1.08              |
| 1:A:635:GLY:HA2  | 4:4:334:GLU:HG2  | 1.16                     | 1.08              |
| 1:D:834:LEU:CD2  | 2:E:54:MET:HG3   | 1.82                     | 1.08              |
| 1:J:639:GLY:CA   | 4:7:345:ILE:HA   | 1.73                     | 1.08              |
| 1:J:84:MLY:HH13  | 1:J:715:VAL:HG13 | 1.28                     | 1.08              |
| 1:J:797:PHE:CD1  | 3:L:149:VAL:HG11 | 1.88                     | 1.08              |
| 1:G:530:MET:HE2  | 4:6:354:GLN:HG2  | 1.27                     | 1.08              |
| 2:E:111:SER:HB3  | 2:E:148:VAL:O    | 1.50                     | 1.08              |
| 1:G:734:GLU:O    | 1:G:738:MET:HG2  | 1.51                     | 1.08              |
| 1:J:202:SER:CA   | 1:J:207:LYS:HE2  | 1.82                     | 1.08              |
| 1:A:639:GLY:HA2  | 4:4:345:ILE:HA   | 1.26                     | 1.08              |
| 1:J:736:GLN:HA   | 1:J:743:ALA:HB3  | 1.35                     | 1.08              |
| 1:A:798:LEU:HD11 | 3:C:126:LEU:CD2  | 1.79                     | 1.08              |
| 2:E:111:SER:OG   | 2:E:148:VAL:O    | 1.71                     | 1.08              |
| 1:J:639:GLY:HA2  | 4:7:345:ILE:HA   | 1.26                     | 1.08              |
| 2:B:121:LEU:C    | 2:B:128:PHE:HB3  | 1.72                     | 1.07              |
| 2:B:111:SER:CB   | 2:B:148:VAL:O    | 0.78                     | 1.07              |
| 2:E:121:LEU:C    | 2:E:128:PHE:HB3  | 1.72                     | 1.07              |
| 2:E:111:SER:CB   | 2:E:148:VAL:O    | 0.78                     | 1.07              |
| 1:G:643:GLY:O    | 1:G:644:SER:OG   | 1.70                     | 1.07              |
| 4:2:287:ILE:HG21 | 4:4:205:GLU:HG2  | 1.17                     | 1.07              |
| 1:J:529:PRO:HB3  | 4:7:353:GLN:OE1  | 1.53                     | 1.07              |
| 1:D:643:GLY:O    | 1:D:644:SER:OG   | 1.70                     | 1.07              |
| 1:G:641:LYS:HE3  | 1:G:647:GLN:OE1  | 1.50                     | 1.07              |
| 1:G:721:LYS:HG3  | 1:G:736:GLN:HG2  | 1.25                     | 1.07              |
| 1:J:768:MLY:HH22 | 1:J:772:LEU:HB2  | 1.36                     | 1.07              |
| 1:A:501:GLU:O    | 1:A:762:HIS:NE2  | 1.87                     | 1.07              |
| 2:H:111:SER:CB   | 2:H:148:VAL:O    | 0.77                     | 1.07              |
| 1:D:529:PRO:HB3  | 4:5:353:GLN:OE1  | 1.53                     | 1.07              |
| 1:A:409:GLY:N    | 1:A:636:LYS:HG3  | 1.69                     | 1.07              |
| 1:D:409:GLY:N    | 1:D:636:LYS:HG3  | 1.69                     | 1.07              |
| 1:D:638:GLY:CA   | 4:5:341:ILE:O    | 2.01                     | 1.07              |
| 1:G:721:LYS:HA   | 1:G:736:GLN:CD   | 1.73                     | 1.07              |
| 1:J:530:MET:HE2  | 4:7:354:GLN:CG   | 1.84                     | 1.07              |
| 1:D:769:ALA:HB1  | 1:D:770:GLY:C    | 1.72                     | 1.07              |
| 2:K:111:SER:CB   | 2:K:148:VAL:O    | 0.78                     | 1.07              |
| 1:J:831:TRP:CZ2  | 2:K:47:LEU:HD22  | 1.88                     | 1.07              |
| 1:G:529:PRO:HB3  | 4:6:353:GLN:OE1  | 1.53                     | 1.07              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:G:641:LYS:CG  | 1:G:647:GLN:CG  | 2.16                     | 1.07              |
| 1:G:641:LYS:HB2 | 1:G:647:GLN:NE2 | 1.68                     | 1.07              |
| 1:G:72:VAL:HG13 | 1:G:76:GLN:HB3  | 1.36                     | 1.07              |
| 1:A:529:PRO:HB3 | 4:4:353:GLN:OE1 | 1.53                     | 1.07              |
| 1:D:541:MET:SD  | 4:5:345:ILE:O   | 2.12                     | 1.07              |
| 1:A:641:LYS:HB2 | 1:A:647:GLN:NE2 | 1.68                     | 1.07              |
| 1:J:541:MET:SD  | 4:7:345:ILE:O   | 2.13                     | 1.07              |
| 2:K:111:SER:CB  | 2:K:148:VAL:C   | 1.93                     | 1.07              |
| 1:J:638:GLY:CA  | 4:7:341:ILE:O   | 2.01                     | 1.07              |
| 1:A:839:MLY:HD2 | 2:B:159:HIS:CG  | 1.88                     | 1.07              |
| 1:G:409:GLY:N   | 1:G:636:LYS:HG3 | 1.69                     | 1.07              |
| 1:A:638:GLY:CA  | 4:4:341:ILE:O   | 2.01                     | 1.07              |
| 1:G:638:GLY:CA  | 4:6:341:ILE:O   | 2.02                     | 1.07              |
| 1:J:793:ARG:HE  | 3:L:147:MET:HA  | 0.93                     | 1.07              |
| 1:J:795:ARG:HD3 | 3:L:35:ARG:HH22 | 1.14                     | 1.07              |
| 1:A:541:MET:SD  | 4:4:345:ILE:O   | 2.12                     | 1.07              |
| 1:J:409:GLY:N   | 1:J:636:LYS:HG3 | 1.69                     | 1.06              |
| 1:A:502:GLU:HG3 | 1:A:761:GLY:HA3 | 1.34                     | 1.06              |
| 1:D:834:LEU:CG  | 2:E:54:MET:CG   | 2.32                     | 1.06              |
| 1:G:635:GLY:HA2 | 4:6:334:GLU:HG2 | 1.16                     | 1.06              |
| 1:A:643:GLY:O   | 1:A:644:SER:OG  | 1.69                     | 1.06              |
| 1:G:831:TRP:HH2 | 2:H:47:LEU:HD21 | 1.13                     | 1.06              |
| 1:J:768:MLY:CH2 | 1:J:772:LEU:CD2 | 2.12                     | 1.06              |
| 1:G:541:MET:SD  | 4:6:345:ILE:O   | 2.13                     | 1.06              |
| 1:A:571:ALA:O   | 1:A:572:LYS:HG3 | 1.52                     | 1.06              |
| 1:A:72:VAL:HG13 | 1:A:76:GLN:HB3  | 1.36                     | 1.06              |
| 1:D:542:PHE:CG  | 4:5:143:TYR:HE1 | 1.73                     | 1.06              |
| 1:D:736:GLN:HA  | 1:D:743:ALA:HB3 | 1.34                     | 1.06              |
| 2:E:114:LYS:HA  | 2:E:146:GLY:O   | 0.89                     | 1.06              |
| 2:H:111:SER:HB3 | 2:H:148:VAL:O   | 1.49                     | 1.06              |
| 2:K:114:LYS:HA  | 2:K:146:GLY:O   | 0.89                     | 1.06              |
| 1:G:797:PHE:CD1 | 3:I:149:VAL:CG1 | 2.03                     | 1.06              |
| 1:D:576:GLU:HG2 | 1:D:577:ALA:N   | 1.66                     | 1.06              |
| 1:J:510:TRP:CZ3 | 1:J:768:MLY:CH1 | 2.39                     | 1.06              |
| 1:A:736:GLN:HA  | 1:A:743:ALA:HB3 | 1.35                     | 1.06              |
| 1:A:795:ARG:CD  | 3:C:35:ARG:HH22 | 1.68                     | 1.06              |
| 1:A:793:ARG:NE  | 3:C:147:MET:HG2 | 1.70                     | 1.06              |
| 2:B:114:LYS:HA  | 2:B:146:GLY:O   | 0.89                     | 1.06              |
| 2:B:111:SER:OG  | 2:B:148:VAL:O   | 1.71                     | 1.06              |
| 1:D:641:LYS:HE3 | 4:5:348:SER:O   | 1.55                     | 1.06              |
| 1:D:768:MLY:O   | 1:D:771:LEU:CD1 | 0.76                     | 1.06              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:571:ALA:O    | 1:G:572:LYS:HG3  | 1.52                     | 1.06              |
| 1:G:635:GLY:HA3  | 4:6:341:ILE:HD13 | 1.36                     | 1.05              |
| 1:A:800:ARG:NH1  | 3:C:149:VAL:C    | 2.08                     | 1.05              |
| 1:D:641:LYS:HB2  | 1:D:647:GLN:NE2  | 1.68                     | 1.05              |
| 2:E:140:PHE:O    | 2:E:141:PRO:O    | 1.74                     | 1.05              |
| 1:J:769:ALA:CB   | 1:J:770:GLY:HA2  | 1.86                     | 1.05              |
| 2:K:140:PHE:O    | 2:K:141:PRO:O    | 1.75                     | 1.05              |
| 1:A:721:LYS:HG3  | 1:A:736:GLN:HG2  | 1.25                     | 1.05              |
| 1:D:831:TRP:CH2  | 2:E:34:ILE:HG23  | 1.89                     | 1.05              |
| 4:1:3:ASP:HA     | 4:1:6:THR:HB     | 1.36                     | 1.05              |
| 1:A:530:MET:CA   | 4:4:354:GLN:HG3  | 1.86                     | 1.05              |
| 1:J:530:MET:CA   | 4:7:354:GLN:HG3  | 1.87                     | 1.05              |
| 1:D:72:VAL:HG13  | 1:D:76:GLN:HB3   | 1.36                     | 1.05              |
| 1:J:641:LYS:HB2  | 1:J:647:GLN:NE2  | 1.68                     | 1.05              |
| 1:A:542:PHE:CG   | 4:4:143:TYR:HE1  | 1.73                     | 1.05              |
| 1:J:638:GLY:HA2  | 4:7:341:ILE:O    | 1.57                     | 1.05              |
| 1:D:795:ARG:HH21 | 3:F:116:GLU:CD   | 1.59                     | 1.05              |
| 1:G:819:ASN:HA   | 2:H:90:GLY:O     | 0.87                     | 1.05              |
| 1:J:641:LYS:HE3  | 4:7:348:SER:O    | 1.55                     | 1.05              |
| 4:Y:3:ASP:HA     | 4:Y:6:THR:HB     | 1.36                     | 1.05              |
| 1:J:793:ARG:NE   | 3:L:147:MET:HA   | 1.71                     | 1.05              |
| 1:J:797:PHE:HD1  | 3:L:149:VAL:HG12 | 1.21                     | 1.05              |
| 1:J:795:ARG:HD2  | 3:L:35:ARG:NH1   | 1.72                     | 1.05              |
| 1:A:797:PHE:CD1  | 3:C:149:VAL:CG1  | 2.33                     | 1.05              |
| 1:G:542:PHE:CG   | 4:6:143:TYR:HE1  | 1.74                     | 1.05              |
| 1:J:819:ASN:CA   | 2:K:90:GLY:O     | 2.04                     | 1.05              |
| 1:A:800:ARG:CB   | 3:C:149:VAL:HG22 | 1.83                     | 1.05              |
| 1:J:641:LYS:HE3  | 1:J:647:GLN:CD   | 1.77                     | 1.05              |
| 1:J:72:VAL:HG13  | 1:J:76:GLN:HB3   | 1.36                     | 1.05              |
| 1:J:800:ARG:HB3  | 3:L:149:VAL:HG21 | 1.35                     | 1.05              |
| 1:A:635:GLY:HA3  | 4:4:341:ILE:HD13 | 1.37                     | 1.04              |
| 1:A:505:MLY:CB   | 1:A:762:HIS:H    | 1.68                     | 1.04              |
| 2:H:114:LYS:HA   | 2:H:146:GLY:O    | 0.88                     | 1.04              |
| 1:D:530:MET:CA   | 4:5:354:GLN:HG3  | 1.87                     | 1.04              |
| 1:D:829:TRP:HE1  | 2:E:67:MET:HG2   | 0.88                     | 1.04              |
| 1:G:829:TRP:CH2  | 2:H:87:LYS:HE2   | 1.91                     | 1.04              |
| 1:D:638:GLY:HA2  | 4:5:341:ILE:O    | 1.57                     | 1.04              |
| 1:A:599:ASN:HA   | 1:A:649:VAL:HB   | 1.06                     | 1.04              |
| 1:A:641:LYS:HE3  | 1:A:647:GLN:CD   | 1.77                     | 1.04              |
| 1:A:834:LEU:CD1  | 2:B:54:MET:HG3   | 1.86                     | 1.04              |
| 3:C:49:ILE:CA    | 3:C:52:ASN:HD22  | 1.70                     | 1.04              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:576:GLU:HG2  | 1:J:577:ALA:N    | 1.66                     | 1.04              |
| 1:J:736:GLN:N    | 1:J:743:ALA:CB   | 2.05                     | 1.04              |
| 1:G:530:MET:HE2  | 4:6:354:GLN:CG   | 1.87                     | 1.04              |
| 1:D:830:PRO:CD   | 2:E:67:MET:HE1   | 1.86                     | 1.04              |
| 1:J:542:PHE:CG   | 4:7:143:TYR:HE1  | 1.73                     | 1.04              |
| 1:J:800:ARG:CZ   | 3:L:149:VAL:HG22 | 1.86                     | 1.04              |
| 1:A:641:LYS:HD2  | 1:A:647:GLN:CD   | 1.70                     | 1.04              |
| 1:G:769:ALA:HB1  | 1:G:770:GLY:HA2  | 1.37                     | 1.04              |
| 1:G:757:GLN:OE1  | 1:G:772:LEU:CG   | 2.03                     | 1.04              |
| 1:J:795:ARG:NH1  | 3:L:35:ARG:HH12  | 1.56                     | 1.04              |
| 4:0:290:ARG:CZ   | 4:2:202:THR:CG2  | 2.36                     | 1.04              |
| 1:G:641:LYS:HE3  | 1:G:647:GLN:CD   | 1.77                     | 1.04              |
| 1:G:817:GLN:HB3  | 2:H:127:ARG:CD   | 1.86                     | 1.04              |
| 4:W:3:ASP:HA     | 4:W:6:THR:HB     | 1.36                     | 1.04              |
| 1:A:757:GLN:HB3  | 1:A:771:LEU:HD13 | 1.32                     | 1.04              |
| 1:A:795:ARG:NH2  | 3:C:116:GLU:HB3  | 1.70                     | 1.04              |
| 1:G:789:ALA:CB   | 3:I:81:GLN:HE21  | 1.68                     | 1.04              |
| 4:2:3:ASP:HA     | 4:2:6:THR:HB     | 1.36                     | 1.04              |
| 1:A:529:PRO:C    | 4:4:354:GLN:HB3  | 1.78                     | 1.04              |
| 2:B:111:SER:HB3  | 2:B:148:VAL:O    | 1.49                     | 1.04              |
| 1:G:93:MET:O     | 1:G:714:ARG:O    | 1.76                     | 1.04              |
| 4:8:290:ARG:CZ   | 4:W:202:THR:CG2  | 2.36                     | 1.04              |
| 1:J:56:GLU:HB2   | 1:J:59:MLY:HB3   | 1.40                     | 1.04              |
| 1:A:538:GLU:OE2  | 4:4:355:MET:HE1  | 1.55                     | 1.03              |
| 1:D:202:SER:CA   | 1:D:207:LYS:CE   | 2.36                     | 1.03              |
| 4:2:290:ARG:CZ   | 4:4:202:THR:CG2  | 2.36                     | 1.03              |
| 1:D:641:LYS:HE3  | 1:D:647:GLN:CD   | 1.77                     | 1.03              |
| 1:G:639:GLY:N    | 4:6:345:ILE:N    | 1.94                     | 1.03              |
| 1:G:641:LYS:HD2  | 1:G:647:GLN:CD   | 1.70                     | 1.03              |
| 2:K:149:ASP:OD2  | 2:K:150:TYR:N    | 1.91                     | 1.03              |
| 4:V:290:ARG:CZ   | 4:X:202:THR:CG2  | 2.36                     | 1.03              |
| 4:4:3:ASP:HA     | 4:4:6:THR:HB     | 1.36                     | 1.03              |
| 4:6:290:ARG:CZ   | 4:8:202:THR:CG2  | 2.36                     | 1.03              |
| 1:A:502:GLU:OE1  | 1:A:763:THR:N    | 1.89                     | 1.03              |
| 1:A:800:ARG:HH11 | 3:C:149:VAL:C    | 1.61                     | 1.03              |
| 1:A:795:ARG:HH21 | 3:C:116:GLU:CB   | 1.71                     | 1.03              |
| 1:G:56:GLU:HB2   | 1:G:59:MLY:HB3   | 1.40                     | 1.03              |
| 1:G:599:ASN:HA   | 1:G:649:VAL:HB   | 1.05                     | 1.03              |
| 4:W:290:ARG:CZ   | 4:Y:202:THR:CG2  | 2.36                     | 1.03              |
| 4:X:290:ARG:CZ   | 4:Z:202:THR:CG2  | 2.36                     | 1.03              |
| 1:G:639:GLY:HA3  | 4:6:344:SER:C    | 1.78                     | 1.03              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:F:49:ILE:CA    | 3:F:52:ASN:HD22  | 1.70                     | 1.03              |
| 3:L:49:ILE:CA    | 3:L:52:ASN:HD22  | 1.71                     | 1.03              |
| 1:A:642:LYS:HG3  | 4:4:23:GLY:H     | 0.87                     | 1.03              |
| 1:A:795:ARG:HD2  | 3:C:35:ARG:HH12  | 0.88                     | 1.03              |
| 1:A:836:PHE:CE2  | 2:B:160:GLY:CA   | 2.40                     | 1.03              |
| 2:H:149:ASP:OD2  | 2:H:150:TYR:N    | 1.91                     | 1.03              |
| 4:3:3:ASP:HA     | 4:3:6:THR:HB     | 1.36                     | 1.03              |
| 1:D:553:MLY:CB   | 4:7:46:GLY:CA    | 2.32                     | 1.03              |
| 1:A:639:GLY:HA3  | 4:4:344:SER:C    | 1.78                     | 1.03              |
| 2:B:140:PHE:O    | 2:B:141:PRO:O    | 1.75                     | 1.03              |
| 3:I:49:ILE:CA    | 3:I:52:ASN:HD22  | 1.70                     | 1.03              |
| 1:J:202:SER:CA   | 1:J:207:LYS:CE   | 2.36                     | 1.03              |
| 1:J:553:MLY:HB3  | 4:V:46:GLY:CA    | 1.51                     | 1.03              |
| 1:A:638:GLY:HA2  | 4:4:341:ILE:O    | 1.56                     | 1.03              |
| 1:J:795:ARG:HE   | 3:L:118:MET:HE1  | 1.16                     | 1.03              |
| 4:4:290:ARG:CZ   | 4:6:202:THR:CG2  | 2.36                     | 1.03              |
| 1:G:557:GLU:N    | 4:8:48:GLY:CA    | 2.12                     | 1.03              |
| 1:G:93:MET:HE3   | 1:G:763:THR:HB   | 1.03                     | 1.03              |
| 1:J:93:MET:HG3   | 1:J:764:MLY:NZ   | 1.72                     | 1.03              |
| 4:7:290:ARG:CZ   | 4:V:202:THR:CG2  | 2.36                     | 1.03              |
| 4:V:3:ASP:HA     | 4:V:6:THR:HB     | 1.36                     | 1.03              |
| 4:X:3:ASP:HA     | 4:X:6:THR:HB     | 1.36                     | 1.03              |
| 4:0:3:ASP:HA     | 4:0:6:THR:HB     | 1.36                     | 1.02              |
| 1:G:529:PRO:C    | 4:6:354:GLN:HB3  | 1.79                     | 1.02              |
| 1:J:541:MET:HB3  | 4:7:143:TYR:OH   | 1.59                     | 1.02              |
| 1:A:202:SER:CA   | 1:A:207:LYS:CE   | 2.36                     | 1.02              |
| 1:A:501:GLU:O    | 1:A:762:HIS:CD2  | 2.12                     | 1.02              |
| 1:A:646:PHE:HE2  | 1:A:652:LEU:HD21 | 1.24                     | 1.02              |
| 1:A:502:GLU:O    | 1:A:761:GLY:HA2  | 1.58                     | 1.02              |
| 1:A:813:ILE:HG23 | 2:B:127:ARG:HD2  | 1.05                     | 1.02              |
| 1:A:834:LEU:HD11 | 2:B:54:MET:HB3   | 1.32                     | 1.02              |
| 2:E:144:VAL:HG13 | 2:E:153:ILE:HD11 | 1.21                     | 1.02              |
| 1:G:817:GLN:CB   | 2:H:127:ARG:HD2  | 1.89                     | 1.02              |
| 1:G:836:PHE:CE2  | 2:H:160:GLY:N    | 2.26                     | 1.02              |
| 1:A:541:MET:HB3  | 4:4:143:TYR:OH   | 1.60                     | 1.02              |
| 1:A:641:LYS:HE3  | 4:4:348:SER:O    | 1.56                     | 1.02              |
| 1:G:642:LYS:HG3  | 4:6:23:GLY:H     | 0.85                     | 1.02              |
| 4:8:3:ASP:HA     | 4:8:6:THR:HB     | 1.36                     | 1.02              |
| 1:A:641:LYS:HG3  | 1:A:647:GLN:HG3  | 1.21                     | 1.02              |
| 2:H:140:PHE:O    | 2:H:141:PRO:O    | 1.75                     | 1.02              |
| 1:G:638:GLY:HA2  | 4:6:341:ILE:O    | 1.58                     | 1.02              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:530:MET:CA   | 4:6:354:GLN:HG3  | 1.88                     | 1.02              |
| 4:6:3:ASP:HA     | 4:6:6:THR:HB     | 1.36                     | 1.02              |
| 4:5:290:ARG:CZ   | 4:7:202:THR:CG2  | 2.36                     | 1.02              |
| 1:D:642:LYS:HG3  | 4:5:23:GLY:H     | 0.86                     | 1.02              |
| 2:E:150:TYR:O    | 2:E:151:LYS:CB   | 2.06                     | 1.02              |
| 4:3:290:ARG:CZ   | 4:5:202:THR:CG2  | 2.36                     | 1.02              |
| 1:J:639:GLY:HA3  | 4:7:344:SER:C    | 1.78                     | 1.02              |
| 2:B:149:ASP:OD2  | 2:B:150:TYR:N    | 1.91                     | 1.02              |
| 1:D:817:GLN:NE2  | 2:E:127:ARG:HG2  | 1.74                     | 1.02              |
| 2:K:144:VAL:HG13 | 2:K:153:ILE:HD11 | 1.21                     | 1.02              |
| 2:K:144:VAL:HG11 | 2:K:153:ILE:HG12 | 1.37                     | 1.02              |
| 1:J:800:ARG:HB2  | 3:L:149:VAL:HG21 | 1.36                     | 1.02              |
| 1:J:553:MLY:CB   | 4:V:46:GLY:CA    | 2.33                     | 1.02              |
| 1:A:800:ARG:CG   | 3:C:149:VAL:HG22 | 1.88                     | 1.02              |
| 1:D:639:GLY:HA3  | 4:5:344:SER:C    | 1.78                     | 1.02              |
| 1:J:599:ASN:CA   | 1:J:649:VAL:HB   | 1.89                     | 1.02              |
| 3:L:24:LYS:CG    | 3:L:63:ILE:O     | 2.08                     | 1.02              |
| 4:1:290:ARG:CZ   | 4:3:202:THR:CG2  | 2.36                     | 1.02              |
| 4:7:3:ASP:HA     | 4:7:6:THR:HB     | 1.36                     | 1.02              |
| 1:D:839:MLY:HH13 | 2:E:159:HIS:CG   | 1.94                     | 1.02              |
| 3:F:24:LYS:HG2   | 3:F:63:ILE:O     | 1.59                     | 1.02              |
| 4:6:287:ILE:HB   | 4:8:204:ALA:H    | 1.25                     | 1.02              |
| 1:A:800:ARG:HB3  | 3:C:149:VAL:HG21 | 1.05                     | 1.02              |
| 1:D:800:ARG:HD2  | 3:F:149:VAL:C    | 1.79                     | 1.02              |
| 4:Z:3:ASP:HA     | 4:Z:6:THR:HB     | 1.36                     | 1.02              |
| 1:D:507:GLY:HA3  | 1:D:762:HIS:CG   | 1.95                     | 1.02              |
| 1:G:736:GLN:HA   | 1:G:743:ALA:HB3  | 1.35                     | 1.02              |
| 1:A:642:LYS:HD3  | 4:4:340:TRP:CH2  | 1.95                     | 1.02              |
| 1:A:642:LYS:HD3  | 4:4:340:TRP:CZ3  | 1.95                     | 1.02              |
| 2:B:121:LEU:HG   | 2:B:128:PHE:CA   | 1.59                     | 1.02              |
| 1:J:754:ASP:HB2  | 1:J:776:GLU:HB3  | 1.38                     | 1.02              |
| 4:1:290:ARG:NH2  | 4:3:202:THR:CG2  | 2.23                     | 1.01              |
| 1:D:557:GLU:N    | 4:7:48:GLY:CA    | 2.12                     | 1.01              |
| 4:8:290:ARG:NH2  | 4:W:202:THR:CG2  | 2.23                     | 1.01              |
| 4:W:290:ARG:NH2  | 4:Y:202:THR:CG2  | 2.23                     | 1.01              |
| 4:3:290:ARG:NH2  | 4:5:202:THR:CG2  | 2.23                     | 1.01              |
| 3:C:24:LYS:HG2   | 3:C:63:ILE:O     | 1.59                     | 1.01              |
| 1:D:814:PHE:CE1  | 2:E:127:ARG:NH2  | 2.26                     | 1.01              |
| 1:G:576:GLU:HG2  | 1:G:577:ALA:H    | 0.85                     | 1.01              |
| 3:I:24:LYS:CG    | 3:I:63:ILE:O     | 2.08                     | 1.01              |
| 1:J:98:HIS:HB3   | 1:J:100:PRO:HD2  | 1.42                     | 1.01              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:1:287:ILE:HB   | 4:3:204:ALA:H    | 1.25                     | 1.01              |
| 4:2:287:ILE:HB   | 4:4:204:ALA:H    | 1.25                     | 1.01              |
| 1:D:599:ASN:CA   | 1:D:649:VAL:HB   | 1.89                     | 1.01              |
| 1:G:751:GLY:HA2  | 3:I:114:LEU:HD13 | 1.40                     | 1.01              |
| 3:I:49:ILE:HA    | 3:I:52:ASN:HD22  | 1.22                     | 1.01              |
| 1:J:757:GLN:NE2  | 1:J:776:GLU:HG2  | 1.75                     | 1.01              |
| 4:6:290:ARG:NH2  | 4:8:202:THR:CG2  | 2.23                     | 1.01              |
| 1:D:830:PRO:CD   | 2:E:67:MET:CE    | 2.37                     | 1.01              |
| 2:H:144:VAL:HG13 | 2:H:153:ILE:HD11 | 1.21                     | 1.01              |
| 4:5:290:ARG:NH2  | 4:7:202:THR:CG2  | 2.23                     | 1.01              |
| 2:B:144:VAL:HG11 | 2:B:153:ILE:HG12 | 1.38                     | 1.01              |
| 1:A:822:SER:CB   | 2:B:88:LEU:HD23  | 1.91                     | 1.01              |
| 2:E:149:ASP:OD2  | 2:E:150:TYR:N    | 1.91                     | 1.01              |
| 1:J:635:GLY:HA3  | 4:7:341:ILE:HD13 | 1.36                     | 1.01              |
| 4:W:287:ILE:HB   | 4:Y:204:ALA:H    | 1.26                     | 1.01              |
| 1:A:639:GLY:N    | 4:4:345:ILE:N    | 1.94                     | 1.01              |
| 1:A:599:ASN:CA   | 1:A:649:VAL:HB   | 1.89                     | 1.01              |
| 2:E:144:VAL:HG11 | 2:E:153:ILE:HG12 | 1.38                     | 1.01              |
| 1:G:797:PHE:CG   | 3:I:149:VAL:HG11 | 1.95                     | 1.01              |
| 1:J:599:ASN:HA   | 1:J:649:VAL:HB   | 1.05                     | 1.01              |
| 2:B:150:TYR:O    | 2:B:151:LYS:CB   | 2.07                     | 1.01              |
| 1:G:202:SER:CA   | 1:G:207:LYS:CE   | 2.36                     | 1.01              |
| 1:D:541:MET:HB3  | 4:5:143:TYR:OH   | 1.60                     | 1.01              |
| 1:D:553:MLY:HG2  | 4:7:44:MET:O     | 1.59                     | 1.01              |
| 1:G:641:LYS:HE3  | 1:G:647:GLN:HB2  | 1.42                     | 1.01              |
| 2:H:144:VAL:HG11 | 2:H:153:ILE:HG12 | 1.38                     | 1.01              |
| 4:4:290:ARG:NH2  | 4:6:202:THR:CG2  | 2.23                     | 1.01              |
| 1:D:635:GLY:HA3  | 4:5:341:ILE:HD13 | 1.37                     | 1.01              |
| 4:7:290:ARG:NH2  | 4:V:202:THR:CG2  | 2.23                     | 1.01              |
| 1:A:793:ARG:HE   | 3:C:147:MET:HG2  | 1.24                     | 1.01              |
| 3:C:48:LYS:O     | 3:C:52:ASN:ND2   | 1.94                     | 1.01              |
| 1:G:84:MLY:HH12  | 1:G:715:VAL:CG1  | 1.83                     | 1.01              |
| 1:J:641:LYS:HE3  | 1:J:647:GLN:HB2  | 1.43                     | 1.01              |
| 2:K:121:LEU:CB   | 2:K:128:PHE:HB3  | 1.69                     | 1.01              |
| 3:L:48:LYS:O     | 3:L:52:ASN:ND2   | 1.94                     | 1.01              |
| 1:G:553:MLY:HG2  | 4:8:44:MET:O     | 1.60                     | 1.01              |
| 1:D:788:THR:HG23 | 3:F:42:THR:HG21  | 1.42                     | 1.01              |
| 2:E:163:ALA:O    | 2:K:22:THR:N     | 1.94                     | 1.01              |
| 3:I:48:LYS:O     | 3:I:52:ASN:ND2   | 1.94                     | 1.01              |
| 1:J:642:LYS:HG3  | 4:7:23:GLY:H     | 0.86                     | 1.01              |
| 4:5:3:ASP:HA     | 4:5:6:THR:HB     | 1.36                     | 1.00              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:D:553:MLY:HB3 | 4:7:46:GLY:CA    | 1.51                     | 1.00              |
| 1:A:502:GLU:CA  | 1:A:761:GLY:HA3  | 1.91                     | 1.00              |
| 1:D:206:LYS:HD2 | 1:D:217:THR:HG23 | 1.41                     | 1.00              |
| 3:I:24:LYS:HG2  | 3:I:63:ILE:O     | 1.59                     | 1.00              |
| 1:J:707:CYS:SG  | 1:J:714:ARG:NH1  | 2.31                     | 1.00              |
| 1:J:642:LYS:HD3 | 4:7:340:TRP:CH2  | 1.96                     | 1.00              |
| 1:G:646:PHE:HE2 | 1:G:652:LEU:HD21 | 1.24                     | 1.00              |
| 1:G:599:ASN:CA  | 1:G:649:VAL:HB   | 1.89                     | 1.00              |
| 1:J:646:PHE:HE2 | 1:J:652:LEU:HD21 | 1.24                     | 1.00              |
| 1:J:84:MLY:HH12 | 1:J:715:VAL:HG13 | 1.03                     | 1.00              |
| 1:J:553:MLY:HG2 | 4:V:44:MET:O     | 1.59                     | 1.00              |
| 1:J:557:GLU:N   | 4:V:48:GLY:CA    | 2.12                     | 1.00              |
| 1:A:534:SER:O   | 4:4:351:THR:HA   | 1.60                     | 1.00              |
| 1:A:149:GLN:HG2 | 1:A:719:ASP:OD1  | 1.57                     | 1.00              |
| 1:A:800:ARG:HD2 | 3:C:149:VAL:C    | 1.81                     | 1.00              |
| 1:D:599:ASN:HA  | 1:D:649:VAL:HB   | 1.05                     | 1.00              |
| 1:D:769:ALA:HA  | 1:D:771:LEU:HA   | 1.42                     | 1.00              |
| 3:L:24:LYS:HG2  | 3:L:63:ILE:O     | 1.59                     | 1.00              |
| 1:A:530:MET:HE2 | 4:4:354:GLN:CG   | 1.91                     | 1.00              |
| 4:5:287:ILE:HB  | 4:7:204:ALA:H    | 1.25                     | 1.00              |
| 1:G:642:LYS:HD3 | 4:6:340:TRP:CH2  | 1.96                     | 1.00              |
| 1:A:206:LYS:HD2 | 1:A:217:THR:HG23 | 1.41                     | 1.00              |
| 1:A:501:GLU:O   | 1:A:762:HIS:CE1  | 2.14                     | 1.00              |
| 1:D:800:ARG:HB3 | 3:F:149:VAL:HG22 | 1.38                     | 1.00              |
| 1:G:93:MET:HE1  | 1:G:763:THR:CG2  | 1.86                     | 1.00              |
| 1:G:800:ARG:HD2 | 3:I:149:VAL:CG2  | 1.90                     | 1.00              |
| 1:J:800:ARG:CG  | 3:L:149:VAL:CG2  | 2.38                     | 1.00              |
| 4:X:287:ILE:HB  | 4:Z:204:ALA:H    | 1.25                     | 1.00              |
| 1:J:529:PRO:C   | 4:7:354:GLN:HB3  | 1.77                     | 1.00              |
| 1:D:174:SER:HB3 | 1:D:667:THR:HG21 | 1.44                     | 1.00              |
| 3:F:49:ILE:HA   | 3:F:52:ASN:HD22  | 1.22                     | 1.00              |
| 3:F:24:LYS:CG   | 3:F:63:ILE:O     | 2.08                     | 1.00              |
| 1:J:90:ASP:CB   | 1:J:764:MLY:HH21 | 1.89                     | 1.00              |
| 4:2:290:ARG:NH2 | 4:4:202:THR:CG2  | 2.23                     | 1.00              |
| 1:J:534:SER:C   | 4:7:351:THR:HA   | 1.81                     | 1.00              |
| 1:A:576:GLU:HG2 | 1:A:577:ALA:H    | 0.85                     | 1.00              |
| 1:A:641:LYS:HE3 | 1:A:647:GLN:CB   | 1.91                     | 1.00              |
| 1:D:809:ARG:NH1 | 2:E:124:GLY:CA   | 2.23                     | 1.00              |
| 1:G:215:GLN:CA  | 1:G:340:ILE:HG23 | 1.92                     | 1.00              |
| 1:G:534:SER:C   | 4:6:351:THR:HA   | 1.82                     | 1.00              |
| 1:G:534:SER:O   | 4:6:351:THR:HA   | 1.60                     | 1.00              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:0:286:ASP:OD1  | 4:2:203:THR:HG22 | 1.62                     | 1.00              |
| 1:J:642:LYS:HD3  | 4:7:340:TRP:CZ3  | 1.96                     | 1.00              |
| 1:A:736:GLN:N    | 1:A:743:ALA:CB   | 2.05                     | 1.00              |
| 3:C:24:LYS:CG    | 3:C:63:ILE:O     | 2.08                     | 1.00              |
| 1:D:642:LYS:HD3  | 4:5:340:TRP:CZ3  | 1.95                     | 1.00              |
| 1:G:576:GLU:CG   | 1:G:577:ALA:H    | 1.75                     | 1.00              |
| 1:G:641:LYS:HE3  | 1:G:647:GLN:CB   | 1.91                     | 1.00              |
| 1:G:642:LYS:HD3  | 4:6:340:TRP:CZ3  | 1.96                     | 1.00              |
| 2:H:150:TYR:O    | 2:H:151:LYS:CB   | 2.06                     | 1.00              |
| 1:J:174:SER:HB3  | 1:J:667:THR:HG21 | 1.44                     | 1.00              |
| 1:A:641:LYS:HE3  | 1:A:647:GLN:HB2  | 1.42                     | 1.00              |
| 1:D:218:LEU:CA   | 1:D:221:GLN:HG3  | 1.91                     | 1.00              |
| 1:D:534:SER:O    | 4:5:351:THR:HA   | 1.60                     | 1.00              |
| 1:D:641:LYS:HE3  | 1:D:647:GLN:HB2  | 1.42                     | 1.00              |
| 1:D:809:ARG:HH12 | 2:E:124:GLY:HA2  | 1.27                     | 1.00              |
| 1:G:541:MET:HB3  | 4:6:143:TYR:OH   | 1.59                     | 1.00              |
| 1:J:757:GLN:OE1  | 1:J:772:LEU:C    | 2.00                     | 1.00              |
| 1:J:93:MET:HG2   | 1:J:764:MLY:CD   | 1.78                     | 1.00              |
| 1:A:56:GLU:HB2   | 1:A:59:MLY:HB3   | 1.40                     | 1.00              |
| 1:D:642:LYS:HD3  | 4:5:340:TRP:CH2  | 1.95                     | 1.00              |
| 1:D:831:TRP:HD1  | 2:E:67:MET:SD    | 1.81                     | 1.00              |
| 1:G:206:LYS:HD2  | 1:G:217:THR:HG23 | 1.41                     | 1.00              |
| 4:6:286:ASP:OD1  | 4:8:203:THR:HG22 | 1.62                     | 1.00              |
| 1:A:576:GLU:CG   | 1:A:577:ALA:H    | 1.75                     | 1.00              |
| 1:G:98:HIS:HB3   | 1:G:100:PRO:HD2  | 1.42                     | 1.00              |
| 4:7:286:ASP:OD1  | 4:V:203:THR:HG22 | 1.62                     | 1.00              |
| 4:V:290:ARG:NH2  | 4:X:202:THR:CG2  | 2.24                     | 1.00              |
| 4:W:286:ASP:OD1  | 4:Y:203:THR:HG22 | 1.62                     | 1.00              |
| 1:D:98:HIS:HB3   | 1:D:100:PRO:HD2  | 1.42                     | 0.99              |
| 4:0:290:ARG:NH2  | 4:2:202:THR:CG2  | 2.23                     | 0.99              |
| 1:A:576:GLU:HG2  | 1:A:577:ALA:N    | 1.66                     | 0.99              |
| 1:A:795:ARG:HD3  | 3:C:35:ARG:HH22  | 1.25                     | 0.99              |
| 1:J:206:LYS:HD2  | 1:J:217:THR:HG23 | 1.41                     | 0.99              |
| 2:K:141:PRO:HB2  | 2:K:142:PRO:HD2  | 1.44                     | 0.99              |
| 4:V:286:ASP:OD1  | 4:X:203:THR:HG22 | 1.62                     | 0.99              |
| 4:2:322:PRO:HB3  | 4:4:244:ASP:OD2  | 1.62                     | 0.99              |
| 1:A:612:GLN:HE22 | 1:A:627:GLY:CA   | 1.75                     | 0.99              |
| 1:A:501:GLU:CG   | 1:A:762:HIS:HD1  | 1.74                     | 0.99              |
| 2:B:139:ALA:O    | 2:B:141:PRO:HD3  | 1.62                     | 0.99              |
| 1:D:56:GLU:HB2   | 1:D:59:MLY:HB3   | 1.40                     | 0.99              |
| 1:D:800:ARG:CB   | 3:F:149:VAL:CG2  | 2.37                     | 0.99              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:F:48:LYS:O     | 3:F:52:ASN:ND2   | 1.94                     | 0.99              |
| 1:J:218:LEU:CA   | 1:J:221:GLN:HG3  | 1.91                     | 0.99              |
| 4:V:287:ILE:HB   | 4:X:204:ALA:H    | 1.25                     | 0.99              |
| 4:X:290:ARG:NH2  | 4:Z:202:THR:CG2  | 2.23                     | 0.99              |
| 4:4:286:ASP:OD1  | 4:6:203:THR:HG22 | 1.62                     | 0.99              |
| 4:4:322:PRO:HB3  | 4:6:244:ASP:OD2  | 1.62                     | 0.99              |
| 1:A:797:PHE:HD1  | 3:C:149:VAL:HG12 | 1.27                     | 0.99              |
| 1:A:534:SER:C    | 4:4:351:THR:HA   | 1.81                     | 0.99              |
| 1:D:639:GLY:CA   | 4:5:345:ILE:CA   | 2.41                     | 0.99              |
| 1:A:502:GLU:CG   | 1:A:761:GLY:HA3  | 1.92                     | 0.99              |
| 1:D:534:SER:C    | 4:5:351:THR:HA   | 1.81                     | 0.99              |
| 2:E:139:ALA:O    | 2:E:141:PRO:HD3  | 1.62                     | 0.99              |
| 1:D:792:ALA:HB1  | 3:F:40:ASN:CB    | 1.92                     | 0.99              |
| 1:G:649:VAL:CG1  | 1:G:649:VAL:HG22 | 1.92                     | 0.99              |
| 2:H:121:LEU:HG   | 2:H:128:PHE:CA   | 1.59                     | 0.99              |
| 1:J:641:LYS:HE3  | 1:J:647:GLN:CB   | 1.91                     | 0.99              |
| 2:K:149:ASP:OD2  | 2:K:150:TYR:O    | 1.80                     | 0.99              |
| 4:1:286:ASP:OD1  | 4:3:203:THR:HG22 | 1.62                     | 0.99              |
| 4:6:322:PRO:HB3  | 4:8:244:ASP:OD2  | 1.62                     | 0.99              |
| 1:A:553:MLY:HG2  | 4:6:44:MET:O     | 1.59                     | 0.99              |
| 1:A:834:LEU:HD11 | 2:B:54:MET:HG3   | 1.35                     | 0.99              |
| 1:D:612:GLN:HE22 | 1:D:627:GLY:CA   | 1.75                     | 0.99              |
| 4:5:286:ASP:OD1  | 4:7:203:THR:HG22 | 1.62                     | 0.99              |
| 4:8:287:ILE:HB   | 4:W:204:ALA:H    | 1.25                     | 0.99              |
| 1:D:834:LEU:HD11 | 2:E:54:MET:CB    | 1.92                     | 0.99              |
| 1:J:639:GLY:CA   | 4:7:345:ILE:CA   | 2.40                     | 0.99              |
| 1:A:836:PHE:HB3  | 2:B:161:GLU:CD   | 1.83                     | 0.99              |
| 1:D:529:PRO:C    | 4:5:354:GLN:HB3  | 1.78                     | 0.99              |
| 2:E:149:ASP:OD2  | 2:E:150:TYR:O    | 1.80                     | 0.99              |
| 1:G:218:LEU:CA   | 1:G:221:GLN:HG3  | 1.91                     | 0.99              |
| 1:J:215:GLN:CA   | 1:J:340:ILE:HG23 | 1.91                     | 0.99              |
| 1:J:798:LEU:CD2  | 3:L:126:LEU:CD1  | 2.36                     | 0.99              |
| 4:0:322:PRO:HB3  | 4:2:244:ASP:OD2  | 1.62                     | 0.99              |
| 1:D:639:GLY:N    | 4:5:345:ILE:N    | 1.94                     | 0.99              |
| 1:J:534:SER:O    | 4:7:351:THR:HG23 | 1.13                     | 0.99              |
| 1:A:98:HIS:HB3   | 1:A:100:PRO:HD2  | 1.42                     | 0.99              |
| 1:A:218:LEU:CA   | 1:A:221:GLN:HG3  | 1.91                     | 0.99              |
| 1:A:215:GLN:CA   | 1:A:340:ILE:HG23 | 1.92                     | 0.99              |
| 1:A:797:PHE:CE2  | 3:C:126:LEU:CD2  | 2.45                     | 0.99              |
| 1:D:576:GLU:HG2  | 1:D:577:ALA:H    | 0.85                     | 0.99              |
| 4:X:286:ASP:OD1  | 4:Z:203:THR:HG22 | 1.62                     | 0.99              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:149:ASP:OD2  | 2:B:150:TYR:O    | 1.80                     | 0.99              |
| 1:A:797:PHE:HE2  | 3:C:126:LEU:HD23 | 1.26                     | 0.99              |
| 1:D:641:LYS:CG   | 4:5:348:SER:HB2  | 1.87                     | 0.99              |
| 1:G:530:MET:CE   | 4:6:354:GLN:CG   | 2.39                     | 0.99              |
| 4:3:287:ILE:HB   | 4:5:204:ALA:H    | 1.26                     | 0.98              |
| 4:8:322:PRO:HB3  | 4:W:244:ASP:OD2  | 1.62                     | 0.98              |
| 1:D:768:MLY:C    | 1:D:771:LEU:HD12 | 1.61                     | 0.98              |
| 1:G:831:TRP:CZ2  | 2:H:67:MET:SD    | 2.56                     | 0.98              |
| 2:K:121:LEU:HG   | 2:K:128:PHE:CA   | 1.60                     | 0.98              |
| 4:1:322:PRO:HB3  | 4:3:244:ASP:OD2  | 1.62                     | 0.98              |
| 1:A:639:GLY:CA   | 4:4:345:ILE:CA   | 2.41                     | 0.98              |
| 1:D:649:VAL:CG1  | 1:D:649:VAL:HG22 | 1.92                     | 0.98              |
| 2:E:112:ILE:O    | 2:E:147:ASN:C    | 2.01                     | 0.98              |
| 1:G:798:LEU:HD23 | 3:I:122:GLU:HB3  | 1.45                     | 0.98              |
| 1:J:649:VAL:HG22 | 1:J:649:VAL:CG1  | 1.92                     | 0.98              |
| 1:J:508:ILE:CD1  | 1:J:759:ALA:CB   | 2.31                     | 0.98              |
| 1:J:831:TRP:CZ2  | 2:K:47:LEU:CD2   | 2.47                     | 0.98              |
| 4:W:322:PRO:HB3  | 4:Y:244:ASP:OD2  | 1.62                     | 0.98              |
| 1:G:639:GLY:CA   | 4:6:345:ILE:CA   | 2.40                     | 0.98              |
| 1:A:649:VAL:CG1  | 1:A:649:VAL:HG22 | 1.92                     | 0.98              |
| 1:A:819:ASN:H    | 2:B:90:GLY:HA3   | 1.28                     | 0.98              |
| 2:B:141:PRO:HB2  | 2:B:142:PRO:HD2  | 1.44                     | 0.98              |
| 1:G:788:THR:O    | 3:I:42:THR:HG22  | 1.62                     | 0.98              |
| 1:J:757:GLN:CD   | 1:J:776:GLU:CG   | 2.32                     | 0.98              |
| 4:2:286:ASP:OD1  | 4:4:203:THR:HG22 | 1.62                     | 0.98              |
| 1:A:530:MET:CE   | 4:4:354:GLN:CG   | 2.41                     | 0.98              |
| 2:B:112:ILE:O    | 2:B:147:ASN:C    | 2.01                     | 0.98              |
| 1:D:215:GLN:CA   | 1:D:340:ILE:HG23 | 1.92                     | 0.98              |
| 1:G:641:LYS:HE3  | 4:6:348:SER:O    | 1.56                     | 0.98              |
| 2:K:150:TYR:O    | 2:K:151:LYS:CB   | 2.06                     | 0.98              |
| 1:A:836:PHE:HB3  | 2:B:161:GLU:OE1  | 1.60                     | 0.98              |
| 3:C:52:ASN:HB2   | 3:C:53:PRO:HD3   | 1.45                     | 0.98              |
| 1:D:530:MET:CE   | 4:5:354:GLN:CG   | 2.40                     | 0.98              |
| 1:D:641:LYS:HE3  | 1:D:647:GLN:CB   | 1.91                     | 0.98              |
| 1:G:612:GLN:HE22 | 1:G:627:GLY:CA   | 1.75                     | 0.98              |
| 2:H:112:ILE:O    | 2:H:147:ASN:C    | 2.01                     | 0.98              |
| 1:J:641:LYS:HG3  | 1:J:647:GLN:NE2  | 1.59                     | 0.98              |
| 1:J:800:ARG:NH1  | 3:L:149:VAL:CG1  | 2.17                     | 0.98              |
| 1:A:206:LYS:CD   | 1:A:217:THR:CG2  | 2.16                     | 0.98              |
| 2:E:121:LEU:HG   | 2:E:128:PHE:CA   | 1.59                     | 0.98              |
| 1:G:817:GLN:HG2  | 2:H:127:ARG:HB2  | 1.40                     | 0.98              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:121:LEU:C    | 2:H:128:PHE:HB3  | 1.71                     | 0.98              |
| 2:K:112:ILE:O    | 2:K:147:ASN:C    | 2.02                     | 0.98              |
| 1:A:641:LYS:CG   | 4:4:348:SER:HB2  | 1.87                     | 0.98              |
| 1:A:505:MLY:HB2  | 1:A:762:HIS:N    | 1.76                     | 0.98              |
| 2:B:117:LEU:CB   | 2:B:147:ASN:CG   | 2.32                     | 0.98              |
| 1:D:576:GLU:CG   | 1:D:577:ALA:H    | 1.75                     | 0.98              |
| 1:D:642:LYS:HD2  | 4:5:24:ASP:O     | 1.64                     | 0.98              |
| 1:D:646:PHE:HE2  | 1:D:652:LEU:HD21 | 1.24                     | 0.98              |
| 2:E:130:PRO:O    | 2:E:133:ILE:N    | 1.96                     | 0.98              |
| 1:G:576:GLU:HG2  | 1:G:577:ALA:N    | 1.66                     | 0.98              |
| 1:J:534:SER:O    | 4:7:351:THR:HA   | 1.60                     | 0.98              |
| 4:4:287:ILE:HB   | 4:6:204:ALA:H    | 1.25                     | 0.98              |
| 3:C:49:ILE:HA    | 3:C:52:ASN:HD22  | 1.22                     | 0.98              |
| 2:E:117:LEU:CB   | 2:E:147:ASN:CG   | 2.32                     | 0.98              |
| 2:E:150:TYR:C    | 2:E:151:LYS:HG3  | 1.83                     | 0.98              |
| 2:E:141:PRO:HB2  | 2:E:142:PRO:HD2  | 1.44                     | 0.98              |
| 2:H:141:PRO:HB2  | 2:H:142:PRO:HD2  | 1.44                     | 0.98              |
| 1:J:612:GLN:HE22 | 1:J:627:GLY:CA   | 1.76                     | 0.98              |
| 3:L:52:ASN:HB2   | 3:L:53:PRO:HD3   | 1.46                     | 0.98              |
| 4:3:322:PRO:HB3  | 4:5:244:ASP:OD2  | 1.62                     | 0.97              |
| 1:A:831:TRP:HH2  | 2:B:50:THR:HB    | 1.25                     | 0.97              |
| 2:K:139:ALA:O    | 2:K:141:PRO:HD3  | 1.62                     | 0.97              |
| 3:L:49:ILE:HA    | 3:L:52:ASN:HD22  | 1.23                     | 0.97              |
| 2:B:130:PRO:O    | 2:B:133:ILE:N    | 1.96                     | 0.97              |
| 1:D:218:LEU:CA   | 1:D:221:GLN:CG   | 2.42                     | 0.97              |
| 1:D:795:ARG:HB3  | 3:F:35:ARG:NE    | 1.35                     | 0.97              |
| 2:H:149:ASP:OD2  | 2:H:150:TYR:O    | 1.80                     | 0.97              |
| 1:J:576:GLU:HG2  | 1:J:577:ALA:H    | 0.85                     | 0.97              |
| 4:3:286:ASP:OD1  | 4:5:203:THR:HG22 | 1.62                     | 0.97              |
| 1:A:174:SER:HB3  | 1:A:667:THR:HG21 | 1.44                     | 0.97              |
| 2:B:150:TYR:C    | 2:B:151:LYS:HG3  | 1.83                     | 0.97              |
| 3:F:46:ILE:O     | 3:F:50:LEU:HG    | 1.65                     | 0.97              |
| 2:H:117:LEU:CB   | 2:H:147:ASN:CG   | 2.32                     | 0.97              |
| 4:X:322:PRO:HB3  | 4:Z:244:ASP:OD2  | 1.62                     | 0.97              |
| 1:A:795:ARG:CD   | 3:C:35:ARG:HH12  | 1.77                     | 0.97              |
| 4:8:286:ASP:OD1  | 4:W:203:THR:HG22 | 1.62                     | 0.97              |
| 1:J:642:LYS:HG2  | 4:7:21:PHE:O     | 1.65                     | 0.97              |
| 1:A:218:LEU:CA   | 1:A:221:GLN:CG   | 2.42                     | 0.97              |
| 1:A:215:GLN:H    | 1:A:340:ILE:CG1  | 1.73                     | 0.97              |
| 1:A:542:PHE:CG   | 4:4:143:TYR:CE1  | 2.52                     | 0.97              |
| 1:A:642:LYS:HG2  | 4:4:21:PHE:O     | 1.65                     | 0.97              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:139:ALA:O    | 2:H:141:PRO:HD3  | 1.62                     | 0.97              |
| 1:G:829:TRP:CZ3  | 2:H:87:LYS:NZ    | 2.30                     | 0.97              |
| 2:K:130:PRO:O    | 2:K:133:ILE:N    | 1.96                     | 0.97              |
| 4:7:287:ILE:HB   | 4:V:204:ALA:H    | 1.25                     | 0.97              |
| 4:0:287:ILE:HB   | 4:2:204:ALA:H    | 1.25                     | 0.97              |
| 1:A:502:GLU:C    | 1:A:761:GLY:HA3  | 1.84                     | 0.97              |
| 2:H:121:LEU:HG   | 2:H:128:PHE:HA   | 1.46                     | 0.97              |
| 2:K:117:LEU:CB   | 2:K:147:ASN:CG   | 2.32                     | 0.97              |
| 1:G:174:SER:HB3  | 1:G:667:THR:HG21 | 1.44                     | 0.97              |
| 1:G:784:ALA:O    | 1:G:788:THR:N    | 1.96                     | 0.97              |
| 1:J:639:GLY:N    | 4:7:345:ILE:N    | 1.94                     | 0.97              |
| 1:J:754:ASP:OD2  | 1:J:776:GLU:C    | 2.03                     | 0.97              |
| 2:K:150:TYR:C    | 2:K:151:LYS:HG3  | 1.83                     | 0.97              |
| 2:E:121:LEU:HG   | 2:E:128:PHE:HA   | 1.46                     | 0.97              |
| 1:G:736:GLN:CA   | 1:G:743:ALA:HB2  | 1.95                     | 0.97              |
| 1:J:649:VAL:CG2  | 1:J:649:VAL:CA   | 2.42                     | 0.97              |
| 1:G:642:LYS:HG2  | 4:6:21:PHE:O     | 1.65                     | 0.97              |
| 1:D:724:TYR:HE1  | 1:D:778:MET:HB3  | 1.24                     | 0.97              |
| 1:J:218:LEU:CA   | 1:J:221:GLN:CG   | 2.42                     | 0.97              |
| 1:J:576:GLU:CG   | 1:J:577:ALA:H    | 1.75                     | 0.97              |
| 1:J:797:PHE:CB   | 3:L:149:VAL:HG11 | 1.94                     | 0.97              |
| 1:D:542:PHE:CG   | 4:5:143:TYR:CE1  | 2.52                     | 0.97              |
| 1:G:218:LEU:CA   | 1:G:221:GLN:CG   | 2.42                     | 0.97              |
| 2:H:130:PRO:O    | 2:H:133:ILE:N    | 1.96                     | 0.97              |
| 1:A:502:GLU:O    | 1:A:761:GLY:CA   | 2.13                     | 0.96              |
| 1:A:501:GLU:HG2  | 1:A:762:HIS:HD1  | 0.83                     | 0.96              |
| 1:A:795:ARG:NH2  | 3:C:116:GLU:CD   | 2.18                     | 0.96              |
| 1:D:724:TYR:C    | 1:D:782:MLY:HH21 | 1.85                     | 0.96              |
| 1:G:819:ASN:HA   | 2:H:90:GLY:C     | 1.85                     | 0.96              |
| 3:L:46:ILE:O     | 3:L:50:LEU:HG    | 1.64                     | 0.96              |
| 1:J:642:LYS:HD2  | 4:7:24:ASP:O     | 1.64                     | 0.96              |
| 2:E:150:TYR:O    | 2:E:151:LYS:HG3  | 1.65                     | 0.96              |
| 1:J:768:MLY:HH12 | 1:J:772:LEU:HD23 | 1.44                     | 0.96              |
| 1:A:534:SER:O    | 4:4:351:THR:HG23 | 1.13                     | 0.96              |
| 1:G:637:LYS:NZ   | 4:6:141:SER:O    | 1.99                     | 0.96              |
| 1:D:553:MLY:HB3  | 4:7:46:GLY:HA2   | 1.47                     | 0.96              |
| 1:A:795:ARG:NE   | 3:C:118:MET:HE1  | 1.80                     | 0.96              |
| 1:D:215:GLN:H    | 1:D:340:ILE:CG1  | 1.73                     | 0.96              |
| 4:V:322:PRO:HB3  | 4:X:244:ASP:OD2  | 1.62                     | 0.96              |
| 2:B:144:VAL:HG13 | 2:B:153:ILE:HD11 | 1.22                     | 0.96              |
| 1:D:649:VAL:CG2  | 1:D:649:VAL:CA   | 2.42                     | 0.96              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:736:GLN:CA   | 1:D:743:ALA:HB2  | 1.95                     | 0.96              |
| 2:H:117:LEU:HD13 | 2:H:147:ASN:OD1  | 1.64                     | 0.96              |
| 1:A:642:LYS:HD2  | 4:4:24:ASP:O     | 1.64                     | 0.96              |
| 2:B:150:TYR:O    | 2:B:151:LYS:HG3  | 1.65                     | 0.96              |
| 1:A:538:GLU:N    | 4:4:349:LEU:CD1  | 2.28                     | 0.96              |
| 1:A:649:VAL:CG2  | 1:A:649:VAL:CG1  | 2.43                     | 0.96              |
| 1:G:635:GLY:HA3  | 4:6:334:GLU:HG2  | 1.47                     | 0.96              |
| 1:G:649:VAL:CA   | 1:G:649:VAL:CG2  | 2.42                     | 0.96              |
| 1:J:821:ARG:HH21 | 2:K:127:ARG:HG2  | 1.21                     | 0.96              |
| 1:D:642:LYS:HG2  | 4:5:21:PHE:O     | 1.65                     | 0.96              |
| 4:5:322:PRO:HB3  | 4:7:244:ASP:OD2  | 1.62                     | 0.96              |
| 1:J:543:PRO:CG   | 4:7:143:TYR:O    | 2.14                     | 0.96              |
| 1:A:649:VAL:CA   | 1:A:649:VAL:CG2  | 2.43                     | 0.96              |
| 1:G:642:LYS:HD2  | 4:6:24:ASP:O     | 1.64                     | 0.96              |
| 1:J:793:ARG:HE   | 3:L:147:MET:CA   | 1.77                     | 0.96              |
| 4:W:288:ASP:HA   | 4:Y:204:ALA:HB2  | 1.48                     | 0.96              |
| 4:V:288:ASP:HA   | 4:X:204:ALA:HB2  | 1.48                     | 0.96              |
| 4:6:288:ASP:HA   | 4:8:204:ALA:HB2  | 1.48                     | 0.96              |
| 4:7:288:ASP:HA   | 4:V:204:ALA:HB2  | 1.48                     | 0.96              |
| 1:D:206:LYS:CD   | 1:D:217:THR:CG2  | 2.16                     | 0.96              |
| 4:8:288:ASP:HA   | 4:W:204:ALA:HB2  | 1.48                     | 0.96              |
| 1:G:641:LYS:HG3  | 1:G:647:GLN:NE2  | 1.58                     | 0.96              |
| 1:G:735:GLY:C    | 1:G:743:ALA:CA   | 2.34                     | 0.96              |
| 3:I:46:ILE:O     | 3:I:50:LEU:HG    | 1.64                     | 0.96              |
| 1:J:542:PHE:CG   | 4:7:143:TYR:CE1  | 2.53                     | 0.96              |
| 4:X:288:ASP:HA   | 4:Z:204:ALA:HB2  | 1.48                     | 0.96              |
| 4:4:288:ASP:HA   | 4:6:204:ALA:HB2  | 1.48                     | 0.96              |
| 4:5:288:ASP:HA   | 4:7:204:ALA:HB2  | 1.48                     | 0.96              |
| 2:B:121:LEU:HG   | 2:B:128:PHE:HA   | 1.47                     | 0.96              |
| 1:A:795:ARG:HH22 | 3:C:116:GLU:CD   | 1.69                     | 0.96              |
| 3:C:46:ILE:O     | 3:C:50:LEU:HG    | 1.65                     | 0.96              |
| 2:H:150:TYR:C    | 2:H:151:LYS:HG3  | 1.83                     | 0.96              |
| 2:K:121:LEU:HG   | 2:K:128:PHE:HA   | 1.47                     | 0.96              |
| 4:0:288:ASP:HA   | 4:2:204:ALA:HB2  | 1.48                     | 0.95              |
| 4:2:288:ASP:HA   | 4:4:204:ALA:HB2  | 1.48                     | 0.95              |
| 1:D:538:GLU:N    | 4:5:349:LEU:CD1  | 2.28                     | 0.95              |
| 1:D:735:GLY:C    | 1:D:743:ALA:CA   | 2.34                     | 0.95              |
| 1:D:792:ALA:C    | 3:F:40:ASN:HB3   | 1.85                     | 0.95              |
| 1:G:206:LYS:CD   | 1:G:217:THR:CG2  | 2.16                     | 0.95              |
| 1:D:726:VAL:CG2  | 1:D:782:MLY:HH22 | 1.96                     | 0.95              |
| 1:J:649:VAL:CG2  | 1:J:649:VAL:CG1  | 2.43                     | 0.95              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:736:GLN:CA   | 1:J:743:ALA:HB2  | 1.95                     | 0.95              |
| 1:D:649:VAL:CG1  | 1:D:649:VAL:CG2  | 2.43                     | 0.95              |
| 1:G:538:GLU:HG3  | 4:6:352:PHE:N    | 1.81                     | 0.95              |
| 1:G:754:ASP:CB   | 1:G:776:GLU:OE2  | 2.14                     | 0.95              |
| 1:J:817:GLN:CG   | 2:K:127:ARG:HD2  | 1.95                     | 0.95              |
| 1:A:635:GLY:HA3  | 4:4:334:GLU:HG2  | 1.47                     | 0.95              |
| 4:3:288:ASP:HA   | 4:5:204:ALA:HB2  | 1.48                     | 0.95              |
| 1:A:721:LYS:CA   | 1:A:736:GLN:CD   | 2.34                     | 0.95              |
| 1:A:735:GLY:C    | 1:A:743:ALA:CA   | 2.34                     | 0.95              |
| 1:D:839:MLY:HH11 | 2:E:159:HIS:HD2  | 1.18                     | 0.95              |
| 1:G:530:MET:HA   | 4:6:354:GLN:HG3  | 0.97                     | 0.95              |
| 1:G:649:VAL:CG1  | 1:G:649:VAL:CG2  | 2.44                     | 0.95              |
| 1:G:790:THR:OG1  | 3:I:87:PHE:CD2   | 2.18                     | 0.95              |
| 1:J:84:MLY:HE2   | 1:J:719:ASP:HB3  | 0.99                     | 0.95              |
| 1:J:735:GLY:C    | 1:J:743:ALA:CA   | 2.34                     | 0.95              |
| 4:1:288:ASP:HA   | 4:3:204:ALA:HB2  | 1.48                     | 0.95              |
| 1:G:542:PHE:CG   | 4:6:143:TYR:CE1  | 2.53                     | 0.95              |
| 1:A:505:MLY:HG3  | 1:A:741:LYS:NZ   | 1.81                     | 0.95              |
| 1:A:834:LEU:CD1  | 2:B:54:MET:CB    | 2.45                     | 0.95              |
| 1:D:721:LYS:CA   | 1:D:736:GLN:CD   | 2.34                     | 0.95              |
| 1:J:553:MLY:HB3  | 4:V:46:GLY:HA2   | 1.48                     | 0.95              |
| 1:A:637:LYS:NZ   | 4:4:141:SER:O    | 1.99                     | 0.95              |
| 1:G:538:GLU:N    | 4:6:349:LEU:CD1  | 2.29                     | 0.95              |
| 1:D:641:LYS:HD2  | 1:D:647:GLN:CD   | 1.70                     | 0.95              |
| 2:H:150:TYR:O    | 2:H:151:LYS:HB2  | 1.67                     | 0.95              |
| 4:7:322:PRO:HB3  | 4:V:244:ASP:OD2  | 1.62                     | 0.95              |
| 1:A:541:MET:N    | 4:4:349:LEU:HD21 | 1.80                     | 0.95              |
| 1:D:724:TYR:HA   | 1:D:782:MLY:NZ   | 1.81                     | 0.95              |
| 1:G:546:THR:HG22 | 1:G:548:THR:H    | 1.32                     | 0.95              |
| 2:K:117:LEU:HD13 | 2:K:147:ASN:OD1  | 1.64                     | 0.95              |
| 1:J:538:GLU:N    | 4:7:349:LEU:CD1  | 2.28                     | 0.95              |
| 1:A:502:GLU:CD   | 1:A:764:MLY:N    | 2.20                     | 0.95              |
| 2:B:117:LEU:HD13 | 2:B:147:ASN:OD1  | 1.64                     | 0.95              |
| 1:D:543:PRO:CG   | 4:5:143:TYR:O    | 2.14                     | 0.95              |
| 1:D:818:TYR:HB2  | 2:E:90:GLY:N     | 1.81                     | 0.95              |
| 2:H:150:TYR:O    | 2:H:151:LYS:HG3  | 1.65                     | 0.95              |
| 1:J:795:ARG:NH1  | 3:L:35:ARG:NH1   | 2.15                     | 0.95              |
| 2:K:150:TYR:O    | 2:K:151:LYS:HG3  | 1.65                     | 0.95              |
| 1:J:637:LYS:NZ   | 4:7:141:SER:O    | 1.98                     | 0.95              |
| 1:A:813:ILE:CG2  | 2:B:127:ARG:NE   | 2.26                     | 0.95              |
| 1:A:819:ASN:N    | 2:B:90:GLY:HA3   | 1.81                     | 0.95              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:150:TYR:O    | 2:E:151:LYS:CG   | 2.15                     | 0.95              |
| 1:J:93:MET:CG    | 1:J:764:MLY:NZ   | 2.22                     | 0.95              |
| 1:A:543:PRO:CG   | 4:4:143:TYR:O    | 2.14                     | 0.95              |
| 1:D:635:GLY:HA3  | 4:5:334:GLU:HG2  | 1.47                     | 0.95              |
| 1:A:768:MLY:C    | 1:A:771:LEU:HB2  | 1.96                     | 0.95              |
| 2:B:121:LEU:CB   | 2:B:128:PHE:HB3  | 1.69                     | 0.95              |
| 1:D:215:GLN:HA   | 1:D:340:ILE:HG23 | 0.95                     | 0.95              |
| 1:D:537:GLU:C    | 4:5:349:LEU:CD1  | 2.20                     | 0.95              |
| 3:F:52:ASN:HB2   | 3:F:53:PRO:HD3   | 1.45                     | 0.95              |
| 1:G:721:LYS:CA   | 1:G:736:GLN:CD   | 2.34                     | 0.95              |
| 1:A:538:GLU:HG3  | 4:4:352:PHE:N    | 1.82                     | 0.94              |
| 1:A:530:MET:HA   | 4:4:354:GLN:HG3  | 0.96                     | 0.94              |
| 1:A:800:ARG:HH11 | 3:C:149:VAL:HG13 | 1.21                     | 0.94              |
| 1:J:721:LYS:CA   | 1:J:736:GLN:CD   | 2.34                     | 0.94              |
| 1:J:749:GLY:O    | 3:L:114:LEU:CD2  | 2.14                     | 0.94              |
| 1:J:783:LEU:O    | 1:J:787:ILE:N    | 1.99                     | 0.94              |
| 1:D:637:LYS:NZ   | 4:5:141:SER:O    | 1.99                     | 0.94              |
| 1:A:709:LYS:C    | 1:A:710:GLY:HA3  | 1.88                     | 0.94              |
| 1:A:757:GLN:CB   | 1:A:771:LEU:CD1  | 2.05                     | 0.94              |
| 2:H:121:LEU:CB   | 2:H:128:PHE:HB3  | 1.69                     | 0.94              |
| 1:A:530:MET:CA   | 4:4:354:GLN:CG   | 2.44                     | 0.94              |
| 1:D:541:MET:N    | 4:5:349:LEU:HD21 | 1.80                     | 0.94              |
| 1:J:538:GLU:HG3  | 4:7:352:PHE:N    | 1.82                     | 0.94              |
| 1:A:768:MLY:HB3  | 1:A:771:LEU:HB2  | 1.46                     | 0.94              |
| 1:J:635:GLY:HA3  | 4:7:334:GLU:HG2  | 1.47                     | 0.94              |
| 2:K:150:TYR:O    | 2:K:151:LYS:CG   | 2.15                     | 0.94              |
| 2:B:150:TYR:O    | 2:B:151:LYS:HB2  | 1.67                     | 0.94              |
| 2:E:150:TYR:O    | 2:E:151:LYS:HB2  | 1.67                     | 0.94              |
| 1:J:795:ARG:HH11 | 3:L:35:ARG:NH1   | 1.65                     | 0.94              |
| 1:G:642:LYS:CG   | 4:6:23:GLY:H     | 1.76                     | 0.94              |
| 1:A:800:ARG:CD   | 3:C:149:VAL:C    | 2.35                     | 0.94              |
| 1:G:84:MLY:CH2   | 1:G:716:LEU:O    | 2.14                     | 0.94              |
| 2:H:150:TYR:O    | 2:H:151:LYS:CG   | 2.15                     | 0.94              |
| 1:A:502:GLU:CG   | 1:A:761:GLY:CA   | 2.45                     | 0.94              |
| 1:D:538:GLU:HG3  | 4:5:352:PHE:N    | 1.82                     | 0.94              |
| 1:G:93:MET:HE2   | 1:G:764:MLY:HG3  | 1.49                     | 0.94              |
| 1:G:218:LEU:CB   | 1:G:221:GLN:CG   | 2.46                     | 0.94              |
| 1:G:831:TRP:CE2  | 2:H:67:MET:SD    | 2.60                     | 0.94              |
| 2:H:144:VAL:HG13 | 2:H:153:ILE:HG12 | 1.14                     | 0.94              |
| 1:A:642:LYS:CG   | 4:4:23:GLY:H     | 1.77                     | 0.94              |
| 1:J:797:PHE:CA   | 3:L:149:VAL:HG11 | 1.98                     | 0.94              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:530:MET:HA   | 4:7:354:GLN:HG3  | 0.96                     | 0.94              |
| 1:A:553:MLY:HB3  | 4:6:46:GLY:HA2   | 1.47                     | 0.94              |
| 1:A:612:GLN:NE2  | 1:A:627:GLY:HA3  | 1.83                     | 0.94              |
| 1:D:530:MET:HA   | 4:5:354:GLN:HG3  | 0.96                     | 0.94              |
| 1:D:546:THR:HG22 | 1:D:548:THR:H    | 1.32                     | 0.94              |
| 1:D:839:MLY:NZ   | 2:E:159:HIS:HB3  | 1.83                     | 0.94              |
| 1:G:834:LEU:HD13 | 2:H:51:PHE:HE1   | 0.79                     | 0.94              |
| 3:I:52:ASN:HB2   | 3:I:53:PRO:HD3   | 1.46                     | 0.94              |
| 1:J:612:GLN:NE2  | 1:J:627:GLY:CA   | 2.31                     | 0.94              |
| 1:J:823:PHE:CE1  | 2:K:156:VAL:O    | 2.21                     | 0.94              |
| 1:A:218:LEU:CB   | 1:A:221:GLN:CG   | 2.46                     | 0.94              |
| 1:A:736:GLN:CA   | 1:A:743:ALA:HB2  | 1.95                     | 0.94              |
| 2:E:163:ALA:C    | 2:K:22:THR:H     | 1.69                     | 0.94              |
| 1:A:768:MLY:HB3  | 1:A:771:LEU:CD1  | 1.97                     | 0.93              |
| 1:D:218:LEU:CB   | 1:D:221:GLN:CG   | 2.46                     | 0.93              |
| 1:J:798:LEU:HD22 | 3:L:126:LEU:HD11 | 0.94                     | 0.93              |
| 1:J:800:ARG:NH1  | 3:L:149:VAL:HG22 | 1.84                     | 0.93              |
| 1:G:541:MET:N    | 4:6:349:LEU:HD21 | 1.80                     | 0.93              |
| 2:B:150:TYR:O    | 2:B:151:LYS:CG   | 2.15                     | 0.93              |
| 1:G:543:PRO:CG   | 4:6:143:TYR:O    | 2.14                     | 0.93              |
| 1:G:612:GLN:NE2  | 1:G:627:GLY:HA3  | 1.83                     | 0.93              |
| 1:G:817:GLN:HG2  | 2:H:127:ARG:CB   | 1.97                     | 0.93              |
| 1:D:507:GLY:O    | 1:D:761:GLY:HA3  | 1.69                     | 0.93              |
| 1:D:798:LEU:CD1  | 3:F:126:LEU:HD21 | 1.97                     | 0.93              |
| 1:D:839:MLY:CH1  | 2:E:159:HIS:HB3  | 1.97                     | 0.93              |
| 1:G:707:CYS:C    | 1:G:714:ARG:HH22 | 1.70                     | 0.93              |
| 1:J:557:GLU:H    | 4:V:48:GLY:HA2   | 1.32                     | 0.93              |
| 1:D:817:GLN:HG3  | 2:E:127:ARG:HD3  | 1.49                     | 0.93              |
| 1:D:830:PRO:HG2  | 2:E:67:MET:HE2   | 1.46                     | 0.93              |
| 2:E:117:LEU:HD13 | 2:E:147:ASN:OD1  | 1.64                     | 0.93              |
| 1:J:530:MET:CE   | 4:7:354:GLN:CG   | 2.40                     | 0.93              |
| 1:J:537:GLU:C    | 4:7:349:LEU:CD1  | 2.20                     | 0.93              |
| 1:J:612:GLN:NE2  | 1:J:627:GLY:HA3  | 1.83                     | 0.93              |
| 1:A:557:GLU:N    | 4:6:48:GLY:CA    | 2.12                     | 0.93              |
| 1:J:530:MET:CA   | 4:7:354:GLN:CG   | 2.44                     | 0.93              |
| 1:A:836:PHE:CE1  | 2:B:159:HIS:C    | 2.42                     | 0.93              |
| 1:D:834:LEU:CD1  | 2:E:54:MET:HB2   | 1.98                     | 0.93              |
| 1:J:508:ILE:HD11 | 1:J:759:ALA:HB1  | 1.48                     | 0.93              |
| 1:G:553:MLY:HB3  | 4:8:46:GLY:HA2   | 1.48                     | 0.93              |
| 1:A:836:PHE:CZ   | 2:B:160:GLY:HA3  | 1.94                     | 0.93              |
| 1:J:786:ILE:HG12 | 3:L:86:ASP:HB3   | 1.51                     | 0.93              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:612:GLN:NE2  | 1:D:627:GLY:CA   | 2.31                     | 0.93              |
| 1:J:538:GLU:N    | 4:7:351:THR:H    | 1.67                     | 0.93              |
| 1:A:502:GLU:HG3  | 1:A:761:GLY:N    | 1.84                     | 0.93              |
| 1:A:629:GLU:CB   | 1:A:643:GLY:O    | 2.17                     | 0.93              |
| 1:A:753:VAL:HA   | 1:A:778:MET:SD   | 2.09                     | 0.93              |
| 1:G:798:LEU:HD11 | 3:I:126:LEU:HD23 | 1.49                     | 0.93              |
| 1:G:789:ALA:HB2  | 3:I:81:GLN:HE21  | 0.77                     | 0.93              |
| 1:A:648:THR:HG21 | 1:A:651:ALA:HB2  | 1.50                     | 0.93              |
| 1:D:831:TRP:CE2  | 2:E:47:LEU:HD23  | 1.94                     | 0.93              |
| 1:G:612:GLN:NE2  | 1:G:627:GLY:CA   | 2.31                     | 0.93              |
| 1:G:819:ASN:CB   | 2:H:90:GLY:O     | 2.16                     | 0.93              |
| 1:J:206:LYS:CD   | 1:J:217:THR:CG2  | 2.16                     | 0.93              |
| 1:J:739:ASP:HB3  | 1:J:742:LYS:CB   | 1.98                     | 0.93              |
| 1:A:549:SER:C    | 4:6:46:GLY:HA3   | 1.90                     | 0.92              |
| 1:G:530:MET:CA   | 4:6:354:GLN:CG   | 2.45                     | 0.92              |
| 1:A:215:GLN:HA   | 1:A:340:ILE:HG23 | 0.96                     | 0.92              |
| 1:A:505:MLY:NZ   | 1:A:762:HIS:C    | 2.16                     | 0.92              |
| 1:A:612:GLN:NE2  | 1:A:627:GLY:CA   | 2.31                     | 0.92              |
| 1:A:793:ARG:HH21 | 3:C:147:MET:HB3  | 1.33                     | 0.92              |
| 1:G:215:GLN:HA   | 1:G:340:ILE:HG23 | 0.95                     | 0.92              |
| 1:G:795:ARG:HB3  | 3:I:35:ARG:NH2   | 1.82                     | 0.92              |
| 1:J:215:GLN:HA   | 1:J:340:ILE:HG23 | 0.95                     | 0.92              |
| 1:J:768:MLY:HD3  | 1:J:772:LEU:HB2  | 1.49                     | 0.92              |
| 1:J:90:ASP:CG    | 1:J:764:MLY:CH1  | 2.37                     | 0.92              |
| 1:G:642:LYS:CB   | 4:6:21:PHE:O     | 2.17                     | 0.92              |
| 1:D:549:SER:C    | 4:7:46:GLY:HA3   | 1.90                     | 0.92              |
| 1:J:541:MET:N    | 4:7:349:LEU:HD21 | 1.80                     | 0.92              |
| 1:J:648:THR:HG21 | 1:J:651:ALA:HB2  | 1.50                     | 0.92              |
| 1:J:768:MLY:HH12 | 1:J:772:LEU:HD21 | 1.49                     | 0.92              |
| 1:J:549:SER:C    | 4:V:46:GLY:HA3   | 1.90                     | 0.92              |
| 1:D:530:MET:CA   | 4:5:354:GLN:CG   | 2.44                     | 0.92              |
| 1:A:641:LYS:HE3  | 1:A:647:GLN:CG   | 2.00                     | 0.92              |
| 1:D:213:LYS:HA   | 1:D:220:ASP:CG   | 1.90                     | 0.92              |
| 1:D:834:LEU:CD1  | 2:E:54:MET:CB    | 2.47                     | 0.92              |
| 1:G:537:GLU:C    | 4:6:349:LEU:CD1  | 2.21                     | 0.92              |
| 1:J:636:LYS:HD2  | 4:7:332:PRO:HB3  | 1.52                     | 0.92              |
| 1:D:557:GLU:H    | 4:7:48:GLY:HA2   | 1.32                     | 0.92              |
| 1:A:739:ASP:HB3  | 1:A:742:LYS:CB   | 1.98                     | 0.92              |
| 1:A:800:ARG:CB   | 3:C:149:VAL:HG21 | 1.89                     | 0.92              |
| 1:J:546:THR:HG22 | 1:J:548:THR:H    | 1.32                     | 0.92              |
| 1:J:821:ARG:HH22 | 2:K:127:ARG:HG2  | 1.31                     | 0.92              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:818:TYR:HB3  | 2:K:90:GLY:HA3   | 1.51                     | 0.92              |
| 1:D:550:PHE:HA   | 4:7:46:GLY:CA    | 2.00                     | 0.92              |
| 1:A:642:LYS:CB   | 4:4:21:PHE:O     | 2.17                     | 0.92              |
| 1:D:612:GLN:NE2  | 1:D:627:GLY:HA3  | 1.83                     | 0.92              |
| 1:D:629:GLU:CB   | 1:D:643:GLY:O    | 2.17                     | 0.92              |
| 1:D:790:THR:HA   | 3:F:87:PHE:CE2   | 2.04                     | 0.92              |
| 1:J:213:LYS:HA   | 1:J:220:ASP:CG   | 1.90                     | 0.92              |
| 1:J:629:GLU:CB   | 1:J:643:GLY:O    | 2.17                     | 0.92              |
| 1:D:278:GLN:HG2  | 1:D:317:GLU:HB2  | 1.52                     | 0.92              |
| 1:D:790:THR:N    | 3:F:87:PHE:HE2   | 1.67                     | 0.92              |
| 1:G:629:GLU:CB   | 1:G:643:GLY:O    | 2.17                     | 0.92              |
| 1:G:783:LEU:O    | 1:G:787:ILE:HB   | 1.70                     | 0.92              |
| 1:A:795:ARG:HD2  | 3:C:35:ARG:CZ    | 1.99                     | 0.92              |
| 1:A:636:LYS:HD2  | 4:4:332:PRO:HB3  | 1.51                     | 0.92              |
| 1:A:546:THR:HG22 | 1:A:548:THR:H    | 1.32                     | 0.92              |
| 1:D:790:THR:CA   | 3:F:87:PHE:CE2   | 2.47                     | 0.92              |
| 1:G:648:THR:HG21 | 1:G:651:ALA:HB2  | 1.51                     | 0.92              |
| 1:J:92:ALA:O     | 1:J:714:ARG:CD   | 2.18                     | 0.92              |
| 1:D:537:GLU:O    | 4:5:349:LEU:HD13 | 0.74                     | 0.92              |
| 1:A:831:TRP:CE2  | 2:B:51:PHE:CE1   | 2.58                     | 0.92              |
| 1:G:641:LYS:HE3  | 1:G:647:GLN:CG   | 2.00                     | 0.92              |
| 1:G:757:GLN:OE1  | 1:G:772:LEU:HG   | 1.70                     | 0.92              |
| 1:G:831:TRP:CH2  | 2:H:47:LEU:HD21  | 1.93                     | 0.92              |
| 1:J:550:PHE:HA   | 4:V:46:GLY:CA    | 2.00                     | 0.92              |
| 1:D:636:LYS:HD2  | 4:5:332:PRO:HB3  | 1.52                     | 0.91              |
| 1:J:537:GLU:O    | 4:7:349:LEU:HD13 | 0.73                     | 0.91              |
| 1:G:549:SER:C    | 4:8:46:GLY:HA3   | 1.90                     | 0.91              |
| 1:D:648:THR:HG21 | 1:D:651:ALA:HB2  | 1.50                     | 0.91              |
| 1:D:739:ASP:HB3  | 1:D:742:LYS:CB   | 1.98                     | 0.91              |
| 1:G:795:ARG:CG   | 3:I:35:ARG:HH22  | 1.82                     | 0.91              |
| 1:J:642:LYS:CB   | 4:7:21:PHE:O     | 2.17                     | 0.91              |
| 1:D:642:LYS:CB   | 4:5:21:PHE:O     | 2.17                     | 0.91              |
| 1:J:538:GLU:N    | 4:7:349:LEU:HD12 | 1.86                     | 0.91              |
| 1:A:735:GLY:C    | 1:A:743:ALA:HA   | 1.90                     | 0.91              |
| 1:G:795:ARG:HB3  | 3:I:35:ARG:HH21  | 1.33                     | 0.91              |
| 1:G:821:ARG:HH21 | 2:H:127:ARG:HG2  | 1.34                     | 0.91              |
| 1:J:797:PHE:CG   | 3:L:149:VAL:HG11 | 2.05                     | 0.91              |
| 1:G:537:GLU:O    | 4:6:349:LEU:HD13 | 0.74                     | 0.91              |
| 1:A:218:LEU:HA   | 1:A:221:GLN:CG   | 2.01                     | 0.91              |
| 1:J:641:LYS:HE3  | 1:J:647:GLN:CG   | 2.00                     | 0.91              |
| 1:A:649:VAL:CG1  | 1:A:649:VAL:C    | 2.38                     | 0.91              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:538:GLU:N    | 4:5:351:THR:H    | 1.68                     | 0.91              |
| 1:G:550:PHE:HA   | 4:8:46:GLY:CA    | 2.00                     | 0.91              |
| 1:G:838:ILE:HD11 | 2:H:54:MET:HE3   | 0.92                     | 0.91              |
| 1:J:278:GLN:HG2  | 1:J:317:GLU:HB2  | 1.52                     | 0.91              |
| 1:A:544:LYS:HD2  | 4:4:147:ARG:HB3  | 1.53                     | 0.91              |
| 1:D:834:LEU:HD11 | 2:E:54:MET:HG2   | 1.53                     | 0.91              |
| 1:G:218:LEU:HA   | 1:G:221:GLN:CG   | 2.01                     | 0.91              |
| 1:J:218:LEU:CB   | 1:J:221:GLN:CG   | 2.46                     | 0.91              |
| 1:J:735:GLY:C    | 1:J:743:ALA:HA   | 1.90                     | 0.91              |
| 1:A:557:GLU:H    | 4:6:48:GLY:HA2   | 1.32                     | 0.91              |
| 3:F:62:ALA:O     | 3:F:63:ILE:CG1   | 2.19                     | 0.91              |
| 1:G:544:LYS:HD2  | 4:6:147:ARG:HB3  | 1.53                     | 0.91              |
| 1:J:736:GLN:HA   | 1:J:743:ALA:HB2  | 1.50                     | 0.91              |
| 1:G:557:GLU:H    | 4:8:48:GLY:HA2   | 1.33                     | 0.91              |
| 1:D:649:VAL:C    | 1:D:649:VAL:CG1  | 2.38                     | 0.91              |
| 1:G:410:ASN:OD1  | 4:6:334:GLU:C    | 2.10                     | 0.91              |
| 2:B:149:ASP:CG   | 2:B:150:TYR:H    | 1.73                     | 0.91              |
| 1:A:819:ASN:ND2  | 2:B:91:ALA:C     | 2.23                     | 0.91              |
| 3:C:62:ALA:O     | 3:C:63:ILE:CG1   | 2.19                     | 0.91              |
| 1:D:735:GLY:C    | 1:D:743:ALA:HA   | 1.91                     | 0.91              |
| 3:F:62:ALA:O     | 3:F:63:ILE:HG12  | 1.71                     | 0.91              |
| 1:G:538:GLU:N    | 4:6:351:THR:H    | 1.68                     | 0.91              |
| 1:G:768:MLY:HH23 | 1:G:772:LEU:HD22 | 1.53                     | 0.91              |
| 1:J:93:MET:HG2   | 1:J:764:MLY:HD3  | 0.92                     | 0.91              |
| 1:A:537:GLU:O    | 4:4:349:LEU:HD13 | 0.74                     | 0.91              |
| 1:A:550:PHE:HA   | 4:6:46:GLY:CA    | 2.00                     | 0.91              |
| 1:A:537:GLU:C    | 4:4:349:LEU:CD1  | 2.20                     | 0.91              |
| 1:D:724:TYR:CE1  | 1:D:778:MET:SD   | 2.64                     | 0.91              |
| 1:G:638:GLY:HA3  | 4:6:341:ILE:O    | 1.70                     | 0.91              |
| 1:G:739:ASP:HB3  | 1:G:742:LYS:CB   | 1.99                     | 0.91              |
| 3:I:62:ALA:O     | 3:I:63:ILE:HG12  | 1.71                     | 0.91              |
| 1:A:538:GLU:N    | 4:4:349:LEU:HD12 | 1.86                     | 0.90              |
| 1:D:553:MLY:HE2  | 4:7:45:VAL:HA    | 1.53                     | 0.90              |
| 1:A:836:PHE:HB3  | 2:B:161:GLU:CG   | 2.01                     | 0.90              |
| 1:D:735:GLY:O    | 1:D:743:ALA:CA   | 2.19                     | 0.90              |
| 1:D:790:THR:N    | 3:F:87:PHE:CE2   | 2.39                     | 0.90              |
| 1:G:649:VAL:CG1  | 1:G:649:VAL:C    | 2.38                     | 0.90              |
| 1:J:800:ARG:HB3  | 3:L:149:VAL:CG2  | 1.94                     | 0.90              |
| 1:G:636:LYS:HD2  | 4:6:332:PRO:HB3  | 1.52                     | 0.90              |
| 1:J:544:LYS:HD2  | 4:7:147:ARG:HB3  | 1.53                     | 0.90              |
| 1:A:538:GLU:N    | 4:4:351:THR:H    | 1.68                     | 0.90              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:649:VAL:CG2  | 1:A:649:VAL:CB   | 2.50                     | 0.90              |
| 1:G:213:LYS:HA   | 1:G:220:ASP:CG   | 1.90                     | 0.90              |
| 1:G:649:VAL:CB   | 1:G:649:VAL:CG2  | 2.49                     | 0.90              |
| 2:H:149:ASP:CG   | 2:H:150:TYR:H    | 1.73                     | 0.90              |
| 1:A:638:GLY:HA3  | 4:4:341:ILE:O    | 1.70                     | 0.90              |
| 1:A:768:MLY:CB   | 1:A:771:LEU:HB2  | 2.00                     | 0.90              |
| 1:D:649:VAL:HG13 | 1:D:649:VAL:CG2  | 2.02                     | 0.90              |
| 1:G:278:GLN:HG2  | 1:G:317:GLU:HB2  | 1.52                     | 0.90              |
| 1:J:649:VAL:CG1  | 1:J:649:VAL:C    | 2.38                     | 0.90              |
| 2:K:150:TYR:O    | 2:K:151:LYS:HB2  | 1.67                     | 0.90              |
| 1:J:798:LEU:HD21 | 3:L:126:LEU:HG   | 1.51                     | 0.90              |
| 1:G:538:GLU:N    | 4:6:349:LEU:HD12 | 1.87                     | 0.90              |
| 1:A:213:LYS:HA   | 1:A:220:ASP:CG   | 1.90                     | 0.90              |
| 1:A:505:MLY:CH2  | 1:A:762:HIS:O    | 2.19                     | 0.90              |
| 1:A:757:GLN:CG   | 1:A:771:LEU:CD1  | 2.44                     | 0.90              |
| 1:D:218:LEU:HA   | 1:D:221:GLN:CG   | 2.01                     | 0.90              |
| 1:D:538:GLU:O    | 4:5:349:LEU:CG   | 2.20                     | 0.90              |
| 1:D:641:LYS:HE3  | 1:D:647:GLN:CG   | 2.00                     | 0.90              |
| 1:D:796:GLY:HA3  | 3:F:40:ASN:OD1   | 1.71                     | 0.90              |
| 1:G:721:LYS:CB   | 1:G:736:GLN:OE1  | 2.20                     | 0.90              |
| 1:G:735:GLY:C    | 1:G:743:ALA:HA   | 1.90                     | 0.90              |
| 1:J:649:VAL:CG2  | 1:J:649:VAL:HG13 | 2.02                     | 0.90              |
| 1:J:553:MLY:HE2  | 4:V:45:VAL:HA    | 1.53                     | 0.90              |
| 1:D:544:LYS:HD2  | 4:5:147:ARG:HB3  | 1.53                     | 0.90              |
| 1:G:557:GLU:H    | 4:8:48:GLY:HA3   | 1.28                     | 0.90              |
| 1:G:754:ASP:OD2  | 1:G:776:GLU:OE2  | 1.89                     | 0.90              |
| 3:I:62:ALA:O     | 3:I:63:ILE:CG1   | 2.19                     | 0.90              |
| 1:J:735:GLY:O    | 1:J:743:ALA:CA   | 2.19                     | 0.90              |
| 1:D:534:SER:O    | 4:5:351:THR:HG23 | 1.13                     | 0.90              |
| 1:D:839:MLY:CH1  | 2:E:159:HIS:CG   | 2.50                     | 0.90              |
| 2:E:121:LEU:CB   | 2:E:128:PHE:HB3  | 1.69                     | 0.90              |
| 1:J:553:MLY:CG   | 4:V:44:MET:O     | 2.20                     | 0.90              |
| 2:H:137:TRP:HA   | 2:H:145:ALA:HB2  | 1.54                     | 0.90              |
| 1:J:818:TYR:HB3  | 2:K:90:GLY:CA    | 2.01                     | 0.90              |
| 1:A:278:GLN:HG2  | 1:A:317:GLU:HB2  | 1.52                     | 0.90              |
| 1:D:550:PHE:CA   | 4:7:46:GLY:HA3   | 2.02                     | 0.90              |
| 2:E:137:TRP:HA   | 2:E:145:ALA:HB2  | 1.53                     | 0.90              |
| 1:J:757:GLN:CD   | 1:J:776:GLU:HG2  | 1.90                     | 0.90              |
| 1:A:410:ASN:OD1  | 4:4:334:GLU:C    | 2.10                     | 0.90              |
| 1:D:538:GLU:N    | 4:5:349:LEU:HD12 | 1.86                     | 0.90              |
| 1:A:629:GLU:HG2  | 1:A:643:GLY:O    | 1.72                     | 0.90              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:D:836:PHE:CB  | 2:E:161:GLU:OE1  | 2.20                     | 0.90              |
| 1:D:795:ARG:CB  | 3:F:35:ARG:NE    | 2.26                     | 0.90              |
| 1:G:629:GLU:HG2 | 1:G:643:GLY:O    | 1.72                     | 0.90              |
| 1:J:218:LEU:HA  | 1:J:221:GLN:CG   | 2.01                     | 0.90              |
| 1:J:410:ASN:OD1 | 4:7:334:GLU:C    | 2.10                     | 0.90              |
| 1:J:530:MET:N   | 4:7:354:GLN:HB3  | 1.87                     | 0.90              |
| 2:E:163:ALA:C   | 2:K:22:THR:OG1   | 2.10                     | 0.90              |
| 1:J:538:GLU:O   | 4:7:349:LEU:CG   | 2.20                     | 0.90              |
| 1:A:817:GLN:HB2 | 2:B:127:ARG:CZ   | 2.02                     | 0.90              |
| 1:G:215:GLN:H   | 1:G:340:ILE:CG1  | 1.72                     | 0.90              |
| 1:G:817:GLN:OE1 | 2:H:127:ARG:HD2  | 1.71                     | 0.90              |
| 1:J:550:PHE:CA  | 4:V:46:GLY:HA3   | 2.02                     | 0.90              |
| 1:A:735:GLY:O   | 1:A:743:ALA:CA   | 2.19                     | 0.89              |
| 1:D:799:MET:CE  | 3:F:32:ASP:HB3   | 2.02                     | 0.89              |
| 2:E:163:ALA:C   | 2:K:22:THR:N     | 2.24                     | 0.89              |
| 1:J:635:GLY:CA  | 4:7:341:ILE:HD13 | 2.02                     | 0.89              |
| 1:D:638:GLY:HA3 | 4:5:341:ILE:O    | 1.70                     | 0.89              |
| 1:G:735:GLY:O   | 1:G:743:ALA:CA   | 2.19                     | 0.89              |
| 1:J:821:ARG:NH2 | 2:K:127:ARG:CD   | 2.35                     | 0.89              |
| 1:J:84:MLY:HE2  | 1:J:719:ASP:CG   | 1.92                     | 0.89              |
| 1:D:553:MLY:CG  | 4:7:44:MET:O     | 2.20                     | 0.89              |
| 3:C:24:LYS:HB3  | 3:C:63:ILE:O     | 1.72                     | 0.89              |
| 3:C:62:ALA:O    | 3:C:63:ILE:HG12  | 1.71                     | 0.89              |
| 1:D:649:VAL:CB  | 1:D:649:VAL:CG2  | 2.49                     | 0.89              |
| 1:A:795:ARG:CZ  | 3:C:116:GLU:OE2  | 2.19                     | 0.89              |
| 1:A:800:ARG:HD2 | 3:C:149:VAL:HG22 | 0.92                     | 0.89              |
| 1:D:815:CYS:O   | 2:E:90:GLY:O     | 1.89                     | 0.89              |
| 1:G:599:ASN:OD1 | 1:G:649:VAL:HB   | 1.72                     | 0.89              |
| 1:J:534:SER:HA  | 4:7:350:SER:O    | 1.71                     | 0.89              |
| 3:L:62:ALA:O    | 3:L:63:ILE:CG1   | 2.19                     | 0.89              |
| 1:A:530:MET:N   | 4:4:354:GLN:HB3  | 1.87                     | 0.89              |
| 1:D:629:GLU:HG2 | 1:D:643:GLY:O    | 1.72                     | 0.89              |
| 1:D:721:LYS:CB  | 1:D:736:GLN:OE1  | 2.20                     | 0.89              |
| 1:J:649:VAL:CG2 | 1:J:649:VAL:CB   | 2.49                     | 0.89              |
| 1:J:721:LYS:CB  | 1:J:736:GLN:OE1  | 2.20                     | 0.89              |
| 1:J:557:GLU:H   | 4:V:48:GLY:HA3   | 1.28                     | 0.89              |
| 1:D:630:ALA:O   | 4:5:25:ASP:CG    | 2.09                     | 0.89              |
| 1:D:410:ASN:OD1 | 4:5:334:GLU:C    | 2.10                     | 0.89              |
| 1:D:635:GLY:CA  | 4:5:341:ILE:HD13 | 2.03                     | 0.89              |
| 1:G:538:GLU:O   | 4:6:349:LEU:CG   | 2.20                     | 0.89              |
| 1:J:630:ALA:O   | 4:7:25:ASP:CG    | 2.09                     | 0.89              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:137:TRP:HA   | 2:K:145:ALA:HB2  | 1.53                     | 0.89              |
| 1:D:534:SER:HA   | 4:5:350:SER:O    | 1.71                     | 0.89              |
| 1:J:503:TYR:OH   | 1:J:711:PHE:HD2  | 1.55                     | 0.89              |
| 1:A:553:MLY:CG   | 4:6:44:MET:O     | 2.20                     | 0.89              |
| 1:A:721:LYS:CB   | 1:A:736:GLN:OE1  | 2.20                     | 0.89              |
| 1:D:507:GLY:CA   | 1:D:762:HIS:CG   | 2.56                     | 0.89              |
| 1:D:530:MET:N    | 4:5:354:GLN:HB3  | 1.87                     | 0.89              |
| 1:D:641:LYS:HD2  | 4:5:348:SER:CB   | 2.02                     | 0.89              |
| 1:G:93:MET:HE3   | 1:G:763:THR:CB   | 1.74                     | 0.89              |
| 1:J:215:GLN:H    | 1:J:340:ILE:CG1  | 1.72                     | 0.89              |
| 1:G:816:ILE:HD11 | 2:H:100:ALA:CB   | 2.02                     | 0.89              |
| 1:A:630:ALA:O    | 4:4:25:ASP:CG    | 2.10                     | 0.89              |
| 1:J:638:GLY:HA3  | 4:7:341:ILE:O    | 1.70                     | 0.89              |
| 1:A:538:GLU:O    | 4:4:349:LEU:CG   | 2.20                     | 0.89              |
| 1:A:505:MLY:HG3  | 1:A:741:LYS:HZ3  | 1.37                     | 0.89              |
| 1:J:641:LYS:HD2  | 4:7:348:SER:CB   | 2.02                     | 0.89              |
| 1:J:826:VAL:HG21 | 2:K:88:LEU:CD2   | 2.03                     | 0.89              |
| 1:G:534:SER:HA   | 4:6:350:SER:O    | 1.71                     | 0.88              |
| 1:A:534:SER:HA   | 4:4:350:SER:O    | 1.71                     | 0.88              |
| 1:A:769:ALA:C    | 1:A:772:LEU:H    | 1.76                     | 0.88              |
| 1:A:795:ARG:CD   | 3:C:35:ARG:NH2   | 2.36                     | 0.88              |
| 2:H:121:LEU:CA   | 2:H:128:PHE:CB   | 2.46                     | 0.88              |
| 1:G:838:ILE:CD1  | 2:H:54:MET:HE1   | 1.96                     | 0.88              |
| 1:A:550:PHE:CA   | 4:6:46:GLY:HA3   | 2.02                     | 0.88              |
| 1:G:530:MET:N    | 4:6:354:GLN:HB3  | 1.88                     | 0.88              |
| 1:J:829:TRP:CZ3  | 2:K:84:PHE:HZ    | 1.85                     | 0.88              |
| 1:D:541:MET:CB   | 4:5:143:TYR:OH   | 2.21                     | 0.88              |
| 2:E:137:TRP:HA   | 2:E:145:ALA:CB   | 2.03                     | 0.88              |
| 1:D:800:ARG:HD2  | 3:F:149:VAL:HG22 | 1.53                     | 0.88              |
| 1:J:769:ALA:HB3  | 1:J:770:GLY:HA2  | 0.90                     | 0.88              |
| 3:L:62:ALA:O     | 3:L:63:ILE:HG12  | 1.71                     | 0.88              |
| 4:X:322:PRO:HB2  | 4:Z:244:ASP:CG   | 1.94                     | 0.88              |
| 1:A:836:PHE:HE1  | 2:B:159:HIS:HA   | 1.37                     | 0.88              |
| 1:D:215:GLN:H    | 1:D:340:ILE:HG12 | 1.06                     | 0.88              |
| 1:D:641:LYS:CD   | 1:D:647:GLN:OE1  | 2.17                     | 0.88              |
| 1:G:541:MET:CB   | 4:6:143:TYR:OH   | 2.21                     | 0.88              |
| 1:G:795:ARG:CG   | 3:I:35:ARG:NH2   | 2.35                     | 0.88              |
| 1:G:553:MLY:HE2  | 4:8:45:VAL:HA    | 1.53                     | 0.88              |
| 1:D:599:ASN:OD1  | 1:D:649:VAL:HB   | 1.73                     | 0.88              |
| 1:J:629:GLU:HG2  | 1:J:643:GLY:O    | 1.72                     | 0.88              |
| 1:J:757:GLN:OE1  | 1:J:772:LEU:O    | 1.92                     | 0.88              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:818:TYR:CE1  | 2:K:127:ARG:NH2  | 2.42                     | 0.88              |
| 4:0:322:PRO:HB2  | 4:2:244:ASP:CG   | 1.94                     | 0.88              |
| 1:A:541:MET:CB   | 4:4:143:TYR:OH   | 2.20                     | 0.88              |
| 1:G:553:MLY:CG   | 4:8:44:MET:O     | 2.20                     | 0.88              |
| 1:G:641:LYS:CD   | 1:G:647:GLN:OE1  | 2.17                     | 0.88              |
| 1:G:728:ASN:HD21 | 3:I:110:VAL:HA   | 1.38                     | 0.88              |
| 1:J:215:GLN:H    | 1:J:340:ILE:HG12 | 1.05                     | 0.88              |
| 1:J:642:LYS:HG2  | 4:7:22:ALA:CA    | 2.03                     | 0.88              |
| 1:J:838:ILE:HD11 | 2:K:54:MET:CE    | 2.04                     | 0.88              |
| 3:L:24:LYS:HB3   | 3:L:63:ILE:O     | 1.72                     | 0.88              |
| 1:A:642:LYS:HG2  | 4:4:22:ALA:CA    | 2.04                     | 0.88              |
| 1:A:707:CYS:SG   | 1:A:714:ARG:NH1  | 2.47                     | 0.88              |
| 1:G:642:LYS:HG2  | 4:6:22:ALA:CA    | 2.03                     | 0.88              |
| 1:G:93:MET:CB    | 1:G:764:MLY:NZ   | 2.27                     | 0.88              |
| 1:J:831:TRP:HZ2  | 2:K:47:LEU:CD2   | 1.83                     | 0.88              |
| 1:A:641:LYS:HD2  | 4:4:348:SER:CB   | 2.02                     | 0.88              |
| 1:A:795:ARG:HB3  | 3:C:35:ARG:CZ    | 2.04                     | 0.88              |
| 1:J:642:LYS:CG   | 4:7:21:PHE:O     | 2.22                     | 0.88              |
| 4:2:322:PRO:HB2  | 4:4:244:ASP:CG   | 1.94                     | 0.88              |
| 1:G:542:PHE:HA   | 4:6:143:TYR:HE1  | 1.34                     | 0.88              |
| 1:A:553:MLY:HE2  | 4:6:45:VAL:HA    | 1.53                     | 0.88              |
| 2:B:137:TRP:HA   | 2:B:145:ALA:HB2  | 1.54                     | 0.88              |
| 1:D:635:GLY:HA2  | 4:5:334:GLU:CG   | 2.03                     | 0.88              |
| 3:F:139:TYR:HA   | 3:F:142:PHE:HB3  | 1.56                     | 0.88              |
| 1:G:510:TRP:CZ3  | 1:G:768:MLY:CH1  | 2.57                     | 0.88              |
| 1:G:642:LYS:CG   | 4:6:21:PHE:O     | 2.22                     | 0.88              |
| 4:V:322:PRO:HB2  | 4:X:244:ASP:CG   | 1.94                     | 0.88              |
| 1:A:817:GLN:OE1  | 2:B:127:ARG:NH2  | 1.81                     | 0.88              |
| 1:A:839:MLY:NZ   | 2:B:159:HIS:HB3  | 1.89                     | 0.88              |
| 1:A:789:ALA:HB1  | 3:C:87:PHE:HE2   | 1.39                     | 0.88              |
| 1:D:646:PHE:CE2  | 1:D:652:LEU:CD1  | 2.57                     | 0.88              |
| 1:G:550:PHE:CA   | 4:8:46:GLY:HA3   | 2.03                     | 0.88              |
| 1:G:707:CYS:O    | 1:G:714:ARG:NH2  | 2.06                     | 0.88              |
| 1:J:541:MET:CB   | 4:7:143:TYR:OH   | 2.20                     | 0.87              |
| 3:C:139:TYR:HA   | 3:C:142:PHE:HB3  | 1.56                     | 0.87              |
| 1:G:649:VAL:CG2  | 1:G:649:VAL:HG13 | 2.02                     | 0.87              |
| 1:G:646:PHE:CE2  | 1:G:652:LEU:CD1  | 2.58                     | 0.87              |
| 1:G:817:GLN:HB3  | 2:H:127:ARG:HH11 | 1.39                     | 0.87              |
| 1:J:795:ARG:HE   | 3:L:118:MET:CE   | 1.87                     | 0.87              |
| 1:D:795:ARG:HB3  | 3:F:35:ARG:CD    | 2.04                     | 0.87              |
| 1:G:817:GLN:CG   | 2:H:127:ARG:CD   | 2.52                     | 0.87              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:84:MLY:HE2   | 1:J:719:ASP:OD2  | 1.73                     | 0.87              |
| 1:J:735:GLY:C    | 1:J:743:ALA:HB2  | 1.82                     | 0.87              |
| 1:J:754:ASP:CB   | 1:J:776:GLU:HB3  | 2.03                     | 0.87              |
| 4:8:322:PRO:HB2  | 4:W:244:ASP:CG   | 1.94                     | 0.87              |
| 1:A:641:LYS:HG3  | 1:A:647:GLN:NE2  | 1.58                     | 0.87              |
| 1:A:72:VAL:CG1   | 1:A:76:GLN:HB3   | 2.05                     | 0.87              |
| 2:B:137:TRP:HA   | 2:B:145:ALA:CB   | 2.04                     | 0.87              |
| 1:J:92:ALA:O     | 1:J:714:ARG:HG3  | 1.74                     | 0.87              |
| 1:D:642:LYS:CG   | 4:5:21:PHE:O     | 2.22                     | 0.87              |
| 1:G:534:SER:O    | 4:6:351:THR:HG23 | 1.12                     | 0.87              |
| 1:G:635:GLY:CA   | 4:6:341:ILE:HD13 | 2.02                     | 0.87              |
| 3:I:24:LYS:HB3   | 3:I:63:ILE:O     | 1.72                     | 0.87              |
| 1:J:768:MLY:CH2  | 1:J:772:LEU:CG   | 2.45                     | 0.87              |
| 3:L:139:TYR:HA   | 3:L:142:PHE:HB3  | 1.56                     | 0.87              |
| 4:4:322:PRO:HB2  | 4:6:244:ASP:CG   | 1.94                     | 0.87              |
| 4:5:322:PRO:HB2  | 4:7:244:ASP:CG   | 1.94                     | 0.87              |
| 1:A:642:LYS:CG   | 4:4:21:PHE:O     | 2.22                     | 0.87              |
| 1:G:752:ASP:OD2  | 1:G:783:LEU:CB   | 2.22                     | 0.87              |
| 1:G:816:ILE:HD11 | 2:H:100:ALA:HB1  | 1.56                     | 0.87              |
| 1:A:635:GLY:CA   | 4:4:341:ILE:HD13 | 2.02                     | 0.87              |
| 1:D:636:LYS:H    | 4:5:334:GLU:CD   | 1.77                     | 0.87              |
| 1:D:792:ALA:HB1  | 3:F:40:ASN:O     | 1.74                     | 0.87              |
| 1:D:795:ARG:NH2  | 3:F:116:GLU:CD   | 2.20                     | 0.87              |
| 1:G:649:VAL:CA   | 1:G:649:VAL:CG1  | 2.53                     | 0.87              |
| 1:J:635:GLY:HA2  | 4:7:334:GLU:CG   | 2.03                     | 0.87              |
| 1:J:646:PHE:CE2  | 1:J:652:LEU:CD1  | 2.58                     | 0.87              |
| 1:A:649:VAL:HG13 | 1:A:649:VAL:CG2  | 2.02                     | 0.87              |
| 1:D:642:LYS:HG2  | 4:5:22:ALA:CA    | 2.04                     | 0.87              |
| 2:K:149:ASP:CG   | 2:K:150:TYR:H    | 1.73                     | 0.87              |
| 4:3:322:PRO:HB2  | 4:5:244:ASP:CG   | 1.94                     | 0.87              |
| 1:A:215:GLN:H    | 1:A:340:ILE:HG12 | 1.06                     | 0.87              |
| 1:A:649:VAL:CA   | 1:A:649:VAL:CG1  | 2.53                     | 0.87              |
| 1:A:819:ASN:OD1  | 2:B:91:ALA:HA    | 0.87                     | 0.87              |
| 1:D:649:VAL:CG1  | 1:D:649:VAL:CA   | 2.53                     | 0.87              |
| 1:G:93:MET:CE    | 1:G:763:THR:HG22 | 2.03                     | 0.87              |
| 1:G:823:PHE:CE1  | 2:H:156:VAL:O    | 2.28                     | 0.87              |
| 1:J:754:ASP:OD2  | 1:J:776:GLU:O    | 1.91                     | 0.87              |
| 1:J:93:MET:HG3   | 1:J:764:MLY:CH1  | 2.04                     | 0.87              |
| 4:W:322:PRO:HB2  | 4:Y:244:ASP:CG   | 1.94                     | 0.87              |
| 1:A:831:TRP:CH2  | 2:B:50:THR:HB    | 2.08                     | 0.87              |
| 1:J:636:LYS:H    | 4:7:334:GLU:CD   | 1.78                     | 0.87              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:641:LYS:CD   | 1:J:647:GLN:OE1  | 2.18                     | 0.87              |
| 1:J:649:VAL:CG1  | 1:J:649:VAL:CA   | 2.53                     | 0.87              |
| 4:7:322:PRO:HB2  | 4:V:244:ASP:CG   | 1.94                     | 0.86              |
| 1:A:798:LEU:CD2  | 3:C:122:GLU:HB3  | 2.05                     | 0.86              |
| 1:G:72:VAL:CG1   | 1:G:76:GLN:HB3   | 2.05                     | 0.86              |
| 1:G:831:TRP:HE1  | 2:H:67:MET:CB    | 1.87                     | 0.86              |
| 1:G:795:ARG:HD2  | 3:I:35:ARG:HH22  | 0.71                     | 0.86              |
| 1:J:84:MLY:HH12  | 1:J:715:VAL:CG1  | 1.75                     | 0.86              |
| 4:1:322:PRO:HB2  | 4:3:244:ASP:CG   | 1.94                     | 0.86              |
| 4:0:287:ILE:CG2  | 4:2:205:GLU:HG2  | 2.05                     | 0.86              |
| 1:D:755:HIS:HA   | 1:D:758:TYR:CE1  | 2.10                     | 0.86              |
| 1:G:817:GLN:HB3  | 2:H:127:ARG:HD3  | 1.56                     | 0.86              |
| 1:A:530:MET:HG2  | 4:4:354:GLN:CG   | 2.05                     | 0.86              |
| 1:D:646:PHE:CD2  | 1:D:652:LEU:HD11 | 2.09                     | 0.86              |
| 1:G:636:LYS:H    | 4:6:334:GLU:CD   | 1.78                     | 0.86              |
| 1:G:641:LYS:HD2  | 4:6:348:SER:CB   | 2.03                     | 0.86              |
| 2:H:137:TRP:HA   | 2:H:145:ALA:CB   | 2.04                     | 0.86              |
| 1:J:508:ILE:HD11 | 1:J:759:ALA:HB2  | 0.87                     | 0.86              |
| 1:J:757:GLN:CD   | 1:J:776:GLU:HG3  | 1.93                     | 0.86              |
| 1:J:797:PHE:CD1  | 3:L:149:VAL:HG12 | 2.06                     | 0.86              |
| 1:A:95:THR:OG1   | 1:A:769:ALA:HA   | 1.74                     | 0.86              |
| 1:D:310:TYR:CZ   | 1:D:320:ILE:HD11 | 2.11                     | 0.86              |
| 1:D:735:GLY:C    | 1:D:743:ALA:HB2  | 1.82                     | 0.86              |
| 1:D:800:ARG:HB3  | 3:F:149:VAL:HG21 | 1.57                     | 0.86              |
| 1:G:646:PHE:CD2  | 1:G:652:LEU:HD11 | 2.09                     | 0.86              |
| 2:K:137:TRP:HA   | 2:K:145:ALA:CB   | 2.04                     | 0.86              |
| 1:A:542:PHE:HA   | 4:4:143:TYR:HE1  | 1.34                     | 0.86              |
| 1:D:530:MET:HG2  | 4:5:354:GLN:CG   | 2.05                     | 0.86              |
| 1:G:107:MLY:HB3  | 1:G:686:MET:HE2  | 1.58                     | 0.86              |
| 1:J:599:ASN:OD1  | 1:J:649:VAL:HB   | 1.73                     | 0.86              |
| 1:J:72:VAL:CG1   | 1:J:76:GLN:HB3   | 2.05                     | 0.86              |
| 1:A:636:LYS:H    | 4:4:334:GLU:CD   | 1.77                     | 0.86              |
| 1:A:502:GLU:HA   | 1:A:762:HIS:N    | 1.90                     | 0.86              |
| 2:E:149:ASP:CG   | 2:E:150:TYR:H    | 1.73                     | 0.86              |
| 3:F:24:LYS:HB3   | 3:F:63:ILE:O     | 1.72                     | 0.86              |
| 1:G:530:MET:HG2  | 4:6:354:GLN:CG   | 2.05                     | 0.86              |
| 1:J:310:TYR:CZ   | 1:J:320:ILE:HD11 | 2.11                     | 0.86              |
| 1:J:530:MET:HG2  | 4:7:354:GLN:CG   | 2.06                     | 0.86              |
| 4:4:287:ILE:CG2  | 4:6:205:GLU:HG2  | 2.05                     | 0.86              |
| 4:6:322:PRO:HB2  | 4:8:244:ASP:CG   | 1.94                     | 0.86              |
| 1:D:206:LYS:HD3  | 1:D:217:THR:CB   | 2.06                     | 0.86              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:72:VAL:CG1   | 1:D:76:GLN:HB3   | 2.05                     | 0.86              |
| 1:D:769:ALA:C    | 1:D:770:GLY:O    | 2.14                     | 0.86              |
| 1:G:206:LYS:HD3  | 1:G:217:THR:CB   | 2.06                     | 0.86              |
| 1:G:755:HIS:HA   | 1:G:758:TYR:CE1  | 2.10                     | 0.86              |
| 1:G:84:MLY:CH1   | 1:G:715:VAL:HG12 | 2.05                     | 0.86              |
| 4:V:287:ILE:CG2  | 4:X:205:GLU:HG2  | 2.05                     | 0.86              |
| 1:D:814:PHE:HD1  | 2:E:127:ARG:NH2  | 1.70                     | 0.86              |
| 1:A:538:GLU:N    | 4:4:351:THR:N    | 2.24                     | 0.86              |
| 1:A:793:ARG:HG3  | 3:C:146:ILE:HG22 | 1.58                     | 0.86              |
| 1:D:724:TYR:HE1  | 1:D:778:MET:CB   | 1.89                     | 0.86              |
| 1:J:755:HIS:HA   | 1:J:758:TYR:CE1  | 2.10                     | 0.86              |
| 1:A:538:GLU:OE2  | 4:4:355:MET:HE3  | 1.73                     | 0.85              |
| 1:A:641:LYS:CD   | 1:A:647:GLN:OE1  | 2.17                     | 0.85              |
| 1:A:755:HIS:HA   | 1:A:758:TYR:CE1  | 2.10                     | 0.85              |
| 2:E:163:ALA:HA   | 2:K:21:GLU:HB3   | 1.55                     | 0.85              |
| 1:G:798:LEU:HD11 | 3:I:126:LEU:CG   | 2.06                     | 0.85              |
| 1:J:206:LYS:HD3  | 1:J:217:THR:CB   | 2.06                     | 0.85              |
| 1:A:599:ASN:OD1  | 1:A:649:VAL:CA   | 2.25                     | 0.85              |
| 2:B:117:LEU:CG   | 2:B:147:ASN:CG   | 2.44                     | 0.85              |
| 1:G:215:GLN:H    | 1:G:340:ILE:HG12 | 1.06                     | 0.85              |
| 1:J:410:ASN:OD1  | 4:7:334:GLU:CA   | 2.24                     | 0.85              |
| 1:A:831:TRP:CD1  | 2:B:51:PHE:CZ    | 2.49                     | 0.85              |
| 1:A:97:LEU:HD22  | 1:A:712:PRO:HB3  | 1.58                     | 0.85              |
| 2:E:117:LEU:CG   | 2:E:147:ASN:CG   | 2.44                     | 0.85              |
| 1:G:204:GLU:H    | 1:G:207:LYS:HE3  | 1.42                     | 0.85              |
| 2:H:117:LEU:CG   | 2:H:147:ASN:CG   | 2.45                     | 0.85              |
| 1:J:646:PHE:CD2  | 1:J:652:LEU:HD11 | 2.09                     | 0.85              |
| 1:J:797:PHE:HA   | 3:L:149:VAL:HG11 | 1.58                     | 0.85              |
| 3:I:139:TYR:HA   | 3:I:142:PHE:HB3  | 1.56                     | 0.85              |
| 1:J:630:ALA:C    | 4:7:25:ASP:OD2   | 2.15                     | 0.85              |
| 1:D:507:GLY:O    | 1:D:761:GLY:HA2  | 1.75                     | 0.85              |
| 1:D:732:ILE:HG23 | 1:D:747:LEU:HB2  | 1.57                     | 0.85              |
| 1:G:202:SER:HA   | 1:G:207:LYS:HE2  | 0.85                     | 0.85              |
| 1:G:599:ASN:OD1  | 1:G:649:VAL:CA   | 2.25                     | 0.85              |
| 1:G:725:ARG:CZ   | 1:G:733:PRO:HB3  | 2.05                     | 0.85              |
| 4:7:287:ILE:CG2  | 4:V:205:GLU:HG2  | 2.05                     | 0.85              |
| 4:6:287:ILE:CG2  | 4:8:205:GLU:HG2  | 2.05                     | 0.85              |
| 1:A:204:GLU:H    | 1:A:207:LYS:HE3  | 1.42                     | 0.85              |
| 1:A:206:LYS:HD3  | 1:A:217:THR:CB   | 2.06                     | 0.85              |
| 1:A:410:ASN:OD1  | 4:4:334:GLU:CA   | 2.25                     | 0.85              |
| 1:G:752:ASP:OD2  | 1:G:783:LEU:HB2  | 1.77                     | 0.85              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:640:LYS:CB   | 1:J:645:SER:OG   | 2.25                     | 0.85              |
| 2:K:117:LEU:CG   | 2:K:147:ASN:CG   | 2.44                     | 0.85              |
| 4:X:287:ILE:CG2  | 4:Z:205:GLU:HG2  | 2.05                     | 0.85              |
| 1:D:630:ALA:C    | 4:5:25:ASP:OD2   | 2.15                     | 0.85              |
| 1:A:202:SER:HA   | 1:A:207:LYS:HE2  | 0.85                     | 0.85              |
| 1:A:800:ARG:HH11 | 3:C:149:VAL:CG1  | 1.90                     | 0.85              |
| 1:D:599:ASN:OD1  | 1:D:649:VAL:CA   | 2.25                     | 0.85              |
| 1:G:310:TYR:CZ   | 1:G:320:ILE:HD11 | 2.11                     | 0.85              |
| 1:G:707:CYS:HB3  | 1:G:714:ARG:HH12 | 0.75                     | 0.85              |
| 1:A:630:ALA:C    | 4:4:25:ASP:OD2   | 2.15                     | 0.85              |
| 1:A:646:PHE:CD2  | 1:A:652:LEU:HD11 | 2.09                     | 0.85              |
| 1:A:797:PHE:CD2  | 3:C:126:LEU:CD2  | 2.59                     | 0.85              |
| 1:D:204:GLU:H    | 1:D:207:LYS:HE3  | 1.42                     | 0.85              |
| 1:D:418:THR:HB   | 1:D:421:GLU:HG3  | 1.59                     | 0.85              |
| 1:D:769:ALA:CB   | 1:D:770:GLY:C    | 2.45                     | 0.85              |
| 1:G:410:ASN:OD1  | 4:6:334:GLU:CA   | 2.24                     | 0.85              |
| 1:J:797:PHE:CB   | 3:L:149:VAL:CG1  | 2.54                     | 0.85              |
| 4:2:287:ILE:CG2  | 4:4:205:GLU:HG2  | 2.05                     | 0.85              |
| 1:D:410:ASN:OD1  | 4:5:334:GLU:CA   | 2.24                     | 0.85              |
| 1:A:725:ARG:CD   | 1:A:733:PRO:HB3  | 2.07                     | 0.85              |
| 1:D:792:ALA:HB1  | 3:F:40:ASN:HB2   | 1.55                     | 0.85              |
| 1:J:725:ARG:CZ   | 1:J:733:PRO:HB3  | 2.06                     | 0.85              |
| 1:A:640:LYS:C    | 4:4:23:GLY:O     | 2.15                     | 0.84              |
| 1:A:530:MET:HE1  | 4:4:355:MET:SD   | 2.17                     | 0.84              |
| 4:5:287:ILE:CG2  | 4:7:205:GLU:HG2  | 2.05                     | 0.84              |
| 1:J:529:PRO:CB   | 4:7:353:GLN:OE1  | 2.25                     | 0.84              |
| 1:G:732:ILE:HG23 | 1:G:747:LEU:HB2  | 1.57                     | 0.84              |
| 1:G:725:ARG:CD   | 1:G:733:PRO:HB3  | 2.07                     | 0.84              |
| 1:J:410:ASN:ND2  | 4:7:336:LYS:HG2  | 1.92                     | 0.84              |
| 2:K:121:LEU:CA   | 2:K:128:PHE:CB   | 2.46                     | 0.84              |
| 4:8:287:ILE:CG2  | 4:W:205:GLU:HG2  | 2.05                     | 0.84              |
| 1:A:836:PHE:HB3  | 2:B:161:GLU:HG2  | 1.57                     | 0.84              |
| 1:D:202:SER:HA   | 1:D:207:LYS:HE2  | 0.85                     | 0.84              |
| 1:J:543:PRO:HG3  | 4:7:143:TYR:O    | 1.77                     | 0.84              |
| 1:J:800:ARG:HD2  | 3:L:149:VAL:HG23 | 0.85                     | 0.84              |
| 1:J:821:ARG:HH22 | 2:K:127:ARG:CD   | 1.89                     | 0.84              |
| 4:3:287:ILE:CG2  | 4:5:205:GLU:HG2  | 2.05                     | 0.84              |
| 1:G:410:ASN:ND2  | 4:6:336:LYS:HG2  | 1.92                     | 0.84              |
| 1:G:538:GLU:N    | 4:6:351:THR:N    | 2.24                     | 0.84              |
| 1:A:822:SER:OG   | 2:B:88:LEU:HA    | 1.77                     | 0.84              |
| 1:A:795:ARG:NH2  | 3:C:116:GLU:CB   | 2.36                     | 0.84              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:553:MLY:HG2  | 4:8:47:MET:H     | 1.43                     | 0.84              |
| 1:J:418:THR:HB   | 1:J:421:GLU:HG3  | 1.60                     | 0.84              |
| 1:J:510:TRP:CZ3  | 1:J:772:LEU:HD21 | 2.11                     | 0.84              |
| 1:J:757:GLN:NE2  | 1:J:776:GLU:CG   | 2.39                     | 0.84              |
| 2:B:121:LEU:CA   | 2:B:128:PHE:CB   | 2.46                     | 0.84              |
| 1:J:202:SER:HA   | 1:J:207:LYS:HE2  | 0.85                     | 0.84              |
| 1:J:640:LYS:C    | 4:7:23:GLY:O     | 2.15                     | 0.84              |
| 1:J:732:ILE:HG23 | 1:J:747:LEU:CB   | 1.85                     | 0.84              |
| 1:A:635:GLY:HA2  | 4:4:334:GLU:CG   | 2.03                     | 0.84              |
| 1:A:800:ARG:NH1  | 3:C:149:VAL:O    | 2.10                     | 0.84              |
| 1:D:732:ILE:HG21 | 1:D:747:LEU:HD13 | 0.91                     | 0.84              |
| 1:D:769:ALA:HA   | 1:D:771:LEU:CB   | 2.07                     | 0.84              |
| 1:D:817:GLN:NE2  | 2:E:127:ARG:CG   | 2.40                     | 0.84              |
| 1:G:735:GLY:C    | 1:G:743:ALA:HB2  | 1.82                     | 0.84              |
| 1:G:768:MLY:CD   | 1:G:772:LEU:HD22 | 2.06                     | 0.84              |
| 1:G:730:SER:OG   | 3:I:109:HIS:NE2  | 2.09                     | 0.84              |
| 1:J:732:ILE:HG23 | 1:J:747:LEU:HB2  | 1.57                     | 0.84              |
| 1:J:754:ASP:OD2  | 1:J:776:GLU:HA   | 1.77                     | 0.84              |
| 1:D:640:LYS:C    | 4:5:23:GLY:O     | 2.15                     | 0.84              |
| 1:D:529:PRO:CB   | 4:5:353:GLN:OE1  | 2.25                     | 0.84              |
| 1:A:310:TYR:CZ   | 1:A:320:ILE:HD11 | 2.11                     | 0.84              |
| 1:A:732:ILE:HG23 | 1:A:747:LEU:HB2  | 1.57                     | 0.84              |
| 1:D:557:GLU:H    | 4:7:48:GLY:HA3   | 1.28                     | 0.84              |
| 1:J:735:GLY:C    | 1:J:743:ALA:HB1  | 1.84                     | 0.84              |
| 4:W:287:ILE:CG2  | 4:Y:205:GLU:HG2  | 2.05                     | 0.84              |
| 1:J:649:VAL:HG12 | 1:J:649:VAL:C    | 1.98                     | 0.84              |
| 4:5:237:GLU:HA   | 4:5:251:GLY:HA2  | 1.60                     | 0.84              |
| 1:G:557:GLU:N    | 4:8:48:GLY:HA2   | 1.91                     | 0.84              |
| 1:A:814:PHE:HA   | 2:B:127:ARG:NH2  | 1.93                     | 0.84              |
| 1:D:641:LYS:HG3  | 1:D:647:GLN:NE2  | 1.59                     | 0.84              |
| 1:D:649:VAL:C    | 1:D:649:VAL:HG12 | 1.98                     | 0.84              |
| 1:G:648:THR:CG2  | 1:G:651:ALA:HB2  | 2.08                     | 0.84              |
| 1:J:204:GLU:H    | 1:J:207:LYS:HE3  | 1.41                     | 0.84              |
| 1:J:753:VAL:HA   | 1:J:780:ASP:OD2  | 1.78                     | 0.84              |
| 4:3:237:GLU:HA   | 4:3:251:GLY:HA2  | 1.60                     | 0.84              |
| 1:A:410:ASN:ND2  | 4:4:336:LYS:HG2  | 1.93                     | 0.84              |
| 4:7:237:GLU:HA   | 4:7:251:GLY:HA2  | 1.60                     | 0.84              |
| 1:D:640:LYS:CB   | 1:D:645:SER:OG   | 2.25                     | 0.84              |
| 1:D:629:GLU:CG   | 1:D:643:GLY:O    | 2.26                     | 0.84              |
| 1:G:788:THR:C    | 3:I:42:THR:CG2   | 2.34                     | 0.84              |
| 1:J:629:GLU:CG   | 1:J:643:GLY:O    | 2.26                     | 0.84              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:X:286:ASP:OD1  | 4:Z:203:THR:CG2  | 2.26                     | 0.84              |
| 4:0:286:ASP:OD1  | 4:2:203:THR:CG2  | 2.26                     | 0.84              |
| 4:1:286:ASP:OD1  | 4:3:203:THR:CG2  | 2.26                     | 0.84              |
| 1:A:542:PHE:CA   | 4:4:143:TYR:CE1  | 2.61                     | 0.84              |
| 2:H:141:PRO:CB   | 2:H:142:PRO:CD   | 2.56                     | 0.84              |
| 4:1:237:GLU:HA   | 4:1:251:GLY:HA2  | 1.60                     | 0.83              |
| 1:D:538:GLU:N    | 4:5:351:THR:N    | 2.25                     | 0.83              |
| 1:A:797:PHE:CE2  | 3:C:126:LEU:HD23 | 2.07                     | 0.83              |
| 1:D:730:SER:O    | 1:D:734:GLU:HG3  | 1.78                     | 0.83              |
| 1:G:635:GLY:HA2  | 4:6:334:GLU:CG   | 2.03                     | 0.83              |
| 1:J:599:ASN:OD1  | 1:J:649:VAL:CA   | 2.25                     | 0.83              |
| 1:J:95:THR:OG1   | 1:J:713:SER:CB   | 2.25                     | 0.83              |
| 1:A:543:PRO:HG3  | 4:4:143:TYR:O    | 1.77                     | 0.83              |
| 4:3:286:ASP:OD1  | 4:5:203:THR:CG2  | 2.26                     | 0.83              |
| 1:D:410:ASN:ND2  | 4:5:336:LYS:HG2  | 1.92                     | 0.83              |
| 1:A:648:THR:CG2  | 1:A:651:ALA:HB2  | 2.08                     | 0.83              |
| 1:A:798:LEU:HD13 | 3:C:126:LEU:CD2  | 1.95                     | 0.83              |
| 1:D:648:THR:CG2  | 1:D:651:ALA:HB2  | 2.08                     | 0.83              |
| 1:D:725:ARG:CD   | 1:D:733:PRO:HB3  | 2.07                     | 0.83              |
| 1:J:783:LEU:O    | 1:J:787:ILE:HB   | 1.79                     | 0.83              |
| 2:K:141:PRO:CB   | 2:K:142:PRO:CD   | 2.56                     | 0.83              |
| 4:V:237:GLU:HA   | 4:V:251:GLY:HA2  | 1.60                     | 0.83              |
| 1:J:542:PHE:CA   | 4:7:143:TYR:CE1  | 2.61                     | 0.83              |
| 1:A:768:MLY:CB   | 1:A:771:LEU:HD13 | 2.08                     | 0.83              |
| 1:D:724:TYR:CE1  | 1:D:778:MET:CB   | 2.61                     | 0.83              |
| 1:G:549:SER:O    | 4:8:46:GLY:HA3   | 1.78                     | 0.83              |
| 1:G:640:LYS:C    | 4:6:23:GLY:O     | 2.16                     | 0.83              |
| 1:G:736:GLN:HA   | 1:G:743:ALA:HB2  | 1.51                     | 0.83              |
| 1:G:819:ASN:CG   | 2:H:92:ASP:CB    | 2.47                     | 0.83              |
| 4:V:286:ASP:OD1  | 4:X:203:THR:CG2  | 2.26                     | 0.83              |
| 1:A:599:ASN:OD1  | 1:A:649:VAL:HB   | 1.72                     | 0.83              |
| 1:G:529:PRO:CB   | 4:6:353:GLN:OE1  | 2.25                     | 0.83              |
| 1:G:795:ARG:HB2  | 3:I:35:ARG:NH2   | 1.91                     | 0.83              |
| 4:2:286:ASP:OD1  | 4:4:203:THR:CG2  | 2.26                     | 0.83              |
| 1:G:542:PHE:CA   | 4:6:143:TYR:CE1  | 2.61                     | 0.83              |
| 1:D:732:ILE:CG2  | 1:D:747:LEU:HD13 | 1.34                     | 0.83              |
| 1:G:640:LYS:CB   | 1:G:645:SER:OG   | 2.25                     | 0.83              |
| 1:J:795:ARG:CZ   | 3:L:35:ARG:HH12  | 1.92                     | 0.83              |
| 4:1:287:ILE:CG2  | 4:3:205:GLU:HG2  | 2.05                     | 0.83              |
| 1:A:549:SER:O    | 4:6:46:GLY:HA3   | 1.77                     | 0.83              |
| 1:A:553:MLY:HG2  | 4:6:47:MET:H     | 1.44                     | 0.83              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:646:PHE:CE2  | 1:A:652:LEU:CD1  | 2.58                     | 0.83              |
| 1:A:831:TRP:HZ3  | 2:B:50:THR:HG21  | 1.44                     | 0.83              |
| 1:J:218:LEU:HB3  | 1:J:221:GLN:HG3  | 1.60                     | 0.83              |
| 1:J:549:SER:O    | 4:V:46:GLY:HA3   | 1.78                     | 0.83              |
| 1:J:817:GLN:HB3  | 2:K:127:ARG:HH11 | 1.44                     | 0.83              |
| 4:X:237:GLU:HA   | 4:X:251:GLY:HA2  | 1.60                     | 0.83              |
| 1:D:549:SER:O    | 4:7:46:GLY:HA3   | 1.77                     | 0.83              |
| 1:A:629:GLU:CG   | 1:A:643:GLY:O    | 2.26                     | 0.83              |
| 2:B:141:PRO:CB   | 2:B:142:PRO:CD   | 2.56                     | 0.83              |
| 1:D:725:ARG:CZ   | 1:D:733:PRO:HB3  | 2.05                     | 0.83              |
| 1:D:834:LEU:HD11 | 2:E:54:MET:HB2   | 1.56                     | 0.83              |
| 1:J:730:SER:O    | 1:J:734:GLU:HG3  | 1.79                     | 0.83              |
| 4:Z:237:GLU:HA   | 4:Z:251:GLY:HA2  | 1.60                     | 0.83              |
| 1:A:529:PRO:CB   | 4:4:353:GLN:OE1  | 2.25                     | 0.83              |
| 4:5:286:ASP:OD1  | 4:7:203:THR:CG2  | 2.26                     | 0.83              |
| 1:J:538:GLU:N    | 4:7:351:THR:N    | 2.24                     | 0.83              |
| 4:6:286:ASP:OD1  | 4:8:203:THR:CG2  | 2.26                     | 0.83              |
| 1:A:506:GLU:H    | 1:A:761:GLY:HA2  | 1.43                     | 0.83              |
| 2:E:141:PRO:CB   | 2:E:142:PRO:CD   | 2.56                     | 0.83              |
| 2:H:144:VAL:HG12 | 2:H:153:ILE:CD1  | 2.09                     | 0.83              |
| 1:A:732:ILE:CG2  | 1:A:747:LEU:HD13 | 1.34                     | 0.83              |
| 1:G:418:THR:HB   | 1:G:421:GLU:HG3  | 1.59                     | 0.83              |
| 1:G:791:GLN:OE1  | 3:I:116:GLU:CB   | 2.27                     | 0.83              |
| 1:J:279:LEU:HB2  | 1:J:282:GLU:HG3  | 1.60                     | 0.83              |
| 4:0:237:GLU:HA   | 4:0:251:GLY:HA2  | 1.60                     | 0.83              |
| 4:7:286:ASP:OD1  | 4:V:203:THR:CG2  | 2.26                     | 0.83              |
| 1:A:836:PHE:HE1  | 2:B:159:HIS:CA   | 1.92                     | 0.83              |
| 1:D:279:LEU:HB2  | 1:D:282:GLU:HG3  | 1.60                     | 0.83              |
| 1:D:553:MLY:HG2  | 4:7:47:MET:H     | 1.44                     | 0.83              |
| 2:E:121:LEU:CA   | 2:E:128:PHE:CB   | 2.46                     | 0.83              |
| 4:8:286:ASP:OD1  | 4:W:203:THR:CG2  | 2.26                     | 0.83              |
| 4:X:290:ARG:NH1  | 4:Z:202:THR:HG21 | 1.94                     | 0.83              |
| 4:0:290:ARG:NH1  | 4:2:202:THR:HG21 | 1.94                     | 0.82              |
| 1:D:641:LYS:HG2  | 1:D:647:GLN:HG3  | 1.61                     | 0.82              |
| 1:G:543:PRO:HG3  | 4:6:143:TYR:O    | 1.78                     | 0.82              |
| 1:J:831:TRP:CH2  | 2:K:34:ILE:HG21  | 2.14                     | 0.82              |
| 4:1:290:ARG:NH1  | 4:3:202:THR:HG21 | 1.95                     | 0.82              |
| 4:2:290:ARG:NH1  | 4:4:202:THR:HG21 | 1.94                     | 0.82              |
| 4:4:290:ARG:NH1  | 4:6:202:THR:HG21 | 1.94                     | 0.82              |
| 1:D:542:PHE:CA   | 4:5:143:TYR:CE1  | 2.61                     | 0.82              |
| 1:G:538:GLU:OE2  | 4:6:355:MET:HE3  | 1.78                     | 0.82              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:8:290:ARG:NH1  | 4:W:202:THR:HG21 | 1.94                     | 0.82              |
| 1:A:499:GLU:OE1  | 1:A:766:PHE:HZ   | 1.61                     | 0.82              |
| 1:A:814:PHE:HD1  | 2:B:127:ARG:HH22 | 1.14                     | 0.82              |
| 1:J:549:SER:O    | 4:V:46:GLY:CA    | 2.27                     | 0.82              |
| 2:K:111:SER:OG   | 2:K:148:VAL:C    | 2.15                     | 0.82              |
| 4:W:286:ASP:OD1  | 4:Y:203:THR:CG2  | 2.26                     | 0.82              |
| 1:J:542:PHE:CA   | 4:7:143:TYR:HE1  | 1.92                     | 0.82              |
| 1:A:418:THR:HB   | 1:A:421:GLU:HG3  | 1.60                     | 0.82              |
| 1:D:831:TRP:HH2  | 2:E:47:LEU:HA    | 1.43                     | 0.82              |
| 4:2:237:GLU:HA   | 4:2:251:GLY:HA2  | 1.60                     | 0.82              |
| 4:6:290:ARG:NH1  | 4:8:202:THR:HG21 | 1.94                     | 0.82              |
| 1:A:557:GLU:H    | 4:6:48:GLY:HA3   | 1.28                     | 0.82              |
| 1:A:578:HIS:HB3  | 1:A:592:ILE:HD12 | 1.62                     | 0.82              |
| 1:A:795:ARG:NH1  | 3:C:43:ASN:H     | 1.78                     | 0.82              |
| 1:J:641:LYS:HG2  | 1:J:647:GLN:HG3  | 1.61                     | 0.82              |
| 1:G:556:ASP:HA   | 4:8:49:GLN:O     | 1.69                     | 0.82              |
| 1:A:735:GLY:C    | 1:A:743:ALA:HB2  | 1.82                     | 0.82              |
| 1:G:629:GLU:CG   | 1:G:643:GLY:O    | 2.26                     | 0.82              |
| 1:G:769:ALA:HB3  | 1:G:770:GLY:HA2  | 0.83                     | 0.82              |
| 1:J:648:THR:CG2  | 1:J:651:ALA:HB2  | 2.08                     | 0.82              |
| 1:J:90:ASP:OD2   | 1:J:764:MLY:CH1  | 2.27                     | 0.82              |
| 4:W:290:ARG:NH1  | 4:Y:202:THR:HG21 | 1.94                     | 0.82              |
| 1:G:549:SER:O    | 4:8:46:GLY:C     | 2.18                     | 0.82              |
| 1:A:107:MLY:HB3  | 1:A:686:MET:HE2  | 1.61                     | 0.82              |
| 1:D:218:LEU:HD22 | 1:D:222:ILE:CG1  | 2.10                     | 0.82              |
| 1:G:218:LEU:HD22 | 1:G:222:ILE:CG1  | 2.09                     | 0.82              |
| 1:G:549:SER:O    | 4:8:46:GLY:CA    | 2.27                     | 0.82              |
| 1:J:127:ASN:HD22 | 1:J:128:PRO:HD2  | 1.44                     | 0.82              |
| 1:J:218:LEU:HD22 | 1:J:222:ILE:CG1  | 2.10                     | 0.82              |
| 1:J:549:SER:O    | 4:V:46:GLY:C     | 2.18                     | 0.82              |
| 4:V:290:ARG:NH1  | 4:X:202:THR:HG21 | 1.95                     | 0.82              |
| 4:Y:237:GLU:HA   | 4:Y:251:GLY:HA2  | 1.60                     | 0.82              |
| 4:4:286:ASP:OD1  | 4:6:203:THR:CG2  | 2.26                     | 0.82              |
| 4:3:290:ARG:NH1  | 4:5:202:THR:HG21 | 1.95                     | 0.82              |
| 1:G:643:GLY:N    | 4:6:24:ASP:HA    | 1.94                     | 0.82              |
| 1:J:643:GLY:N    | 4:7:24:ASP:HA    | 1.93                     | 0.82              |
| 1:D:543:PRO:HG3  | 4:5:143:TYR:O    | 1.77                     | 0.82              |
| 1:D:817:GLN:NE2  | 2:E:127:ARG:HE   | 1.77                     | 0.82              |
| 1:G:279:LEU:HB2  | 1:G:282:GLU:HG3  | 1.60                     | 0.82              |
| 1:G:578:HIS:HB3  | 1:G:592:ILE:HD12 | 1.62                     | 0.82              |
| 1:J:218:LEU:HA   | 1:J:221:GLN:HG2  | 1.62                     | 0.82              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:542:PHE:CA   | 4:4:143:TYR:HE1  | 1.92                     | 0.82              |
| 1:A:127:ASN:HD22 | 1:A:128:PRO:HD2  | 1.45                     | 0.82              |
| 1:A:279:LEU:HB2  | 1:A:282:GLU:HG3  | 1.60                     | 0.82              |
| 1:D:817:GLN:OE1  | 2:E:127:ARG:CZ   | 2.28                     | 0.82              |
| 1:D:834:LEU:HD21 | 2:E:54:MET:CG    | 2.09                     | 0.82              |
| 1:J:725:ARG:CD   | 1:J:733:PRO:HB3  | 2.07                     | 0.82              |
| 1:J:816:ILE:HD11 | 2:K:100:ALA:HB1  | 1.59                     | 0.82              |
| 1:A:641:LYS:HG2  | 1:A:647:GLN:HG3  | 1.61                     | 0.82              |
| 1:A:768:MLY:C    | 1:A:771:LEU:CB   | 2.57                     | 0.82              |
| 1:G:95:THR:OG1   | 1:G:713:SER:HB3  | 1.79                     | 0.82              |
| 1:J:599:ASN:CA   | 1:J:649:VAL:CB   | 2.53                     | 0.82              |
| 1:J:721:LYS:CA   | 1:J:736:GLN:NE2  | 2.43                     | 0.82              |
| 1:J:757:GLN:HG2  | 1:J:776:GLU:HG3  | 0.82                     | 0.82              |
| 1:A:218:LEU:HD22 | 1:A:222:ILE:CG1  | 2.10                     | 0.82              |
| 1:D:218:LEU:HB3  | 1:D:221:GLN:HG3  | 1.60                     | 0.82              |
| 1:D:809:ARG:CZ   | 2:E:124:GLY:HA3  | 2.10                     | 0.82              |
| 1:D:817:GLN:NE2  | 2:E:127:ARG:NE   | 2.28                     | 0.82              |
| 1:G:730:SER:O    | 1:G:734:GLU:HG3  | 1.78                     | 0.82              |
| 1:A:639:GLY:CA   | 4:4:344:SER:C    | 2.48                     | 0.81              |
| 1:D:549:SER:O    | 4:7:46:GLY:C     | 2.18                     | 0.81              |
| 1:J:734:GLU:O    | 1:J:738:MET:CG   | 2.28                     | 0.81              |
| 1:J:821:ARG:HH22 | 2:K:127:ARG:CG   | 1.84                     | 0.81              |
| 4:4:237:GLU:HA   | 4:4:251:GLY:HA2  | 1.60                     | 0.81              |
| 4:7:290:ARG:NH1  | 4:V:202:THR:HG21 | 1.94                     | 0.81              |
| 1:D:549:SER:O    | 4:7:46:GLY:CA    | 2.27                     | 0.81              |
| 1:A:640:LYS:CB   | 1:A:645:SER:OG   | 2.25                     | 0.81              |
| 1:A:730:SER:O    | 1:A:734:GLU:HG3  | 1.78                     | 0.81              |
| 1:D:734:GLU:O    | 1:D:738:MET:CG   | 2.28                     | 0.81              |
| 4:W:237:GLU:HA   | 4:W:251:GLY:HA2  | 1.60                     | 0.81              |
| 1:D:643:GLY:N    | 4:5:24:ASP:HA    | 1.93                     | 0.81              |
| 4:6:237:GLU:HA   | 4:6:251:GLY:HA2  | 1.60                     | 0.81              |
| 1:A:553:MLY:CB   | 4:6:46:GLY:CA    | 2.32                     | 0.81              |
| 1:A:831:TRP:CZ3  | 2:B:50:THR:HG21  | 2.15                     | 0.81              |
| 1:D:834:LEU:HD21 | 2:E:54:MET:HG3   | 1.62                     | 0.81              |
| 1:G:734:GLU:O    | 1:G:738:MET:CG   | 2.28                     | 0.81              |
| 1:J:480:ILE:HG22 | 1:J:481:ASN:HD22 | 1.45                     | 0.81              |
| 1:A:549:SER:O    | 4:6:46:GLY:CA    | 2.28                     | 0.81              |
| 4:8:237:GLU:HA   | 4:8:251:GLY:HA2  | 1.60                     | 0.81              |
| 2:B:111:SER:OG   | 2:B:148:VAL:C    | 2.15                     | 0.81              |
| 1:A:798:LEU:HD12 | 3:C:126:LEU:HD21 | 1.58                     | 0.81              |
| 1:D:571:ALA:O    | 1:D:572:LYS:CG   | 2.28                     | 0.81              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:639:GLY:CA   | 4:5:344:SER:C    | 2.48                     | 0.81              |
| 1:D:830:PRO:HD2  | 2:E:67:MET:HE1   | 1.63                     | 0.81              |
| 1:G:232:PHE:CZ   | 1:G:287:ILE:HD13 | 2.16                     | 0.81              |
| 1:J:578:HIS:HB3  | 1:J:592:ILE:HD12 | 1.62                     | 0.81              |
| 2:K:121:LEU:CG   | 2:K:128:PHE:CA   | 2.48                     | 0.81              |
| 1:J:639:GLY:CA   | 4:7:344:SER:C    | 2.48                     | 0.81              |
| 1:A:549:SER:O    | 4:6:46:GLY:C     | 2.19                     | 0.81              |
| 1:D:127:ASN:HD22 | 1:D:128:PRO:HD2  | 1.45                     | 0.81              |
| 1:D:557:GLU:N    | 4:7:48:GLY:HA2   | 1.90                     | 0.81              |
| 1:D:792:ALA:HB1  | 3:F:40:ASN:HB3   | 1.62                     | 0.81              |
| 1:G:641:LYS:HG2  | 1:G:647:GLN:HG3  | 1.61                     | 0.81              |
| 1:G:800:ARG:HD2  | 3:I:149:VAL:HG22 | 1.61                     | 0.81              |
| 1:J:510:TRP:CZ2  | 1:J:768:MLY:CH1  | 2.58                     | 0.81              |
| 1:J:768:MLY:CH2  | 1:J:772:LEU:CB   | 2.35                     | 0.81              |
| 1:A:218:LEU:HA   | 1:A:221:GLN:HG2  | 1.62                     | 0.81              |
| 1:A:834:LEU:CD1  | 2:B:54:MET:HB3   | 2.08                     | 0.81              |
| 1:A:789:ALA:CB   | 3:C:87:PHE:HE2   | 1.94                     | 0.81              |
| 1:D:550:PHE:CA   | 4:7:46:GLY:CA    | 2.59                     | 0.81              |
| 1:D:578:HIS:HD2  | 1:D:591:ASN:HA   | 1.45                     | 0.81              |
| 1:G:127:ASN:HD22 | 1:G:128:PRO:HD2  | 1.45                     | 0.81              |
| 1:J:550:PHE:CA   | 4:V:46:GLY:CA    | 2.59                     | 0.81              |
| 1:D:542:PHE:CA   | 4:5:143:TYR:HE1  | 1.92                     | 0.81              |
| 4:5:290:ARG:NH1  | 4:7:202:THR:HG21 | 1.94                     | 0.81              |
| 1:D:538:GLU:CA   | 4:5:351:THR:H    | 1.93                     | 0.81              |
| 1:A:643:GLY:N    | 4:4:24:ASP:HA    | 1.93                     | 0.81              |
| 1:J:553:MLY:HG2  | 4:V:47:MET:H     | 1.44                     | 0.81              |
| 4:5:223:PHE:HE1  | 4:5:255:PHE:HB2  | 1.46                     | 0.81              |
| 1:D:641:LYS:HD2  | 4:5:348:SER:CA   | 2.09                     | 0.81              |
| 1:A:538:GLU:CA   | 4:4:351:THR:H    | 1.93                     | 0.81              |
| 1:A:721:LYS:CA   | 1:A:736:GLN:NE2  | 2.43                     | 0.81              |
| 1:G:480:ILE:HG22 | 1:G:481:ASN:HD22 | 1.45                     | 0.81              |
| 4:2:223:PHE:HE1  | 4:2:255:PHE:HB2  | 1.46                     | 0.81              |
| 4:4:223:PHE:HE1  | 4:4:255:PHE:HB2  | 1.46                     | 0.81              |
| 4:7:223:PHE:HE1  | 4:7:255:PHE:HB2  | 1.46                     | 0.81              |
| 1:A:793:ARG:HE   | 3:C:147:MET:CG   | 1.94                     | 0.81              |
| 2:B:121:LEU:CG   | 2:B:128:PHE:CA   | 2.48                     | 0.81              |
| 1:D:218:LEU:CA   | 1:D:221:GLN:HG2  | 2.10                     | 0.81              |
| 1:D:107:MLY:HB3  | 1:D:686:MET:HE2  | 1.63                     | 0.81              |
| 1:D:723:ARG:O    | 1:D:782:MLY:NZ   | 2.13                     | 0.81              |
| 1:G:530:MET:HE1  | 4:6:355:MET:SD   | 2.20                     | 0.81              |
| 1:G:721:LYS:CA   | 1:G:736:GLN:NE2  | 2.43                     | 0.81              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:144:VAL:HG12 | 2:K:153:ILE:CD1  | 2.10                     | 0.81              |
| 4:3:223:PHE:HE1  | 4:3:255:PHE:HB2  | 1.46                     | 0.81              |
| 1:G:639:GLY:CA   | 4:6:344:SER:C    | 2.48                     | 0.81              |
| 1:A:734:GLU:O    | 1:A:738:MET:CG   | 2.28                     | 0.81              |
| 1:D:724:TYR:CZ   | 1:D:778:MET:SD   | 2.73                     | 0.81              |
| 1:D:507:GLY:HA2  | 1:D:762:HIS:CE1  | 2.16                     | 0.81              |
| 1:D:792:ALA:CB   | 3:F:40:ASN:O     | 2.29                     | 0.81              |
| 1:D:831:TRP:CZ2  | 2:E:47:LEU:CG    | 2.63                     | 0.81              |
| 1:J:641:LYS:HD2  | 4:7:348:SER:CA   | 2.09                     | 0.81              |
| 1:A:232:PHE:CZ   | 1:A:287:ILE:HD13 | 2.16                     | 0.81              |
| 1:A:709:LYS:O    | 1:A:710:GLY:HA3  | 1.81                     | 0.81              |
| 1:D:218:LEU:HA   | 1:D:221:GLN:HG2  | 1.62                     | 0.81              |
| 1:D:724:TYR:O    | 1:D:782:MLY:HH11 | 1.80                     | 0.81              |
| 4:V:223:PHE:HE1  | 4:V:255:PHE:HB2  | 1.46                     | 0.81              |
| 4:0:223:PHE:HE1  | 4:0:255:PHE:HB2  | 1.46                     | 0.80              |
| 1:A:646:PHE:CE2  | 1:A:652:LEU:HD21 | 2.14                     | 0.80              |
| 1:G:641:LYS:HD2  | 4:6:348:SER:CA   | 2.10                     | 0.80              |
| 1:G:646:PHE:CE2  | 1:G:652:LEU:HD21 | 2.14                     | 0.80              |
| 1:J:218:LEU:CA   | 1:J:221:GLN:HG2  | 2.10                     | 0.80              |
| 1:J:538:GLU:CA   | 4:7:351:THR:H    | 1.93                     | 0.80              |
| 1:J:578:HIS:HD2  | 1:J:591:ASN:HA   | 1.45                     | 0.80              |
| 4:X:223:PHE:HE1  | 4:X:255:PHE:HB2  | 1.46                     | 0.80              |
| 1:A:641:LYS:HD2  | 4:4:348:SER:CA   | 2.09                     | 0.80              |
| 1:A:550:PHE:CA   | 4:6:46:GLY:CA    | 2.59                     | 0.80              |
| 1:A:725:ARG:CZ   | 1:A:733:PRO:HB3  | 2.06                     | 0.80              |
| 1:A:813:ILE:HG23 | 2:B:127:ARG:CD   | 1.94                     | 0.80              |
| 1:D:374:GLN:HG3  | 1:D:375:ALA:N    | 1.96                     | 0.80              |
| 1:D:721:LYS:CA   | 1:D:736:GLN:NE2  | 2.43                     | 0.80              |
| 1:G:571:ALA:O    | 1:G:572:LYS:CG   | 2.28                     | 0.80              |
| 1:G:836:PHE:CZ   | 2:H:159:HIS:HA   | 2.15                     | 0.80              |
| 1:J:800:ARG:HD2  | 3:L:149:VAL:CB   | 2.10                     | 0.80              |
| 4:Y:223:PHE:HE1  | 4:Y:255:PHE:HB2  | 1.46                     | 0.80              |
| 1:D:215:GLN:N    | 1:D:340:ILE:CD1  | 2.44                     | 0.80              |
| 1:D:723:ARG:O    | 1:D:782:MLY:CE   | 2.30                     | 0.80              |
| 2:K:141:PRO:CB   | 2:K:142:PRO:HD2  | 2.11                     | 0.80              |
| 1:J:798:LEU:CD2  | 3:L:126:LEU:CG   | 2.59                     | 0.80              |
| 1:G:553:MLY:NZ   | 4:8:45:VAL:HA    | 1.84                     | 0.80              |
| 2:B:144:VAL:CA   | 2:B:153:ILE:HD11 | 2.11                     | 0.80              |
| 1:D:818:TYR:CB   | 2:E:90:GLY:N     | 2.45                     | 0.80              |
| 1:G:93:MET:CE    | 1:G:763:THR:C    | 2.48                     | 0.80              |
| 1:J:215:GLN:N    | 1:J:340:ILE:CD1  | 2.44                     | 0.80              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:374:GLN:HG3  | 1:J:375:ALA:N    | 1.96                     | 0.80              |
| 4:Z:223:PHE:HE1  | 4:Z:255:PHE:HB2  | 1.46                     | 0.80              |
| 1:G:538:GLU:HG3  | 4:6:351:THR:C    | 2.02                     | 0.80              |
| 2:B:141:PRO:CB   | 2:B:142:PRO:HD2  | 2.11                     | 0.80              |
| 1:D:732:ILE:HG22 | 1:D:747:LEU:HD12 | 0.81                     | 0.80              |
| 1:D:831:TRP:HA   | 2:E:51:PHE:HE1   | 1.45                     | 0.80              |
| 1:D:797:PHE:HE2  | 3:F:126:LEU:CD2  | 1.93                     | 0.80              |
| 1:G:538:GLU:CA   | 4:6:351:THR:H    | 1.93                     | 0.80              |
| 1:A:215:GLN:N    | 1:A:340:ILE:CD1  | 2.44                     | 0.80              |
| 1:A:732:ILE:HG21 | 1:A:747:LEU:HD13 | 0.91                     | 0.80              |
| 1:D:578:HIS:HB3  | 1:D:592:ILE:HD12 | 1.62                     | 0.80              |
| 2:E:111:SER:OG   | 2:E:148:VAL:C    | 2.15                     | 0.80              |
| 1:D:822:SER:CB   | 2:E:88:LEU:CD2   | 2.52                     | 0.80              |
| 1:G:829:TRP:CH2  | 2:H:87:LYS:CE    | 2.63                     | 0.80              |
| 2:K:141:PRO:HB2  | 2:K:142:PRO:CD   | 2.11                     | 0.80              |
| 1:A:480:ILE:HG22 | 1:A:481:ASN:HD22 | 1.45                     | 0.80              |
| 1:J:93:MET:SD    | 1:J:716:LEU:CD1  | 2.67                     | 0.80              |
| 1:J:93:MET:HG3   | 1:J:764:MLY:CD   | 2.11                     | 0.80              |
| 1:G:542:PHE:CA   | 4:6:143:TYR:HE1  | 1.93                     | 0.80              |
| 4:6:223:PHE:HE1  | 4:6:255:PHE:HB2  | 1.46                     | 0.80              |
| 1:G:578:HIS:HD2  | 1:G:591:ASN:HA   | 1.44                     | 0.80              |
| 1:G:599:ASN:CA   | 1:G:649:VAL:CB   | 2.53                     | 0.80              |
| 1:G:732:ILE:HG22 | 1:G:747:LEU:HD12 | 0.81                     | 0.80              |
| 3:L:49:ILE:N     | 3:L:52:ASN:ND2   | 2.29                     | 0.80              |
| 4:1:223:PHE:HE1  | 4:1:255:PHE:HB2  | 1.46                     | 0.80              |
| 1:A:374:GLN:HG3  | 1:A:375:ALA:N    | 1.96                     | 0.80              |
| 1:A:578:HIS:HD2  | 1:A:591:ASN:HA   | 1.45                     | 0.80              |
| 1:D:232:PHE:CZ   | 1:D:287:ILE:HD13 | 2.16                     | 0.80              |
| 1:G:215:GLN:N    | 1:G:340:ILE:CD1  | 2.44                     | 0.80              |
| 1:G:798:LEU:CD2  | 3:I:122:GLU:HB3  | 2.10                     | 0.80              |
| 1:J:571:ALA:O    | 1:J:572:LYS:CG   | 2.28                     | 0.80              |
| 2:K:144:VAL:CA   | 2:K:153:ILE:HD11 | 2.11                     | 0.80              |
| 1:J:797:PHE:HB2  | 3:L:149:VAL:CG1  | 2.12                     | 0.80              |
| 1:G:218:LEU:HA   | 1:G:221:GLN:HG2  | 1.62                     | 0.80              |
| 1:G:550:PHE:CA   | 4:8:46:GLY:CA    | 2.59                     | 0.80              |
| 1:G:769:ALA:HB2  | 1:G:770:GLY:CA   | 2.12                     | 0.80              |
| 1:G:553:MLY:CB   | 4:8:46:GLY:CA    | 2.33                     | 0.79              |
| 1:A:732:ILE:HG22 | 1:A:747:LEU:HD12 | 0.81                     | 0.79              |
| 1:A:752:ASP:O    | 1:A:778:MET:SD   | 2.39                     | 0.79              |
| 3:C:49:ILE:N     | 3:C:52:ASN:ND2   | 2.29                     | 0.79              |
| 1:D:830:PRO:HB2  | 2:E:51:PHE:CE2   | 2.16                     | 0.79              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:F:49:ILE:N     | 3:F:52:ASN:ND2   | 2.29                     | 0.79              |
| 1:G:374:GLN:HG3  | 1:G:375:ALA:N    | 1.96                     | 0.79              |
| 1:J:232:PHE:CZ   | 1:J:287:ILE:HD13 | 2.16                     | 0.79              |
| 1:J:732:ILE:HG22 | 1:J:747:LEU:HD12 | 0.81                     | 0.79              |
| 1:J:838:ILE:CD1  | 2:K:54:MET:CE    | 2.61                     | 0.79              |
| 1:J:820:VAL:HG11 | 2:K:136:MET:HE3  | 1.64                     | 0.79              |
| 1:D:480:ILE:HG22 | 1:D:481:ASN:HD22 | 1.45                     | 0.79              |
| 1:J:84:MLY:HE2   | 1:J:719:ASP:CB   | 1.63                     | 0.79              |
| 1:J:784:ALA:O    | 1:J:788:THR:N    | 2.14                     | 0.79              |
| 4:6:287:ILE:HB   | 4:8:204:ALA:N    | 1.97                     | 0.79              |
| 1:A:571:ALA:O    | 1:A:572:LYS:CG   | 2.28                     | 0.79              |
| 1:D:736:GLN:HA   | 1:D:743:ALA:HB2  | 1.51                     | 0.79              |
| 2:E:144:VAL:HG12 | 2:E:153:ILE:CD1  | 2.10                     | 0.79              |
| 1:G:752:ASP:C    | 1:G:779:ARG:NH1  | 2.34                     | 0.79              |
| 1:J:732:ILE:CG2  | 1:J:747:LEU:HD13 | 1.34                     | 0.79              |
| 1:J:732:ILE:HG21 | 1:J:747:LEU:HD13 | 0.90                     | 0.79              |
| 1:A:599:ASN:CA   | 1:A:649:VAL:CB   | 2.54                     | 0.79              |
| 1:A:732:ILE:HG23 | 1:A:747:LEU:CB   | 1.85                     | 0.79              |
| 1:D:769:ALA:HA   | 1:D:771:LEU:N    | 1.97                     | 0.79              |
| 2:E:144:VAL:CA   | 2:E:153:ILE:HD11 | 2.11                     | 0.79              |
| 2:H:121:LEU:CG   | 2:H:128:PHE:CA   | 2.49                     | 0.79              |
| 1:G:819:ASN:ND2  | 2:H:92:ASP:HB2   | 1.96                     | 0.79              |
| 3:I:49:ILE:N     | 3:I:52:ASN:ND2   | 2.29                     | 0.79              |
| 4:W:223:PHE:HE1  | 4:W:255:PHE:HB2  | 1.46                     | 0.79              |
| 4:4:287:ILE:HB   | 4:6:204:ALA:N    | 1.97                     | 0.79              |
| 1:A:557:GLU:N    | 4:6:48:GLY:HA2   | 1.90                     | 0.79              |
| 1:A:174:SER:CB   | 1:A:667:THR:HG21 | 2.13                     | 0.79              |
| 1:A:641:LYS:CE   | 1:A:647:GLN:CG   | 2.60                     | 0.79              |
| 2:H:144:VAL:CA   | 2:H:153:ILE:HD11 | 2.11                     | 0.79              |
| 2:E:150:TYR:C    | 2:E:151:LYS:CG   | 2.48                     | 0.79              |
| 1:G:754:ASP:HB2  | 1:G:776:GLU:CD   | 2.02                     | 0.79              |
| 1:J:530:MET:HE1  | 4:7:355:MET:SD   | 2.23                     | 0.79              |
| 1:J:817:GLN:OE1  | 2:K:127:ARG:HD2  | 1.82                     | 0.79              |
| 1:A:538:GLU:HG3  | 4:4:351:THR:C    | 2.03                     | 0.79              |
| 1:A:218:LEU:CA   | 1:A:221:GLN:HG2  | 2.10                     | 0.79              |
| 2:E:141:PRO:CB   | 2:E:142:PRO:HD2  | 2.12                     | 0.79              |
| 1:D:830:PRO:HD2  | 2:E:67:MET:CE    | 2.11                     | 0.79              |
| 2:H:141:PRO:CB   | 2:H:142:PRO:HD2  | 2.12                     | 0.79              |
| 1:G:537:GLU:O    | 4:6:350:SER:N    | 2.16                     | 0.79              |
| 1:A:550:PHE:N    | 4:6:46:GLY:HA3   | 1.97                     | 0.79              |
| 1:A:537:GLU:O    | 4:4:350:SER:N    | 2.16                     | 0.79              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:409:GLY:N    | 1:A:636:LYS:CG   | 2.44                     | 0.79              |
| 2:B:141:PRO:HB2  | 2:B:142:PRO:CD   | 2.11                     | 0.79              |
| 1:D:641:LYS:CE   | 1:D:647:GLN:HB2  | 2.13                     | 0.79              |
| 1:D:768:MLY:CA   | 1:D:771:LEU:HD13 | 2.12                     | 0.79              |
| 1:G:550:PHE:N    | 4:8:46:GLY:HA3   | 1.97                     | 0.79              |
| 1:G:641:LYS:HD2  | 4:6:348:SER:HB2  | 1.54                     | 0.79              |
| 1:D:550:PHE:HA   | 4:7:46:GLY:HA2   | 1.64                     | 0.79              |
| 1:D:409:GLY:N    | 1:D:636:LYS:CG   | 2.44                     | 0.79              |
| 1:D:407:GLY:HA2  | 1:D:412:ALA:HA   | 1.65                     | 0.79              |
| 1:D:537:GLU:O    | 4:5:350:SER:N    | 2.16                     | 0.79              |
| 2:E:141:PRO:HB2  | 2:E:142:PRO:CD   | 2.12                     | 0.79              |
| 1:D:793:ARG:HA   | 3:F:40:ASN:ND2   | 1.96                     | 0.79              |
| 3:I:50:LEU:C     | 3:I:53:PRO:HD2   | 2.03                     | 0.79              |
| 1:J:407:GLY:HA2  | 1:J:412:ALA:HA   | 1.65                     | 0.79              |
| 3:L:50:LEU:C     | 3:L:53:PRO:HD2   | 2.03                     | 0.79              |
| 4:W:287:ILE:HB   | 4:Y:204:ALA:N    | 1.98                     | 0.79              |
| 1:A:641:LYS:HD2  | 4:4:348:SER:HB2  | 1.54                     | 0.79              |
| 1:A:769:ALA:C    | 1:A:772:LEU:N    | 2.33                     | 0.79              |
| 1:D:792:ALA:CA   | 3:F:40:ASN:HB3   | 2.12                     | 0.79              |
| 1:D:834:LEU:HG   | 2:E:54:MET:CG    | 2.03                     | 0.79              |
| 1:G:174:SER:CB   | 1:G:667:THR:HG21 | 2.13                     | 0.79              |
| 1:G:218:LEU:CA   | 1:G:221:GLN:HG2  | 2.10                     | 0.79              |
| 1:G:550:PHE:HA   | 4:8:46:GLY:HA2   | 1.64                     | 0.79              |
| 1:J:92:ALA:O     | 1:J:714:ARG:CG   | 2.31                     | 0.79              |
| 4:1:287:ILE:HB   | 4:3:204:ALA:N    | 1.97                     | 0.78              |
| 1:J:642:LYS:CG   | 4:7:23:GLY:H     | 1.77                     | 0.78              |
| 2:B:144:VAL:HG12 | 2:B:153:ILE:CD1  | 2.09                     | 0.78              |
| 1:D:732:ILE:HG23 | 1:D:747:LEU:CB   | 1.85                     | 0.78              |
| 1:A:817:GLN:HB2  | 2:B:127:ARG:NH1  | 1.97                     | 0.78              |
| 1:D:291:ILE:HA   | 1:D:331:LEU:HD11 | 1.64                     | 0.78              |
| 3:F:50:LEU:C     | 3:F:53:PRO:HD2   | 2.03                     | 0.78              |
| 1:G:407:GLY:HA2  | 1:G:412:ALA:HA   | 1.65                     | 0.78              |
| 1:A:553:MLY:NZ   | 4:6:45:VAL:HA    | 1.84                     | 0.78              |
| 1:J:538:GLU:HG3  | 4:7:351:THR:C    | 2.03                     | 0.78              |
| 1:A:550:PHE:HA   | 4:6:46:GLY:HA2   | 1.65                     | 0.78              |
| 1:J:409:GLY:N    | 1:J:636:LYS:CG   | 2.44                     | 0.78              |
| 1:J:550:PHE:HA   | 4:V:46:GLY:HA2   | 1.64                     | 0.78              |
| 1:J:754:ASP:OD2  | 1:J:776:GLU:CB   | 2.32                     | 0.78              |
| 4:V:287:ILE:HB   | 4:X:204:ALA:N    | 1.97                     | 0.78              |
| 1:J:639:GLY:CA   | 4:7:345:ILE:N    | 2.47                     | 0.78              |
| 1:A:51:THR:O     | 1:A:62:VAL:HG13  | 1.84                     | 0.78              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:50:LEU:C     | 3:C:53:PRO:HD2   | 2.03                     | 0.78              |
| 1:D:481:ASN:N    | 1:D:481:ASN:HD22 | 1.82                     | 0.78              |
| 2:E:162:ASP:HB3  | 2:K:20:ASP:HB2   | 1.64                     | 0.78              |
| 1:J:291:ILE:HA   | 1:J:331:LEU:HD11 | 1.64                     | 0.78              |
| 1:J:641:LYS:CE   | 1:J:647:GLN:HB2  | 2.13                     | 0.78              |
| 4:5:287:ILE:HB   | 4:7:204:ALA:N    | 1.97                     | 0.78              |
| 1:D:550:PHE:N    | 4:7:46:GLY:HA3   | 1.97                     | 0.78              |
| 1:A:642:LYS:HG2  | 4:4:22:ALA:HA    | 1.66                     | 0.78              |
| 1:D:815:CYS:SG   | 2:E:92:ASP:HB2   | 2.24                     | 0.78              |
| 1:G:642:LYS:HG2  | 4:6:22:ALA:HA    | 1.65                     | 0.78              |
| 1:G:646:PHE:HE2  | 1:G:652:LEU:CD2  | 1.97                     | 0.78              |
| 4:3:287:ILE:HB   | 4:5:204:ALA:N    | 1.98                     | 0.78              |
| 4:8:287:ILE:HB   | 4:W:204:ALA:N    | 1.97                     | 0.78              |
| 1:G:537:GLU:HG3  | 4:6:350:SER:O    | 1.79                     | 0.78              |
| 1:J:537:GLU:O    | 4:7:350:SER:N    | 2.16                     | 0.78              |
| 1:A:556:ASP:HA   | 4:6:49:GLN:O     | 1.70                     | 0.78              |
| 3:C:49:ILE:N     | 3:C:52:ASN:HD22  | 1.82                     | 0.78              |
| 1:G:291:ILE:HA   | 1:G:331:LEU:HD11 | 1.64                     | 0.78              |
| 1:G:51:THR:O     | 1:G:62:VAL:HG13  | 1.84                     | 0.78              |
| 1:G:93:MET:SD    | 1:G:763:THR:HG22 | 2.24                     | 0.78              |
| 1:J:646:PHE:HE2  | 1:J:652:LEU:CD2  | 1.97                     | 0.78              |
| 1:J:174:SER:CB   | 1:J:667:THR:HG21 | 2.13                     | 0.78              |
| 1:J:797:PHE:HA   | 3:L:149:VAL:CG1  | 2.12                     | 0.78              |
| 4:2:287:ILE:HB   | 4:4:204:ALA:N    | 1.98                     | 0.78              |
| 1:A:537:GLU:HG3  | 4:4:350:SER:O    | 1.79                     | 0.78              |
| 1:J:530:MET:CG   | 4:7:354:GLN:CB   | 2.30                     | 0.78              |
| 4:8:223:PHE:HE1  | 4:8:255:PHE:HB2  | 1.46                     | 0.78              |
| 2:B:121:LEU:CG   | 2:B:128:PHE:HA   | 2.14                     | 0.78              |
| 1:D:800:ARG:CD   | 3:F:149:VAL:C    | 2.53                     | 0.78              |
| 1:G:732:ILE:HG21 | 1:G:747:LEU:HD13 | 0.91                     | 0.78              |
| 1:G:93:MET:CA    | 1:G:764:MLY:NZ   | 2.35                     | 0.78              |
| 1:J:51:THR:O     | 1:J:62:VAL:HG13  | 1.84                     | 0.78              |
| 1:J:550:PHE:N    | 4:V:46:GLY:HA3   | 1.97                     | 0.78              |
| 1:J:798:LEU:HD21 | 3:L:126:LEU:CG   | 2.14                     | 0.78              |
| 1:A:496:PHE:CD2  | 1:A:514:ASP:HA   | 2.19                     | 0.78              |
| 1:D:831:TRP:HA   | 2:E:51:PHE:CE1   | 2.19                     | 0.78              |
| 1:D:831:TRP:N    | 2:E:51:PHE:CZ    | 2.52                     | 0.78              |
| 1:J:95:THR:HA    | 1:J:713:SER:HA   | 1.66                     | 0.78              |
| 1:G:639:GLY:CA   | 4:6:345:ILE:N    | 2.47                     | 0.78              |
| 2:B:117:LEU:HB2  | 2:B:147:ASN:HD21 | 1.47                     | 0.78              |
| 1:A:789:ALA:HB1  | 3:C:87:PHE:CE2   | 2.18                     | 0.78              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:646:PHE:CE2  | 1:D:652:LEU:HD21 | 2.14                     | 0.78              |
| 1:D:793:ARG:HE   | 3:F:147:MET:HA   | 1.47                     | 0.78              |
| 1:D:839:MLY:CH1  | 2:E:159:HIS:CB   | 2.61                     | 0.78              |
| 1:G:219:GLU:O    | 1:G:223:ILE:HG13 | 1.84                     | 0.78              |
| 1:G:496:PHE:CD2  | 1:G:514:ASP:HA   | 2.19                     | 0.78              |
| 1:J:496:PHE:CD2  | 1:J:514:ASP:HA   | 2.19                     | 0.78              |
| 1:J:107:MLY:HB3  | 1:J:686:MET:HE2  | 1.66                     | 0.78              |
| 1:J:84:MLY:HH11  | 1:J:715:VAL:HG11 | 1.66                     | 0.78              |
| 1:A:219:GLU:O    | 1:A:223:ILE:HG13 | 1.84                     | 0.77              |
| 1:A:795:ARG:CB   | 3:C:35:ARG:NH2   | 2.43                     | 0.77              |
| 1:D:538:GLU:HG3  | 4:5:351:THR:C    | 2.03                     | 0.77              |
| 1:D:639:GLY:CA   | 4:5:345:ILE:N    | 2.47                     | 0.77              |
| 1:G:409:GLY:N    | 1:G:636:LYS:CG   | 2.44                     | 0.77              |
| 1:G:727:LEU:O    | 3:I:113:THR:OG1  | 2.02                     | 0.77              |
| 1:J:829:TRP:CZ3  | 2:K:84:PHE:CE2   | 2.51                     | 0.77              |
| 4:5:223:PHE:HD2  | 4:5:312:ARG:HH21 | 1.32                     | 0.77              |
| 1:A:530:MET:HE3  | 4:4:354:GLN:HG2  | 1.65                     | 0.77              |
| 1:D:496:PHE:CD2  | 1:D:514:ASP:HA   | 2.19                     | 0.77              |
| 1:D:724:TYR:C    | 1:D:782:MLY:HH11 | 2.04                     | 0.77              |
| 1:D:831:TRP:CH2  | 2:E:34:ILE:CG2   | 2.65                     | 0.77              |
| 2:K:117:LEU:HB2  | 2:K:147:ASN:HD21 | 1.47                     | 0.77              |
| 4:V:223:PHE:HD2  | 4:V:312:ARG:HH21 | 1.33                     | 0.77              |
| 4:Z:223:PHE:HD2  | 4:Z:312:ARG:HH21 | 1.33                     | 0.77              |
| 1:D:530:MET:HE1  | 4:5:355:MET:SD   | 2.24                     | 0.77              |
| 1:A:407:GLY:HA2  | 1:A:412:ALA:HA   | 1.65                     | 0.77              |
| 1:A:502:GLU:CG   | 1:A:764:MLY:O    | 2.31                     | 0.77              |
| 1:D:831:TRP:CH2  | 2:E:47:LEU:CA    | 2.37                     | 0.77              |
| 1:J:116:TYR:O    | 1:J:153:PRO:HB2  | 1.85                     | 0.77              |
| 4:X:223:PHE:HD2  | 4:X:312:ARG:HH21 | 1.33                     | 0.77              |
| 1:A:291:ILE:HA   | 1:A:331:LEU:HD11 | 1.64                     | 0.77              |
| 1:D:51:THR:O     | 1:D:62:VAL:HG13  | 1.84                     | 0.77              |
| 1:D:809:ARG:CZ   | 2:E:124:GLY:CA   | 2.61                     | 0.77              |
| 1:G:836:PHE:CZ   | 2:H:160:GLY:N    | 2.50                     | 0.77              |
| 1:G:93:MET:CE    | 1:G:764:MLY:HE3  | 2.14                     | 0.77              |
| 1:A:793:ARG:HH21 | 3:C:147:MET:CB   | 1.97                     | 0.77              |
| 1:D:831:TRP:HZ3  | 2:E:34:ILE:HG23  | 1.42                     | 0.77              |
| 3:I:49:ILE:N     | 3:I:52:ASN:HD22  | 1.82                     | 0.77              |
| 1:J:725:ARG:HG3  | 1:J:733:PRO:HA   | 1.67                     | 0.77              |
| 4:7:223:PHE:HD2  | 4:7:312:ARG:HH21 | 1.33                     | 0.77              |
| 1:A:639:GLY:CA   | 4:4:345:ILE:N    | 2.47                     | 0.77              |
| 1:D:629:GLU:HA   | 1:D:643:GLY:C    | 2.05                     | 0.77              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:116:TYR:O    | 1:G:153:PRO:HB2  | 1.85                     | 0.77              |
| 1:G:218:LEU:HD22 | 1:G:222:ILE:HG12 | 1.66                     | 0.77              |
| 1:G:641:LYS:CE   | 1:G:647:GLN:HB2  | 2.13                     | 0.77              |
| 1:G:831:TRP:CZ2  | 2:H:47:LEU:HD22  | 2.17                     | 0.77              |
| 1:J:93:MET:HG3   | 1:J:764:MLY:HD3  | 1.60                     | 0.77              |
| 1:A:736:GLN:HA   | 1:A:743:ALA:HB2  | 1.51                     | 0.77              |
| 1:D:116:TYR:O    | 1:D:153:PRO:HB2  | 1.85                     | 0.77              |
| 1:D:174:SER:CB   | 1:D:667:THR:HG21 | 2.13                     | 0.77              |
| 1:G:728:ASN:ND2  | 3:I:113:THR:OG1  | 2.18                     | 0.77              |
| 1:G:732:ILE:CG2  | 1:G:747:LEU:HD13 | 1.34                     | 0.77              |
| 1:G:736:GLN:HA   | 1:G:743:ALA:HB1  | 1.26                     | 0.77              |
| 4:0:223:PHE:HD2  | 4:0:312:ARG:HH21 | 1.33                     | 0.77              |
| 1:D:94:MET:CE    | 1:D:101:ALA:HB1  | 2.15                     | 0.77              |
| 1:D:646:PHE:HE2  | 1:D:652:LEU:CD2  | 1.97                     | 0.77              |
| 3:I:3:SER:O      | 3:I:4:LYS:HB2    | 1.84                     | 0.77              |
| 1:J:629:GLU:HA   | 1:J:643:GLY:C    | 2.05                     | 0.77              |
| 2:K:121:LEU:CG   | 2:K:128:PHE:HA   | 2.14                     | 0.77              |
| 4:1:223:PHE:HD2  | 4:1:312:ARG:HH21 | 1.33                     | 0.77              |
| 4:3:223:PHE:HD2  | 4:3:312:ARG:HH21 | 1.33                     | 0.77              |
| 4:4:223:PHE:HD2  | 4:4:312:ARG:HH21 | 1.33                     | 0.77              |
| 1:A:641:LYS:CE   | 1:A:647:GLN:HB2  | 2.13                     | 0.77              |
| 1:A:646:PHE:HE2  | 1:A:652:LEU:CD2  | 1.97                     | 0.77              |
| 1:A:725:ARG:HG3  | 1:A:733:PRO:HA   | 1.67                     | 0.77              |
| 1:A:757:GLN:HB2  | 1:A:771:LEU:HD11 | 1.58                     | 0.77              |
| 4:X:287:ILE:HB   | 4:Z:204:ALA:N    | 1.97                     | 0.77              |
| 1:D:642:LYS:HG2  | 4:5:22:ALA:HA    | 1.65                     | 0.77              |
| 1:D:508:ILE:HA   | 1:D:761:GLY:HA3  | 1.65                     | 0.77              |
| 1:D:721:LYS:CA   | 1:D:736:GLN:OE1  | 2.33                     | 0.77              |
| 1:D:818:TYR:CG   | 2:E:89:LYS:HB2   | 2.20                     | 0.77              |
| 1:G:725:ARG:HG3  | 1:G:733:PRO:HA   | 1.67                     | 0.77              |
| 1:G:733:PRO:C    | 1:G:737:PHE:HD1  | 1.88                     | 0.77              |
| 1:G:769:ALA:O    | 1:G:773:GLY:CA   | 2.33                     | 0.77              |
| 2:H:141:PRO:HB2  | 2:H:142:PRO:CD   | 2.11                     | 0.77              |
| 1:J:219:GLU:O    | 1:J:223:ILE:HG13 | 1.84                     | 0.77              |
| 1:J:218:LEU:HD22 | 1:J:222:ILE:HG12 | 1.67                     | 0.77              |
| 1:J:646:PHE:CE2  | 1:J:652:LEU:HD21 | 2.14                     | 0.77              |
| 4:2:223:PHE:HD2  | 4:2:312:ARG:HH21 | 1.33                     | 0.76              |
| 1:D:635:GLY:HA3  | 4:5:341:ILE:CD1  | 2.14                     | 0.76              |
| 1:A:721:LYS:CA   | 1:A:736:GLN:OE1  | 2.33                     | 0.76              |
| 1:A:502:GLU:CB   | 1:A:761:GLY:HA3  | 2.16                     | 0.76              |
| 1:A:793:ARG:NH2  | 3:C:147:MET:CE   | 2.48                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:733:PRO:C    | 1:D:737:PHE:HD1  | 1.88                     | 0.76              |
| 3:F:49:ILE:N     | 3:F:52:ASN:HD22  | 1.82                     | 0.76              |
| 1:G:732:ILE:N    | 1:G:733:PRO:HD2  | 2.00                     | 0.76              |
| 1:J:641:LYS:CE   | 1:J:647:GLN:CG   | 2.60                     | 0.76              |
| 3:L:3:SER:O      | 3:L:4:LYS:HB2    | 1.85                     | 0.76              |
| 4:0:287:ILE:HB   | 4:2:204:ALA:N    | 1.97                     | 0.76              |
| 1:J:635:GLY:HA3  | 4:7:341:ILE:CD1  | 2.14                     | 0.76              |
| 1:A:732:ILE:N    | 1:A:733:PRO:HD2  | 2.00                     | 0.76              |
| 1:D:599:ASN:CA   | 1:D:649:VAL:CB   | 2.53                     | 0.76              |
| 1:G:798:LEU:HD22 | 3:I:126:LEU:HD11 | 1.66                     | 0.76              |
| 1:J:94:MET:CE    | 1:J:101:ALA:HB1  | 2.15                     | 0.76              |
| 1:A:94:MET:CE    | 1:A:101:ALA:HB1  | 2.15                     | 0.76              |
| 1:D:219:GLU:O    | 1:D:223:ILE:HG13 | 1.84                     | 0.76              |
| 1:D:641:LYS:CE   | 1:D:647:GLN:CG   | 2.60                     | 0.76              |
| 2:E:121:LEU:CG   | 2:E:128:PHE:HA   | 2.14                     | 0.76              |
| 1:J:721:LYS:CA   | 1:J:736:GLN:OE1  | 2.33                     | 0.76              |
| 1:G:530:MET:CG   | 4:6:354:GLN:CB   | 2.30                     | 0.76              |
| 4:7:287:ILE:HB   | 4:V:204:ALA:N    | 1.97                     | 0.76              |
| 1:A:623:PHE:CG   | 1:A:623:PHE:CA   | 2.68                     | 0.76              |
| 1:A:629:GLU:HA   | 1:A:643:GLY:C    | 2.05                     | 0.76              |
| 1:A:795:ARG:NH1  | 3:C:43:ASN:N     | 2.31                     | 0.76              |
| 1:D:534:SER:O    | 4:5:351:THR:N    | 2.19                     | 0.76              |
| 1:G:218:LEU:HB2  | 1:G:221:GLN:CG   | 2.09                     | 0.76              |
| 1:J:721:LYS:HG2  | 1:J:736:GLN:CD   | 1.86                     | 0.76              |
| 4:6:290:ARG:HH22 | 4:8:202:THR:HG23 | 1.50                     | 0.76              |
| 1:A:218:LEU:HD22 | 1:A:222:ILE:HG12 | 1.67                     | 0.76              |
| 1:D:732:ILE:N    | 1:D:733:PRO:HD2  | 2.00                     | 0.76              |
| 1:G:629:GLU:HA   | 1:G:643:GLY:C    | 2.05                     | 0.76              |
| 1:G:641:LYS:HD2  | 1:G:647:GLN:OE1  | 1.81                     | 0.76              |
| 2:H:121:LEU:CG   | 2:H:128:PHE:HA   | 2.14                     | 0.76              |
| 2:H:150:TYR:C    | 2:H:151:LYS:CG   | 2.48                     | 0.76              |
| 1:J:732:ILE:N    | 1:J:733:PRO:HD2  | 2.01                     | 0.76              |
| 1:J:733:PRO:C    | 1:J:737:PHE:HD1  | 1.88                     | 0.76              |
| 1:J:831:TRP:CH2  | 2:K:47:LEU:CD2   | 2.68                     | 0.76              |
| 4:Y:223:PHE:HD2  | 4:Y:312:ARG:HH21 | 1.33                     | 0.76              |
| 4:6:223:PHE:HD2  | 4:6:312:ARG:HH21 | 1.33                     | 0.76              |
| 1:G:530:MET:HE3  | 4:6:354:GLN:HG2  | 1.66                     | 0.76              |
| 4:8:223:PHE:HD2  | 4:8:312:ARG:HH21 | 1.32                     | 0.76              |
| 1:A:721:LYS:HG2  | 1:A:736:GLN:CD   | 1.86                     | 0.76              |
| 1:D:529:PRO:C    | 4:5:354:GLN:CB   | 2.49                     | 0.76              |
| 1:D:831:TRP:CG   | 2:E:51:PHE:CZ    | 2.74                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:797:PHE:HD1  | 3:I:149:VAL:CB   | 1.97                     | 0.76              |
| 1:G:817:GLN:HB3  | 2:H:127:ARG:HD2  | 1.53                     | 0.76              |
| 1:J:481:ASN:N    | 1:J:481:ASN:HD22 | 1.82                     | 0.76              |
| 1:J:623:PHE:CA   | 1:J:623:PHE:CG   | 2.68                     | 0.76              |
| 4:V:290:ARG:NH1  | 4:X:202:THR:CG2  | 2.49                     | 0.76              |
| 4:8:290:ARG:NH1  | 4:W:202:THR:CG2  | 2.49                     | 0.76              |
| 4:8:290:ARG:HH22 | 4:W:202:THR:HG23 | 1.50                     | 0.76              |
| 4:W:223:PHE:HD2  | 4:W:312:ARG:HH21 | 1.32                     | 0.76              |
| 4:0:290:ARG:NH1  | 4:2:202:THR:CG2  | 2.49                     | 0.76              |
| 4:5:290:ARG:NH1  | 4:7:202:THR:CG2  | 2.49                     | 0.76              |
| 1:J:550:PHE:HA   | 4:V:46:GLY:HA3   | 1.66                     | 0.76              |
| 1:D:553:MLY:NZ   | 4:7:45:VAL:HA    | 1.84                     | 0.76              |
| 1:D:623:PHE:CA   | 1:D:623:PHE:CG   | 2.68                     | 0.76              |
| 2:E:117:LEU:HB2  | 2:E:147:ASN:HD21 | 1.47                     | 0.76              |
| 4:4:290:ARG:NH1  | 4:6:202:THR:CG2  | 2.49                     | 0.76              |
| 1:D:550:PHE:HA   | 4:7:46:GLY:HA3   | 1.66                     | 0.76              |
| 1:A:116:TYR:O    | 1:A:153:PRO:HB2  | 1.85                     | 0.76              |
| 1:A:218:LEU:HB2  | 1:A:221:GLN:CG   | 2.09                     | 0.76              |
| 1:D:649:VAL:CB   | 1:D:649:VAL:CG1  | 2.64                     | 0.76              |
| 1:D:664:LEU:O    | 1:D:667:THR:HB   | 1.86                     | 0.76              |
| 1:G:649:VAL:CB   | 1:G:649:VAL:CG1  | 2.64                     | 0.76              |
| 1:G:735:GLY:C    | 1:G:743:ALA:HB1  | 1.84                     | 0.76              |
| 1:J:820:VAL:HG11 | 2:K:136:MET:CE   | 2.16                     | 0.76              |
| 4:X:290:ARG:NH1  | 4:Z:202:THR:CG2  | 2.49                     | 0.76              |
| 1:D:538:GLU:OE2  | 4:5:355:MET:HE3  | 1.86                     | 0.76              |
| 1:A:218:LEU:HB3  | 1:A:221:GLN:HG3  | 1.61                     | 0.76              |
| 1:G:94:MET:CE    | 1:G:101:ALA:HB1  | 2.15                     | 0.76              |
| 1:A:768:MLY:HB3  | 1:A:771:LEU:CB   | 2.16                     | 0.75              |
| 1:G:534:SER:O    | 4:6:351:THR:N    | 2.20                     | 0.75              |
| 1:G:641:LYS:CE   | 1:G:647:GLN:CG   | 2.61                     | 0.75              |
| 3:L:49:ILE:N     | 3:L:52:ASN:HD22  | 1.82                     | 0.75              |
| 1:A:502:GLU:CD   | 1:A:763:THR:H    | 1.88                     | 0.75              |
| 1:D:831:TRP:CZ2  | 2:E:47:LEU:HB3   | 2.19                     | 0.75              |
| 1:G:798:LEU:CD1  | 3:I:126:LEU:CG   | 2.65                     | 0.75              |
| 1:J:818:TYR:CZ   | 2:K:127:ARG:NH2  | 2.54                     | 0.75              |
| 1:A:793:ARG:HE   | 3:C:147:MET:HA   | 1.49                     | 0.75              |
| 1:G:481:ASN:HD22 | 1:G:481:ASN:N    | 1.82                     | 0.75              |
| 1:J:556:ASP:HA   | 4:V:49:GLN:O     | 1.69                     | 0.75              |
| 1:J:95:THR:HG1   | 1:J:713:SER:HB3  | 1.47                     | 0.75              |
| 1:J:90:ASP:HB3   | 1:J:764:MLY:HH21 | 1.69                     | 0.75              |
| 1:D:642:LYS:CG   | 4:5:23:GLY:H     | 1.77                     | 0.75              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:649:VAL:CB  | 1:A:649:VAL:CG1  | 2.64                     | 0.75              |
| 1:A:664:LEU:O   | 1:A:667:THR:HB   | 1.86                     | 0.75              |
| 1:A:831:TRP:HH2 | 2:B:50:THR:CB    | 2.00                     | 0.75              |
| 1:D:537:GLU:HG3 | 4:5:350:SER:O    | 1.79                     | 0.75              |
| 1:G:751:GLY:CA  | 3:I:114:LEU:HD13 | 2.16                     | 0.75              |
| 1:D:166:MET:HE1 | 1:D:254:PHE:HB2  | 1.68                     | 0.75              |
| 1:J:541:MET:O   | 4:7:143:TYR:CZ   | 2.40                     | 0.75              |
| 1:J:642:LYS:HG2 | 4:7:22:ALA:HA    | 1.65                     | 0.75              |
| 1:G:623:PHE:CA  | 1:G:623:PHE:CG   | 2.68                     | 0.75              |
| 1:G:721:LYS:CA  | 1:G:736:GLN:OE1  | 2.33                     | 0.75              |
| 1:J:649:VAL:CG1 | 1:J:649:VAL:CB   | 2.64                     | 0.75              |
| 1:A:502:GLU:CA  | 1:A:761:GLY:CA   | 2.65                     | 0.75              |
| 4:X:288:ASP:H   | 4:Z:203:THR:HG22 | 1.52                     | 0.75              |
| 4:O:288:ASP:H   | 4:2:203:THR:HG22 | 1.52                     | 0.75              |
| 1:A:534:SER:O   | 4:4:351:THR:N    | 2.18                     | 0.75              |
| 1:A:530:MET:CG  | 4:4:354:GLN:CB   | 2.30                     | 0.75              |
| 3:C:3:SER:O     | 3:C:4:LYS:HB2    | 1.84                     | 0.75              |
| 1:D:724:TYR:HA  | 1:D:782:MLY:CH1  | 2.16                     | 0.75              |
| 1:D:725:ARG:HG3 | 1:D:733:PRO:HA   | 1.67                     | 0.75              |
| 1:D:818:TYR:HB2 | 2:E:90:GLY:CA    | 2.17                     | 0.75              |
| 1:D:839:MLY:CH1 | 2:E:159:HIS:HD2  | 1.76                     | 0.75              |
| 1:G:664:LEU:O   | 1:G:667:THR:HB   | 1.86                     | 0.75              |
| 1:G:817:GLN:CD  | 2:H:127:ARG:CD   | 2.54                     | 0.75              |
| 1:J:538:GLU:OE2 | 4:7:355:MET:HE3  | 1.87                     | 0.75              |
| 1:A:481:ASN:N   | 1:A:481:ASN:HD22 | 1.82                     | 0.75              |
| 1:A:636:LYS:O   | 1:A:637:LYS:HB2  | 1.86                     | 0.75              |
| 1:D:538:GLU:O   | 4:5:349:LEU:HG   | 1.86                     | 0.75              |
| 1:G:817:GLN:HG3 | 2:H:128:PHE:CE1  | 2.22                     | 0.75              |
| 1:J:350:ALA:O   | 1:J:354:LEU:HB2  | 1.87                     | 0.75              |
| 1:J:664:LEU:O   | 1:J:667:THR:HB   | 1.86                     | 0.75              |
| 1:J:823:PHE:CE1 | 2:K:156:VAL:HG12 | 2.21                     | 0.75              |
| 1:A:350:ALA:O   | 1:A:354:LEU:HB2  | 1.87                     | 0.74              |
| 1:J:310:TYR:CE2 | 1:J:320:ILE:HD11 | 2.22                     | 0.74              |
| 1:J:736:GLN:HA  | 1:J:743:ALA:HB1  | 1.26                     | 0.74              |
| 4:7:290:ARG:NH1 | 4:V:202:THR:CG2  | 2.49                     | 0.74              |
| 4:W:288:ASP:H   | 4:Y:203:THR:HG22 | 1.52                     | 0.74              |
| 4:5:253:GLU:HA  | 4:5:256:ARG:HG3  | 1.69                     | 0.74              |
| 4:5:288:ASP:H   | 4:7:203:THR:HG22 | 1.52                     | 0.74              |
| 1:A:793:ARG:NH2 | 3:C:147:MET:HE3  | 2.02                     | 0.74              |
| 1:A:836:PHE:HZ  | 2:B:160:GLY:N    | 1.80                     | 0.74              |
| 3:F:3:SER:O     | 3:F:4:LYS:HB2    | 1.84                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:783:LEU:O    | 1:G:787:ILE:CB   | 2.35                     | 0.74              |
| 2:H:117:LEU:HB2  | 2:H:147:ASN:HD21 | 1.47                     | 0.74              |
| 1:J:93:MET:HG3   | 1:J:764:MLY:HH12 | 1.69                     | 0.74              |
| 1:J:90:ASP:OD2   | 1:J:764:MLY:CH2  | 2.35                     | 0.74              |
| 4:Y:253:GLU:HA   | 4:Y:256:ARG:HG3  | 1.69                     | 0.74              |
| 4:1:253:GLU:HA   | 4:1:256:ARG:HG3  | 1.70                     | 0.74              |
| 4:3:288:ASP:H    | 4:5:203:THR:HG22 | 1.52                     | 0.74              |
| 1:A:502:GLU:C    | 1:A:761:GLY:CA   | 2.54                     | 0.74              |
| 1:D:350:ALA:O    | 1:D:354:LEU:HB2  | 1.87                     | 0.74              |
| 1:D:272:MLY:HH13 | 1:D:435:GLU:OE1  | 1.87                     | 0.74              |
| 1:D:732:ILE:N    | 1:D:733:PRO:CD   | 2.51                     | 0.74              |
| 1:G:541:MET:O    | 4:6:143:TYR:CZ   | 2.40                     | 0.74              |
| 1:J:636:LYS:O    | 1:J:637:LYS:HB2  | 1.86                     | 0.74              |
| 4:1:290:ARG:NH1  | 4:3:202:THR:CG2  | 2.49                     | 0.74              |
| 1:A:541:MET:O    | 4:4:143:TYR:CZ   | 2.40                     | 0.74              |
| 4:3:290:ARG:HH22 | 4:5:202:THR:HG23 | 1.50                     | 0.74              |
| 4:7:253:GLU:HA   | 4:7:256:ARG:HG3  | 1.69                     | 0.74              |
| 1:A:215:GLN:NE2  | 1:A:336:SER:O    | 2.21                     | 0.74              |
| 1:A:732:ILE:N    | 1:A:733:PRO:CD   | 2.51                     | 0.74              |
| 1:G:350:ALA:O    | 1:G:354:LEU:HB2  | 1.87                     | 0.74              |
| 1:G:735:GLY:CA   | 1:G:743:ALA:HA   | 2.17                     | 0.74              |
| 2:H:111:SER:OG   | 2:H:148:VAL:C    | 2.15                     | 0.74              |
| 4:8:288:ASP:H    | 4:W:203:THR:HG22 | 1.52                     | 0.74              |
| 1:A:538:GLU:O    | 4:4:349:LEU:HG   | 1.86                     | 0.74              |
| 4:4:288:ASP:H    | 4:6:203:THR:HG22 | 1.52                     | 0.74              |
| 1:G:538:GLU:HA   | 4:6:349:LEU:HD12 | 0.74                     | 0.74              |
| 1:J:640:LYS:O    | 4:7:23:GLY:O     | 2.06                     | 0.74              |
| 1:J:538:GLU:HA   | 4:7:349:LEU:HD12 | 0.75                     | 0.74              |
| 4:8:253:GLU:HA   | 4:8:256:ARG:HG3  | 1.69                     | 0.74              |
| 1:A:499:GLU:OE1  | 1:A:766:PHE:CZ   | 2.40                     | 0.74              |
| 1:D:218:LEU:HD22 | 1:D:222:ILE:HG12 | 1.67                     | 0.74              |
| 1:D:310:TYR:CE2  | 1:D:320:ILE:HD11 | 2.22                     | 0.74              |
| 1:G:218:LEU:HB3  | 1:G:221:GLN:HG3  | 1.60                     | 0.74              |
| 1:J:641:LYS:HD2  | 1:J:647:GLN:OE1  | 1.81                     | 0.74              |
| 4:3:253:GLU:HA   | 4:3:256:ARG:HG3  | 1.69                     | 0.74              |
| 4:6:288:ASP:H    | 4:8:203:THR:HG22 | 1.52                     | 0.74              |
| 1:A:436:MLY:HE3  | 1:A:626:TYR:CE1  | 2.23                     | 0.74              |
| 1:D:215:GLN:NE2  | 1:D:336:SER:O    | 2.20                     | 0.74              |
| 1:D:541:MET:O    | 4:5:143:TYR:CZ   | 2.40                     | 0.74              |
| 1:D:636:LYS:O    | 1:D:637:LYS:HB2  | 1.86                     | 0.74              |
| 1:G:636:LYS:O    | 1:G:637:LYS:HB2  | 1.86                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:831:TRP:NE1  | 2:H:67:MET:SD    | 2.60                     | 0.74              |
| 3:I:4:LYS:N      | 3:I:5:ALA:O      | 2.16                     | 0.74              |
| 1:J:534:SER:O    | 4:7:351:THR:N    | 2.19                     | 0.74              |
| 1:J:739:ASP:CB   | 1:J:742:LYS:HB3  | 2.12                     | 0.74              |
| 4:W:253:GLU:HA   | 4:W:256:ARG:HG3  | 1.69                     | 0.74              |
| 1:A:409:GLY:HA3  | 4:4:333:PRO:N    | 2.02                     | 0.74              |
| 1:A:640:LYS:O    | 4:4:23:GLY:O     | 2.06                     | 0.74              |
| 1:J:797:PHE:CA   | 3:L:149:VAL:CG1  | 2.65                     | 0.74              |
| 4:1:288:ASP:H    | 4:3:203:THR:HG22 | 1.52                     | 0.74              |
| 4:2:290:ARG:NH1  | 4:4:202:THR:CG2  | 2.49                     | 0.74              |
| 1:A:635:GLY:HA3  | 4:4:341:ILE:CD1  | 2.14                     | 0.74              |
| 1:D:538:GLU:HA   | 4:5:349:LEU:HD12 | 0.74                     | 0.74              |
| 1:A:793:ARG:NE   | 3:C:147:MET:HA   | 2.03                     | 0.74              |
| 1:D:769:ALA:CA   | 1:D:771:LEU:HA   | 2.17                     | 0.74              |
| 1:D:834:LEU:HD13 | 2:E:51:PHE:HD1   | 1.53                     | 0.74              |
| 1:G:310:TYR:CE2  | 1:G:320:ILE:HD11 | 2.22                     | 0.74              |
| 1:G:730:SER:CB   | 3:I:109:HIS:NE2  | 2.50                     | 0.74              |
| 1:J:272:MLY:HH13 | 1:J:435:GLU:OE1  | 1.87                     | 0.74              |
| 1:J:768:MLY:CD   | 1:J:772:LEU:HB2  | 2.18                     | 0.74              |
| 4:V:253:GLU:HA   | 4:V:256:ARG:HG3  | 1.69                     | 0.74              |
| 4:V:290:ARG:HH22 | 4:X:202:THR:HG23 | 1.50                     | 0.74              |
| 4:V:288:ASP:H    | 4:X:203:THR:HG22 | 1.52                     | 0.74              |
| 1:A:538:GLU:HA   | 4:4:349:LEU:HD12 | 0.74                     | 0.74              |
| 1:A:538:GLU:CD   | 4:4:355:MET:HE3  | 2.08                     | 0.74              |
| 1:A:757:GLN:HG3  | 1:A:771:LEU:HD11 | 1.70                     | 0.74              |
| 1:D:436:MLY:HE3  | 1:D:626:TYR:CE1  | 2.23                     | 0.74              |
| 1:J:538:GLU:O    | 4:7:349:LEU:HG   | 1.86                     | 0.74              |
| 4:2:288:ASP:H    | 4:4:203:THR:HG22 | 1.52                     | 0.74              |
| 1:A:530:MET:CE   | 4:4:355:MET:SD   | 2.76                     | 0.74              |
| 4:4:290:ARG:HH22 | 4:6:202:THR:HG23 | 1.50                     | 0.74              |
| 1:A:733:PRO:C    | 1:A:737:PHE:HD1  | 1.88                     | 0.74              |
| 1:D:640:LYS:O    | 4:5:23:GLY:O     | 2.06                     | 0.74              |
| 4:X:253:GLU:HA   | 4:X:256:ARG:HG3  | 1.69                     | 0.74              |
| 4:W:290:ARG:NH1  | 4:Y:202:THR:CG2  | 2.49                     | 0.74              |
| 1:D:530:MET:CG   | 4:5:354:GLN:CB   | 2.30                     | 0.73              |
| 1:A:486:MLY:HH13 | 1:A:527:GLU:OE1  | 1.88                     | 0.73              |
| 1:A:839:MLY:CD   | 2:B:159:HIS:CB   | 2.65                     | 0.73              |
| 3:I:24:LYS:CA    | 3:I:63:ILE:O     | 2.36                     | 0.73              |
| 1:J:84:MLY:CH1   | 1:J:715:VAL:HG12 | 2.15                     | 0.73              |
| 2:K:130:PRO:O    | 2:K:132:GLU:N    | 2.21                     | 0.73              |
| 4:4:253:GLU:HA   | 4:4:256:ARG:HG3  | 1.69                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:6:253:GLU:HA   | 4:6:256:ARG:HG3  | 1.69                     | 0.73              |
| 1:J:735:GLY:CA   | 1:J:743:ALA:HA   | 2.18                     | 0.73              |
| 1:A:542:PHE:CD2  | 4:4:143:TYR:CE1  | 2.76                     | 0.73              |
| 1:D:409:GLY:HA3  | 4:5:333:PRO:N    | 2.03                     | 0.73              |
| 1:D:487:LEU:O    | 1:D:490:PHE:HB3  | 1.89                     | 0.73              |
| 1:G:732:ILE:N    | 1:G:733:PRO:CD   | 2.51                     | 0.73              |
| 1:G:795:ARG:CD   | 3:I:35:ARG:NH2   | 2.17                     | 0.73              |
| 1:J:166:MET:HE3  | 1:J:254:PHE:CD2  | 2.23                     | 0.73              |
| 1:J:529:PRO:C    | 4:7:354:GLN:CB   | 2.48                     | 0.73              |
| 1:J:557:GLU:N    | 4:V:48:GLY:HA3   | 1.90                     | 0.73              |
| 1:D:534:SER:CA   | 4:5:351:THR:HA   | 2.19                     | 0.73              |
| 1:A:709:LYS:O    | 1:A:710:GLY:CA   | 2.37                     | 0.73              |
| 1:G:215:GLN:NE2  | 1:G:336:SER:O    | 2.20                     | 0.73              |
| 1:J:441:MET:O    | 1:J:445:ILE:HG13 | 1.88                     | 0.73              |
| 1:J:93:MET:HA    | 1:J:714:ARG:HG3  | 1.70                     | 0.73              |
| 4:1:290:ARG:HH22 | 4:3:202:THR:HG23 | 1.50                     | 0.73              |
| 1:J:534:SER:CA   | 4:7:351:THR:HA   | 2.19                     | 0.73              |
| 4:6:290:ARG:NH1  | 4:8:202:THR:CG2  | 2.49                     | 0.73              |
| 1:A:310:TYR:CE2  | 1:A:320:ILE:HD11 | 2.22                     | 0.73              |
| 1:A:529:PRO:C    | 4:4:354:GLN:CB   | 2.49                     | 0.73              |
| 1:A:735:GLY:C    | 1:A:743:ALA:HB1  | 1.84                     | 0.73              |
| 1:D:721:LYS:CB   | 1:D:736:GLN:CD   | 2.56                     | 0.73              |
| 1:D:726:VAL:H    | 1:D:782:MLY:CH2  | 2.01                     | 0.73              |
| 1:J:487:LEU:O    | 1:J:490:PHE:HB3  | 1.88                     | 0.73              |
| 1:J:486:MLY:HH13 | 1:J:527:GLU:OE1  | 1.88                     | 0.73              |
| 1:J:818:TYR:CE1  | 2:K:127:ARG:NH1  | 2.57                     | 0.73              |
| 1:D:542:PHE:CD2  | 4:5:143:TYR:CE1  | 2.77                     | 0.73              |
| 1:G:409:GLY:HA3  | 4:6:333:PRO:N    | 2.03                     | 0.73              |
| 1:A:237:THR:HG22 | 1:A:239:ARG:H    | 1.53                     | 0.73              |
| 1:A:707:CYS:HA   | 1:A:714:ARG:CZ   | 2.18                     | 0.73              |
| 1:A:831:TRP:CD2  | 2:B:51:PHE:CE1   | 2.77                     | 0.73              |
| 2:E:130:PRO:O    | 2:E:132:GLU:N    | 2.21                     | 0.73              |
| 1:G:486:MLY:HH13 | 1:G:527:GLU:OE1  | 1.87                     | 0.73              |
| 1:G:487:LEU:O    | 1:G:490:PHE:HB3  | 1.89                     | 0.73              |
| 1:G:536:LEU:HD13 | 1:G:550:PHE:CZ   | 2.24                     | 0.73              |
| 1:G:93:MET:HE2   | 1:G:764:MLY:HE3  | 1.69                     | 0.73              |
| 2:H:130:PRO:O    | 2:H:132:GLU:N    | 2.21                     | 0.73              |
| 4:0:253:GLU:HA   | 4:0:256:ARG:HG3  | 1.69                     | 0.73              |
| 1:D:530:MET:CE   | 4:5:355:MET:SD   | 2.77                     | 0.73              |
| 1:G:410:ASN:OD1  | 4:6:335:ARG:N    | 2.21                     | 0.73              |
| 1:J:530:MET:CE   | 4:7:355:MET:SD   | 2.77                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:131:TRP:C    | 1:A:132:LEU:HD12 | 2.09                     | 0.73              |
| 2:B:130:PRO:O    | 2:B:132:GLU:N    | 2.21                     | 0.73              |
| 1:D:802:GLU:O    | 1:D:806:MET:HG3  | 1.89                     | 0.73              |
| 1:D:829:TRP:CD1  | 2:E:67:MET:HG2   | 2.24                     | 0.73              |
| 3:F:24:LYS:CA    | 3:F:63:ILE:O     | 2.36                     | 0.73              |
| 1:J:640:LYS:O    | 1:J:645:SER:OG   | 2.06                     | 0.73              |
| 1:J:790:THR:N    | 3:L:87:PHE:CE2   | 2.57                     | 0.73              |
| 4:7:288:ASP:H    | 4:V:203:THR:HG22 | 1.52                     | 0.73              |
| 1:G:635:GLY:HA3  | 4:6:341:ILE:CD1  | 2.14                     | 0.73              |
| 1:D:557:GLU:N    | 4:7:48:GLY:HA3   | 1.90                     | 0.73              |
| 1:A:536:LEU:HD13 | 1:A:550:PHE:CZ   | 2.24                     | 0.73              |
| 1:A:97:LEU:CD2   | 1:A:712:PRO:HB3  | 2.19                     | 0.73              |
| 1:G:190:MLY:HE3  | 1:G:230:GLU:OE2  | 1.89                     | 0.73              |
| 1:G:93:MET:HE2   | 1:G:764:MLY:CG   | 2.13                     | 0.73              |
| 1:J:436:MLY:HE3  | 1:J:626:TYR:CE1  | 2.23                     | 0.73              |
| 1:A:410:ASN:OD1  | 4:4:335:ARG:N    | 2.22                     | 0.73              |
| 4:5:290:ARG:HH22 | 4:7:202:THR:HG23 | 1.50                     | 0.73              |
| 1:D:441:MET:O    | 1:D:445:ILE:HG13 | 1.88                     | 0.73              |
| 1:D:486:MLY:HH13 | 1:D:527:GLU:OE1  | 1.88                     | 0.73              |
| 1:G:733:PRO:C    | 1:G:737:PHE:CD1  | 2.62                     | 0.73              |
| 2:H:144:VAL:CB   | 2:H:153:ILE:HD11 | 2.19                     | 0.73              |
| 1:D:410:ASN:OD1  | 4:5:335:ARG:N    | 2.22                     | 0.73              |
| 1:A:735:GLY:CA   | 1:A:743:ALA:HA   | 2.18                     | 0.73              |
| 1:D:190:MLY:HE3  | 1:D:230:GLU:OE2  | 1.89                     | 0.73              |
| 1:D:618:THR:O    | 1:D:622:LEU:HD13 | 1.89                     | 0.73              |
| 1:D:769:ALA:HB1  | 1:D:770:GLY:HA3  | 1.71                     | 0.73              |
| 1:G:410:ASN:CG   | 4:6:334:GLU:CA   | 2.47                     | 0.73              |
| 1:G:272:MLY:HH13 | 1:G:435:GLU:OE1  | 1.88                     | 0.73              |
| 1:G:640:LYS:O    | 4:6:23:GLY:O     | 2.06                     | 0.73              |
| 1:G:802:GLU:O    | 1:G:806:MET:HG3  | 1.88                     | 0.73              |
| 1:J:190:MLY:HE3  | 1:J:230:GLU:OE2  | 1.89                     | 0.73              |
| 1:J:237:THR:HG22 | 1:J:239:ARG:H    | 1.54                     | 0.73              |
| 1:J:732:ILE:N    | 1:J:733:PRO:CD   | 2.51                     | 0.73              |
| 4:Z:253:GLU:HA   | 4:Z:256:ARG:HG3  | 1.69                     | 0.73              |
| 1:J:410:ASN:OD1  | 4:7:335:ARG:N    | 2.21                     | 0.72              |
| 1:D:214:MET:HA   | 1:D:340:ILE:HD11 | 1.71                     | 0.72              |
| 1:D:36:SER:O     | 1:D:52:ILE:HG12  | 1.89                     | 0.72              |
| 1:D:640:LYS:O    | 1:D:645:SER:OG   | 2.06                     | 0.72              |
| 1:G:436:MLY:HE3  | 1:G:626:TYR:CE1  | 2.23                     | 0.72              |
| 1:G:538:GLU:O    | 4:6:349:LEU:HG   | 1.87                     | 0.72              |
| 1:G:817:GLN:CG   | 2:H:127:ARG:HB2  | 2.16                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:215:GLN:NE2  | 1:J:336:SER:O    | 2.21                     | 0.72              |
| 1:J:553:MLY:NZ   | 4:V:45:VAL:HA    | 1.84                     | 0.72              |
| 4:2:253:GLU:HA   | 4:2:256:ARG:HG3  | 1.69                     | 0.72              |
| 1:A:441:MET:O    | 1:A:445:ILE:HG13 | 1.88                     | 0.72              |
| 1:A:721:LYS:CB   | 1:A:736:GLN:CD   | 2.56                     | 0.72              |
| 1:A:802:GLU:O    | 1:A:806:MET:HG3  | 1.89                     | 0.72              |
| 1:A:834:LEU:HD21 | 2:B:54:MET:SD    | 2.29                     | 0.72              |
| 1:D:237:THR:HG22 | 1:D:239:ARG:H    | 1.54                     | 0.72              |
| 1:G:21:GLU:O     | 1:G:25:ILE:HG13  | 1.89                     | 0.72              |
| 1:J:21:GLU:O     | 1:J:25:ILE:HG13  | 1.89                     | 0.72              |
| 1:J:36:SER:O     | 1:J:52:ILE:HG12  | 1.89                     | 0.72              |
| 1:J:618:THR:O    | 1:J:622:LEU:HD13 | 1.89                     | 0.72              |
| 1:J:802:GLU:O    | 1:J:806:MET:HG3  | 1.88                     | 0.72              |
| 3:L:24:LYS:CA    | 3:L:63:ILE:O     | 2.37                     | 0.72              |
| 1:J:557:GLU:N    | 4:V:48:GLY:HA2   | 1.90                     | 0.72              |
| 1:J:409:GLY:HA3  | 4:7:333:PRO:N    | 2.03                     | 0.72              |
| 1:A:272:MLY:HH13 | 1:A:435:GLU:OE1  | 1.88                     | 0.72              |
| 1:A:534:SER:CA   | 4:4:351:THR:HA   | 2.18                     | 0.72              |
| 1:A:641:LYS:HD2  | 1:A:647:GLN:OE1  | 1.81                     | 0.72              |
| 1:D:536:LEU:HD13 | 1:D:550:PHE:CZ   | 2.24                     | 0.72              |
| 2:E:144:VAL:CB   | 2:E:153:ILE:HD11 | 2.19                     | 0.72              |
| 1:J:542:PHE:CD2  | 4:7:143:TYR:CE1  | 2.77                     | 0.72              |
| 1:J:754:ASP:HB3  | 1:J:757:GLN:HG2  | 1.71                     | 0.72              |
| 1:D:735:GLY:CA   | 1:D:743:ALA:HA   | 2.18                     | 0.72              |
| 2:E:117:LEU:CB   | 2:E:147:ASN:ND2  | 2.35                     | 0.72              |
| 1:G:214:MET:HA   | 1:G:340:ILE:HD11 | 1.70                     | 0.72              |
| 1:G:618:THR:O    | 1:G:622:LEU:HD13 | 1.89                     | 0.72              |
| 1:G:640:LYS:O    | 1:G:645:SER:OG   | 2.06                     | 0.72              |
| 1:J:214:MET:HA   | 1:J:340:ILE:HD11 | 1.70                     | 0.72              |
| 1:J:295:MLY:HG3  | 1:J:332:MET:CE   | 2.19                     | 0.72              |
| 1:J:536:LEU:HD13 | 1:J:550:PHE:CZ   | 2.24                     | 0.72              |
| 1:J:95:THR:CB    | 1:J:713:SER:HB3  | 2.20                     | 0.72              |
| 3:L:4:LYS:N      | 3:L:5:ALA:O      | 2.16                     | 0.72              |
| 4:0:290:ARG:HH22 | 4:2:202:THR:HG23 | 1.50                     | 0.72              |
| 4:4:3:ASP:HA     | 4:4:6:THR:CB     | 2.18                     | 0.72              |
| 3:C:24:LYS:CA    | 3:C:63:ILE:O     | 2.37                     | 0.72              |
| 1:D:295:MLY:HG3  | 1:D:332:MET:CE   | 2.20                     | 0.72              |
| 1:D:789:ALA:HB2  | 3:F:81:GLN:HG2   | 1.72                     | 0.72              |
| 1:G:176:LEU:N    | 1:G:176:LEU:HD12 | 2.05                     | 0.72              |
| 1:G:754:ASP:HB3  | 1:G:757:GLN:HG2  | 1.72                     | 0.72              |
| 1:G:817:GLN:CB   | 2:H:127:ARG:HH11 | 2.02                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:721:LYS:CB   | 1:J:736:GLN:CD   | 2.56                     | 0.72              |
| 1:A:21:GLU:O     | 1:A:25:ILE:HG13  | 1.88                     | 0.72              |
| 1:A:519:LEU:HD12 | 1:A:519:LEU:N    | 2.04                     | 0.72              |
| 1:A:486:MLY:HH22 | 1:A:527:GLU:OE2  | 1.90                     | 0.72              |
| 1:A:36:SER:O     | 1:A:52:ILE:HG12  | 1.89                     | 0.72              |
| 1:G:93:MET:HE1   | 1:G:763:THR:HG22 | 1.67                     | 0.72              |
| 1:J:769:ALA:HB3  | 1:J:770:GLY:N    | 2.04                     | 0.72              |
| 2:K:144:VAL:CB   | 2:K:153:ILE:HD11 | 2.19                     | 0.72              |
| 4:Y:3:ASP:HA     | 4:Y:6:THR:CB     | 2.18                     | 0.72              |
| 1:A:290:GLN:C    | 1:A:331:LEU:HD12 | 2.09                     | 0.72              |
| 1:A:707:CYS:CA   | 1:A:714:ARG:NH1  | 2.50                     | 0.72              |
| 1:D:21:GLU:O     | 1:D:25:ILE:HG13  | 1.88                     | 0.72              |
| 1:D:817:GLN:OE1  | 2:E:127:ARG:NE   | 2.22                     | 0.72              |
| 1:G:486:MLY:HH22 | 1:G:527:GLU:OE2  | 1.90                     | 0.72              |
| 1:G:530:MET:CE   | 4:6:355:MET:SD   | 2.78                     | 0.72              |
| 1:G:731:ALA:HB2  | 3:I:109:HIS:ND1  | 2.04                     | 0.72              |
| 2:H:117:LEU:HD12 | 2:H:147:ASN:CA   | 2.19                     | 0.72              |
| 4:W:3:ASP:HA     | 4:W:6:THR:CB     | 2.18                     | 0.72              |
| 1:G:237:THR:HG22 | 1:G:239:ARG:H    | 1.54                     | 0.72              |
| 1:G:290:GLN:C    | 1:G:331:LEU:HD12 | 2.09                     | 0.72              |
| 1:G:441:MET:O    | 1:G:445:ILE:HG13 | 1.88                     | 0.72              |
| 1:J:131:TRP:C    | 1:J:132:LEU:HD12 | 2.09                     | 0.72              |
| 1:J:510:TRP:CZ3  | 1:J:768:MLY:HH12 | 2.23                     | 0.72              |
| 1:J:795:ARG:HD2  | 3:L:35:ARG:HH12  | 1.54                     | 0.72              |
| 4:3:290:ARG:NH1  | 4:5:202:THR:CG2  | 2.49                     | 0.72              |
| 1:D:217:THR:C    | 1:D:221:GLN:HE21 | 1.92                     | 0.72              |
| 1:D:292:MET:HE3  | 1:D:309:PRO:HA   | 1.71                     | 0.72              |
| 1:D:290:GLN:C    | 1:D:331:LEU:HD12 | 2.09                     | 0.72              |
| 1:D:641:LYS:HD2  | 1:D:647:GLN:OE1  | 1.81                     | 0.72              |
| 1:D:754:ASP:HB3  | 1:D:757:GLN:HG2  | 1.72                     | 0.72              |
| 1:G:732:ILE:HG23 | 1:G:747:LEU:CB   | 1.84                     | 0.72              |
| 2:K:136:MET:O    | 2:K:140:PHE:HB2  | 1.90                     | 0.72              |
| 4:W:290:ARG:HH22 | 4:Y:202:THR:HG23 | 1.51                     | 0.72              |
| 1:A:14:ALA:HB3   | 1:A:15:PRO:HD3   | 1.72                     | 0.72              |
| 2:B:144:VAL:CB   | 2:B:153:ILE:HD11 | 2.19                     | 0.72              |
| 1:D:486:MLY:HH22 | 1:D:527:GLU:OE2  | 1.90                     | 0.72              |
| 1:G:14:ALA:HB3   | 1:G:15:PRO:HD3   | 1.72                     | 0.72              |
| 1:G:721:LYS:CB   | 1:G:736:GLN:CD   | 2.56                     | 0.72              |
| 4:1:3:ASP:HA     | 4:1:6:THR:CB     | 2.18                     | 0.71              |
| 4:5:3:ASP:HA     | 4:5:6:THR:CB     | 2.18                     | 0.71              |
| 1:A:217:THR:C    | 1:A:221:GLN:HE21 | 1.93                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:754:ASP:HB3  | 1:A:757:GLN:HG2  | 1.72                     | 0.71              |
| 1:A:795:ARG:HD2  | 3:C:35:ARG:NH2   | 2.01                     | 0.71              |
| 1:D:834:LEU:HD13 | 2:E:51:PHE:HA    | 1.71                     | 0.71              |
| 1:J:176:LEU:N    | 1:J:176:LEU:HD12 | 2.05                     | 0.71              |
| 1:A:217:THR:O    | 1:A:220:ASP:HB2  | 1.91                     | 0.71              |
| 1:A:487:LEU:O    | 1:A:490:PHE:HB3  | 1.88                     | 0.71              |
| 1:D:176:LEU:HD12 | 1:D:176:LEU:N    | 2.05                     | 0.71              |
| 1:D:519:LEU:N    | 1:D:519:LEU:HD12 | 2.05                     | 0.71              |
| 1:G:131:TRP:C    | 1:G:132:LEU:HD12 | 2.09                     | 0.71              |
| 1:G:519:LEU:N    | 1:G:519:LEU:HD12 | 2.05                     | 0.71              |
| 1:G:542:PHE:CD2  | 4:6:143:TYR:CE1  | 2.78                     | 0.71              |
| 1:G:739:ASP:CB   | 1:G:742:LYS:HB3  | 2.12                     | 0.71              |
| 1:J:486:MLY:HH22 | 1:J:527:GLU:OE2  | 1.90                     | 0.71              |
| 1:J:816:ILE:HD11 | 2:K:100:ALA:CB   | 2.19                     | 0.71              |
| 1:J:800:ARG:CG   | 3:L:149:VAL:HG23 | 2.12                     | 0.71              |
| 4:8:3:ASP:HA     | 4:8:6:THR:CB     | 2.18                     | 0.71              |
| 1:A:190:MLY:HE3  | 1:A:230:GLU:OE2  | 1.89                     | 0.71              |
| 1:A:836:PHE:CE1  | 2:B:159:HIS:CA   | 2.71                     | 0.71              |
| 1:D:131:TRP:C    | 1:D:132:LEU:HD12 | 2.09                     | 0.71              |
| 1:D:217:THR:O    | 1:D:220:ASP:HB2  | 1.90                     | 0.71              |
| 2:E:136:MET:O    | 2:E:140:PHE:HB2  | 1.90                     | 0.71              |
| 1:G:84:MLY:HH11  | 1:G:715:VAL:HG11 | 1.70                     | 0.71              |
| 1:G:798:LEU:HD13 | 3:I:126:LEU:HD21 | 0.72                     | 0.71              |
| 1:J:290:GLN:C    | 1:J:331:LEU:HD12 | 2.09                     | 0.71              |
| 1:G:534:SER:CA   | 4:6:351:THR:HA   | 2.20                     | 0.71              |
| 1:A:793:ARG:HG3  | 3:C:146:ILE:CG2  | 2.21                     | 0.71              |
| 1:G:795:ARG:CB   | 3:I:35:ARG:HH21  | 1.91                     | 0.71              |
| 1:J:72:VAL:HG13  | 1:J:76:GLN:CB    | 2.19                     | 0.71              |
| 1:J:510:TRP:CE3  | 1:J:768:MLY:CH1  | 2.72                     | 0.71              |
| 1:A:214:MET:HA   | 1:A:340:ILE:HD11 | 1.71                     | 0.71              |
| 1:D:245:ARG:HD3  | 1:D:271:GLU:OE1  | 1.90                     | 0.71              |
| 1:D:792:ALA:CB   | 3:F:40:ASN:HB3   | 2.19                     | 0.71              |
| 1:G:36:SER:O     | 1:G:52:ILE:HG12  | 1.90                     | 0.71              |
| 1:J:217:THR:C    | 1:J:221:GLN:HE21 | 1.92                     | 0.71              |
| 1:J:823:PHE:CD1  | 2:K:156:VAL:O    | 2.44                     | 0.71              |
| 1:A:166:MET:HE3  | 1:A:254:PHE:CD2  | 2.25                     | 0.71              |
| 1:A:618:THR:O    | 1:A:622:LEU:HD13 | 1.89                     | 0.71              |
| 1:A:640:LYS:O    | 1:A:645:SER:OG   | 2.06                     | 0.71              |
| 2:B:136:MET:O    | 2:B:140:PHE:HB2  | 1.90                     | 0.71              |
| 1:D:724:TYR:CA   | 1:D:782:MLY:NZ   | 2.53                     | 0.71              |
| 1:D:86:ASP:OD2   | 1:D:87:MLY:HH13  | 1.91                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:F:4:LYS:N      | 3:F:5:ALA:O      | 2.16                     | 0.71              |
| 1:G:217:THR:C    | 1:G:221:GLN:HE21 | 1.92                     | 0.71              |
| 1:J:295:MLY:HG3  | 1:J:332:MET:HE1  | 1.72                     | 0.71              |
| 1:J:410:ASN:CG   | 4:7:334:GLU:CA   | 2.47                     | 0.71              |
| 1:J:519:LEU:HD12 | 1:J:519:LEU:N    | 2.04                     | 0.71              |
| 4:X:290:ARG:HH22 | 4:Z:202:THR:HG23 | 1.50                     | 0.71              |
| 4:Z:3:ASP:HA     | 4:Z:6:THR:CB     | 2.18                     | 0.71              |
| 1:G:553:MLY:HG2  | 4:8:47:MET:N     | 2.06                     | 0.71              |
| 1:A:206:LYS:HD3  | 1:A:217:THR:HG23 | 0.71                     | 0.71              |
| 1:A:295:MLY:HG3  | 1:A:332:MET:CE   | 2.19                     | 0.71              |
| 1:A:798:LEU:HD11 | 3:C:126:LEU:CG   | 2.20                     | 0.71              |
| 1:A:831:TRP:CZ3  | 2:B:50:THR:CG2   | 2.72                     | 0.71              |
| 1:A:830:PRO:HG2  | 2:B:67:MET:CE    | 2.20                     | 0.71              |
| 1:D:56:GLU:CB    | 1:D:59:MLY:HB3   | 2.19                     | 0.71              |
| 1:J:831:TRP:HH2  | 2:K:34:ILE:HG21  | 1.55                     | 0.71              |
| 1:A:819:ASN:N    | 2:B:90:GLY:CA    | 2.53                     | 0.71              |
| 1:D:800:ARG:HB3  | 3:F:149:VAL:HG23 | 1.67                     | 0.71              |
| 1:D:817:GLN:HG3  | 2:E:127:ARG:CD   | 2.19                     | 0.71              |
| 1:G:274:ARG:NH2  | 1:G:282:GLU:OE1  | 2.24                     | 0.71              |
| 1:J:56:GLU:CB    | 1:J:59:MLY:HB3   | 2.19                     | 0.71              |
| 1:J:84:MLY:CH2   | 1:J:716:LEU:O    | 2.38                     | 0.71              |
| 1:J:757:GLN:HG3  | 1:J:776:GLU:HG3  | 1.64                     | 0.71              |
| 4:7:290:ARG:HH22 | 4:V:202:THR:HG23 | 1.50                     | 0.71              |
| 4:3:3:ASP:HA     | 4:3:6:THR:CB     | 2.18                     | 0.71              |
| 1:D:14:ALA:HB3   | 1:D:15:PRO:HD3   | 1.72                     | 0.71              |
| 1:D:831:TRP:CD1  | 2:E:51:PHE:HZ    | 2.09                     | 0.71              |
| 1:D:834:LEU:HD12 | 2:E:54:MET:HB2   | 1.73                     | 0.71              |
| 1:G:166:MET:HE1  | 1:G:254:PHE:HB2  | 1.72                     | 0.71              |
| 1:G:717:TYR:HD1  | 1:G:744:SER:HG   | 1.39                     | 0.71              |
| 1:G:834:LEU:CD1  | 2:H:51:PHE:CD1   | 2.74                     | 0.71              |
| 1:J:274:ARG:NH2  | 1:J:282:GLU:OE1  | 2.24                     | 0.71              |
| 1:J:762:HIS:CD2  | 1:J:762:HIS:H    | 2.07                     | 0.71              |
| 4:2:290:ARG:HH22 | 4:4:202:THR:HG23 | 1.50                     | 0.71              |
| 1:D:831:TRP:CD1  | 2:E:51:PHE:CZ    | 2.79                     | 0.71              |
| 1:G:86:ASP:OD2   | 1:G:87:MLY:HH13  | 1.91                     | 0.71              |
| 1:J:14:ALA:HB3   | 1:J:15:PRO:HD3   | 1.72                     | 0.71              |
| 1:J:245:ARG:HD3  | 1:J:271:GLU:OE1  | 1.90                     | 0.71              |
| 1:A:505:MLY:HB2  | 1:A:761:GLY:C    | 2.11                     | 0.70              |
| 1:G:245:ARG:HD3  | 1:G:271:GLU:OE1  | 1.90                     | 0.70              |
| 1:D:530:MET:HE2  | 4:5:354:GLN:HG3  | 1.73                     | 0.70              |
| 4:6:3:ASP:HA     | 4:6:6:THR:CB     | 2.18                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:176:LEU:HD12 | 1:A:176:LEU:N    | 2.05                     | 0.70              |
| 1:A:72:VAL:HG13  | 1:A:76:GLN:CB    | 2.19                     | 0.70              |
| 1:D:579:PHE:HD2  | 1:D:592:ILE:HD11 | 1.56                     | 0.70              |
| 1:G:295:MLY:HG3  | 1:G:332:MET:CE   | 2.20                     | 0.70              |
| 1:G:550:PHE:HA   | 4:8:46:GLY:HA3   | 1.66                     | 0.70              |
| 1:G:792:ALA:HA   | 3:I:35:ARG:NH1   | 2.04                     | 0.70              |
| 1:G:793:ARG:NH1  | 3:I:40:ASN:HD21  | 1.90                     | 0.70              |
| 1:G:810:ARG:HH11 | 1:G:810:ARG:HG2  | 1.56                     | 0.70              |
| 1:J:206:LYS:HD3  | 1:J:217:THR:HG23 | 0.71                     | 0.70              |
| 1:J:217:THR:O    | 1:J:220:ASP:HB2  | 1.91                     | 0.70              |
| 1:J:93:MET:SD    | 1:J:764:MLY:CH2  | 2.65                     | 0.70              |
| 3:C:48:LYS:HB3   | 3:C:52:ASN:HD21  | 1.57                     | 0.70              |
| 1:D:577:ALA:O    | 1:D:578:HIS:CG   | 2.45                     | 0.70              |
| 1:D:643:GLY:N    | 4:5:24:ASP:CA    | 2.46                     | 0.70              |
| 1:D:800:ARG:CD   | 3:F:149:VAL:HG22 | 2.21                     | 0.70              |
| 1:J:754:ASP:CG   | 1:J:776:GLU:CA   | 2.59                     | 0.70              |
| 1:J:787:ILE:HG22 | 1:J:788:THR:N    | 2.07                     | 0.70              |
| 1:J:86:ASP:OD2   | 1:J:87:MLY:HH13  | 1.91                     | 0.70              |
| 1:J:826:VAL:CG2  | 2:K:88:LEU:HD21  | 2.12                     | 0.70              |
| 1:A:245:ARG:HD3  | 1:A:271:GLU:OE1  | 1.90                     | 0.70              |
| 1:A:274:ARG:NH2  | 1:A:282:GLU:OE1  | 2.24                     | 0.70              |
| 1:A:787:ILE:HG22 | 1:A:788:THR:N    | 2.07                     | 0.70              |
| 1:D:641:LYS:HD2  | 4:5:348:SER:HA   | 1.73                     | 0.70              |
| 1:D:769:ALA:HB1  | 1:D:770:GLY:N    | 2.05                     | 0.70              |
| 1:G:579:PHE:HD2  | 1:G:592:ILE:HD11 | 1.56                     | 0.70              |
| 1:G:721:LYS:HG2  | 1:G:736:GLN:CD   | 1.86                     | 0.70              |
| 1:J:213:LYS:HA   | 1:J:220:ASP:OD1  | 1.92                     | 0.70              |
| 1:J:630:ALA:O    | 4:7:25:ASP:HB2   | 1.91                     | 0.70              |
| 1:A:123:CYS:HB2  | 1:A:158:ILE:HD11 | 1.73                     | 0.70              |
| 1:A:818:TYR:HB2  | 2:B:90:GLY:CA    | 2.22                     | 0.70              |
| 1:A:86:ASP:OD2   | 1:A:87:MLY:HH13  | 1.91                     | 0.70              |
| 1:D:274:ARG:NH2  | 1:D:282:GLU:OE1  | 2.24                     | 0.70              |
| 1:D:72:VAL:HG13  | 1:D:76:GLN:CB    | 2.19                     | 0.70              |
| 1:D:831:TRP:CG   | 2:E:51:PHE:HZ    | 2.10                     | 0.70              |
| 1:D:789:ALA:CB   | 3:F:81:GLN:O     | 2.39                     | 0.70              |
| 1:G:217:THR:O    | 1:G:220:ASP:HB2  | 1.91                     | 0.70              |
| 2:H:136:MET:O    | 2:H:140:PHE:HB2  | 1.90                     | 0.70              |
| 1:D:213:LYS:HA   | 1:D:220:ASP:OD1  | 1.92                     | 0.70              |
| 1:D:834:LEU:CD1  | 2:E:51:PHE:HA    | 2.20                     | 0.70              |
| 3:F:25:ILE:O     | 3:F:63:ILE:HB    | 1.92                     | 0.70              |
| 1:A:579:PHE:HD2  | 1:A:592:ILE:HD11 | 1.56                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:839:MLY:CD   | 2:B:159:HIS:CG   | 2.70                     | 0.70              |
| 3:F:48:LYS:HB3   | 3:F:52:ASN:HD21  | 1.57                     | 0.70              |
| 1:G:56:GLU:CB    | 1:G:59:MLY:HB3   | 2.19                     | 0.70              |
| 1:J:123:CYS:HB2  | 1:J:158:ILE:HD11 | 1.73                     | 0.70              |
| 1:J:641:LYS:HD2  | 4:7:348:SER:HA   | 1.73                     | 0.70              |
| 1:J:810:ARG:HH11 | 1:J:810:ARG:HG2  | 1.57                     | 0.70              |
| 1:A:839:MLY:HD2  | 2:B:159:HIS:CB   | 2.21                     | 0.70              |
| 1:A:814:PHE:HD1  | 2:B:127:ARG:NH2  | 1.70                     | 0.70              |
| 1:D:789:ALA:HB1  | 3:F:81:GLN:O     | 1.92                     | 0.70              |
| 1:G:123:CYS:HB2  | 1:G:158:ILE:HD11 | 1.73                     | 0.70              |
| 1:G:798:LEU:HD23 | 3:I:122:GLU:CB   | 2.20                     | 0.70              |
| 1:J:577:ALA:O    | 1:J:578:HIS:CG   | 2.45                     | 0.70              |
| 3:L:25:ILE:O     | 3:L:63:ILE:HB    | 1.92                     | 0.70              |
| 1:A:546:THR:HG22 | 1:A:548:THR:N    | 2.05                     | 0.70              |
| 1:A:732:ILE:HG21 | 1:A:747:LEU:HD11 | 0.73                     | 0.70              |
| 1:G:762:HIS:H    | 1:G:762:HIS:CD2  | 2.07                     | 0.70              |
| 1:J:800:ARG:HB2  | 3:L:149:VAL:CG2  | 2.07                     | 0.70              |
| 1:J:818:TYR:CE1  | 2:K:127:ARG:CZ   | 2.75                     | 0.70              |
| 1:D:630:ALA:O    | 4:5:25:ASP:HB2   | 1.92                     | 0.70              |
| 1:A:813:ILE:HG22 | 2:B:127:ARG:NH1  | 2.06                     | 0.70              |
| 2:B:111:SER:OG   | 2:B:148:VAL:HG12 | 1.92                     | 0.70              |
| 1:D:123:CYS:HB2  | 1:D:158:ILE:HD11 | 1.73                     | 0.70              |
| 1:D:206:LYS:HD3  | 1:D:217:THR:HG23 | 0.71                     | 0.70              |
| 1:D:782:MLY:C    | 1:D:783:LEU:HD12 | 2.22                     | 0.70              |
| 1:D:810:ARG:HG2  | 1:D:810:ARG:HH11 | 1.57                     | 0.70              |
| 1:G:782:MLY:C    | 1:G:783:LEU:HD12 | 2.22                     | 0.70              |
| 3:I:25:ILE:O     | 3:I:63:ILE:HB    | 1.92                     | 0.70              |
| 1:J:215:GLN:CA   | 1:J:340:ILE:CG2  | 2.62                     | 0.70              |
| 4:8:1:ASP:HA     | 4:8:4:GLU:HB3    | 1.74                     | 0.69              |
| 1:A:733:PRO:C    | 1:A:737:PHE:CD1  | 2.62                     | 0.69              |
| 1:A:769:ALA:N    | 1:A:771:LEU:HB2  | 2.07                     | 0.69              |
| 1:A:802:GLU:OE1  | 1:A:802:GLU:HA   | 1.92                     | 0.69              |
| 1:D:726:VAL:H    | 1:D:782:MLY:HH22 | 1.55                     | 0.69              |
| 1:G:546:THR:HG22 | 1:G:548:THR:N    | 2.05                     | 0.69              |
| 1:J:838:ILE:HD11 | 2:K:54:MET:HE1   | 1.74                     | 0.69              |
| 4:W:1:ASP:HA     | 4:W:4:GLU:HB3    | 1.74                     | 0.69              |
| 4:0:3:ASP:HA     | 4:0:6:THR:CB     | 2.18                     | 0.69              |
| 1:A:800:ARG:CG   | 3:C:149:VAL:CG2  | 2.60                     | 0.69              |
| 1:G:643:GLY:N    | 4:6:24:ASP:CA    | 2.47                     | 0.69              |
| 3:L:48:LYS:HB3   | 3:L:52:ASN:HD21  | 1.57                     | 0.69              |
| 1:A:577:ALA:O    | 1:A:578:HIS:CG   | 2.45                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:117:LEU:CB   | 2:B:147:ASN:OD1  | 2.39                     | 0.69              |
| 2:E:117:LEU:HD12 | 2:E:147:ASN:CA   | 2.19                     | 0.69              |
| 1:J:530:MET:HE2  | 4:7:354:GLN:HG3  | 1.74                     | 0.69              |
| 1:J:579:PHE:HD2  | 1:J:592:ILE:HD11 | 1.56                     | 0.69              |
| 1:J:630:ALA:O    | 4:7:25:ASP:CB    | 2.41                     | 0.69              |
| 1:J:733:PRO:C    | 1:J:737:PHE:CD1  | 2.62                     | 0.69              |
| 4:Y:1:ASP:HA     | 4:Y:4:GLU:HB3    | 1.74                     | 0.69              |
| 4:1:1:ASP:HA     | 4:1:4:GLU:HB3    | 1.74                     | 0.69              |
| 1:A:834:LEU:CD2  | 2:B:54:MET:HG3   | 2.22                     | 0.69              |
| 1:G:72:VAL:HG13  | 1:G:76:GLN:CB    | 2.19                     | 0.69              |
| 1:G:800:ARG:HD2  | 3:I:149:VAL:HG23 | 1.72                     | 0.69              |
| 2:H:111:SER:OG   | 2:H:148:VAL:HG12 | 1.92                     | 0.69              |
| 2:K:111:SER:OG   | 2:K:148:VAL:HG12 | 1.92                     | 0.69              |
| 1:A:641:LYS:HD2  | 4:4:348:SER:HA   | 1.73                     | 0.69              |
| 1:A:782:MLY:C    | 1:A:783:LEU:HD12 | 2.22                     | 0.69              |
| 1:A:810:ARG:HG2  | 1:A:810:ARG:HH11 | 1.57                     | 0.69              |
| 3:C:3:SER:O      | 3:C:4:LYS:CB     | 2.41                     | 0.69              |
| 1:D:218:LEU:HB2  | 1:D:221:GLN:CG   | 2.09                     | 0.69              |
| 1:G:93:MET:SD    | 1:G:716:LEU:HD11 | 2.32                     | 0.69              |
| 1:J:768:MLY:HH23 | 1:J:772:LEU:CD1  | 2.21                     | 0.69              |
| 1:J:823:PHE:CZ   | 2:K:156:VAL:HG12 | 2.27                     | 0.69              |
| 4:6:1:ASP:HA     | 4:6:4:GLU:HB3    | 1.74                     | 0.69              |
| 1:A:123:CYS:HB2  | 1:A:158:ILE:CD1  | 2.23                     | 0.69              |
| 1:A:166:MET:HE3  | 1:A:254:PHE:HD2  | 1.58                     | 0.69              |
| 1:D:553:MLY:HG2  | 4:7:47:MET:N     | 2.07                     | 0.69              |
| 1:G:787:ILE:HG22 | 1:G:788:THR:N    | 2.07                     | 0.69              |
| 1:G:817:GLN:CB   | 2:H:127:ARG:CD   | 2.53                     | 0.69              |
| 4:3:1:ASP:HA     | 4:3:4:GLU:HB3    | 1.74                     | 0.69              |
| 4:7:3:ASP:HA     | 4:7:6:THR:CB     | 2.18                     | 0.69              |
| 1:A:553:MLY:HG2  | 4:6:47:MET:N     | 2.07                     | 0.69              |
| 1:A:818:TYR:CB   | 2:B:90:GLY:N     | 2.56                     | 0.69              |
| 1:D:541:MET:CG   | 4:5:345:ILE:O    | 2.41                     | 0.69              |
| 1:G:206:LYS:HD3  | 1:G:217:THR:HG23 | 0.70                     | 0.69              |
| 1:G:577:ALA:O    | 1:G:578:HIS:CG   | 2.45                     | 0.69              |
| 1:G:815:CYS:O    | 1:G:819:ASN:HB2  | 1.93                     | 0.69              |
| 1:J:752:ASP:O    | 1:J:780:ASP:CG   | 2.31                     | 0.69              |
| 1:J:807:VAL:O    | 1:J:810:ARG:HB2  | 1.93                     | 0.69              |
| 4:2:3:ASP:HA     | 4:2:6:THR:CB     | 2.18                     | 0.69              |
| 1:D:642:LYS:HB3  | 4:5:21:PHE:O     | 1.93                     | 0.69              |
| 4:5:1:ASP:HA     | 4:5:4:GLU:HB3    | 1.74                     | 0.69              |
| 1:D:556:ASP:HA   | 4:7:49:GLN:O     | 1.70                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:630:ALA:O    | 4:4:25:ASP:HB2   | 1.92                     | 0.69              |
| 1:A:798:LEU:HD21 | 3:C:122:GLU:HB3  | 1.73                     | 0.69              |
| 1:A:793:ARG:CG   | 3:C:146:ILE:HG22 | 2.21                     | 0.69              |
| 1:D:807:VAL:O    | 1:D:810:ARG:HB2  | 1.93                     | 0.69              |
| 1:J:218:LEU:HB2  | 1:J:221:GLN:CG   | 2.09                     | 0.69              |
| 3:L:3:SER:O      | 3:L:4:LYS:CB     | 2.41                     | 0.69              |
| 4:V:3:ASP:HA     | 4:V:6:THR:CB     | 2.18                     | 0.69              |
| 1:J:530:MET:HE3  | 4:7:354:GLN:HG2  | 1.71                     | 0.69              |
| 1:D:510:TRP:CH2  | 1:D:711:PHE:HE2  | 2.11                     | 0.69              |
| 1:D:769:ALA:CA   | 1:D:770:GLY:C    | 2.61                     | 0.69              |
| 1:D:800:ARG:HD2  | 3:F:149:VAL:CG2  | 2.22                     | 0.69              |
| 1:G:123:CYS:HB2  | 1:G:158:ILE:CD1  | 2.23                     | 0.69              |
| 1:J:802:GLU:OE1  | 1:J:802:GLU:HA   | 1.93                     | 0.69              |
| 1:A:642:LYS:HB3  | 4:4:21:PHE:O     | 1.93                     | 0.69              |
| 1:G:641:LYS:HD2  | 4:6:348:SER:HA   | 1.73                     | 0.69              |
| 1:G:752:ASP:C    | 1:G:779:ARG:HH12 | 1.96                     | 0.69              |
| 1:G:820:VAL:HG11 | 2:H:136:MET:HE3  | 1.73                     | 0.69              |
| 4:4:1:ASP:HA     | 4:4:4:GLU:HB3    | 1.74                     | 0.69              |
| 1:A:550:PHE:HA   | 4:6:46:GLY:HA3   | 1.66                     | 0.69              |
| 4:7:1:ASP:HA     | 4:7:4:GLU:HB3    | 1.74                     | 0.69              |
| 1:G:93:MET:HE2   | 1:G:763:THR:HB   | 1.61                     | 0.69              |
| 1:G:832:MET:SD   | 2:H:84:PHE:HE2   | 2.17                     | 0.69              |
| 1:J:732:ILE:CG2  | 1:J:747:LEU:HD11 | 1.26                     | 0.69              |
| 1:J:786:ILE:CG1  | 3:L:86:ASP:HB3   | 2.23                     | 0.69              |
| 1:D:630:ALA:O    | 4:5:25:ASP:CB    | 2.41                     | 0.68              |
| 1:J:538:GLU:CD   | 4:7:355:MET:HE1  | 2.12                     | 0.68              |
| 1:D:733:PRO:C    | 1:D:737:PHE:CD1  | 2.62                     | 0.68              |
| 1:D:817:GLN:CD   | 2:E:127:ARG:CD   | 2.61                     | 0.68              |
| 2:E:117:LEU:CB   | 2:E:147:ASN:OD1  | 2.39                     | 0.68              |
| 1:D:797:PHE:CE2  | 3:F:126:LEU:CD2  | 2.75                     | 0.68              |
| 1:G:652:LEU:O    | 1:G:655:GLU:N    | 2.27                     | 0.68              |
| 3:I:3:SER:O      | 3:I:4:LYS:CB     | 2.41                     | 0.68              |
| 1:J:546:THR:HG22 | 1:J:548:THR:N    | 2.05                     | 0.68              |
| 1:J:769:ALA:CB   | 1:J:770:GLY:N    | 2.57                     | 0.68              |
| 4:5:160:THR:HG21 | 4:5:274:ILE:HD11 | 1.76                     | 0.68              |
| 1:J:541:MET:CG   | 4:7:345:ILE:O    | 2.40                     | 0.68              |
| 1:A:502:GLU:HG2  | 1:A:764:MLY:O    | 1.93                     | 0.68              |
| 1:A:52:ILE:HD13  | 1:A:52:ILE:N     | 2.08                     | 0.68              |
| 1:A:815:CYS:O    | 1:A:819:ASN:HB2  | 1.93                     | 0.68              |
| 2:B:117:LEU:HD12 | 2:B:147:ASN:CA   | 2.20                     | 0.68              |
| 1:D:732:ILE:HG21 | 1:D:747:LEU:HD11 | 0.72                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:815:CYS:O    | 1:D:819:ASN:HB2  | 1.93                     | 0.68              |
| 4:V:1:ASP:HA     | 4:V:4:GLU:HB3    | 1.74                     | 0.68              |
| 4:1:160:THR:HG21 | 4:1:274:ILE:HD11 | 1.76                     | 0.68              |
| 4:3:160:THR:HG21 | 4:3:274:ILE:HD11 | 1.76                     | 0.68              |
| 1:A:213:LYS:HA   | 1:A:220:ASP:OD1  | 1.92                     | 0.68              |
| 1:D:62:VAL:HG12  | 1:D:63:MLY:O     | 1.93                     | 0.68              |
| 2:E:111:SER:OG   | 2:E:148:VAL:HG12 | 1.92                     | 0.68              |
| 3:F:48:LYS:C     | 3:F:52:ASN:HD21  | 1.96                     | 0.68              |
| 1:G:213:LYS:HA   | 1:G:220:ASP:OD1  | 1.92                     | 0.68              |
| 1:G:533:PHE:O    | 1:G:537:GLU:HG2  | 1.93                     | 0.68              |
| 1:G:807:VAL:O    | 1:G:810:ARG:HB2  | 1.93                     | 0.68              |
| 1:J:538:GLU:CD   | 4:7:355:MET:CE   | 2.62                     | 0.68              |
| 1:J:90:ASP:OD1   | 1:J:764:MLY:HH11 | 1.92                     | 0.68              |
| 4:2:1:ASP:HA     | 4:2:4:GLU:HB3    | 1.74                     | 0.68              |
| 4:7:160:THR:HG21 | 4:7:274:ILE:HD11 | 1.76                     | 0.68              |
| 1:A:166:MET:HE1  | 1:A:254:PHE:HB2  | 1.75                     | 0.68              |
| 1:A:652:LEU:O    | 1:A:655:GLU:N    | 2.27                     | 0.68              |
| 2:E:117:LEU:HD11 | 2:E:147:ASN:HB3  | 1.75                     | 0.68              |
| 3:F:3:SER:O      | 3:F:4:LYS:CB     | 2.41                     | 0.68              |
| 1:G:52:ILE:HD13  | 1:G:52:ILE:N     | 2.09                     | 0.68              |
| 2:H:117:LEU:CB   | 2:H:147:ASN:OD1  | 2.39                     | 0.68              |
| 1:J:553:MLY:HG2  | 4:V:47:MET:N     | 2.07                     | 0.68              |
| 1:J:90:ASP:HB2   | 1:J:764:MLY:HH21 | 1.74                     | 0.68              |
| 4:Z:1:ASP:HA     | 4:Z:4:GLU:HB3    | 1.74                     | 0.68              |
| 1:A:732:ILE:CG2  | 1:A:747:LEU:HD11 | 1.26                     | 0.68              |
| 1:D:533:PHE:O    | 1:D:537:GLU:HG2  | 1.93                     | 0.68              |
| 1:D:762:HIS:H    | 1:D:762:HIS:CD2  | 2.08                     | 0.68              |
| 1:D:787:ILE:HG22 | 1:D:788:THR:N    | 2.07                     | 0.68              |
| 2:H:114:LYS:HA   | 2:H:146:GLY:C    | 2.02                     | 0.68              |
| 3:I:48:LYS:C     | 3:I:52:ASN:HD21  | 1.96                     | 0.68              |
| 1:J:533:PHE:O    | 1:J:537:GLU:HG2  | 1.93                     | 0.68              |
| 2:K:117:LEU:HD12 | 2:K:147:ASN:CA   | 2.19                     | 0.68              |
| 4:V:160:THR:HG21 | 4:V:274:ILE:HD11 | 1.75                     | 0.68              |
| 4:X:3:ASP:HA     | 4:X:6:THR:CB     | 2.18                     | 0.68              |
| 4:X:1:ASP:HA     | 4:X:4:GLU:HB3    | 1.74                     | 0.68              |
| 4:Y:160:THR:HG21 | 4:Y:274:ILE:HD11 | 1.76                     | 0.68              |
| 4:0:1:ASP:HA     | 4:0:4:GLU:HB3    | 1.74                     | 0.68              |
| 1:A:807:VAL:O    | 1:A:810:ARG:HB2  | 1.93                     | 0.68              |
| 3:C:25:ILE:O     | 3:C:63:ILE:HB    | 1.92                     | 0.68              |
| 1:J:166:MET:HE3  | 1:J:254:PHE:HD2  | 1.56                     | 0.68              |
| 1:J:798:LEU:HD21 | 3:L:126:LEU:CD1  | 2.21                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:117:LEU:CB   | 2:K:147:ASN:ND2  | 2.35                     | 0.68              |
| 4:Z:153:LEU:HD11 | 4:Z:274:ILE:HG13 | 1.76                     | 0.68              |
| 4:2:153:LEU:HD11 | 4:2:274:ILE:HG13 | 1.76                     | 0.68              |
| 1:A:408:VAL:HG12 | 4:4:332:PRO:HB3  | 1.76                     | 0.68              |
| 1:G:408:VAL:HG12 | 4:6:332:PRO:HB3  | 1.76                     | 0.68              |
| 3:C:4:LYS:N      | 3:C:5:ALA:O      | 2.16                     | 0.68              |
| 1:D:123:CYS:HB2  | 1:D:158:ILE:CD1  | 2.23                     | 0.68              |
| 1:D:550:PHE:HE2  | 1:D:592:ILE:HG23 | 1.59                     | 0.68              |
| 3:I:48:LYS:HB3   | 3:I:52:ASN:HD21  | 1.57                     | 0.68              |
| 1:J:707:CYS:CA   | 1:J:714:ARG:HH22 | 2.07                     | 0.68              |
| 1:J:817:GLN:HG3  | 2:K:128:PHE:CE1  | 2.29                     | 0.68              |
| 1:J:800:ARG:NH1  | 3:L:149:VAL:CG2  | 2.35                     | 0.68              |
| 1:A:630:ALA:O    | 4:4:25:ASP:CB    | 2.41                     | 0.68              |
| 2:B:117:LEU:CB   | 2:B:147:ASN:ND2  | 2.35                     | 0.68              |
| 1:D:538:GLU:CD   | 4:5:355:MET:CE   | 2.62                     | 0.68              |
| 1:D:507:GLY:O    | 1:D:762:HIS:N    | 2.27                     | 0.68              |
| 1:D:802:GLU:HA   | 1:D:802:GLU:OE1  | 1.93                     | 0.68              |
| 3:F:102:VAL:HG23 | 3:F:139:TYR:HD1  | 1.59                     | 0.68              |
| 1:D:789:ALA:C    | 3:F:87:PHE:CE2   | 2.67                     | 0.68              |
| 1:G:166:MET:HE3  | 1:G:254:PHE:CD2  | 2.29                     | 0.68              |
| 1:G:541:MET:CG   | 4:6:345:ILE:O    | 2.41                     | 0.68              |
| 1:G:550:PHE:HE2  | 1:G:592:ILE:HG23 | 1.59                     | 0.68              |
| 1:G:819:ASN:OD1  | 2:H:90:GLY:O     | 2.12                     | 0.68              |
| 1:J:537:GLU:HG3  | 4:7:350:SER:O    | 1.78                     | 0.68              |
| 1:J:782:MLY:C    | 1:J:783:LEU:HD12 | 2.22                     | 0.68              |
| 4:0:153:LEU:HD11 | 4:0:274:ILE:HG13 | 1.76                     | 0.68              |
| 1:D:530:MET:HE3  | 4:5:354:GLN:HG2  | 1.73                     | 0.68              |
| 1:G:642:LYS:HB3  | 4:6:21:PHE:O     | 1.92                     | 0.68              |
| 1:A:793:ARG:HE   | 3:C:147:MET:CA   | 2.06                     | 0.68              |
| 1:D:817:GLN:CG   | 2:E:127:ARG:HD3  | 2.22                     | 0.68              |
| 2:E:117:LEU:CG   | 2:E:147:ASN:HB3  | 2.24                     | 0.68              |
| 1:D:831:TRP:CH2  | 2:E:47:LEU:HD23  | 2.26                     | 0.68              |
| 1:D:830:PRO:CB   | 2:E:51:PHE:CZ    | 2.68                     | 0.68              |
| 1:J:62:VAL:HG12  | 1:J:63:MLY:O     | 1.93                     | 0.68              |
| 1:J:815:CYS:O    | 1:J:819:ASN:HB2  | 1.93                     | 0.68              |
| 2:K:117:LEU:CB   | 2:K:147:ASN:OD1  | 2.39                     | 0.68              |
| 1:A:541:MET:CG   | 4:4:345:ILE:O    | 2.40                     | 0.67              |
| 1:A:56:GLU:CB    | 1:A:59:MLY:HB3   | 2.20                     | 0.67              |
| 1:A:58:GLY:HA2   | 1:A:74:GLU:OE1   | 1.94                     | 0.67              |
| 1:D:215:GLN:HA   | 1:D:340:ILE:CB   | 2.23                     | 0.67              |
| 1:D:652:LEU:O    | 1:D:655:GLU:N    | 2.27                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:735:GLY:C    | 1:D:743:ALA:HB1  | 1.84                     | 0.67              |
| 1:G:768:MLY:CD   | 1:G:772:LEU:CD2  | 2.68                     | 0.67              |
| 2:H:117:LEU:CG   | 2:H:147:ASN:HB3  | 2.24                     | 0.67              |
| 1:G:792:ALA:HB3  | 3:I:40:ASN:HB3   | 1.76                     | 0.67              |
| 1:J:612:GLN:NE2  | 1:J:627:GLY:N    | 2.43                     | 0.67              |
| 4:V:153:LEU:HD11 | 4:V:274:ILE:HG13 | 1.76                     | 0.67              |
| 4:W:160:THR:HG21 | 4:W:274:ILE:HD11 | 1.76                     | 0.67              |
| 4:X:153:LEU:HD11 | 4:X:274:ILE:HG13 | 1.76                     | 0.67              |
| 4:X:160:THR:HG21 | 4:X:274:ILE:HD11 | 1.76                     | 0.67              |
| 1:A:762:HIS:CD2  | 1:A:762:HIS:H    | 2.08                     | 0.67              |
| 1:A:836:PHE:CE1  | 2:B:159:HIS:HA   | 2.26                     | 0.67              |
| 1:A:800:ARG:CZ   | 3:C:149:VAL:C    | 2.62                     | 0.67              |
| 1:D:52:ILE:N     | 1:D:52:ILE:HD13  | 2.09                     | 0.67              |
| 1:D:788:THR:HG23 | 3:F:42:THR:CG2   | 2.20                     | 0.67              |
| 1:J:123:CYS:HB2  | 1:J:158:ILE:CD1  | 2.23                     | 0.67              |
| 1:J:546:THR:H    | 1:J:549:SER:HB3  | 1.59                     | 0.67              |
| 4:8:160:THR:HG21 | 4:8:274:ILE:HD11 | 1.76                     | 0.67              |
| 2:B:141:PRO:O    | 2:B:145:ALA:CB   | 2.43                     | 0.67              |
| 1:A:797:PHE:CD2  | 3:C:126:LEU:HD22 | 2.29                     | 0.67              |
| 1:D:723:ARG:NH2  | 1:D:783:LEU:HD11 | 2.08                     | 0.67              |
| 1:D:795:ARG:CZ   | 3:F:43:ASN:CG    | 2.62                     | 0.67              |
| 1:G:538:GLU:CD   | 4:6:355:MET:CE   | 2.62                     | 0.67              |
| 3:I:24:LYS:HA    | 3:I:63:ILE:O     | 1.95                     | 0.67              |
| 1:J:795:ARG:HB3  | 3:L:35:ARG:NH2   | 2.09                     | 0.67              |
| 2:K:114:LYS:HA   | 2:K:146:GLY:C    | 2.03                     | 0.67              |
| 1:J:750:GLY:HA2  | 3:L:114:LEU:CD2  | 2.25                     | 0.67              |
| 1:D:538:GLU:CD   | 4:5:355:MET:HE1  | 2.13                     | 0.67              |
| 1:J:642:LYS:HB3  | 4:7:21:PHE:O     | 1.92                     | 0.67              |
| 1:A:546:THR:H    | 1:A:549:SER:HB3  | 1.60                     | 0.67              |
| 1:J:374:GLN:HG3  | 1:J:375:ALA:H    | 1.59                     | 0.67              |
| 1:J:821:ARG:HH22 | 2:K:127:ARG:NE   | 1.91                     | 0.67              |
| 2:E:162:ASP:O    | 2:K:21:GLU:CB    | 2.41                     | 0.67              |
| 1:J:838:ILE:HD11 | 2:K:54:MET:SD    | 2.34                     | 0.67              |
| 4:4:153:LEU:HD11 | 4:4:274:ILE:HG13 | 1.76                     | 0.67              |
| 4:6:153:LEU:HD11 | 4:6:274:ILE:HG13 | 1.76                     | 0.67              |
| 1:D:546:THR:H    | 1:D:549:SER:HB3  | 1.59                     | 0.67              |
| 1:G:58:GLY:HA2   | 1:G:74:GLU:OE1   | 1.95                     | 0.67              |
| 1:J:769:ALA:HB3  | 1:J:770:GLY:HA3  | 1.68                     | 0.67              |
| 2:K:117:LEU:CG   | 2:K:147:ASN:HB3  | 2.25                     | 0.67              |
| 3:L:102:VAL:HG23 | 3:L:139:TYR:HD1  | 1.59                     | 0.67              |
| 1:J:798:LEU:HD23 | 3:L:122:GLU:HB3  | 1.75                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:643:GLY:N    | 4:7:24:ASP:CA    | 2.46                     | 0.67              |
| 4:7:153:LEU:HD11 | 4:7:274:ILE:HG13 | 1.76                     | 0.67              |
| 1:D:831:TRP:CZ3  | 2:E:50:THR:HB    | 2.29                     | 0.67              |
| 1:G:217:THR:O    | 1:G:221:GLN:HG2  | 1.95                     | 0.67              |
| 1:G:784:ALA:O    | 1:G:788:THR:HB   | 1.94                     | 0.67              |
| 1:G:84:MLY:HH12  | 1:G:715:VAL:HG12 | 1.67                     | 0.67              |
| 1:J:480:ILE:HG22 | 1:J:481:ASN:ND2  | 2.09                     | 0.67              |
| 1:J:795:ARG:CD   | 3:L:35:ARG:NH1   | 2.53                     | 0.67              |
| 1:A:217:THR:O    | 1:A:221:GLN:HG2  | 1.95                     | 0.67              |
| 3:C:102:VAL:HG23 | 3:C:139:TYR:HD1  | 1.60                     | 0.67              |
| 1:D:480:ILE:HG22 | 1:D:481:ASN:ND2  | 2.09                     | 0.67              |
| 1:D:732:ILE:HG22 | 1:D:747:LEU:CD1  | 1.55                     | 0.67              |
| 1:D:769:ALA:CA   | 1:D:771:LEU:N    | 2.57                     | 0.67              |
| 1:J:652:LEU:O    | 1:J:655:GLU:N    | 2.27                     | 0.67              |
| 3:L:24:LYS:HA    | 3:L:63:ILE:O     | 1.95                     | 0.67              |
| 4:Z:160:THR:HG21 | 4:Z:274:ILE:HD11 | 1.76                     | 0.67              |
| 3:C:24:LYS:HA    | 3:C:63:ILE:O     | 1.95                     | 0.67              |
| 1:D:131:TRP:O    | 1:D:132:LEU:HD12 | 1.95                     | 0.67              |
| 1:D:546:THR:HG22 | 1:D:548:THR:N    | 2.05                     | 0.67              |
| 1:G:202:SER:HA   | 1:G:207:LYS:HE3  | 1.72                     | 0.67              |
| 1:G:292:MET:HE3  | 1:G:309:PRO:HA   | 1.77                     | 0.67              |
| 1:G:62:VAL:HG12  | 1:G:63:MLY:O     | 1.94                     | 0.67              |
| 1:J:290:GLN:O    | 1:J:331:LEU:HD12 | 1.95                     | 0.67              |
| 1:J:58:GLY:HA2   | 1:J:74:GLU:OE1   | 1.95                     | 0.67              |
| 1:D:642:LYS:CD   | 4:5:24:ASP:O     | 2.42                     | 0.67              |
| 4:6:160:THR:HG21 | 4:6:274:ILE:HD11 | 1.76                     | 0.67              |
| 1:A:533:PHE:O    | 1:A:537:GLU:HG2  | 1.93                     | 0.67              |
| 1:A:62:VAL:HG12  | 1:A:63:MLY:O     | 1.93                     | 0.67              |
| 1:A:61:THR:HG23  | 1:A:71:THR:OG1   | 1.94                     | 0.67              |
| 2:B:144:VAL:CG1  | 2:B:153:ILE:HD13 | 2.20                     | 0.67              |
| 1:D:612:GLN:NE2  | 1:D:627:GLY:N    | 2.43                     | 0.67              |
| 1:D:739:ASP:CB   | 1:D:742:LYS:HB3  | 2.12                     | 0.67              |
| 1:G:290:GLN:O    | 1:G:331:LEU:HD12 | 1.95                     | 0.67              |
| 1:G:802:GLU:OE1  | 1:G:802:GLU:HA   | 1.93                     | 0.67              |
| 2:K:141:PRO:O    | 2:K:145:ALA:CB   | 2.43                     | 0.67              |
| 4:0:160:THR:HG21 | 4:0:274:ILE:HD11 | 1.76                     | 0.67              |
| 4:2:160:THR:HG21 | 4:2:274:ILE:HD11 | 1.76                     | 0.67              |
| 4:4:160:THR:HG21 | 4:4:274:ILE:HD11 | 1.76                     | 0.67              |
| 1:G:537:GLU:C    | 4:6:351:THR:H    | 1.99                     | 0.67              |
| 1:A:550:PHE:HE2  | 1:A:592:ILE:HG23 | 1.59                     | 0.67              |
| 1:A:504:MLY:C    | 1:A:762:HIS:NE2  | 2.57                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:818:TYR:CB   | 2:B:89:LYS:C     | 2.63                     | 0.67              |
| 1:D:58:GLY:HA2   | 1:D:74:GLU:OE1   | 1.95                     | 0.67              |
| 1:G:546:THR:H    | 1:G:549:SER:HB3  | 1.59                     | 0.67              |
| 1:G:78:PHE:HB3   | 1:G:98:HIS:CD2   | 2.30                     | 0.67              |
| 1:J:131:TRP:O    | 1:J:132:LEU:HD12 | 1.95                     | 0.67              |
| 1:J:749:GLY:C    | 3:L:114:LEU:HD21 | 2.15                     | 0.67              |
| 1:J:541:MET:O    | 4:7:143:TYR:OH   | 2.14                     | 0.66              |
| 1:J:408:VAL:HG12 | 4:7:332:PRO:HB3  | 1.76                     | 0.66              |
| 1:A:78:PHE:HB3   | 1:A:98:HIS:CD2   | 2.30                     | 0.66              |
| 1:D:374:GLN:HG3  | 1:D:375:ALA:H    | 1.60                     | 0.66              |
| 1:D:648:THR:CB   | 4:5:350:SER:OG   | 2.43                     | 0.66              |
| 2:E:141:PRO:O    | 2:E:145:ALA:CB   | 2.43                     | 0.66              |
| 2:H:141:PRO:O    | 2:H:145:ALA:CB   | 2.43                     | 0.66              |
| 1:J:635:GLY:O    | 4:7:341:ILE:HG21 | 1.95                     | 0.66              |
| 1:J:831:TRP:CE3  | 2:K:34:ILE:CD1   | 2.77                     | 0.66              |
| 4:5:153:LEU:HD11 | 4:5:274:ILE:HG13 | 1.76                     | 0.66              |
| 1:A:290:GLN:O    | 1:A:331:LEU:HD12 | 1.95                     | 0.66              |
| 1:A:795:ARG:CD   | 3:C:35:ARG:NH1   | 2.43                     | 0.66              |
| 1:D:418:THR:HG22 | 1:D:419:VAL:N    | 2.11                     | 0.66              |
| 1:D:724:TYR:HE1  | 1:D:778:MET:CG   | 2.08                     | 0.66              |
| 1:G:174:SER:O    | 1:G:670:HIS:HB2  | 1.96                     | 0.66              |
| 1:G:599:ASN:OD1  | 1:G:649:VAL:N    | 2.29                     | 0.66              |
| 2:K:117:LEU:HD11 | 2:K:147:ASN:HB3  | 1.76                     | 0.66              |
| 1:A:648:THR:CB   | 4:4:350:SER:OG   | 2.43                     | 0.66              |
| 4:8:153:LEU:HD11 | 4:8:274:ILE:HG13 | 1.76                     | 0.66              |
| 1:A:174:SER:O    | 1:A:670:HIS:HB2  | 1.96                     | 0.66              |
| 1:G:131:TRP:O    | 1:G:132:LEU:HD12 | 1.95                     | 0.66              |
| 1:G:93:MET:HE1   | 1:G:763:THR:O    | 1.94                     | 0.66              |
| 1:G:783:LEU:O    | 1:G:787:ILE:CA   | 2.43                     | 0.66              |
| 1:J:322:VAL:HB   | 1:J:325:ILE:CD1  | 2.26                     | 0.66              |
| 1:J:52:ILE:HD13  | 1:J:52:ILE:N     | 2.09                     | 0.66              |
| 1:J:550:PHE:HE2  | 1:J:592:ILE:HG23 | 1.59                     | 0.66              |
| 4:1:153:LEU:HD11 | 4:1:274:ILE:HG13 | 1.76                     | 0.66              |
| 1:A:418:THR:HG22 | 1:A:419:VAL:N    | 2.11                     | 0.66              |
| 1:A:817:GLN:HE21 | 2:B:127:ARG:HG2  | 1.59                     | 0.66              |
| 2:B:117:LEU:CG   | 2:B:147:ASN:HB3  | 2.24                     | 0.66              |
| 2:E:141:PRO:O    | 2:E:145:ALA:HB2  | 1.96                     | 0.66              |
| 1:G:61:THR:HG23  | 1:G:71:THR:OG1   | 1.94                     | 0.66              |
| 1:J:339:ASP:OD1  | 1:J:348:MLY:HH13 | 1.95                     | 0.66              |
| 1:A:537:GLU:C    | 4:4:351:THR:H    | 1.99                     | 0.66              |
| 1:A:502:GLU:HA   | 1:A:761:GLY:C    | 2.15                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:834:LEU:HD21 | 2:B:54:MET:HG3   | 1.76                     | 0.66              |
| 1:D:226:ASN:HB2  | 1:D:227:PRO:HD3  | 1.78                     | 0.66              |
| 1:D:290:GLN:O    | 1:D:331:LEU:HD12 | 1.95                     | 0.66              |
| 1:D:339:ASP:OD1  | 1:D:348:MLY:HH13 | 1.95                     | 0.66              |
| 1:D:408:VAL:HG12 | 4:5:332:PRO:HB3  | 1.76                     | 0.66              |
| 1:D:599:ASN:OD1  | 1:D:649:VAL:N    | 2.28                     | 0.66              |
| 1:G:648:THR:CB   | 4:6:350:SER:OG   | 2.44                     | 0.66              |
| 1:J:707:CYS:CB   | 1:J:714:ARG:HH22 | 2.08                     | 0.66              |
| 1:J:754:ASP:CB   | 1:J:776:GLU:CB   | 2.56                     | 0.66              |
| 4:3:153:LEU:HD11 | 4:3:274:ILE:HG13 | 1.76                     | 0.66              |
| 1:A:642:LYS:CD   | 4:4:24:ASP:O     | 2.42                     | 0.66              |
| 1:A:480:ILE:HG22 | 1:A:481:ASN:ND2  | 2.10                     | 0.66              |
| 1:A:541:MET:HG2  | 4:4:345:ILE:C    | 2.16                     | 0.66              |
| 1:D:507:GLY:HA3  | 1:D:762:HIS:CB   | 2.24                     | 0.66              |
| 1:D:537:GLU:C    | 4:5:351:THR:H    | 1.98                     | 0.66              |
| 1:D:174:SER:O    | 1:D:670:HIS:HB2  | 1.96                     | 0.66              |
| 1:G:612:GLN:NE2  | 1:G:627:GLY:N    | 2.42                     | 0.66              |
| 1:G:800:ARG:NH1  | 3:I:149:VAL:C    | 2.49                     | 0.66              |
| 3:I:102:VAL:HG23 | 3:I:139:TYR:HD1  | 1.59                     | 0.66              |
| 1:J:166:MET:HE1  | 1:J:254:PHE:HB2  | 1.78                     | 0.66              |
| 1:J:174:SER:O    | 1:J:670:HIS:HB2  | 1.96                     | 0.66              |
| 1:J:648:THR:CB   | 4:7:350:SER:OG   | 2.43                     | 0.66              |
| 1:J:754:ASP:HB2  | 1:J:776:GLU:CB   | 2.14                     | 0.66              |
| 1:J:831:TRP:CH2  | 2:K:47:LEU:HD23  | 2.31                     | 0.66              |
| 2:K:146:GLY:O    | 2:K:147:ASN:HB2  | 1.96                     | 0.66              |
| 1:A:131:TRP:O    | 1:A:132:LEU:HD12 | 1.95                     | 0.66              |
| 1:A:91:MET:HE3   | 1:A:119:SER:HB2  | 1.78                     | 0.66              |
| 2:B:141:PRO:O    | 2:B:145:ALA:HB2  | 1.96                     | 0.66              |
| 1:D:322:VAL:HB   | 1:D:325:ILE:CD1  | 2.26                     | 0.66              |
| 3:F:48:LYS:O     | 3:F:52:ASN:CG    | 2.34                     | 0.66              |
| 1:G:374:GLN:HG3  | 1:G:375:ALA:H    | 1.60                     | 0.66              |
| 1:G:553:MLY:CE   | 4:8:45:VAL:CA    | 2.49                     | 0.66              |
| 1:G:797:PHE:CD1  | 3:I:149:VAL:HG12 | 2.25                     | 0.66              |
| 1:J:78:PHE:HB3   | 1:J:98:HIS:CD2   | 2.30                     | 0.66              |
| 1:J:790:THR:CA   | 3:L:87:PHE:CE2   | 2.79                     | 0.66              |
| 2:K:141:PRO:O    | 2:K:145:ALA:HB2  | 1.96                     | 0.66              |
| 1:J:795:ARG:NE   | 3:L:118:MET:HE1  | 2.01                     | 0.66              |
| 1:A:538:GLU:HA   | 4:4:349:LEU:HB3  | 1.78                     | 0.66              |
| 1:A:612:GLN:NE2  | 1:A:627:GLY:N    | 2.43                     | 0.66              |
| 1:A:717:TYR:HD1  | 1:A:744:SER:HG   | 1.44                     | 0.66              |
| 1:A:818:TYR:HB3  | 2:B:89:LYS:C     | 2.16                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:541:MET:O    | 4:5:143:TYR:OH   | 2.14                     | 0.66              |
| 2:E:146:GLY:O    | 2:E:147:ASN:HB2  | 1.96                     | 0.66              |
| 1:G:757:GLN:CD   | 1:G:772:LEU:HG   | 2.15                     | 0.66              |
| 1:G:831:TRP:NE1  | 2:H:67:MET:CB    | 2.55                     | 0.66              |
| 2:H:146:GLY:O    | 2:H:147:ASN:HB2  | 1.96                     | 0.66              |
| 2:H:117:LEU:CB   | 2:H:147:ASN:ND2  | 2.35                     | 0.66              |
| 1:J:226:ASN:HB2  | 1:J:227:PRO:HD3  | 1.78                     | 0.66              |
| 1:J:541:MET:HG2  | 4:7:345:ILE:C    | 2.16                     | 0.66              |
| 4:W:153:LEU:HD11 | 4:W:274:ILE:HG13 | 1.76                     | 0.66              |
| 1:A:530:MET:CG   | 4:4:354:GLN:CG   | 2.71                     | 0.66              |
| 1:G:635:GLY:O    | 4:6:341:ILE:HG21 | 1.95                     | 0.66              |
| 1:J:537:GLU:C    | 4:7:351:THR:H    | 1.98                     | 0.66              |
| 1:G:226:ASN:HB2  | 1:G:227:PRO:HD3  | 1.78                     | 0.66              |
| 1:J:599:ASN:OD1  | 1:J:649:VAL:N    | 2.28                     | 0.66              |
| 2:K:150:TYR:C    | 2:K:151:LYS:CG   | 2.49                     | 0.66              |
| 1:A:144:ARG:NH1  | 1:A:160:ASP:OD1  | 2.29                     | 0.66              |
| 1:A:161:ASN:O    | 1:A:165:PHE:HB2  | 1.96                     | 0.66              |
| 1:A:339:ASP:OD1  | 1:A:348:MLY:HH13 | 1.95                     | 0.66              |
| 1:A:530:MET:CA   | 4:4:354:GLN:CB   | 2.74                     | 0.66              |
| 3:C:45:GLU:O     | 3:C:49:ILE:HG13  | 1.96                     | 0.66              |
| 1:G:541:MET:HG2  | 4:6:345:ILE:C    | 2.17                     | 0.66              |
| 2:H:117:LEU:HD11 | 2:H:147:ASN:HB3  | 1.75                     | 0.66              |
| 1:J:144:ARG:NH1  | 1:J:160:ASP:OD1  | 2.29                     | 0.66              |
| 1:D:635:GLY:O    | 4:5:341:ILE:HG21 | 1.95                     | 0.65              |
| 1:G:530:MET:HE2  | 4:6:354:GLN:HG3  | 1.76                     | 0.65              |
| 1:A:296:MLY:HH11 | 1:A:348:MLY:HH21 | 1.78                     | 0.65              |
| 1:A:643:GLY:N    | 4:4:24:ASP:CA    | 2.46                     | 0.65              |
| 1:D:466:GLY:HA2  | 1:D:484:ASN:HD21 | 1.61                     | 0.65              |
| 1:D:769:ALA:CA   | 1:D:771:LEU:CA   | 2.63                     | 0.65              |
| 1:G:144:ARG:NH1  | 1:G:160:ASP:OD1  | 2.29                     | 0.65              |
| 1:G:480:ILE:HG22 | 1:G:481:ASN:ND2  | 2.10                     | 0.65              |
| 1:G:480:ILE:HG22 | 1:G:481:ASN:N    | 2.11                     | 0.65              |
| 1:G:557:GLU:N    | 4:8:48:GLY:HA3   | 1.90                     | 0.65              |
| 3:I:48:LYS:O     | 3:I:52:ASN:CG    | 2.34                     | 0.65              |
| 1:J:418:THR:HG22 | 1:J:419:VAL:N    | 2.11                     | 0.65              |
| 1:J:90:ASP:OD2   | 1:J:764:MLY:HH13 | 1.96                     | 0.65              |
| 3:L:45:GLU:O     | 3:L:49:ILE:HG13  | 1.96                     | 0.65              |
| 3:L:48:LYS:C     | 3:L:52:ASN:HD21  | 1.96                     | 0.65              |
| 1:G:541:MET:O    | 4:6:143:TYR:OH   | 2.13                     | 0.65              |
| 1:A:538:GLU:CD   | 4:4:355:MET:CE   | 2.62                     | 0.65              |
| 1:D:217:THR:O    | 1:D:221:GLN:HG2  | 1.94                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:691:VAL:O    | 1:D:695:LEU:HD13 | 1.97                     | 0.65              |
| 1:D:818:TYR:CB   | 2:E:89:LYS:C     | 2.65                     | 0.65              |
| 1:G:161:ASN:O    | 1:G:165:PHE:HB2  | 1.96                     | 0.65              |
| 1:G:769:ALA:O    | 1:G:773:GLY:HA3  | 1.95                     | 0.65              |
| 1:J:217:THR:O    | 1:J:221:GLN:HG2  | 1.95                     | 0.65              |
| 1:J:642:LYS:HA   | 4:7:21:PHE:O     | 1.96                     | 0.65              |
| 1:J:691:VAL:O    | 1:J:695:LEU:HD13 | 1.96                     | 0.65              |
| 1:J:61:THR:HG23  | 1:J:71:THR:OG1   | 1.95                     | 0.65              |
| 1:G:538:GLU:CD   | 4:6:355:MET:HE3  | 2.17                     | 0.65              |
| 1:A:502:GLU:HA   | 1:A:761:GLY:CA   | 2.26                     | 0.65              |
| 1:A:831:TRP:CH2  | 2:B:34:ILE:HG23  | 2.31                     | 0.65              |
| 1:A:822:SER:HG   | 2:B:88:LEU:HA    | 1.60                     | 0.65              |
| 1:D:709:LYS:O    | 1:D:710:GLY:HA2  | 1.96                     | 0.65              |
| 1:D:61:THR:HG23  | 1:D:71:THR:OG1   | 1.95                     | 0.65              |
| 1:D:78:PHE:HB3   | 1:D:98:HIS:CD2   | 2.30                     | 0.65              |
| 1:G:339:ASP:OD1  | 1:G:348:MLY:HH13 | 1.95                     | 0.65              |
| 1:G:296:MLY:HH11 | 1:G:348:MLY:HH21 | 1.78                     | 0.65              |
| 1:G:466:GLY:HA2  | 1:G:484:ASN:HD21 | 1.61                     | 0.65              |
| 2:H:141:PRO:O    | 2:H:145:ALA:HB2  | 1.96                     | 0.65              |
| 4:Y:153:LEU:HD11 | 4:Y:274:ILE:HG13 | 1.76                     | 0.65              |
| 1:D:530:MET:CA   | 4:5:354:GLN:CB   | 2.74                     | 0.65              |
| 2:E:114:LYS:HA   | 2:E:146:GLY:C    | 2.03                     | 0.65              |
| 3:F:24:LYS:HA    | 3:F:63:ILE:O     | 1.95                     | 0.65              |
| 3:I:45:GLU:O     | 3:I:49:ILE:HG13  | 1.97                     | 0.65              |
| 1:D:530:MET:CG   | 4:5:354:GLN:CG   | 2.71                     | 0.65              |
| 1:A:635:GLY:O    | 4:4:341:ILE:HG21 | 1.95                     | 0.65              |
| 1:A:691:VAL:O    | 1:A:695:LEU:HD13 | 1.97                     | 0.65              |
| 1:A:739:ASP:CB   | 1:A:742:LYS:HB3  | 2.12                     | 0.65              |
| 1:D:541:MET:HG2  | 4:5:345:ILE:C    | 2.16                     | 0.65              |
| 1:G:691:VAL:O    | 1:G:695:LEU:HD13 | 1.97                     | 0.65              |
| 1:G:769:ALA:CB   | 1:G:770:GLY:N    | 2.59                     | 0.65              |
| 1:G:822:SER:O    | 1:G:825:ASN:HB2  | 1.97                     | 0.65              |
| 1:G:820:VAL:HG11 | 2:H:136:MET:CE   | 2.26                     | 0.65              |
| 1:J:161:ASN:O    | 1:J:165:PHE:HB2  | 1.96                     | 0.65              |
| 1:J:84:MLY:NZ    | 1:J:719:ASP:O    | 2.13                     | 0.65              |
| 1:J:818:TYR:HB3  | 2:K:90:GLY:HA2   | 1.75                     | 0.65              |
| 3:L:3:SER:HG     | 3:L:5:ALA:N      | 1.95                     | 0.65              |
| 1:A:107:MLY:HB3  | 1:A:686:MET:CE   | 2.27                     | 0.65              |
| 1:A:480:ILE:HG22 | 1:A:481:ASN:N    | 2.11                     | 0.65              |
| 1:A:501:GLU:O    | 1:A:762:HIS:CG   | 2.48                     | 0.65              |
| 1:A:599:ASN:OD1  | 1:A:649:VAL:N    | 2.29                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:793:ARG:CZ   | 3:C:147:MET:HG2  | 2.27                     | 0.65              |
| 1:D:612:GLN:HE22 | 1:D:627:GLY:N    | 1.94                     | 0.65              |
| 1:D:822:SER:O    | 1:D:825:ASN:HB2  | 1.97                     | 0.65              |
| 1:G:769:ALA:HB2  | 1:G:770:GLY:N    | 2.09                     | 0.65              |
| 1:J:530:MET:CA   | 4:7:354:GLN:CB   | 2.74                     | 0.65              |
| 1:A:226:ASN:HB2  | 1:A:227:PRO:HD3  | 1.77                     | 0.65              |
| 1:A:322:VAL:HB   | 1:A:325:ILE:CD1  | 2.26                     | 0.65              |
| 3:F:45:GLU:O     | 3:F:49:ILE:HG13  | 1.97                     | 0.65              |
| 1:G:466:GLY:HA2  | 1:G:484:ASN:ND2  | 2.12                     | 0.65              |
| 1:G:530:MET:CG   | 4:6:354:GLN:CG   | 2.72                     | 0.65              |
| 1:G:725:ARG:NE   | 1:G:737:PHE:HE1  | 1.95                     | 0.65              |
| 3:I:48:LYS:C     | 3:I:52:ASN:HD22  | 1.97                     | 0.65              |
| 1:J:95:THR:CA    | 1:J:713:SER:HB3  | 2.27                     | 0.65              |
| 1:J:725:ARG:NE   | 1:J:737:PHE:HE1  | 1.95                     | 0.65              |
| 1:A:217:THR:HB   | 1:A:220:ASP:OD2  | 1.97                     | 0.65              |
| 1:A:818:TYR:HB3  | 2:B:90:GLY:N     | 2.12                     | 0.65              |
| 1:D:94:MET:HE1   | 1:D:101:ALA:HB1  | 1.79                     | 0.65              |
| 1:D:725:ARG:NE   | 1:D:737:PHE:HE1  | 1.95                     | 0.65              |
| 1:G:418:THR:HG22 | 1:G:419:VAL:N    | 2.11                     | 0.65              |
| 1:G:798:LEU:HD11 | 3:I:126:LEU:HG   | 1.78                     | 0.65              |
| 1:J:792:ALA:HB1  | 3:L:40:ASN:HB3   | 0.73                     | 0.65              |
| 1:D:642:LYS:CD   | 4:5:340:TRP:CZ3  | 2.79                     | 0.65              |
| 1:A:374:GLN:HG3  | 1:A:375:ALA:H    | 1.60                     | 0.65              |
| 1:A:636:LYS:HG3  | 4:4:334:GLU:CD   | 2.17                     | 0.65              |
| 1:A:822:SER:O    | 1:A:825:ASN:HB2  | 1.97                     | 0.65              |
| 3:C:49:ILE:HA    | 3:C:52:ASN:ND2   | 2.05                     | 0.65              |
| 1:J:822:SER:O    | 1:J:825:ASN:HB2  | 1.97                     | 0.65              |
| 1:A:642:LYS:HA   | 4:4:21:PHE:O     | 1.96                     | 0.65              |
| 1:J:636:LYS:HG3  | 4:7:334:GLU:CD   | 2.17                     | 0.65              |
| 1:A:94:MET:HE1   | 1:A:101:ALA:HB1  | 1.79                     | 0.65              |
| 1:D:144:ARG:NH1  | 1:D:160:ASP:OD1  | 2.29                     | 0.65              |
| 1:D:202:SER:CA   | 1:D:207:LYS:HE3  | 2.27                     | 0.65              |
| 1:G:90:ASP:O     | 1:G:764:MLY:CH2  | 2.44                     | 0.65              |
| 1:G:93:MET:HE3   | 1:G:763:THR:CG2  | 2.08                     | 0.65              |
| 1:G:818:TYR:CD1  | 2:H:127:ARG:NH1  | 2.65                     | 0.65              |
| 2:K:144:VAL:CG1  | 2:K:153:ILE:HD13 | 2.20                     | 0.65              |
| 1:A:642:LYS:CD   | 4:4:340:TRP:CZ3  | 2.79                     | 0.64              |
| 1:A:292:MET:HE3  | 1:A:309:PRO:HA   | 1.78                     | 0.64              |
| 1:A:466:GLY:HA2  | 1:A:484:ASN:ND2  | 2.12                     | 0.64              |
| 1:D:479:CYS:HB3  | 1:D:653:PHE:CE2  | 2.32                     | 0.64              |
| 1:D:636:LYS:O    | 1:D:637:LYS:CB   | 2.45                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:642:LYS:HA   | 4:5:21:PHE:O     | 1.96                     | 0.64              |
| 1:D:831:TRP:NE1  | 2:E:47:LEU:CD2   | 2.36                     | 0.64              |
| 1:G:107:MLY:HB3  | 1:G:686:MET:CE   | 2.26                     | 0.64              |
| 1:J:823:PHE:CE2  | 2:K:140:PHE:CZ   | 2.86                     | 0.64              |
| 3:L:48:LYS:O     | 3:L:52:ASN:CG    | 2.34                     | 0.64              |
| 1:G:538:GLU:HA   | 4:6:349:LEU:HB3  | 1.79                     | 0.64              |
| 1:A:505:MLY:HG3  | 1:A:741:LYS:HZ2  | 1.63                     | 0.64              |
| 1:A:93:MET:O     | 1:A:713:SER:HB3  | 1.97                     | 0.64              |
| 1:A:814:PHE:HA   | 2:B:127:ARG:HH22 | 1.54                     | 0.64              |
| 1:D:161:ASN:O    | 1:D:165:PHE:HB2  | 1.96                     | 0.64              |
| 1:D:480:ILE:HG22 | 1:D:481:ASN:N    | 2.11                     | 0.64              |
| 1:D:636:LYS:HG3  | 4:5:334:GLU:CD   | 2.17                     | 0.64              |
| 1:D:834:LEU:HD21 | 2:E:54:MET:CE    | 2.27                     | 0.64              |
| 1:G:322:VAL:HB   | 1:G:325:ILE:CD1  | 2.26                     | 0.64              |
| 1:G:642:LYS:CD   | 4:6:24:ASP:O     | 2.43                     | 0.64              |
| 1:A:466:GLY:HA2  | 1:A:484:ASN:HD21 | 1.61                     | 0.64              |
| 1:D:806:MET:O    | 1:D:809:ARG:HB2  | 1.98                     | 0.64              |
| 3:F:3:SER:HG     | 3:F:5:ALA:N      | 1.95                     | 0.64              |
| 1:G:642:LYS:HA   | 4:6:21:PHE:O     | 1.97                     | 0.64              |
| 1:J:107:MLY:HB3  | 1:J:686:MET:CE   | 2.27                     | 0.64              |
| 1:J:133:PRO:O    | 1:J:136:ASN:HB2  | 1.98                     | 0.64              |
| 1:J:466:GLY:HA2  | 1:J:484:ASN:ND2  | 2.12                     | 0.64              |
| 1:J:612:GLN:HE22 | 1:J:627:GLY:N    | 1.94                     | 0.64              |
| 1:J:783:LEU:N    | 1:J:783:LEU:HD12 | 2.13                     | 0.64              |
| 1:J:793:ARG:HG3  | 3:L:146:ILE:HG22 | 1.79                     | 0.64              |
| 1:J:795:ARG:HH11 | 3:L:35:ARG:CZ    | 2.09                     | 0.64              |
| 1:A:557:GLU:N    | 4:6:48:GLY:HA3   | 1.90                     | 0.64              |
| 1:A:133:PRO:O    | 1:A:136:ASN:HB2  | 1.97                     | 0.64              |
| 1:A:218:LEU:CD2  | 1:A:222:ILE:HG12 | 2.28                     | 0.64              |
| 1:A:612:GLN:HE22 | 1:A:627:GLY:N    | 1.94                     | 0.64              |
| 2:B:140:PHE:HB3  | 2:B:144:VAL:CG1  | 2.28                     | 0.64              |
| 1:D:466:GLY:HA2  | 1:D:484:ASN:ND2  | 2.12                     | 0.64              |
| 1:G:210:GLN:O    | 1:G:211:SER:OG   | 2.15                     | 0.64              |
| 1:G:84:MLY:HH11  | 1:G:720:PHE:N    | 2.13                     | 0.64              |
| 1:J:217:THR:HB   | 1:J:220:ASP:OD2  | 1.97                     | 0.64              |
| 1:J:479:CYS:HB3  | 1:J:653:PHE:CE2  | 2.33                     | 0.64              |
| 2:K:117:LEU:CG   | 2:K:147:ASN:CB   | 2.76                     | 0.64              |
| 1:A:202:SER:CA   | 1:A:207:LYS:HE3  | 2.27                     | 0.64              |
| 1:D:217:THR:HB   | 1:D:220:ASP:OD2  | 1.97                     | 0.64              |
| 1:D:296:MLY:HH11 | 1:D:348:MLY:HH21 | 1.78                     | 0.64              |
| 1:D:107:MLY:HB3  | 1:D:686:MET:CE   | 2.26                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:133:PRO:O    | 1:G:136:ASN:HB2  | 1.98                     | 0.64              |
| 1:G:217:THR:HB   | 1:G:220:ASP:OD2  | 1.97                     | 0.64              |
| 1:J:466:GLY:HA2  | 1:J:484:ASN:HD21 | 1.61                     | 0.64              |
| 1:J:806:MET:O    | 1:J:809:ARG:HB2  | 1.98                     | 0.64              |
| 1:J:819:ASN:N    | 2:K:90:GLY:O     | 2.29                     | 0.64              |
| 1:J:90:ASP:CG    | 1:J:764:MLY:HH21 | 2.18                     | 0.64              |
| 1:J:831:TRP:HH2  | 2:K:47:LEU:HD23  | 1.61                     | 0.64              |
| 1:J:642:LYS:CA   | 4:7:21:PHE:O     | 2.45                     | 0.64              |
| 1:J:538:GLU:HA   | 4:7:349:LEU:HB3  | 1.78                     | 0.64              |
| 1:A:553:MLY:CE   | 4:6:45:VAL:CA    | 2.49                     | 0.64              |
| 1:A:642:LYS:CA   | 4:4:21:PHE:O     | 2.46                     | 0.64              |
| 3:C:48:LYS:O     | 3:C:52:ASN:CG    | 2.34                     | 0.64              |
| 2:E:140:PHE:O    | 2:E:141:PRO:C    | 2.33                     | 0.64              |
| 1:G:218:LEU:CD2  | 1:G:222:ILE:HG12 | 2.28                     | 0.64              |
| 1:G:406:VAL:HG12 | 1:G:407:GLY:N    | 2.13                     | 0.64              |
| 1:G:530:MET:CA   | 4:6:354:GLN:CB   | 2.75                     | 0.64              |
| 1:G:612:GLN:HE22 | 1:G:627:GLY:N    | 1.94                     | 0.64              |
| 1:G:636:LYS:HG3  | 4:6:334:GLU:CD   | 2.18                     | 0.64              |
| 2:H:140:PHE:HB3  | 2:H:144:VAL:CG1  | 2.28                     | 0.64              |
| 1:G:730:SER:CB   | 3:I:109:HIS:CD2  | 2.80                     | 0.64              |
| 1:J:296:MLY:HH11 | 1:J:348:MLY:HH21 | 1.78                     | 0.64              |
| 2:K:140:PHE:HB3  | 2:K:144:VAL:CG1  | 2.28                     | 0.64              |
| 1:A:534:SER:C    | 4:4:351:THR:CA   | 2.47                     | 0.64              |
| 1:A:725:ARG:NE   | 1:A:737:PHE:HE1  | 1.95                     | 0.64              |
| 2:E:140:PHE:HB3  | 2:E:144:VAL:CG1  | 2.27                     | 0.64              |
| 2:E:149:ASP:OD2  | 2:E:150:TYR:C    | 2.36                     | 0.64              |
| 1:G:541:MET:HG2  | 4:6:345:ILE:O    | 1.98                     | 0.64              |
| 1:J:537:GLU:C    | 4:7:351:THR:N    | 2.51                     | 0.64              |
| 1:J:636:LYS:O    | 1:J:637:LYS:CB   | 2.45                     | 0.64              |
| 1:J:510:TRP:CZ3  | 1:J:772:LEU:CD2  | 2.80                     | 0.64              |
| 1:J:795:ARG:CD   | 3:L:35:ARG:HH12  | 2.11                     | 0.64              |
| 2:K:144:VAL:HA   | 2:K:153:ILE:HD11 | 1.80                     | 0.64              |
| 4:4:190:MET:SD   | 4:4:209:VAL:HG11 | 2.38                     | 0.64              |
| 1:G:642:LYS:CA   | 4:6:21:PHE:O     | 2.46                     | 0.64              |
| 1:A:479:CYS:HB3  | 1:A:653:PHE:CE2  | 2.32                     | 0.64              |
| 1:A:636:LYS:O    | 1:A:637:LYS:CB   | 2.45                     | 0.64              |
| 1:D:795:ARG:NH2  | 3:F:116:GLU:OE1  | 2.29                     | 0.64              |
| 2:E:117:LEU:CG   | 2:E:147:ASN:CB   | 2.76                     | 0.64              |
| 1:D:830:PRO:CB   | 2:E:67:MET:HE3   | 2.23                     | 0.64              |
| 1:G:166:MET:HE3  | 1:G:254:PHE:HD2  | 1.61                     | 0.64              |
| 1:J:127:ASN:HD22 | 1:J:128:PRO:CD   | 2.11                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:541:MET:O    | 4:4:143:TYR:OH   | 2.14                     | 0.64              |
| 1:J:636:LYS:N    | 4:7:334:GLU:OE1  | 2.31                     | 0.64              |
| 1:J:642:LYS:CD   | 4:7:340:TRP:CZ3  | 2.79                     | 0.64              |
| 1:D:127:ASN:HD22 | 1:D:128:PRO:CD   | 2.11                     | 0.64              |
| 1:D:537:GLU:HB3  | 1:D:648:THR:HB   | 1.80                     | 0.64              |
| 1:D:818:TYR:HB2  | 2:E:89:LYS:C     | 2.18                     | 0.64              |
| 1:G:479:CYS:HB3  | 1:G:653:PHE:CE2  | 2.32                     | 0.64              |
| 1:G:751:GLY:N    | 3:I:114:LEU:CD1  | 2.61                     | 0.64              |
| 1:J:292:MET:HE3  | 1:J:309:PRO:HA   | 1.78                     | 0.64              |
| 1:J:838:ILE:CD1  | 2:K:54:MET:HE3   | 2.27                     | 0.64              |
| 4:V:190:MET:SD   | 4:V:209:VAL:HG11 | 2.38                     | 0.64              |
| 4:X:190:MET:SD   | 4:X:209:VAL:HG11 | 2.38                     | 0.64              |
| 4:2:190:MET:SD   | 4:2:209:VAL:HG11 | 2.38                     | 0.64              |
| 1:A:530:MET:HE3  | 4:4:354:GLN:CG   | 2.23                     | 0.64              |
| 1:A:806:MET:O    | 1:A:809:ARG:HB2  | 1.98                     | 0.64              |
| 1:A:831:TRP:NE1  | 2:B:51:PHE:CE2   | 2.63                     | 0.64              |
| 1:G:529:PRO:C    | 4:6:354:GLN:CB   | 2.50                     | 0.64              |
| 1:G:724:TYR:HB3  | 1:G:727:LEU:HD12 | 1.80                     | 0.64              |
| 1:G:784:ALA:O    | 1:G:788:THR:CB   | 2.45                     | 0.64              |
| 3:I:49:ILE:HA    | 3:I:52:ASN:ND2   | 2.05                     | 0.64              |
| 1:J:406:VAL:HG12 | 1:J:407:GLY:N    | 2.13                     | 0.64              |
| 4:5:190:MET:SD   | 4:5:209:VAL:HG11 | 2.38                     | 0.63              |
| 1:A:538:GLU:HA   | 4:4:349:LEU:CG   | 2.27                     | 0.63              |
| 1:D:830:PRO:CB   | 2:E:67:MET:CE    | 2.74                     | 0.63              |
| 1:J:480:ILE:HG22 | 1:J:481:ASN:N    | 2.11                     | 0.63              |
| 1:J:577:ALA:O    | 1:J:578:HIS:CD2  | 2.51                     | 0.63              |
| 1:A:636:LYS:N    | 4:4:334:GLU:OE1  | 2.31                     | 0.63              |
| 1:A:724:TYR:HB3  | 1:A:727:LEU:HD12 | 1.80                     | 0.63              |
| 2:B:132:GLU:O    | 2:B:136:MET:HG2  | 1.99                     | 0.63              |
| 2:B:146:GLY:O    | 2:B:147:ASN:HB2  | 1.96                     | 0.63              |
| 1:G:215:GLN:CA   | 1:G:340:ILE:CG2  | 2.63                     | 0.63              |
| 1:G:577:ALA:O    | 1:G:578:HIS:CD2  | 2.52                     | 0.63              |
| 1:G:724:TYR:HD1  | 1:G:727:LEU:HD11 | 1.64                     | 0.63              |
| 1:G:91:MET:HE3   | 1:G:119:SER:HB2  | 1.80                     | 0.63              |
| 1:G:829:TRP:CZ2  | 2:H:87:LYS:HE2   | 2.34                     | 0.63              |
| 1:J:725:ARG:NE   | 1:J:737:PHE:CE1  | 2.66                     | 0.63              |
| 1:A:502:GLU:OE2  | 1:A:764:MLY:N    | 2.31                     | 0.63              |
| 1:A:822:SER:CB   | 2:B:88:LEU:CD2   | 2.67                     | 0.63              |
| 1:A:795:ARG:CB   | 3:C:35:ARG:CZ    | 2.75                     | 0.63              |
| 1:D:218:LEU:CD2  | 1:D:222:ILE:HG12 | 2.28                     | 0.63              |
| 1:D:577:ALA:O    | 1:D:578:HIS:CD2  | 2.51                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:537:GLU:HB3  | 1:G:648:THR:HB   | 1.80                     | 0.63              |
| 1:G:754:ASP:CG   | 1:G:776:GLU:OE2  | 2.36                     | 0.63              |
| 1:G:783:LEU:HD12 | 1:G:783:LEU:N    | 2.13                     | 0.63              |
| 1:J:642:LYS:CG   | 4:7:22:ALA:C     | 2.67                     | 0.63              |
| 4:0:190:MET:SD   | 4:0:209:VAL:HG11 | 2.38                     | 0.63              |
| 1:G:642:LYS:CG   | 4:6:22:ALA:C     | 2.67                     | 0.63              |
| 1:G:643:GLY:H    | 4:6:23:GLY:C     | 2.02                     | 0.63              |
| 4:7:190:MET:SD   | 4:7:209:VAL:HG11 | 2.38                     | 0.63              |
| 1:A:406:VAL:HG12 | 1:A:407:GLY:N    | 2.13                     | 0.63              |
| 1:A:530:MET:HA   | 4:4:354:GLN:CB   | 2.29                     | 0.63              |
| 1:A:725:ARG:NE   | 1:A:737:PHE:CE1  | 2.67                     | 0.63              |
| 1:D:133:PRO:O    | 1:D:136:ASN:HB2  | 1.98                     | 0.63              |
| 1:D:783:LEU:HD12 | 1:D:783:LEU:N    | 2.13                     | 0.63              |
| 1:D:817:GLN:CD   | 2:E:127:ARG:HE   | 1.90                     | 0.63              |
| 1:J:534:SER:C    | 4:7:351:THR:CA   | 2.47                     | 0.63              |
| 4:0:257:CYS:HB3  | 4:0:258:PRO:HD3  | 1.81                     | 0.63              |
| 1:D:538:GLU:HA   | 4:5:349:LEU:HB3  | 1.78                     | 0.63              |
| 1:J:541:MET:CA   | 4:7:143:TYR:OH   | 2.46                     | 0.63              |
| 4:7:257:CYS:HB3  | 4:7:258:PRO:HD3  | 1.81                     | 0.63              |
| 1:A:577:ALA:O    | 1:A:578:HIS:CD2  | 2.52                     | 0.63              |
| 2:B:117:LEU:CG   | 2:B:147:ASN:CB   | 2.76                     | 0.63              |
| 1:G:827:MLY:HH21 | 2:H:139:ALA:HB3  | 1.81                     | 0.63              |
| 1:G:829:TRP:CH2  | 2:H:87:LYS:NZ    | 2.66                     | 0.63              |
| 1:J:724:TYR:HB3  | 1:J:727:LEU:HD12 | 1.80                     | 0.63              |
| 2:K:146:GLY:O    | 2:K:147:ASN:CB   | 2.46                     | 0.63              |
| 4:V:257:CYS:HB3  | 4:V:258:PRO:HD3  | 1.81                     | 0.63              |
| 4:3:257:CYS:HB3  | 4:3:258:PRO:HD3  | 1.81                     | 0.63              |
| 1:A:537:GLU:C    | 4:4:351:THR:N    | 2.52                     | 0.63              |
| 1:A:542:PHE:CZ   | 1:A:553:MLY:HH11 | 2.34                     | 0.63              |
| 1:A:724:TYR:HD1  | 1:A:727:LEU:HD11 | 1.64                     | 0.63              |
| 1:A:800:ARG:HD2  | 3:C:149:VAL:CB   | 2.27                     | 0.63              |
| 2:B:144:VAL:HA   | 2:B:153:ILE:HD11 | 1.80                     | 0.63              |
| 1:D:793:ARG:HE   | 3:F:147:MET:CA   | 2.11                     | 0.63              |
| 1:D:829:TRP:NE1  | 2:E:67:MET:CG    | 2.39                     | 0.63              |
| 2:E:132:GLU:O    | 2:E:136:MET:HG2  | 1.99                     | 0.63              |
| 1:G:636:LYS:O    | 1:G:637:LYS:CB   | 2.45                     | 0.63              |
| 1:G:771:LEU:O    | 1:G:774:LEU:N    | 2.32                     | 0.63              |
| 2:H:117:LEU:CG   | 2:H:147:ASN:CB   | 2.76                     | 0.63              |
| 1:J:141:LEU:HD12 | 1:J:141:LEU:H    | 1.64                     | 0.63              |
| 1:J:278:GLN:CG   | 1:J:317:GLU:HB2  | 2.27                     | 0.63              |
| 3:L:49:ILE:HA    | 3:L:52:ASN:ND2   | 2.06                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:X:257:CYS:HB3  | 4:X:258:PRO:HD3  | 1.81                     | 0.63              |
| 4:Z:257:CYS:HB3  | 4:Z:258:PRO:HD3  | 1.81                     | 0.63              |
| 1:A:541:MET:HG2  | 4:4:345:ILE:O    | 1.98                     | 0.63              |
| 1:J:541:MET:HG2  | 4:7:345:ILE:O    | 1.98                     | 0.63              |
| 2:E:146:GLY:O    | 2:E:147:ASN:CB   | 2.46                     | 0.63              |
| 1:D:818:TYR:HD2  | 2:E:89:LYS:O     | 1.81                     | 0.63              |
| 3:F:24:LYS:HB3   | 3:F:63:ILE:H     | 1.64                     | 0.63              |
| 1:G:806:MET:O    | 1:G:809:ARG:HB2  | 1.98                     | 0.63              |
| 1:J:218:LEU:CD2  | 1:J:222:ILE:HG12 | 2.28                     | 0.63              |
| 1:J:537:GLU:HB3  | 1:J:648:THR:HB   | 1.80                     | 0.63              |
| 1:J:768:MLY:HH21 | 1:J:772:LEU:HD22 | 1.66                     | 0.63              |
| 1:G:541:MET:CA   | 4:6:143:TYR:OH   | 2.47                     | 0.63              |
| 1:A:127:ASN:HD22 | 1:A:128:PRO:CD   | 2.11                     | 0.63              |
| 1:A:831:TRP:HZ3  | 2:B:50:THR:CG2   | 2.11                     | 0.63              |
| 2:B:121:LEU:HA   | 2:B:128:PHE:CG   | 2.34                     | 0.63              |
| 2:B:146:GLY:O    | 2:B:147:ASN:CB   | 2.46                     | 0.63              |
| 1:D:538:GLU:HA   | 4:5:349:LEU:CG   | 2.28                     | 0.63              |
| 1:D:725:ARG:NE   | 1:D:737:PHE:CE1  | 2.66                     | 0.63              |
| 1:G:141:LEU:H    | 1:G:141:LEU:HD12 | 1.64                     | 0.63              |
| 1:J:641:LYS:CE   | 1:J:647:GLN:CB   | 2.75                     | 0.63              |
| 1:J:84:MLY:HH11  | 1:J:715:VAL:HG12 | 1.76                     | 0.63              |
| 2:K:132:GLU:O    | 2:K:136:MET:HG2  | 1.99                     | 0.63              |
| 4:1:190:MET:SD   | 4:1:209:VAL:HG11 | 2.38                     | 0.63              |
| 4:2:257:CYS:HB3  | 4:2:258:PRO:HD3  | 1.81                     | 0.63              |
| 4:5:257:CYS:HB3  | 4:5:258:PRO:HD3  | 1.81                     | 0.63              |
| 1:A:707:CYS:CA   | 1:A:714:ARG:CZ   | 2.77                     | 0.63              |
| 1:A:93:MET:HE1   | 1:A:716:LEU:H    | 1.64                     | 0.63              |
| 3:C:24:LYS:HB3   | 3:C:63:ILE:H     | 1.64                     | 0.63              |
| 1:D:166:MET:HE3  | 1:D:254:PHE:CD2  | 2.34                     | 0.63              |
| 1:D:278:GLN:CG   | 1:D:317:GLU:HB2  | 2.27                     | 0.63              |
| 1:D:411:GLU:N    | 4:5:333:PRO:HB2  | 2.11                     | 0.63              |
| 1:D:541:MET:HG2  | 4:5:345:ILE:O    | 1.98                     | 0.63              |
| 1:D:642:LYS:CG   | 4:5:22:ALA:C     | 2.67                     | 0.63              |
| 1:D:771:LEU:O    | 1:D:774:LEU:N    | 2.32                     | 0.63              |
| 1:D:726:VAL:HB   | 1:D:782:MLY:HH13 | 0.82                     | 0.63              |
| 1:G:251:ARG:HB2  | 1:G:264:ASP:CB   | 2.29                     | 0.63              |
| 1:G:537:GLU:C    | 4:6:351:THR:N    | 2.51                     | 0.63              |
| 1:G:831:TRP:NE1  | 2:H:67:MET:HB3   | 2.14                     | 0.63              |
| 1:J:553:MLY:O    | 4:V:48:GLY:HA2   | 1.99                     | 0.63              |
| 4:W:190:MET:SD   | 4:W:209:VAL:HG11 | 2.38                     | 0.63              |
| 4:3:190:MET:SD   | 4:3:209:VAL:HG11 | 2.38                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:541:MET:CA   | 4:4:143:TYR:OH   | 2.47                     | 0.62              |
| 1:G:636:LYS:N    | 4:6:334:GLU:OE1  | 2.31                     | 0.62              |
| 1:D:551:MLY:C    | 4:7:46:GLY:O     | 2.47                     | 0.62              |
| 4:8:190:MET:SD   | 4:8:209:VAL:HG11 | 2.38                     | 0.62              |
| 1:A:578:HIS:CB   | 1:A:592:ILE:HD12 | 2.29                     | 0.62              |
| 1:A:817:GLN:HE21 | 2:B:127:ARG:CG   | 2.12                     | 0.62              |
| 1:D:210:GLN:O    | 1:D:211:SER:OG   | 2.15                     | 0.62              |
| 1:D:793:ARG:NE   | 3:F:147:MET:HA   | 2.14                     | 0.62              |
| 1:G:728:ASN:HD22 | 3:I:113:THR:HG1  | 1.46                     | 0.62              |
| 1:G:725:ARG:NE   | 1:G:737:PHE:CE1  | 2.67                     | 0.62              |
| 2:H:149:ASP:OD2  | 2:H:150:TYR:C    | 2.36                     | 0.62              |
| 1:G:791:GLN:CD   | 3:I:116:GLU:HB2  | 2.20                     | 0.62              |
| 3:I:3:SER:HG     | 3:I:5:ALA:N      | 1.96                     | 0.62              |
| 1:J:541:MET:HE1  | 4:7:346:LEU:HD12 | 1.81                     | 0.62              |
| 4:Z:190:MET:SD   | 4:Z:209:VAL:HG11 | 2.38                     | 0.62              |
| 1:A:643:GLY:H    | 4:4:23:GLY:C     | 2.02                     | 0.62              |
| 1:A:274:ARG:HB2  | 1:A:285:TYR:CE2  | 2.34                     | 0.62              |
| 1:A:542:PHE:N    | 4:4:143:TYR:OH   | 2.33                     | 0.62              |
| 1:A:502:GLU:CD   | 1:A:764:MLY:O    | 2.37                     | 0.62              |
| 1:A:783:LEU:N    | 1:A:783:LEU:HD12 | 2.13                     | 0.62              |
| 1:D:724:TYR:HB3  | 1:D:727:LEU:HD12 | 1.80                     | 0.62              |
| 1:D:724:TYR:HD1  | 1:D:727:LEU:HD11 | 1.64                     | 0.62              |
| 1:D:767:PHE:HB3  | 1:D:771:LEU:HD11 | 1.80                     | 0.62              |
| 2:E:121:LEU:HA   | 2:E:128:PHE:CG   | 2.34                     | 0.62              |
| 1:D:800:ARG:HB2  | 3:F:149:VAL:HG22 | 1.80                     | 0.62              |
| 1:G:544:LYS:HB2  | 4:6:147:ARG:HA   | 1.80                     | 0.62              |
| 2:H:111:SER:OG   | 2:H:148:VAL:CG1  | 2.47                     | 0.62              |
| 2:H:121:LEU:HA   | 2:H:128:PHE:CG   | 2.34                     | 0.62              |
| 1:J:94:MET:HE1   | 1:J:101:ALA:HB1  | 1.80                     | 0.62              |
| 1:J:817:GLN:HG2  | 2:K:127:ARG:HB2  | 1.81                     | 0.62              |
| 4:1:257:CYS:HB3  | 4:1:258:PRO:HD3  | 1.81                     | 0.62              |
| 4:4:257:CYS:HB3  | 4:4:258:PRO:HD3  | 1.81                     | 0.62              |
| 4:6:190:MET:SD   | 4:6:209:VAL:HG11 | 2.38                     | 0.62              |
| 1:A:551:MLY:C    | 4:6:46:GLY:O     | 2.47                     | 0.62              |
| 1:A:251:ARG:HB2  | 1:A:264:ASP:CB   | 2.29                     | 0.62              |
| 1:A:537:GLU:HB3  | 1:A:648:THR:HB   | 1.80                     | 0.62              |
| 1:A:501:GLU:CG   | 1:A:762:HIS:ND1  | 2.45                     | 0.62              |
| 1:D:251:ARG:HB2  | 1:D:264:ASP:CB   | 2.29                     | 0.62              |
| 1:D:642:LYS:CA   | 4:5:21:PHE:O     | 2.46                     | 0.62              |
| 1:D:507:GLY:HA2  | 1:D:762:HIS:ND1  | 2.15                     | 0.62              |
| 1:D:795:ARG:C    | 3:F:35:ARG:HD3   | 2.20                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:202:SER:CA   | 1:G:207:LYS:HE3  | 2.28                     | 0.62              |
| 1:G:508:ILE:HG21 | 1:G:711:PHE:HZ   | 1.64                     | 0.62              |
| 1:J:278:GLN:HG3  | 1:J:318:GLY:N    | 2.15                     | 0.62              |
| 1:J:771:LEU:O    | 1:J:774:LEU:N    | 2.32                     | 0.62              |
| 1:D:636:LYS:N    | 4:5:334:GLU:OE1  | 2.31                     | 0.62              |
| 4:6:361:GLU:HB3  | 4:6:369:ILE:HG12 | 1.82                     | 0.62              |
| 1:J:544:LYS:HB2  | 4:7:147:ARG:HA   | 1.80                     | 0.62              |
| 1:A:302:MET:HG2  | 1:A:303:LEU:CD1  | 2.30                     | 0.62              |
| 1:A:797:PHE:CE2  | 3:C:126:LEU:HD22 | 2.33                     | 0.62              |
| 2:B:149:ASP:OD2  | 2:B:150:TYR:C    | 2.37                     | 0.62              |
| 1:D:541:MET:HE2  | 4:5:346:LEU:HD12 | 1.82                     | 0.62              |
| 1:D:542:PHE:CZ   | 1:D:553:MLY:HH11 | 2.34                     | 0.62              |
| 1:D:580:SER:HA   | 1:D:588:VAL:O    | 2.00                     | 0.62              |
| 2:H:146:GLY:O    | 2:H:147:ASN:CB   | 2.46                     | 0.62              |
| 3:I:24:LYS:HB3   | 3:I:63:ILE:H     | 1.64                     | 0.62              |
| 1:J:551:MLY:C    | 4:V:46:GLY:O     | 2.47                     | 0.62              |
| 1:J:724:TYR:HD1  | 1:J:727:LEU:HD11 | 1.64                     | 0.62              |
| 3:L:24:LYS:HB3   | 3:L:63:ILE:H     | 1.64                     | 0.62              |
| 4:0:361:GLU:HB3  | 4:0:369:ILE:HG12 | 1.82                     | 0.62              |
| 1:A:543:PRO:HG2  | 4:4:143:TYR:O    | 1.98                     | 0.62              |
| 4:4:361:GLU:HB3  | 4:4:369:ILE:HG12 | 1.82                     | 0.62              |
| 1:G:542:PHE:N    | 4:6:143:TYR:OH   | 2.33                     | 0.62              |
| 1:A:544:LYS:HB2  | 4:4:147:ARG:HA   | 1.80                     | 0.62              |
| 1:A:506:GLU:N    | 1:A:761:GLY:HA2  | 2.13                     | 0.62              |
| 1:J:251:ARG:HB2  | 1:J:264:ASP:CB   | 2.29                     | 0.62              |
| 1:J:580:SER:HA   | 1:J:588:VAL:O    | 2.00                     | 0.62              |
| 2:K:149:ASP:OD2  | 2:K:150:TYR:C    | 2.36                     | 0.62              |
| 4:2:361:GLU:HB3  | 4:2:369:ILE:HG12 | 1.82                     | 0.62              |
| 4:5:361:GLU:HB3  | 4:5:369:ILE:HG12 | 1.82                     | 0.62              |
| 4:6:257:CYS:HB3  | 4:6:258:PRO:HD3  | 1.81                     | 0.62              |
| 4:7:361:GLU:HB3  | 4:7:369:ILE:HG12 | 1.82                     | 0.62              |
| 4:8:361:GLU:HB3  | 4:8:369:ILE:HG12 | 1.82                     | 0.62              |
| 2:B:114:LYS:HA   | 2:B:146:GLY:C    | 2.03                     | 0.62              |
| 1:D:730:SER:C    | 1:D:733:PRO:HD2  | 2.20                     | 0.62              |
| 1:J:161:ASN:HA   | 1:J:164:GLN:HE21 | 1.63                     | 0.62              |
| 2:K:111:SER:OG   | 2:K:148:VAL:CG1  | 2.47                     | 0.62              |
| 1:A:541:MET:HE2  | 4:4:346:LEU:HD12 | 1.82                     | 0.62              |
| 1:G:543:PRO:HG2  | 4:6:143:TYR:O    | 1.98                     | 0.62              |
| 1:J:530:MET:CG   | 4:7:354:GLN:CG   | 2.72                     | 0.62              |
| 1:G:553:MLY:O    | 4:8:48:GLY:HA2   | 1.99                     | 0.62              |
| 1:A:161:ASN:HA   | 1:A:164:GLN:HE21 | 1.63                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:520:ALA:O    | 1:A:524:GLU:HG2  | 2.00                     | 0.62              |
| 1:D:537:GLU:C    | 4:5:351:THR:N    | 2.51                     | 0.62              |
| 1:D:578:HIS:CB   | 1:D:592:ILE:HD12 | 2.30                     | 0.62              |
| 1:D:91:MET:HE3   | 1:D:119:SER:HB2  | 1.82                     | 0.62              |
| 2:E:111:SER:OG   | 2:E:148:VAL:CG1  | 2.48                     | 0.62              |
| 1:G:127:ASN:HD22 | 1:G:128:PRO:CD   | 2.11                     | 0.62              |
| 1:G:154:HIS:CE1  | 1:G:156:PHE:CD2  | 2.88                     | 0.62              |
| 1:G:580:SER:HA   | 1:G:588:VAL:O    | 2.00                     | 0.62              |
| 1:G:798:LEU:HD21 | 3:I:122:GLU:O    | 2.00                     | 0.62              |
| 1:J:538:GLU:HA   | 4:7:349:LEU:CG   | 2.28                     | 0.62              |
| 1:J:542:PHE:CZ   | 1:J:553:MLY:HH11 | 2.34                     | 0.62              |
| 1:J:732:ILE:HG21 | 1:J:747:LEU:HD11 | 0.73                     | 0.62              |
| 1:J:754:ASP:CG   | 1:J:776:GLU:HA   | 2.20                     | 0.62              |
| 2:K:121:LEU:HA   | 2:K:128:PHE:CG   | 2.34                     | 0.62              |
| 4:W:361:GLU:HB3  | 4:W:369:ILE:HG12 | 1.82                     | 0.62              |
| 4:Y:190:MET:SD   | 4:Y:209:VAL:HG11 | 2.38                     | 0.62              |
| 4:1:361:GLU:HB3  | 4:1:369:ILE:HG12 | 1.82                     | 0.62              |
| 1:D:542:PHE:CB   | 4:5:143:TYR:HE1  | 2.13                     | 0.62              |
| 1:D:295:MLY:HG3  | 1:D:332:MET:HE1  | 1.80                     | 0.62              |
| 1:D:831:TRP:N    | 2:E:51:PHE:CE1   | 2.68                     | 0.62              |
| 1:G:278:GLN:HG3  | 1:G:318:GLY:N    | 2.14                     | 0.62              |
| 1:G:541:MET:C    | 4:6:143:TYR:CZ   | 2.73                     | 0.62              |
| 1:G:578:HIS:CB   | 1:G:592:ILE:HD12 | 2.30                     | 0.62              |
| 1:G:510:TRP:CE3  | 1:G:768:MLY:CH1  | 2.83                     | 0.62              |
| 1:G:98:HIS:HB3   | 1:G:100:PRO:CD   | 2.25                     | 0.62              |
| 1:J:541:MET:C    | 4:7:143:TYR:CZ   | 2.72                     | 0.62              |
| 1:J:707:CYS:HB3  | 1:J:714:ARG:NH2  | 2.14                     | 0.62              |
| 4:V:361:GLU:HB3  | 4:V:369:ILE:HG12 | 1.82                     | 0.62              |
| 4:X:361:GLU:HB3  | 4:X:369:ILE:HG12 | 1.82                     | 0.62              |
| 4:Y:257:CYS:HB3  | 4:Y:258:PRO:HD3  | 1.81                     | 0.62              |
| 4:Y:361:GLU:HB3  | 4:Y:369:ILE:HG12 | 1.82                     | 0.62              |
| 4:Z:361:GLU:HB3  | 4:Z:369:ILE:HG12 | 1.82                     | 0.62              |
| 1:D:541:MET:CA   | 4:5:143:TYR:OH   | 2.47                     | 0.62              |
| 1:A:643:GLY:O    | 1:A:644:SER:CB   | 2.48                     | 0.62              |
| 1:A:98:HIS:HB3   | 1:A:100:PRO:CD   | 2.25                     | 0.62              |
| 1:D:161:ASN:HA   | 1:D:164:GLN:HE21 | 1.64                     | 0.62              |
| 1:D:302:MET:HG2  | 1:D:303:LEU:CD1  | 2.30                     | 0.62              |
| 1:D:406:VAL:HG12 | 1:D:407:GLY:N    | 2.13                     | 0.62              |
| 1:D:520:ALA:O    | 1:D:524:GLU:HG2  | 2.00                     | 0.62              |
| 1:D:830:PRO:CG   | 2:E:67:MET:HE2   | 2.15                     | 0.62              |
| 1:G:302:MET:HG2  | 1:G:303:LEU:CD1  | 2.30                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:542:PHE:CZ   | 1:G:553:MLY:HH11 | 2.34                     | 0.62              |
| 1:G:730:SER:C    | 1:G:733:PRO:HD2  | 2.20                     | 0.62              |
| 1:G:768:MLY:CH2  | 1:G:772:LEU:HD22 | 2.27                     | 0.62              |
| 1:G:791:GLN:OE1  | 3:I:116:GLU:CG   | 2.48                     | 0.62              |
| 4:3:361:GLU:HB3  | 4:3:369:ILE:HG12 | 1.82                     | 0.62              |
| 1:A:553:MLY:O    | 4:6:48:GLY:HA2   | 1.99                     | 0.62              |
| 1:A:580:SER:HA   | 1:A:588:VAL:O    | 2.00                     | 0.62              |
| 1:A:730:SER:C    | 1:A:733:PRO:HD2  | 2.20                     | 0.62              |
| 1:A:771:LEU:O    | 1:A:774:LEU:N    | 2.32                     | 0.62              |
| 3:C:50:LEU:O     | 3:C:53:PRO:HD2   | 2.00                     | 0.62              |
| 1:D:202:SER:HA   | 1:D:207:LYS:HE3  | 1.72                     | 0.62              |
| 1:J:557:GLU:O    | 1:J:557:GLU:HG3  | 2.00                     | 0.62              |
| 1:J:730:SER:C    | 1:J:733:PRO:HD2  | 2.20                     | 0.62              |
| 1:J:817:GLN:CG   | 2:K:127:ARG:CD   | 2.75                     | 0.62              |
| 1:D:543:PRO:HG2  | 4:5:143:TYR:O    | 1.98                     | 0.61              |
| 4:8:257:CYS:HB3  | 4:8:258:PRO:HD3  | 1.81                     | 0.61              |
| 1:A:141:LEU:H    | 1:A:141:LEU:HD12 | 1.64                     | 0.61              |
| 1:A:278:GLN:HG3  | 1:A:318:GLY:N    | 2.15                     | 0.61              |
| 1:A:579:PHE:CE1  | 1:A:581:LEU:HD13 | 2.35                     | 0.61              |
| 1:A:732:ILE:HG22 | 1:A:747:LEU:CD1  | 1.55                     | 0.61              |
| 1:A:818:TYR:HB2  | 2:B:90:GLY:N     | 2.15                     | 0.61              |
| 1:A:81:ASN:OD1   | 1:A:96:HIS:HB2   | 2.00                     | 0.61              |
| 1:D:278:GLN:HG3  | 1:D:318:GLY:N    | 2.15                     | 0.61              |
| 1:D:507:GLY:HA2  | 1:D:762:HIS:CG   | 2.34                     | 0.61              |
| 1:G:551:MLY:C    | 4:8:46:GLY:O     | 2.48                     | 0.61              |
| 4:W:257:CYS:HB3  | 4:W:258:PRO:HD3  | 1.81                     | 0.61              |
| 1:J:542:PHE:CB   | 4:7:143:TYR:HE1  | 2.13                     | 0.61              |
| 1:A:154:HIS:CE1  | 1:A:156:PHE:CD2  | 2.88                     | 0.61              |
| 1:A:278:GLN:CG   | 1:A:317:GLU:HB2  | 2.27                     | 0.61              |
| 1:D:544:LYS:HB2  | 4:5:147:ARG:HA   | 1.80                     | 0.61              |
| 3:F:50:LEU:O     | 3:F:53:PRO:HD2   | 2.00                     | 0.61              |
| 1:G:278:GLN:CG   | 1:G:317:GLU:HB2  | 2.26                     | 0.61              |
| 2:H:132:GLU:O    | 2:H:136:MET:HG2  | 1.99                     | 0.61              |
| 3:I:50:LEU:O     | 3:I:53:PRO:HD2   | 2.00                     | 0.61              |
| 1:J:732:ILE:HG22 | 1:J:747:LEU:CD1  | 1.55                     | 0.61              |
| 1:J:411:GLU:N    | 4:7:333:PRO:HB2  | 2.11                     | 0.61              |
| 1:D:553:MLY:O    | 4:7:48:GLY:HA2   | 1.99                     | 0.61              |
| 1:A:642:LYS:CG   | 4:4:22:ALA:C     | 2.67                     | 0.61              |
| 1:A:686:MET:HG3  | 1:A:691:VAL:HG21 | 1.83                     | 0.61              |
| 1:A:797:PHE:CD2  | 3:C:126:LEU:HD21 | 2.35                     | 0.61              |
| 3:C:48:LYS:C     | 3:C:52:ASN:HD21  | 1.97                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:3:SER:HG     | 3:C:5:ALA:N      | 1.97                     | 0.61              |
| 1:D:141:LEU:H    | 1:D:141:LEU:HD12 | 1.64                     | 0.61              |
| 1:D:831:TRP:CZ2  | 2:E:47:LEU:C     | 2.70                     | 0.61              |
| 1:G:728:ASN:HD21 | 3:I:110:VAL:CA   | 2.13                     | 0.61              |
| 1:G:797:PHE:CB   | 3:I:149:VAL:HG11 | 2.29                     | 0.61              |
| 1:D:634:GLY:N    | 4:5:25:ASP:O     | 2.31                     | 0.61              |
| 1:J:642:LYS:CD   | 4:7:24:ASP:O     | 2.43                     | 0.61              |
| 1:A:99:GLU:OE2   | 1:A:696:ARG:NH2  | 2.30                     | 0.61              |
| 1:D:274:ARG:HB2  | 1:D:285:TYR:CE2  | 2.34                     | 0.61              |
| 2:E:114:LYS:HG3  | 2:E:146:GLY:HA2  | 1.82                     | 0.61              |
| 1:G:161:ASN:HA   | 1:G:164:GLN:HE21 | 1.63                     | 0.61              |
| 1:G:579:PHE:CE1  | 1:G:581:LEU:HD13 | 2.35                     | 0.61              |
| 1:G:639:GLY:N    | 4:6:344:SER:C    | 2.54                     | 0.61              |
| 1:G:732:ILE:HG22 | 1:G:747:LEU:CD1  | 1.55                     | 0.61              |
| 1:G:81:ASN:OD1   | 1:G:96:HIS:HB2   | 2.00                     | 0.61              |
| 2:H:144:VAL:HA   | 2:H:153:ILE:HD11 | 1.80                     | 0.61              |
| 1:J:578:HIS:CB   | 1:J:592:ILE:HD12 | 2.30                     | 0.61              |
| 2:K:114:LYS:HG3  | 2:K:146:GLY:HA2  | 1.82                     | 0.61              |
| 3:L:52:ASN:N     | 3:L:53:PRO:HD2   | 2.16                     | 0.61              |
| 1:A:800:ARG:CD   | 3:C:149:VAL:CG2  | 2.41                     | 0.61              |
| 2:B:117:LEU:HD11 | 2:B:147:ASN:HB3  | 1.76                     | 0.61              |
| 1:D:831:TRP:CA   | 2:E:51:PHE:CE1   | 2.83                     | 0.61              |
| 2:E:144:VAL:HA   | 2:E:153:ILE:HD11 | 1.80                     | 0.61              |
| 1:G:541:MET:HE2  | 4:6:346:LEU:HD12 | 1.82                     | 0.61              |
| 1:J:274:ARG:HB2  | 1:J:285:TYR:CE2  | 2.34                     | 0.61              |
| 1:J:579:PHE:CE1  | 1:J:581:LEU:HD13 | 2.35                     | 0.61              |
| 1:J:643:GLY:H    | 4:7:23:GLY:C     | 2.01                     | 0.61              |
| 1:D:541:MET:C    | 4:5:143:TYR:CZ   | 2.73                     | 0.61              |
| 1:A:798:LEU:HD23 | 3:C:122:GLU:HB3  | 1.83                     | 0.61              |
| 1:D:557:GLU:O    | 1:D:557:GLU:HG3  | 2.00                     | 0.61              |
| 1:D:724:TYR:C    | 1:D:782:MLY:CH2  | 2.66                     | 0.61              |
| 1:D:507:GLY:CA   | 1:D:762:HIS:CD2  | 2.84                     | 0.61              |
| 1:G:274:ARG:HB2  | 1:G:285:TYR:CE2  | 2.34                     | 0.61              |
| 1:G:643:GLY:O    | 1:G:644:SER:CB   | 2.48                     | 0.61              |
| 1:J:623:PHE:CG   | 1:J:623:PHE:HA   | 2.35                     | 0.61              |
| 1:J:813:ILE:O    | 1:J:817:GLN:N    | 2.30                     | 0.61              |
| 1:J:95:THR:HA    | 1:J:713:SER:HB3  | 1.82                     | 0.61              |
| 1:J:99:GLU:OE2   | 1:J:696:ARG:NH2  | 2.30                     | 0.61              |
| 1:A:542:PHE:CB   | 4:4:143:TYR:HE1  | 2.12                     | 0.61              |
| 1:A:530:MET:HE2  | 4:4:354:GLN:HG3  | 1.80                     | 0.61              |
| 2:B:111:SER:OG   | 2:B:148:VAL:CG1  | 2.47                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:541:MET:SD   | 4:5:346:LEU:O    | 2.48                     | 0.61              |
| 1:D:686:MET:HG3  | 1:D:691:VAL:HG21 | 1.83                     | 0.61              |
| 3:F:52:ASN:HB2   | 3:F:53:PRO:CD    | 2.28                     | 0.61              |
| 1:G:524:GLU:O    | 1:G:528:MLY:HB3  | 2.01                     | 0.61              |
| 1:G:821:ARG:HH22 | 2:H:127:ARG:HG2  | 0.78                     | 0.61              |
| 1:J:302:MET:HG2  | 1:J:303:LEU:CD1  | 2.30                     | 0.61              |
| 1:J:639:GLY:N    | 4:7:344:SER:C    | 2.54                     | 0.61              |
| 1:J:643:GLY:O    | 1:J:644:SER:CB   | 2.49                     | 0.61              |
| 2:B:34:ILE:O     | 2:B:46:ASP:HB3   | 2.01                     | 0.61              |
| 1:D:217:THR:C    | 1:D:221:GLN:HG2  | 2.21                     | 0.61              |
| 2:H:144:VAL:CG1  | 2:H:153:ILE:HD13 | 2.19                     | 0.61              |
| 1:G:792:ALA:HA   | 3:I:35:ARG:CZ    | 2.31                     | 0.61              |
| 1:J:93:MET:SD    | 1:J:764:MLY:HH23 | 2.33                     | 0.61              |
| 4:5:223:PHE:HD2  | 4:5:312:ARG:NH2  | 1.99                     | 0.61              |
| 2:B:114:LYS:HG3  | 2:B:146:GLY:HA2  | 1.82                     | 0.61              |
| 3:C:63:ILE:HG22  | 3:C:64:THR:O     | 2.01                     | 0.61              |
| 1:D:154:HIS:CE1  | 1:D:156:PHE:CD2  | 2.88                     | 0.61              |
| 1:D:576:GLU:CG   | 1:D:577:ALA:N    | 2.44                     | 0.61              |
| 1:D:579:PHE:CE1  | 1:D:581:LEU:HD13 | 2.35                     | 0.61              |
| 3:F:49:ILE:HA    | 3:F:52:ASN:ND2   | 2.05                     | 0.61              |
| 1:G:557:GLU:O    | 1:G:557:GLU:HG3  | 2.01                     | 0.61              |
| 1:G:730:SER:OG   | 3:I:109:HIS:CE1  | 2.53                     | 0.61              |
| 1:J:154:HIS:CE1  | 1:J:156:PHE:CD2  | 2.88                     | 0.61              |
| 1:J:202:SER:HA   | 1:J:207:LYS:HE3  | 1.72                     | 0.61              |
| 1:J:769:ALA:CB   | 1:J:770:GLY:HA3  | 2.28                     | 0.61              |
| 4:4:223:PHE:HD2  | 4:4:312:ARG:NH2  | 1.99                     | 0.61              |
| 1:A:411:GLU:N    | 4:4:333:PRO:HB2  | 2.11                     | 0.61              |
| 1:D:643:GLY:H    | 4:5:23:GLY:C     | 2.02                     | 0.61              |
| 1:D:643:GLY:O    | 1:D:644:SER:CB   | 2.48                     | 0.61              |
| 3:F:52:ASN:N     | 3:F:53:PRO:HD2   | 2.15                     | 0.61              |
| 1:G:94:MET:HE1   | 1:G:101:ALA:HB1  | 1.80                     | 0.61              |
| 1:G:530:MET:HE3  | 4:6:354:GLN:CG   | 2.25                     | 0.61              |
| 1:G:686:MET:HG3  | 1:G:691:VAL:HG21 | 1.83                     | 0.61              |
| 1:G:732:ILE:HG21 | 1:G:747:LEU:HD11 | 0.72                     | 0.61              |
| 1:G:769:ALA:O    | 1:G:773:GLY:HA2  | 2.01                     | 0.61              |
| 1:G:838:ILE:CG1  | 2:H:54:MET:HE1   | 2.30                     | 0.61              |
| 1:J:798:LEU:CD2  | 3:L:126:LEU:HG   | 2.18                     | 0.61              |
| 3:L:50:LEU:O     | 3:L:53:PRO:HD2   | 2.00                     | 0.61              |
| 1:D:530:MET:CG   | 4:5:354:GLN:HG3  | 2.30                     | 0.60              |
| 1:A:156:PHE:CD1  | 1:A:195:TYR:CD1  | 2.89                     | 0.60              |
| 1:A:40:VAL:HG22  | 1:A:41:VAL:N     | 2.16                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:578:HIS:CD2  | 1:D:591:ASN:HA   | 2.32                     | 0.60              |
| 1:D:623:PHE:HA   | 1:D:623:PHE:CG   | 2.36                     | 0.60              |
| 1:G:520:ALA:O    | 1:G:524:GLU:HG2  | 2.00                     | 0.60              |
| 1:G:755:HIS:HA   | 1:G:758:TYR:HE1  | 1.64                     | 0.60              |
| 2:H:114:LYS:HG3  | 2:H:146:GLY:HA2  | 1.82                     | 0.60              |
| 1:J:524:GLU:O    | 1:J:528:MLY:HB3  | 2.01                     | 0.60              |
| 1:J:795:ARG:CD   | 3:L:35:ARG:CZ    | 2.53                     | 0.60              |
| 4:Z:223:PHE:HD2  | 4:Z:312:ARG:NH2  | 1.99                     | 0.60              |
| 4:2:223:PHE:HD2  | 4:2:312:ARG:NH2  | 1.99                     | 0.60              |
| 1:A:217:THR:C    | 1:A:221:GLN:HG2  | 2.21                     | 0.60              |
| 1:A:524:GLU:O    | 1:A:528:MLY:HB3  | 2.01                     | 0.60              |
| 1:A:813:ILE:CG2  | 2:B:127:ARG:CZ   | 2.68                     | 0.60              |
| 3:C:52:ASN:N     | 3:C:53:PRO:HD2   | 2.16                     | 0.60              |
| 1:D:38:VAL:HB    | 1:D:52:ILE:HD11  | 1.84                     | 0.60              |
| 1:D:81:ASN:OD1   | 1:D:96:HIS:HB2   | 2.00                     | 0.60              |
| 1:G:124:VAL:CG1  | 1:G:675:ILE:HD13 | 2.31                     | 0.60              |
| 1:G:40:VAL:HG22  | 1:G:41:VAL:N     | 2.16                     | 0.60              |
| 1:G:553:MLY:NZ   | 4:8:45:VAL:HG13  | 2.16                     | 0.60              |
| 1:J:520:ALA:O    | 1:J:524:GLU:HG2  | 2.00                     | 0.60              |
| 1:J:543:PRO:HG2  | 4:7:143:TYR:O    | 1.98                     | 0.60              |
| 1:J:665:ARG:C    | 1:J:667:THR:H    | 2.05                     | 0.60              |
| 1:J:686:MET:HG3  | 1:J:691:VAL:HG21 | 1.83                     | 0.60              |
| 1:J:81:ASN:OD1   | 1:J:96:HIS:HB2   | 2.00                     | 0.60              |
| 1:J:95:THR:HG23  | 1:J:96:HIS:ND1   | 2.17                     | 0.60              |
| 2:K:34:ILE:O     | 2:K:46:ASP:HB3   | 2.01                     | 0.60              |
| 1:A:557:GLU:O    | 1:A:557:GLU:HG3  | 2.00                     | 0.60              |
| 1:A:665:ARG:C    | 1:A:667:THR:H    | 2.05                     | 0.60              |
| 1:D:166:MET:HE3  | 1:D:254:PHE:HD2  | 1.66                     | 0.60              |
| 1:D:410:ASN:CG   | 4:5:334:GLU:CA   | 2.47                     | 0.60              |
| 1:D:721:LYS:HG2  | 1:D:736:GLN:CD   | 1.86                     | 0.60              |
| 1:D:837:MLY:O    | 1:D:840:PRO:HD2  | 2.02                     | 0.60              |
| 1:J:217:THR:C    | 1:J:221:GLN:HG2  | 2.21                     | 0.60              |
| 1:A:553:MLY:NZ   | 4:6:45:VAL:HG13  | 2.16                     | 0.60              |
| 1:J:530:MET:CG   | 4:7:354:GLN:HG3  | 2.30                     | 0.60              |
| 4:6:223:PHE:HD2  | 4:6:312:ARG:NH2  | 1.99                     | 0.60              |
| 1:A:124:VAL:CG1  | 1:A:675:ILE:HD13 | 2.31                     | 0.60              |
| 1:A:40:VAL:HG22  | 1:A:41:VAL:H     | 1.67                     | 0.60              |
| 1:A:546:THR:HG22 | 1:A:547:ASP:N    | 2.17                     | 0.60              |
| 1:D:124:VAL:CG1  | 1:D:675:ILE:HD13 | 2.31                     | 0.60              |
| 1:D:40:VAL:HG22  | 1:D:41:VAL:N     | 2.16                     | 0.60              |
| 1:D:612:GLN:HE22 | 1:D:627:GLY:HA2  | 1.66                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:817:GLN:CG   | 2:E:127:ARG:CD   | 2.78                     | 0.60              |
| 1:G:38:VAL:HB    | 1:G:52:ILE:HD11  | 1.83                     | 0.60              |
| 1:G:623:PHE:CG   | 1:G:623:PHE:HA   | 2.36                     | 0.60              |
| 1:G:730:SER:HB2  | 3:I:109:HIS:NE2  | 2.17                     | 0.60              |
| 1:J:38:VAL:HB    | 1:J:52:ILE:HD11  | 1.83                     | 0.60              |
| 1:J:546:THR:HG22 | 1:J:547:ASP:N    | 2.17                     | 0.60              |
| 1:J:837:MLY:O    | 1:J:840:PRO:HD2  | 2.02                     | 0.60              |
| 2:K:130:PRO:HA   | 2:K:133:ILE:HD12 | 1.83                     | 0.60              |
| 1:J:823:PHE:CD1  | 2:K:157:ILE:HA   | 2.36                     | 0.60              |
| 3:L:63:ILE:HG22  | 3:L:64:THR:O     | 2.01                     | 0.60              |
| 4:Y:287:ILE:HD12 | 4:Y:287:ILE:H    | 1.67                     | 0.60              |
| 4:2:287:ILE:H    | 4:2:287:ILE:HD12 | 1.67                     | 0.60              |
| 4:3:223:PHE:HD2  | 4:3:312:ARG:NH2  | 1.99                     | 0.60              |
| 1:D:542:PHE:N    | 4:5:143:TYR:OH   | 2.32                     | 0.60              |
| 4:5:287:ILE:H    | 4:5:287:ILE:HD12 | 1.67                     | 0.60              |
| 1:G:542:PHE:CB   | 4:6:143:TYR:HE1  | 2.13                     | 0.60              |
| 1:J:542:PHE:N    | 4:7:143:TYR:OH   | 2.33                     | 0.60              |
| 1:A:38:VAL:HB    | 1:A:52:ILE:HD11  | 1.84                     | 0.60              |
| 1:A:787:ILE:O    | 1:A:790:THR:N    | 2.35                     | 0.60              |
| 1:D:530:MET:HA   | 4:5:354:GLN:CB   | 2.29                     | 0.60              |
| 2:E:34:ILE:O     | 2:E:46:ASP:HB3   | 2.01                     | 0.60              |
| 1:G:837:MLY:O    | 1:G:840:PRO:HD2  | 2.02                     | 0.60              |
| 1:J:124:VAL:HG13 | 1:J:675:ILE:HD13 | 1.84                     | 0.60              |
| 1:J:202:SER:CA   | 1:J:207:LYS:HE3  | 2.27                     | 0.60              |
| 1:J:60:VAL:O     | 1:J:71:THR:HA    | 2.02                     | 0.60              |
| 4:V:287:ILE:HD12 | 4:V:287:ILE:H    | 1.67                     | 0.60              |
| 4:X:223:PHE:HD2  | 4:X:312:ARG:NH2  | 1.99                     | 0.60              |
| 4:3:287:ILE:H    | 4:3:287:ILE:HD12 | 1.67                     | 0.60              |
| 1:A:504:MLY:HB2  | 1:A:762:HIS:CE1  | 2.37                     | 0.60              |
| 1:A:550:PHE:CE2  | 1:A:592:ILE:HG23 | 2.37                     | 0.60              |
| 1:A:837:MLY:O    | 1:A:840:PRO:HD2  | 2.02                     | 0.60              |
| 1:D:524:GLU:O    | 1:D:528:MLY:HB3  | 2.01                     | 0.60              |
| 1:D:639:GLY:N    | 4:5:344:SER:C    | 2.54                     | 0.60              |
| 1:D:796:GLY:HA2  | 3:F:35:ARG:HB3   | 1.83                     | 0.60              |
| 2:E:130:PRO:HA   | 2:E:133:ILE:HD12 | 1.84                     | 0.60              |
| 2:E:144:VAL:CG1  | 2:E:153:ILE:HD13 | 2.19                     | 0.60              |
| 1:G:156:PHE:CD1  | 1:G:195:TYR:CD1  | 2.90                     | 0.60              |
| 1:G:84:MLY:CH1   | 1:G:716:LEU:O    | 2.50                     | 0.60              |
| 1:G:60:VAL:O     | 1:G:71:THR:HA    | 2.02                     | 0.60              |
| 1:J:40:VAL:HG22  | 1:J:41:VAL:N     | 2.16                     | 0.60              |
| 1:J:578:HIS:CD2  | 1:J:591:ASN:HA   | 2.31                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:124:VAL:CG1  | 1:J:675:ILE:HD13 | 2.31                     | 0.60              |
| 1:J:787:ILE:O    | 1:J:790:THR:N    | 2.35                     | 0.60              |
| 4:X:287:ILE:H    | 4:X:287:ILE:HD12 | 1.67                     | 0.60              |
| 4:Y:223:PHE:HD2  | 4:Y:312:ARG:NH2  | 1.99                     | 0.60              |
| 4:7:287:ILE:HD12 | 4:7:287:ILE:H    | 1.67                     | 0.60              |
| 1:A:60:VAL:O     | 1:A:71:THR:HA    | 2.02                     | 0.60              |
| 1:A:634:GLY:N    | 4:4:25:ASP:O     | 2.31                     | 0.60              |
| 1:J:827:MLY:HH21 | 2:K:139:ALA:HB3  | 1.83                     | 0.60              |
| 4:0:223:PHE:HD2  | 4:0:312:ARG:NH2  | 1.99                     | 0.60              |
| 4:0:287:ILE:HD12 | 4:0:287:ILE:H    | 1.67                     | 0.60              |
| 1:D:553:MLY:NZ   | 4:7:45:VAL:HG13  | 2.16                     | 0.60              |
| 1:A:542:PHE:CD1  | 4:4:143:TYR:CE1  | 2.90                     | 0.60              |
| 1:A:506:GLU:OE2  | 1:A:760:PHE:CD2  | 2.49                     | 0.60              |
| 3:C:46:ILE:O     | 3:C:50:LEU:CG    | 2.47                     | 0.60              |
| 3:C:52:ASN:N     | 3:C:53:PRO:CD    | 2.65                     | 0.60              |
| 1:D:49:MLY:HH13  | 1:D:108:GLU:OE2  | 2.02                     | 0.60              |
| 1:D:124:VAL:HG13 | 1:D:675:ILE:HD13 | 1.84                     | 0.60              |
| 1:D:665:ARG:C    | 1:D:667:THR:H    | 2.05                     | 0.60              |
| 1:D:769:ALA:HA   | 1:D:771:LEU:HB2  | 1.81                     | 0.60              |
| 1:D:789:ALA:O    | 3:F:87:PHE:CZ    | 2.55                     | 0.60              |
| 1:J:786:ILE:HG12 | 3:L:86:ASP:CB    | 2.30                     | 0.60              |
| 3:L:52:ASN:N     | 3:L:53:PRO:CD    | 2.65                     | 0.60              |
| 4:Z:287:ILE:H    | 4:Z:287:ILE:HD12 | 1.67                     | 0.60              |
| 1:A:95:THR:HG23  | 1:A:96:HIS:ND1   | 2.16                     | 0.60              |
| 1:G:217:THR:C    | 1:G:221:GLN:HG2  | 2.21                     | 0.60              |
| 1:G:578:HIS:CD2  | 1:G:591:ASN:HA   | 2.31                     | 0.60              |
| 4:4:287:ILE:H    | 4:4:287:ILE:HD12 | 1.67                     | 0.59              |
| 1:A:505:MLY:HH23 | 1:A:762:HIS:O    | 2.02                     | 0.59              |
| 1:A:541:MET:SD   | 4:4:346:LEU:O    | 2.48                     | 0.59              |
| 3:C:49:ILE:CA    | 3:C:52:ASN:ND2   | 2.53                     | 0.59              |
| 1:D:536:LEU:HD13 | 1:D:550:PHE:CE1  | 2.37                     | 0.59              |
| 1:D:755:HIS:HA   | 1:D:758:TYR:HE1  | 1.64                     | 0.59              |
| 3:F:63:ILE:HG22  | 3:F:64:THR:O     | 2.01                     | 0.59              |
| 1:G:665:ARG:C    | 1:G:667:THR:H    | 2.05                     | 0.59              |
| 2:H:34:ILE:O     | 2:H:46:ASP:HB3   | 2.01                     | 0.59              |
| 3:I:63:ILE:HG22  | 3:I:64:THR:O     | 2.01                     | 0.59              |
| 1:J:768:MLY:CH2  | 1:J:772:LEU:HD13 | 2.32                     | 0.59              |
| 1:J:820:VAL:CG1  | 2:K:136:MET:CE   | 2.80                     | 0.59              |
| 4:1:287:ILE:H    | 4:1:287:ILE:HD12 | 1.67                     | 0.59              |
| 1:D:60:VAL:O     | 1:D:71:THR:HA    | 2.02                     | 0.59              |
| 1:D:95:THR:HG23  | 1:D:96:HIS:ND1   | 2.17                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:536:LEU:HD13 | 1:G:550:PHE:CE1  | 2.37                     | 0.59              |
| 3:I:52:ASN:HB2   | 3:I:53:PRO:CD    | 2.28                     | 0.59              |
| 3:I:52:ASN:N     | 3:I:53:PRO:CD    | 2.65                     | 0.59              |
| 3:L:49:ILE:CA    | 3:L:52:ASN:ND2   | 2.54                     | 0.59              |
| 4:W:287:ILE:H    | 4:W:287:ILE:HD12 | 1.67                     | 0.59              |
| 1:A:530:MET:CG   | 4:4:354:GLN:HG3  | 2.30                     | 0.59              |
| 1:G:541:MET:SD   | 4:6:346:LEU:O    | 2.48                     | 0.59              |
| 1:A:536:LEU:HD13 | 1:A:550:PHE:CE1  | 2.37                     | 0.59              |
| 1:D:549:SER:OG   | 1:D:550:PHE:N    | 2.36                     | 0.59              |
| 1:G:546:THR:HG22 | 1:G:547:ASP:N    | 2.17                     | 0.59              |
| 1:J:549:SER:OG   | 1:J:550:PHE:N    | 2.35                     | 0.59              |
| 4:8:223:PHE:HD2  | 4:8:312:ARG:NH2  | 1.99                     | 0.59              |
| 1:A:135:TYR:N    | 1:A:135:TYR:CD1  | 2.70                     | 0.59              |
| 1:A:116:TYR:HB2  | 1:A:153:PRO:O    | 2.03                     | 0.59              |
| 1:A:195:TYR:O    | 1:A:199:ILE:HG23 | 2.03                     | 0.59              |
| 1:D:7:MET:HE3    | 1:D:14:ALA:HB1   | 1.84                     | 0.59              |
| 1:D:599:ASN:CB   | 1:D:649:VAL:HB   | 2.32                     | 0.59              |
| 1:D:776:GLU:O    | 1:D:779:ARG:HB3  | 2.03                     | 0.59              |
| 1:D:783:LEU:O    | 1:D:787:ILE:N    | 2.28                     | 0.59              |
| 1:D:787:ILE:O    | 1:D:790:THR:N    | 2.35                     | 0.59              |
| 1:G:7:MET:HE3    | 1:G:14:ALA:HB1   | 1.83                     | 0.59              |
| 1:G:550:PHE:CE2  | 1:G:592:ILE:HG23 | 2.37                     | 0.59              |
| 1:G:787:ILE:O    | 1:G:790:THR:N    | 2.35                     | 0.59              |
| 1:G:792:ALA:CB   | 3:I:40:ASN:HB3   | 2.32                     | 0.59              |
| 1:J:156:PHE:CD1  | 1:J:195:TYR:CD1  | 2.90                     | 0.59              |
| 1:J:530:MET:HA   | 4:7:354:GLN:CB   | 2.28                     | 0.59              |
| 1:G:530:MET:CG   | 4:6:354:GLN:HG3  | 2.30                     | 0.59              |
| 1:J:542:PHE:CD1  | 4:7:143:TYR:CE1  | 2.91                     | 0.59              |
| 1:A:578:HIS:CD2  | 1:A:591:ASN:HA   | 2.31                     | 0.59              |
| 1:A:623:PHE:HA   | 1:A:623:PHE:CG   | 2.36                     | 0.59              |
| 1:A:776:GLU:O    | 1:A:779:ARG:HB3  | 2.03                     | 0.59              |
| 1:G:538:GLU:HA   | 4:6:349:LEU:CG   | 2.28                     | 0.59              |
| 1:G:728:ASN:HA   | 3:I:113:THR:OG1  | 2.03                     | 0.59              |
| 1:G:817:GLN:OE1  | 2:H:127:ARG:CD   | 2.47                     | 0.59              |
| 1:G:818:TYR:CG   | 2:H:127:ARG:NH1  | 2.70                     | 0.59              |
| 3:I:52:ASN:N     | 3:I:53:PRO:HD2   | 2.16                     | 0.59              |
| 4:W:223:PHE:HD2  | 4:W:312:ARG:NH2  | 1.99                     | 0.59              |
| 1:A:529:PRO:HG3  | 4:4:353:GLN:OE1  | 2.03                     | 0.59              |
| 1:A:295:MLY:HG3  | 1:A:332:MET:HE1  | 1.85                     | 0.59              |
| 1:D:156:PHE:CD1  | 1:D:195:TYR:CD1  | 2.90                     | 0.59              |
| 1:D:464:ILE:HG22 | 1:D:465:ALA:N    | 2.18                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:534:SER:C    | 4:5:351:THR:CA   | 2.47                     | 0.59              |
| 1:G:599:ASN:CB   | 1:G:649:VAL:HB   | 2.32                     | 0.59              |
| 1:J:230:GLU:O    | 1:J:234:ASN:HB2  | 2.03                     | 0.59              |
| 1:J:49:MLY:HH13  | 1:J:108:GLU:OE2  | 2.02                     | 0.59              |
| 4:1:223:PHE:HD2  | 4:1:312:ARG:NH2  | 1.99                     | 0.59              |
| 1:D:542:PHE:CD1  | 4:5:143:TYR:CE1  | 2.90                     | 0.59              |
| 1:A:735:GLY:O    | 1:A:743:ALA:HA   | 1.94                     | 0.59              |
| 1:D:40:VAL:HG22  | 1:D:41:VAL:H     | 1.67                     | 0.59              |
| 1:D:831:TRP:CH2  | 2:E:50:THR:HB    | 2.37                     | 0.59              |
| 3:F:52:ASN:N     | 3:F:53:PRO:CD    | 2.65                     | 0.59              |
| 1:G:195:TYR:O    | 1:G:199:ILE:HG23 | 2.03                     | 0.59              |
| 1:G:40:VAL:HG22  | 1:G:41:VAL:H     | 1.67                     | 0.59              |
| 1:G:549:SER:OG   | 1:G:550:PHE:N    | 2.36                     | 0.59              |
| 1:G:646:PHE:CD2  | 1:G:652:LEU:CD1  | 2.85                     | 0.59              |
| 1:G:715:VAL:HG11 | 1:G:720:PHE:HD1  | 1.68                     | 0.59              |
| 1:G:836:PHE:CE1  | 2:H:159:HIS:CA   | 2.63                     | 0.59              |
| 1:G:93:MET:CB    | 1:G:716:LEU:HD12 | 2.33                     | 0.59              |
| 1:J:265:ILE:HG22 | 1:J:266:GLU:N    | 2.18                     | 0.59              |
| 1:J:550:PHE:CE2  | 1:J:592:ILE:HG23 | 2.37                     | 0.59              |
| 1:J:817:GLN:HG2  | 2:K:127:ARG:CB   | 2.32                     | 0.59              |
| 1:G:542:PHE:CD1  | 4:6:143:TYR:CE1  | 2.91                     | 0.59              |
| 1:A:265:ILE:HG22 | 1:A:266:GLU:N    | 2.18                     | 0.59              |
| 1:A:48:VAL:HG22  | 1:A:49:MLY:N     | 2.18                     | 0.59              |
| 1:D:601:ASP:N    | 1:D:602:PRO:HD3  | 2.18                     | 0.59              |
| 1:D:724:TYR:CE1  | 1:D:778:MET:CG   | 2.86                     | 0.59              |
| 1:J:599:ASN:CB   | 1:J:649:VAL:HB   | 2.32                     | 0.59              |
| 1:A:230:GLU:O    | 1:A:234:ASN:HB2  | 2.03                     | 0.59              |
| 1:D:792:ALA:CB   | 3:F:40:ASN:CB    | 2.75                     | 0.59              |
| 1:G:116:TYR:HB2  | 1:G:153:PRO:O    | 2.03                     | 0.59              |
| 1:J:776:GLU:O    | 1:J:779:ARG:HB3  | 2.02                     | 0.59              |
| 1:J:784:ALA:O    | 1:J:788:THR:HB   | 2.02                     | 0.59              |
| 4:V:223:PHE:HD2  | 4:V:312:ARG:NH2  | 1.99                     | 0.59              |
| 1:A:601:ASP:N    | 1:A:602:PRO:HD3  | 2.18                     | 0.59              |
| 1:A:599:ASN:CB   | 1:A:649:VAL:HB   | 2.32                     | 0.59              |
| 1:A:755:HIS:HA   | 1:A:758:TYR:HE1  | 1.64                     | 0.59              |
| 1:D:135:TYR:N    | 1:D:135:TYR:CD1  | 2.69                     | 0.59              |
| 1:D:141:LEU:O    | 1:D:144:ARG:HB3  | 2.03                     | 0.59              |
| 1:D:649:VAL:HA   | 1:D:649:VAL:HG22 | 1.80                     | 0.59              |
| 1:D:817:GLN:NE2  | 2:E:127:ARG:CD   | 2.66                     | 0.59              |
| 1:D:831:TRP:N    | 2:E:51:PHE:HZ    | 1.98                     | 0.59              |
| 1:J:195:TYR:O    | 1:J:199:ILE:HG23 | 2.03                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:536:LEU:HD13 | 1:J:550:PHE:CE1  | 2.37                     | 0.59              |
| 1:J:715:VAL:HG11 | 1:J:720:PHE:HD1  | 1.68                     | 0.59              |
| 4:6:287:ILE:HD12 | 4:6:287:ILE:H    | 1.67                     | 0.58              |
| 1:J:643:GLY:HA2  | 4:7:24:ASP:OD1   | 2.04                     | 0.58              |
| 1:D:769:ALA:CB   | 1:D:771:LEU:N    | 2.66                     | 0.58              |
| 1:D:722:GLN:O    | 1:D:782:MLY:HH23 | 2.02                     | 0.58              |
| 1:G:124:VAL:HG13 | 1:G:675:ILE:HD13 | 1.84                     | 0.58              |
| 1:G:135:TYR:CD1  | 1:G:135:TYR:N    | 2.69                     | 0.58              |
| 1:G:230:GLU:O    | 1:G:234:ASN:HB2  | 2.03                     | 0.58              |
| 1:G:95:THR:HG23  | 1:G:96:HIS:ND1   | 2.17                     | 0.58              |
| 1:J:210:GLN:O    | 1:J:211:SER:OG   | 2.15                     | 0.58              |
| 1:J:601:ASP:N    | 1:J:602:PRO:HD3  | 2.18                     | 0.58              |
| 1:J:7:MET:HE3    | 1:J:14:ALA:HB1   | 1.85                     | 0.58              |
| 1:A:538:GLU:O    | 1:A:541:MET:HB2  | 2.04                     | 0.58              |
| 1:A:794:CYS:O    | 1:A:798:LEU:N    | 2.37                     | 0.58              |
| 1:A:831:TRP:CH2  | 2:B:50:THR:CB    | 2.81                     | 0.58              |
| 1:D:124:VAL:HG13 | 1:D:675:ILE:CD1  | 2.33                     | 0.58              |
| 1:D:550:PHE:CE2  | 1:D:592:ILE:HG23 | 2.37                     | 0.58              |
| 1:D:629:GLU:HB3  | 1:D:645:SER:N    | 2.18                     | 0.58              |
| 1:J:553:MLY:NZ   | 4:V:45:VAL:HG13  | 2.17                     | 0.58              |
| 1:J:754:ASP:OD2  | 1:J:776:GLU:HB3  | 2.01                     | 0.58              |
| 1:A:410:ASN:CG   | 4:4:334:GLU:CA   | 2.48                     | 0.58              |
| 1:A:549:SER:OG   | 1:A:550:PHE:N    | 2.36                     | 0.58              |
| 1:D:529:PRO:HG3  | 4:5:353:GLN:OE1  | 2.03                     | 0.58              |
| 1:D:794:CYS:O    | 1:D:798:LEU:N    | 2.36                     | 0.58              |
| 1:G:265:ILE:HG22 | 1:G:266:GLU:N    | 2.18                     | 0.58              |
| 1:G:464:ILE:HG22 | 1:G:465:ALA:N    | 2.18                     | 0.58              |
| 2:H:130:PRO:HA   | 2:H:133:ILE:HD12 | 1.84                     | 0.58              |
| 1:J:116:TYR:HB2  | 1:J:153:PRO:O    | 2.03                     | 0.58              |
| 1:J:646:PHE:CD2  | 1:J:652:LEU:CD1  | 2.85                     | 0.58              |
| 1:J:820:VAL:CG1  | 2:K:136:MET:HE1  | 2.33                     | 0.58              |
| 1:G:642:LYS:CG   | 4:6:22:ALA:CA    | 2.80                     | 0.58              |
| 1:A:7:MET:HE3    | 1:A:14:ALA:HB1   | 1.84                     | 0.58              |
| 1:A:715:VAL:HG11 | 1:A:720:PHE:HD1  | 1.68                     | 0.58              |
| 2:B:140:PHE:O    | 2:B:141:PRO:C    | 2.33                     | 0.58              |
| 1:A:831:TRP:CZ3  | 2:B:34:ILE:HG12  | 2.39                     | 0.58              |
| 1:D:218:LEU:N    | 1:D:221:GLN:HE21 | 2.01                     | 0.58              |
| 1:D:643:GLY:HA2  | 4:5:24:ASP:OD1   | 2.04                     | 0.58              |
| 1:D:813:ILE:O    | 1:D:817:GLN:N    | 2.30                     | 0.58              |
| 1:G:601:ASP:N    | 1:G:602:PRO:HD3  | 2.18                     | 0.58              |
| 1:J:40:VAL:HG22  | 1:J:41:VAL:H     | 1.67                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:629:GLU:HB3  | 1:J:645:SER:N    | 2.18                     | 0.58              |
| 1:J:649:VAL:HG22 | 1:J:649:VAL:HA   | 1.80                     | 0.58              |
| 3:L:52:ASN:HB2   | 3:L:53:PRO:CD    | 2.28                     | 0.58              |
| 1:J:529:PRO:HG3  | 4:7:353:GLN:OE1  | 2.04                     | 0.58              |
| 4:8:287:ILE:HD12 | 4:8:287:ILE:H    | 1.67                     | 0.58              |
| 1:A:124:VAL:HG13 | 1:A:675:ILE:HD13 | 1.84                     | 0.58              |
| 1:D:220:ASP:O    | 1:D:224:SER:N    | 2.27                     | 0.58              |
| 1:D:48:VAL:HG22  | 1:D:49:MLY:N     | 2.18                     | 0.58              |
| 1:D:546:THR:HG22 | 1:D:547:ASP:N    | 2.17                     | 0.58              |
| 1:D:715:VAL:HG11 | 1:D:720:PHE:HD1  | 1.68                     | 0.58              |
| 1:G:629:GLU:HB3  | 1:G:645:SER:N    | 2.18                     | 0.58              |
| 1:G:751:GLY:HA2  | 3:I:114:LEU:CD1  | 2.24                     | 0.58              |
| 1:G:836:PHE:CE2  | 2:H:160:GLY:CA   | 2.86                     | 0.58              |
| 1:J:135:TYR:CD1  | 1:J:135:TYR:N    | 2.69                     | 0.58              |
| 1:J:48:VAL:HG22  | 1:J:49:MLY:N     | 2.18                     | 0.58              |
| 1:A:839:MLY:CD   | 2:B:159:HIS:HB3  | 2.33                     | 0.58              |
| 1:D:127:ASN:ND2  | 1:D:128:PRO:HD2  | 2.16                     | 0.58              |
| 1:D:230:GLU:O    | 1:D:234:ASN:HB2  | 2.03                     | 0.58              |
| 1:D:538:GLU:O    | 1:D:541:MET:HB2  | 2.04                     | 0.58              |
| 1:G:124:VAL:HG13 | 1:G:675:ILE:CD1  | 2.33                     | 0.58              |
| 1:G:538:GLU:O    | 1:G:541:MET:HB2  | 2.04                     | 0.58              |
| 1:G:508:ILE:CD1  | 1:G:759:ALA:CB   | 2.49                     | 0.58              |
| 1:G:776:GLU:O    | 1:G:779:ARG:HB3  | 2.03                     | 0.58              |
| 1:J:218:LEU:N    | 1:J:221:GLN:HE21 | 2.01                     | 0.58              |
| 1:J:510:TRP:CE2  | 1:J:768:MLY:CH1  | 2.86                     | 0.58              |
| 1:A:124:VAL:HG13 | 1:A:675:ILE:CD1  | 2.33                     | 0.58              |
| 1:A:64:THR:HG22  | 1:A:65:GLU:N     | 2.19                     | 0.58              |
| 1:D:175:ILE:HA   | 1:D:670:HIS:O    | 2.03                     | 0.58              |
| 1:G:254:PHE:CE2  | 1:G:459:ILE:HD12 | 2.39                     | 0.58              |
| 1:G:64:THR:HG22  | 1:G:65:GLU:N     | 2.19                     | 0.58              |
| 1:G:831:TRP:CE2  | 2:H:67:MET:CG    | 2.86                     | 0.58              |
| 1:G:831:TRP:CE2  | 2:H:67:MET:HB3   | 2.38                     | 0.58              |
| 1:J:127:ASN:ND2  | 1:J:128:PRO:HD2  | 2.16                     | 0.58              |
| 1:J:175:ILE:HA   | 1:J:670:HIS:O    | 2.03                     | 0.58              |
| 1:J:755:HIS:HA   | 1:J:758:TYR:HE1  | 1.64                     | 0.58              |
| 3:L:102:VAL:HG11 | 3:L:107:LEU:HB2  | 1.84                     | 0.58              |
| 2:B:130:PRO:HA   | 2:B:133:ILE:HD12 | 1.84                     | 0.58              |
| 1:D:818:TYR:HB2  | 2:E:90:GLY:HA3   | 1.86                     | 0.58              |
| 1:J:279:LEU:HB3  | 1:J:280:PRO:HD2  | 1.86                     | 0.58              |
| 1:J:464:ILE:HG22 | 1:J:465:ALA:N    | 2.18                     | 0.58              |
| 1:J:481:ASN:N    | 1:J:481:ASN:ND2  | 2.51                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:541:MET:C    | 4:4:143:TYR:CZ   | 2.73                     | 0.58              |
| 1:A:642:LYS:CG   | 4:4:22:ALA:CA    | 2.81                     | 0.58              |
| 1:A:49:MLY:HH13  | 1:A:108:GLU:OE2  | 2.03                     | 0.58              |
| 1:A:141:LEU:O    | 1:A:144:ARG:HB3  | 2.03                     | 0.58              |
| 1:A:175:ILE:HA   | 1:A:670:HIS:O    | 2.04                     | 0.58              |
| 1:A:409:GLY:HA3  | 4:4:333:PRO:CD   | 2.34                     | 0.58              |
| 1:D:279:LEU:HB3  | 1:D:280:PRO:HD2  | 1.86                     | 0.58              |
| 1:D:724:TYR:CA   | 1:D:782:MLY:CH2  | 2.81                     | 0.58              |
| 1:D:735:GLY:O    | 1:D:743:ALA:HA   | 1.94                     | 0.58              |
| 1:G:529:PRO:HG3  | 4:6:353:GLN:OE1  | 2.04                     | 0.58              |
| 1:G:568:PRO:HG3  | 1:G:578:HIS:H    | 1.69                     | 0.58              |
| 1:D:254:PHE:CE2  | 1:D:459:ILE:HD12 | 2.39                     | 0.58              |
| 1:D:506:GLU:OE2  | 1:D:764:MLY:HH22 | 2.04                     | 0.58              |
| 1:G:48:VAL:HG22  | 1:G:49:MLY:N     | 2.18                     | 0.58              |
| 1:J:538:GLU:O    | 1:J:541:MET:HB2  | 2.03                     | 0.58              |
| 1:J:541:MET:SD   | 4:7:346:LEU:O    | 2.48                     | 0.57              |
| 1:A:813:ILE:O    | 1:A:817:GLN:N    | 2.30                     | 0.57              |
| 1:A:814:PHE:CA   | 2:B:127:ARG:HH22 | 2.17                     | 0.57              |
| 3:C:102:VAL:HG11 | 3:C:107:LEU:HB2  | 1.85                     | 0.57              |
| 1:D:817:GLN:OE1  | 2:E:127:ARG:NH2  | 2.37                     | 0.57              |
| 2:E:112:ILE:C    | 2:E:147:ASN:O    | 2.42                     | 0.57              |
| 1:G:49:MLY:HH13  | 1:G:108:GLU:OE2  | 2.03                     | 0.57              |
| 1:G:141:LEU:O    | 1:G:144:ARG:HB3  | 2.03                     | 0.57              |
| 1:G:84:MLY:CH1   | 1:G:719:ASP:C    | 2.50                     | 0.57              |
| 1:J:124:VAL:HG13 | 1:J:675:ILE:CD1  | 2.33                     | 0.57              |
| 1:J:95:THR:HA    | 1:J:713:SER:CA   | 2.32                     | 0.57              |
| 1:A:464:ILE:HG22 | 1:A:465:ALA:N    | 2.18                     | 0.57              |
| 1:A:629:GLU:HB3  | 1:A:645:SER:N    | 2.18                     | 0.57              |
| 1:A:676:ILE:O    | 1:A:676:ILE:HG23 | 2.03                     | 0.57              |
| 1:A:831:TRP:CZ2  | 2:B:51:PHE:CZ    | 2.88                     | 0.57              |
| 1:D:265:ILE:HG22 | 1:D:266:GLU:N    | 2.18                     | 0.57              |
| 1:D:322:VAL:HG11 | 1:D:325:ILE:HD11 | 1.86                     | 0.57              |
| 1:D:676:ILE:HG23 | 1:D:676:ILE:O    | 2.03                     | 0.57              |
| 1:D:717:TYR:HD1  | 1:D:744:SER:HG   | 1.52                     | 0.57              |
| 1:G:279:LEU:HB3  | 1:G:280:PRO:HD2  | 1.86                     | 0.57              |
| 1:G:411:GLU:N    | 4:6:333:PRO:HB2  | 2.10                     | 0.57              |
| 1:G:99:GLU:OE2   | 1:G:696:ARG:NH2  | 2.30                     | 0.57              |
| 1:A:254:PHE:CE2  | 1:A:459:ILE:HD12 | 2.39                     | 0.57              |
| 1:A:783:LEU:O    | 1:A:787:ILE:N    | 2.28                     | 0.57              |
| 1:D:541:MET:HG2  | 4:5:345:ILE:CG2  | 2.35                     | 0.57              |
| 1:D:831:TRP:CD2  | 2:E:51:PHE:CZ    | 2.92                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:F:102:VAL:HG11 | 3:F:107:LEU:HB2  | 1.84                     | 0.57              |
| 1:G:295:MLY:HG3  | 1:G:332:MET:HE1  | 1.87                     | 0.57              |
| 1:J:322:VAL:HG11 | 1:J:325:ILE:HD11 | 1.86                     | 0.57              |
| 1:J:717:TYR:HD1  | 1:J:744:SER:HG   | 1.52                     | 0.57              |
| 1:G:409:GLY:HA3  | 4:6:333:PRO:CD   | 2.35                     | 0.57              |
| 1:A:279:LEU:HB3  | 1:A:280:PRO:HD2  | 1.86                     | 0.57              |
| 1:A:418:THR:HG22 | 1:A:419:VAL:H    | 1.69                     | 0.57              |
| 1:A:831:TRP:CD2  | 2:B:51:PHE:CZ    | 2.88                     | 0.57              |
| 1:D:418:THR:HG22 | 1:D:419:VAL:H    | 1.69                     | 0.57              |
| 1:G:813:ILE:O    | 1:G:816:ILE:N    | 2.37                     | 0.57              |
| 3:I:102:VAL:HG11 | 3:I:107:LEU:HB2  | 1.85                     | 0.57              |
| 1:J:254:PHE:CE2  | 1:J:459:ILE:HD12 | 2.39                     | 0.57              |
| 1:J:64:THR:HG22  | 1:J:65:GLU:N     | 2.19                     | 0.57              |
| 1:J:676:ILE:O    | 1:J:676:ILE:HG23 | 2.03                     | 0.57              |
| 1:J:784:ALA:O    | 1:J:788:THR:CB   | 2.52                     | 0.57              |
| 1:J:409:GLY:HA3  | 4:7:333:PRO:CD   | 2.35                     | 0.57              |
| 1:A:220:ASP:O    | 1:A:224:SER:N    | 2.27                     | 0.57              |
| 1:A:635:GLY:HA3  | 4:4:334:GLU:CG   | 2.30                     | 0.57              |
| 1:A:768:MLY:C    | 1:A:771:LEU:HB3  | 2.35                     | 0.57              |
| 2:B:112:ILE:C    | 2:B:147:ASN:O    | 2.42                     | 0.57              |
| 1:D:195:TYR:O    | 1:D:199:ILE:HG23 | 2.03                     | 0.57              |
| 1:D:64:THR:HG22  | 1:D:65:GLU:N     | 2.19                     | 0.57              |
| 1:D:831:TRP:CA   | 2:E:51:PHE:HE1   | 2.17                     | 0.57              |
| 1:G:218:LEU:N    | 1:G:221:GLN:HE21 | 2.01                     | 0.57              |
| 1:G:508:ILE:HD11 | 1:G:759:ALA:HB2  | 0.75                     | 0.57              |
| 1:J:794:CYS:O    | 1:J:798:LEU:N    | 2.36                     | 0.57              |
| 1:J:91:MET:HE3   | 1:J:119:SER:HB2  | 1.85                     | 0.57              |
| 1:J:541:MET:HG2  | 4:7:345:ILE:CG2  | 2.35                     | 0.57              |
| 1:A:541:MET:HG2  | 4:4:345:ILE:CG2  | 2.35                     | 0.57              |
| 1:A:173:GLN:C    | 1:A:667:THR:HG23 | 2.25                     | 0.57              |
| 1:A:818:TYR:HB2  | 2:B:90:GLY:HA3   | 1.86                     | 0.57              |
| 3:C:102:VAL:HG23 | 3:C:139:TYR:CD1  | 2.39                     | 0.57              |
| 1:D:22:LYS:O     | 1:D:26:GLU:N     | 2.29                     | 0.57              |
| 1:D:579:PHE:CD2  | 1:D:592:ILE:HD11 | 2.39                     | 0.57              |
| 1:D:173:GLN:C    | 1:D:667:THR:HG23 | 2.25                     | 0.57              |
| 1:D:822:SER:HG   | 2:E:87:LYS:C     | 2.07                     | 0.57              |
| 3:F:102:VAL:HG23 | 3:F:139:TYR:CD1  | 2.39                     | 0.57              |
| 1:G:599:ASN:CG   | 1:G:649:VAL:HB   | 2.25                     | 0.57              |
| 1:G:813:ILE:O    | 1:G:817:GLN:N    | 2.30                     | 0.57              |
| 1:J:141:LEU:O    | 1:J:144:ARG:HB3  | 2.04                     | 0.57              |
| 1:J:82:PRO:HD2   | 1:J:85:TYR:CD2   | 2.40                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:789:ALA:HB2  | 3:L:81:GLN:HG2   | 1.86                     | 0.57              |
| 1:A:218:LEU:N    | 1:A:221:GLN:HE21 | 2.02                     | 0.57              |
| 1:D:409:GLY:HA3  | 4:5:333:PRO:CD   | 2.35                     | 0.57              |
| 1:D:834:LEU:HD21 | 2:E:54:MET:HE2   | 1.86                     | 0.57              |
| 1:G:175:ILE:HA   | 1:G:670:HIS:O    | 2.04                     | 0.57              |
| 1:J:173:GLN:C    | 1:J:667:THR:HG23 | 2.25                     | 0.57              |
| 1:J:752:ASP:O    | 1:J:780:ASP:OD2  | 2.23                     | 0.57              |
| 1:G:642:LYS:CD   | 4:6:340:TRP:CZ3  | 2.80                     | 0.57              |
| 1:A:322:VAL:HG11 | 1:A:325:ILE:HD11 | 1.86                     | 0.57              |
| 1:A:502:GLU:CG   | 1:A:761:GLY:C    | 2.69                     | 0.57              |
| 1:A:639:GLY:N    | 4:4:344:SER:C    | 2.54                     | 0.57              |
| 1:D:116:TYR:HB2  | 1:D:153:PRO:O    | 2.03                     | 0.57              |
| 1:D:813:ILE:O    | 1:D:816:ILE:N    | 2.38                     | 0.57              |
| 1:D:82:PRO:HD2   | 1:D:85:TYR:CD2   | 2.40                     | 0.57              |
| 1:D:830:PRO:C    | 2:E:51:PHE:CE1   | 2.78                     | 0.57              |
| 1:G:173:GLN:C    | 1:G:667:THR:HG23 | 2.25                     | 0.57              |
| 1:A:643:GLY:HA2  | 4:4:24:ASP:OD1   | 2.04                     | 0.57              |
| 1:J:530:MET:CA   | 4:7:354:GLN:HB3  | 2.35                     | 0.57              |
| 1:A:109:ARG:O    | 1:A:114:MET:N    | 2.37                     | 0.57              |
| 1:A:813:ILE:O    | 1:A:816:ILE:N    | 2.37                     | 0.57              |
| 1:D:481:ASN:N    | 1:D:481:ASN:ND2  | 2.51                     | 0.57              |
| 1:D:530:MET:CA   | 4:5:354:GLN:HB3  | 2.35                     | 0.57              |
| 1:J:579:PHE:CD2  | 1:J:592:ILE:HD11 | 2.40                     | 0.57              |
| 1:J:783:LEU:O    | 1:J:787:ILE:CB   | 2.52                     | 0.57              |
| 1:A:529:PRO:CG   | 4:4:353:GLN:OE1  | 2.53                     | 0.57              |
| 1:A:768:MLY:HB3  | 1:A:771:LEU:CG   | 2.35                     | 0.57              |
| 1:A:795:ARG:NH2  | 3:C:116:GLU:CG   | 2.68                     | 0.57              |
| 1:D:646:PHE:CD2  | 1:D:652:LEU:CD1  | 2.85                     | 0.57              |
| 1:D:724:TYR:OH   | 1:D:778:MET:SD   | 2.63                     | 0.57              |
| 1:G:612:GLN:HE22 | 1:G:627:GLY:HA2  | 1.66                     | 0.57              |
| 1:G:820:VAL:CG1  | 2:H:136:MET:HE1  | 2.34                     | 0.57              |
| 1:G:82:PRO:HD2   | 1:G:85:TYR:CD2   | 2.40                     | 0.57              |
| 1:J:747:LEU:HD23 | 1:J:747:LEU:O    | 2.05                     | 0.57              |
| 1:G:541:MET:HG2  | 4:6:345:ILE:CG2  | 2.35                     | 0.56              |
| 1:A:599:ASN:CG   | 1:A:649:VAL:HB   | 2.25                     | 0.56              |
| 1:A:82:PRO:HD2   | 1:A:85:TYR:CD2   | 2.40                     | 0.56              |
| 1:A:830:PRO:HG2  | 2:B:67:MET:HE1   | 1.87                     | 0.56              |
| 1:A:795:ARG:CG   | 3:C:118:MET:CE   | 2.82                     | 0.56              |
| 1:D:599:ASN:CG   | 1:D:649:VAL:HB   | 2.25                     | 0.56              |
| 1:D:831:TRP:HE1  | 2:E:47:LEU:HD22  | 1.58                     | 0.56              |
| 1:G:747:LEU:HD23 | 1:G:747:LEU:O    | 2.05                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:797:PHE:HE2  | 3:I:126:LEU:HD23 | 1.69                     | 0.56              |
| 1:G:831:TRP:CZ2  | 2:H:67:MET:HB3   | 2.40                     | 0.56              |
| 1:J:677:PRO:HB2  | 1:J:678:ASN:ND2  | 2.20                     | 0.56              |
| 1:J:768:MLY:NZ   | 1:J:772:LEU:CD2  | 2.40                     | 0.56              |
| 1:D:411:GLU:H    | 4:5:333:PRO:HG2  | 1.70                     | 0.56              |
| 1:A:481:ASN:ND2  | 1:A:481:ASN:N    | 2.51                     | 0.56              |
| 1:A:753:VAL:HG12 | 1:A:775:LEU:HG   | 1.86                     | 0.56              |
| 1:A:834:LEU:HD21 | 2:B:54:MET:CG    | 2.35                     | 0.56              |
| 1:D:568:PRO:HG3  | 1:D:578:HIS:H    | 1.69                     | 0.56              |
| 1:D:733:PRO:CB   | 1:D:737:PHE:HE1  | 2.19                     | 0.56              |
| 1:D:724:TYR:CZ   | 1:D:778:MET:HB3  | 2.37                     | 0.56              |
| 1:J:821:ARG:NH2  | 2:K:127:ARG:HD3  | 2.18                     | 0.56              |
| 3:L:102:VAL:HG23 | 3:L:139:TYR:CD1  | 2.39                     | 0.56              |
| 3:L:46:ILE:O     | 3:L:50:LEU:CG    | 2.47                     | 0.56              |
| 1:G:642:LYS:CA   | 4:6:22:ALA:C     | 2.70                     | 0.56              |
| 4:7:223:PHE:HD2  | 4:7:312:ARG:NH2  | 1.99                     | 0.56              |
| 1:A:411:GLU:H    | 4:4:333:PRO:HG2  | 1.71                     | 0.56              |
| 1:A:568:PRO:HG3  | 1:A:578:HIS:H    | 1.69                     | 0.56              |
| 1:D:22:LYS:HA    | 1:D:25:ILE:HB    | 1.87                     | 0.56              |
| 1:D:733:PRO:CA   | 1:D:737:PHE:HE1  | 2.18                     | 0.56              |
| 1:G:338:ILE:HG21 | 1:G:348:MLY:HB3  | 1.87                     | 0.56              |
| 2:H:112:ILE:C    | 2:H:147:ASN:O    | 2.42                     | 0.56              |
| 3:I:102:VAL:HG23 | 3:I:139:TYR:CD1  | 2.39                     | 0.56              |
| 1:G:643:GLY:N    | 4:6:23:GLY:C     | 2.55                     | 0.56              |
| 1:A:135:TYR:N    | 1:A:135:TYR:HD1  | 2.04                     | 0.56              |
| 1:A:302:MET:HG2  | 1:A:303:LEU:HD13 | 1.87                     | 0.56              |
| 1:A:640:LYS:C    | 4:4:23:GLY:CA    | 2.64                     | 0.56              |
| 1:A:733:PRO:CA   | 1:A:737:PHE:HE1  | 2.19                     | 0.56              |
| 1:A:831:TRP:CH2  | 2:B:50:THR:CG2   | 2.88                     | 0.56              |
| 1:D:831:TRP:NE1  | 2:E:67:MET:SD    | 2.77                     | 0.56              |
| 1:G:302:MET:HG2  | 1:G:303:LEU:HD13 | 1.88                     | 0.56              |
| 1:G:322:VAL:HG11 | 1:G:325:ILE:HD11 | 1.86                     | 0.56              |
| 1:G:676:ILE:O    | 1:G:676:ILE:HG23 | 2.03                     | 0.56              |
| 1:G:677:PRO:HB2  | 1:G:678:ASN:ND2  | 2.20                     | 0.56              |
| 1:G:757:GLN:NE2  | 1:G:772:LEU:HG   | 2.20                     | 0.56              |
| 1:J:568:PRO:HG3  | 1:J:578:HIS:H    | 1.69                     | 0.56              |
| 1:J:735:GLY:O    | 1:J:743:ALA:HA   | 1.94                     | 0.56              |
| 1:J:813:ILE:O    | 1:J:816:ILE:N    | 2.37                     | 0.56              |
| 2:E:163:ALA:C    | 2:K:22:THR:CB    | 2.74                     | 0.56              |
| 1:A:630:ALA:CA   | 4:4:25:ASP:OD2   | 2.53                     | 0.56              |
| 1:J:638:GLY:CA   | 4:7:345:ILE:H    | 2.18                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:210:GLN:O    | 1:A:211:SER:OG   | 2.15                     | 0.56              |
| 1:A:768:MLY:HG2  | 1:A:771:LEU:HD13 | 1.87                     | 0.56              |
| 1:A:800:ARG:HD2  | 3:C:149:VAL:CA   | 2.35                     | 0.56              |
| 1:A:839:MLY:HD2  | 2:B:159:HIS:CD2  | 2.38                     | 0.56              |
| 1:A:830:PRO:HG2  | 2:B:67:MET:HE2   | 1.87                     | 0.56              |
| 1:D:135:TYR:N    | 1:D:135:TYR:HD1  | 2.04                     | 0.56              |
| 1:D:677:PRO:HB2  | 1:D:678:ASN:ND2  | 2.20                     | 0.56              |
| 1:D:815:CYS:HA   | 2:E:90:GLY:HA2   | 1.87                     | 0.56              |
| 1:D:786:ILE:HG12 | 3:F:86:ASP:HB3   | 1.87                     | 0.56              |
| 1:J:418:THR:HG22 | 1:J:419:VAL:H    | 1.69                     | 0.56              |
| 1:A:649:VAL:HG23 | 1:A:649:VAL:HA   | 1.83                     | 0.56              |
| 1:A:677:PRO:HB2  | 1:A:678:ASN:ND2  | 2.20                     | 0.56              |
| 1:A:753:VAL:CG1  | 1:A:775:LEU:HG   | 2.36                     | 0.56              |
| 1:A:834:LEU:HD21 | 2:B:54:MET:CE    | 2.36                     | 0.56              |
| 3:C:48:LYS:C     | 3:C:52:ASN:HD22  | 1.97                     | 0.56              |
| 1:D:116:TYR:CE2  | 1:D:154:HIS:CD2  | 2.94                     | 0.56              |
| 1:D:406:VAL:HG12 | 1:D:407:GLY:H    | 1.71                     | 0.56              |
| 1:G:733:PRO:CA   | 1:G:737:PHE:HE1  | 2.19                     | 0.56              |
| 1:G:817:GLN:HG2  | 2:H:127:ARG:CD   | 2.34                     | 0.56              |
| 1:J:116:TYR:CE2  | 1:J:154:HIS:CD2  | 2.94                     | 0.56              |
| 1:J:338:ILE:HG21 | 1:J:348:MLY:HB3  | 1.87                     | 0.56              |
| 1:A:338:ILE:HG21 | 1:A:348:MLY:HB3  | 1.87                     | 0.56              |
| 1:A:546:THR:HG21 | 1:A:548:THR:HB   | 1.88                     | 0.56              |
| 1:A:649:VAL:HG22 | 1:A:649:VAL:HA   | 1.80                     | 0.56              |
| 1:A:646:PHE:CD2  | 1:A:652:LEU:CD1  | 2.85                     | 0.56              |
| 1:A:733:PRO:CB   | 1:A:737:PHE:HE1  | 2.19                     | 0.56              |
| 2:B:150:TYR:C    | 2:B:151:LYS:CG   | 2.49                     | 0.56              |
| 1:G:135:TYR:N    | 1:G:135:TYR:HD1  | 2.04                     | 0.56              |
| 1:J:599:ASN:CG   | 1:J:649:VAL:HB   | 2.25                     | 0.56              |
| 1:G:643:GLY:HA2  | 4:6:24:ASP:OD1   | 2.04                     | 0.56              |
| 1:G:638:GLY:CA   | 4:6:345:ILE:H    | 2.18                     | 0.56              |
| 1:A:116:TYR:CE2  | 1:A:154:HIS:CD2  | 2.94                     | 0.56              |
| 1:A:747:LEU:HD23 | 1:A:747:LEU:O    | 2.05                     | 0.56              |
| 1:A:768:MLY:CG   | 1:A:771:LEU:HD13 | 2.35                     | 0.56              |
| 1:A:797:PHE:HD2  | 3:C:126:LEU:CD2  | 2.18                     | 0.56              |
| 1:D:215:GLN:CA   | 1:D:340:ILE:CG2  | 2.63                     | 0.56              |
| 1:D:834:LEU:HD22 | 2:E:50:THR:HG22  | 1.87                     | 0.56              |
| 1:G:84:MLY:HH11  | 1:G:720:PHE:CA   | 2.35                     | 0.56              |
| 1:J:135:TYR:HD1  | 1:J:135:TYR:N    | 2.04                     | 0.56              |
| 1:J:630:ALA:CA   | 4:7:25:ASP:OD2   | 2.53                     | 0.56              |
| 1:J:503:TYR:OH   | 1:J:711:PHE:CD2  | 2.40                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:95:THR:HA    | 1:J:713:SER:CB   | 2.36                     | 0.56              |
| 1:J:754:ASP:OD1  | 1:J:779:ARG:HD2  | 2.06                     | 0.56              |
| 1:A:530:MET:CA   | 4:4:354:GLN:HB3  | 2.34                     | 0.56              |
| 1:G:538:GLU:CG   | 4:6:351:THR:C    | 2.73                     | 0.56              |
| 1:A:206:LYS:HB3  | 1:A:217:THR:OG1  | 2.06                     | 0.56              |
| 1:A:502:GLU:HA   | 1:A:762:HIS:H    | 1.71                     | 0.56              |
| 1:A:795:ARG:HG2  | 3:C:118:MET:CE   | 2.35                     | 0.56              |
| 1:D:435:GLU:O    | 1:D:438:PHE:HB3  | 2.06                     | 0.56              |
| 1:D:747:LEU:O    | 1:D:747:LEU:HD23 | 2.05                     | 0.56              |
| 1:D:834:LEU:CD2  | 2:E:54:MET:CG    | 2.61                     | 0.56              |
| 1:G:109:ARG:O    | 1:G:114:MET:N    | 2.37                     | 0.56              |
| 1:D:529:PRO:CB   | 4:5:354:GLN:HA   | 2.36                     | 0.56              |
| 1:G:410:ASN:CG   | 4:6:334:GLU:C    | 2.64                     | 0.56              |
| 1:J:530:MET:CB   | 4:7:354:GLN:HG3  | 2.36                     | 0.56              |
| 1:A:217:THR:HG22 | 1:A:218:LEU:O    | 2.05                     | 0.56              |
| 1:D:529:PRO:CG   | 4:5:353:GLN:OE1  | 2.53                     | 0.56              |
| 1:D:99:GLU:OE2   | 1:D:696:ARG:NH2  | 2.31                     | 0.56              |
| 1:G:529:PRO:CG   | 4:6:353:GLN:OE1  | 2.54                     | 0.56              |
| 1:G:649:VAL:CG1  | 1:G:649:VAL:HA   | 2.35                     | 0.56              |
| 1:G:733:PRO:CB   | 1:G:737:PHE:HE1  | 2.19                     | 0.56              |
| 1:J:503:TYR:HH   | 1:J:711:PHE:HD2  | 0.72                     | 0.56              |
| 1:D:630:ALA:CA   | 4:5:25:ASP:OD2   | 2.53                     | 0.56              |
| 1:A:22:LYS:O     | 1:A:26:GLU:HG3   | 2.06                     | 0.56              |
| 1:A:546:THR:HB   | 1:A:549:SER:H    | 1.71                     | 0.56              |
| 1:D:290:GLN:HG2  | 1:D:331:LEU:HA   | 1.87                     | 0.56              |
| 1:D:640:LYS:C    | 1:D:645:SER:OG   | 2.44                     | 0.56              |
| 1:G:217:THR:HG22 | 1:G:218:LEU:O    | 2.06                     | 0.56              |
| 1:G:22:LYS:O     | 1:G:26:GLU:HG3   | 2.06                     | 0.56              |
| 1:G:418:THR:HG22 | 1:G:419:VAL:H    | 1.69                     | 0.56              |
| 1:G:435:GLU:O    | 1:G:438:PHE:HB3  | 2.06                     | 0.56              |
| 1:G:537:GLU:HB3  | 1:G:648:THR:CB   | 2.36                     | 0.56              |
| 1:G:794:CYS:O    | 1:G:798:LEU:N    | 2.37                     | 0.56              |
| 3:I:46:ILE:O     | 3:I:50:LEU:CG    | 2.47                     | 0.56              |
| 1:J:530:MET:HE3  | 4:7:354:GLN:CG   | 2.30                     | 0.56              |
| 1:J:629:GLU:O    | 1:J:643:GLY:HA3  | 2.06                     | 0.56              |
| 1:J:733:PRO:CA   | 1:J:737:PHE:HE1  | 2.19                     | 0.56              |
| 1:G:411:GLU:H    | 4:6:333:PRO:HG2  | 1.70                     | 0.55              |
| 4:7:365:ALA:HB3  | 4:7:369:ILE:HB   | 1.88                     | 0.55              |
| 1:A:290:GLN:HG2  | 1:A:331:LEU:HA   | 1.87                     | 0.55              |
| 1:A:530:MET:HE3  | 4:4:354:GLN:CB   | 2.37                     | 0.55              |
| 1:A:798:LEU:CD1  | 3:C:126:LEU:CG   | 2.79                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:97:LEU:HD22  | 1:A:712:PRO:CB   | 2.32                     | 0.55              |
| 1:A:797:PHE:HD2  | 3:C:126:LEU:HD21 | 1.71                     | 0.55              |
| 1:D:32:PHE:CG    | 1:D:83:PRO:HD3   | 2.41                     | 0.55              |
| 1:D:789:ALA:C    | 3:F:87:PHE:CZ    | 2.79                     | 0.55              |
| 1:G:206:LYS:HB3  | 1:G:217:THR:OG1  | 2.06                     | 0.55              |
| 1:G:530:MET:CA   | 4:6:354:GLN:HB3  | 2.35                     | 0.55              |
| 1:G:649:VAL:HG22 | 1:G:649:VAL:HA   | 1.80                     | 0.55              |
| 1:G:820:VAL:CG1  | 2:H:136:MET:CE   | 2.84                     | 0.55              |
| 1:J:90:ASP:OD2   | 1:J:764:MLY:HH22 | 2.05                     | 0.55              |
| 1:A:538:GLU:CG   | 4:4:351:THR:C    | 2.74                     | 0.55              |
| 1:D:638:GLY:CA   | 4:5:345:ILE:H    | 2.19                     | 0.55              |
| 1:A:529:PRO:CB   | 4:4:354:GLN:HA   | 2.36                     | 0.55              |
| 1:A:640:LYS:C    | 1:A:645:SER:OG   | 2.44                     | 0.55              |
| 1:D:725:ARG:H    | 1:D:782:MLY:HH21 | 1.65                     | 0.55              |
| 1:G:116:TYR:CE2  | 1:G:154:HIS:CD2  | 2.94                     | 0.55              |
| 1:G:84:MLY:HH12  | 1:G:716:LEU:O    | 2.05                     | 0.55              |
| 1:J:217:THR:HG22 | 1:J:218:LEU:O    | 2.05                     | 0.55              |
| 1:J:750:GLY:HA2  | 3:L:114:LEU:HD23 | 1.87                     | 0.55              |
| 4:V:365:ALA:HB3  | 4:V:369:ILE:HB   | 1.88                     | 0.55              |
| 1:D:530:MET:HE3  | 4:5:355:MET:SD   | 2.46                     | 0.55              |
| 1:J:634:GLY:N    | 4:7:25:ASP:O     | 2.31                     | 0.55              |
| 1:A:32:PHE:CG    | 1:A:83:PRO:HD3   | 2.42                     | 0.55              |
| 1:D:537:GLU:HB3  | 1:D:648:THR:CB   | 2.36                     | 0.55              |
| 1:D:546:THR:HG21 | 1:D:548:THR:HB   | 1.88                     | 0.55              |
| 1:J:206:LYS:HB3  | 1:J:217:THR:OG1  | 2.06                     | 0.55              |
| 1:J:579:PHE:HE1  | 1:J:581:LEU:HD13 | 1.72                     | 0.55              |
| 1:J:733:PRO:CB   | 1:J:737:PHE:HE1  | 2.19                     | 0.55              |
| 2:E:162:ASP:O    | 2:K:21:GLU:HB2   | 2.07                     | 0.55              |
| 3:L:123:VAL:O    | 3:L:127:MET:HG2  | 2.06                     | 0.55              |
| 4:5:365:ALA:HB3  | 4:5:369:ILE:HB   | 1.88                     | 0.55              |
| 1:J:643:GLY:N    | 4:7:23:GLY:C     | 2.55                     | 0.55              |
| 1:A:290:GLN:NE2  | 1:A:334:THR:OG1  | 2.40                     | 0.55              |
| 1:A:345:ALA:O    | 1:A:349:THR:N    | 2.40                     | 0.55              |
| 1:A:537:GLU:HB3  | 1:A:648:THR:CB   | 2.36                     | 0.55              |
| 1:A:629:GLU:O    | 1:A:643:GLY:HA3  | 2.06                     | 0.55              |
| 1:A:765:VAL:HG12 | 1:A:766:PHE:N    | 2.22                     | 0.55              |
| 1:A:793:ARG:NH2  | 3:C:147:MET:HE2  | 2.22                     | 0.55              |
| 1:D:217:THR:HG22 | 1:D:218:LEU:O    | 2.06                     | 0.55              |
| 1:D:629:GLU:O    | 1:D:643:GLY:HA3  | 2.06                     | 0.55              |
| 1:D:789:ALA:HB2  | 3:F:81:GLN:O     | 2.06                     | 0.55              |
| 1:G:127:ASN:ND2  | 1:G:128:PRO:HD2  | 2.17                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:732:ILE:CG2  | 1:G:747:LEU:HD11 | 1.26                     | 0.55              |
| 1:J:646:PHE:CE2  | 1:J:652:LEU:CG   | 2.90                     | 0.55              |
| 4:1:365:ALA:HB3  | 4:1:369:ILE:HB   | 1.88                     | 0.55              |
| 1:A:7:MET:HE3    | 1:A:14:ALA:CB    | 2.36                     | 0.55              |
| 1:A:406:VAL:HG12 | 1:A:407:GLY:H    | 1.71                     | 0.55              |
| 1:A:604:ASN:OD1  | 1:A:607:VAL:HG23 | 2.06                     | 0.55              |
| 1:D:604:ASN:OD1  | 1:D:607:VAL:HG23 | 2.06                     | 0.55              |
| 1:D:646:PHE:CE2  | 1:D:652:LEU:CG   | 2.90                     | 0.55              |
| 1:G:22:LYS:HA    | 1:G:25:ILE:HB    | 1.87                     | 0.55              |
| 1:G:629:GLU:O    | 1:G:643:GLY:HA3  | 2.06                     | 0.55              |
| 1:G:646:PHE:CE2  | 1:G:652:LEU:CG   | 2.90                     | 0.55              |
| 1:G:93:MET:HB2   | 1:G:764:MLY:NZ   | 2.18                     | 0.55              |
| 1:J:302:MET:HG2  | 1:J:303:LEU:HD13 | 1.87                     | 0.55              |
| 1:J:406:VAL:HG12 | 1:J:407:GLY:H    | 1.71                     | 0.55              |
| 1:J:640:LYS:C    | 1:J:645:SER:OG   | 2.44                     | 0.55              |
| 1:J:768:MLY:CH2  | 1:J:772:LEU:CD1  | 2.83                     | 0.55              |
| 1:J:7:MET:HE3    | 1:J:14:ALA:CB    | 2.36                     | 0.55              |
| 3:L:35:ARG:HA    | 3:L:39:GLN:O     | 2.07                     | 0.55              |
| 1:A:612:GLN:HE22 | 1:A:627:GLY:HA2  | 1.66                     | 0.55              |
| 2:E:156:VAL:HA   | 2:E:159:HIS:O    | 2.07                     | 0.55              |
| 1:G:579:PHE:HE1  | 1:G:581:LEU:HD13 | 1.72                     | 0.55              |
| 1:G:604:ASN:OD1  | 1:G:607:VAL:HG23 | 2.06                     | 0.55              |
| 1:G:795:ARG:HE   | 3:I:118:MET:HE1  | 1.72                     | 0.55              |
| 1:J:32:PHE:CG    | 1:J:83:PRO:HD3   | 2.41                     | 0.55              |
| 1:J:410:ASN:CG   | 4:7:334:GLU:C    | 2.65                     | 0.55              |
| 1:J:435:GLU:O    | 1:J:438:PHE:HB3  | 2.06                     | 0.55              |
| 4:X:365:ALA:HB3  | 4:X:369:ILE:HB   | 1.88                     | 0.55              |
| 4:3:365:ALA:HB3  | 4:3:369:ILE:HB   | 1.88                     | 0.55              |
| 1:A:530:MET:CB   | 4:4:354:GLN:HG3  | 2.36                     | 0.55              |
| 1:D:530:MET:CB   | 4:5:354:GLN:HG3  | 2.36                     | 0.55              |
| 1:J:529:PRO:CB   | 4:7:354:GLN:HA   | 2.36                     | 0.55              |
| 1:A:642:LYS:CA   | 4:4:22:ALA:C     | 2.71                     | 0.55              |
| 1:A:725:ARG:HG3  | 1:A:733:PRO:CA   | 2.36                     | 0.55              |
| 1:A:757:GLN:OE1  | 1:A:771:LEU:HD12 | 2.06                     | 0.55              |
| 1:D:338:ILE:HG21 | 1:D:348:MLY:HB3  | 1.87                     | 0.55              |
| 1:G:290:GLN:NE2  | 1:G:334:THR:OG1  | 2.40                     | 0.55              |
| 1:G:546:THR:HB   | 1:G:549:SER:H    | 1.71                     | 0.55              |
| 1:G:7:MET:HE3    | 1:G:14:ALA:CB    | 2.37                     | 0.55              |
| 3:I:35:ARG:HA    | 3:I:39:GLN:O     | 2.07                     | 0.55              |
| 1:J:22:LYS:HA    | 1:J:25:ILE:HB    | 1.87                     | 0.55              |
| 1:J:345:ALA:O    | 1:J:349:THR:N    | 2.40                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:725:ARG:HG3  | 1:J:733:PRO:CA   | 2.36                     | 0.55              |
| 1:J:82:PRO:HD2   | 1:J:85:TYR:HD2   | 1.72                     | 0.55              |
| 1:D:302:MET:HG2  | 1:D:303:LEU:HD13 | 1.87                     | 0.55              |
| 1:D:723:ARG:HH21 | 1:D:783:LEU:HD11 | 1.71                     | 0.55              |
| 1:G:640:LYS:C    | 1:G:645:SER:OG   | 2.44                     | 0.55              |
| 2:H:156:VAL:HA   | 2:H:159:HIS:O    | 2.07                     | 0.55              |
| 1:J:411:GLU:H    | 4:7:333:PRO:HG2  | 1.71                     | 0.55              |
| 1:J:635:GLY:HA3  | 4:7:334:GLU:CG   | 2.30                     | 0.55              |
| 2:K:156:VAL:HA   | 2:K:159:HIS:O    | 2.07                     | 0.55              |
| 1:J:529:PRO:CG   | 4:7:353:GLN:OE1  | 2.54                     | 0.55              |
| 1:A:292:MET:HE1  | 1:A:309:PRO:CD   | 2.37                     | 0.55              |
| 1:A:646:PHE:CE2  | 1:A:652:LEU:CG   | 2.90                     | 0.55              |
| 1:A:817:GLN:NE2  | 2:B:127:ARG:CG   | 2.70                     | 0.55              |
| 3:C:35:ARG:HA    | 3:C:39:GLN:O     | 2.07                     | 0.55              |
| 1:D:7:MET:HE3    | 1:D:14:ALA:CB    | 2.36                     | 0.55              |
| 1:D:135:TYR:HD2  | 1:D:191:ARG:HG2  | 1.72                     | 0.55              |
| 1:D:206:LYS:HB3  | 1:D:217:THR:OG1  | 2.07                     | 0.55              |
| 2:E:121:LEU:CA   | 2:E:128:PHE:CG   | 2.89                     | 0.55              |
| 3:F:46:ILE:O     | 3:F:50:LEU:CG    | 2.47                     | 0.55              |
| 1:G:290:GLN:HG2  | 1:G:331:LEU:HA   | 1.87                     | 0.55              |
| 1:G:751:GLY:N    | 3:I:114:LEU:HD11 | 2.21                     | 0.55              |
| 2:H:121:LEU:CA   | 2:H:128:PHE:CG   | 2.89                     | 0.55              |
| 2:H:140:PHE:O    | 2:H:141:PRO:C    | 2.33                     | 0.55              |
| 1:G:730:SER:HG   | 3:I:109:HIS:CG   | 2.20                     | 0.55              |
| 1:J:290:GLN:HG2  | 1:J:331:LEU:HA   | 1.88                     | 0.55              |
| 1:J:723:ARG:HH11 | 1:J:723:ARG:CG   | 2.20                     | 0.55              |
| 4:Y:365:ALA:HB3  | 4:Y:369:ILE:HB   | 1.88                     | 0.55              |
| 1:A:643:GLY:N    | 4:4:23:GLY:C     | 2.55                     | 0.55              |
| 1:G:553:MLY:HG3  | 4:8:44:MET:O     | 2.07                     | 0.55              |
| 1:A:127:ASN:ND2  | 1:A:128:PRO:HD2  | 2.16                     | 0.55              |
| 1:A:723:ARG:HH11 | 1:A:723:ARG:CG   | 2.20                     | 0.55              |
| 1:G:638:GLY:HA2  | 4:6:345:ILE:H    | 1.71                     | 0.55              |
| 1:G:723:ARG:CG   | 1:G:723:ARG:HH11 | 2.20                     | 0.55              |
| 1:J:84:MLY:CH1   | 1:J:719:ASP:C    | 2.63                     | 0.55              |
| 4:W:365:ALA:HB3  | 4:W:369:ILE:HB   | 1.88                     | 0.55              |
| 1:A:630:ALA:HA   | 4:4:25:ASP:OD2   | 2.07                     | 0.54              |
| 1:D:638:GLY:HA2  | 4:5:345:ILE:H    | 1.72                     | 0.54              |
| 1:A:10:PHE:O     | 1:A:12:GLU:N     | 2.41                     | 0.54              |
| 1:A:22:LYS:HA    | 1:A:25:ILE:HB    | 1.88                     | 0.54              |
| 1:A:435:GLU:O    | 1:A:438:PHE:HB3  | 2.06                     | 0.54              |
| 1:A:638:GLY:CA   | 4:4:345:ILE:H    | 2.19                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:638:GLY:HA2  | 4:4:345:ILE:H    | 1.72                     | 0.54              |
| 1:A:795:ARG:CG   | 3:C:118:MET:HE3  | 2.37                     | 0.54              |
| 1:D:305:ILE:HG22 | 1:D:312:TYR:CE2  | 2.42                     | 0.54              |
| 1:D:635:GLY:HA3  | 4:5:334:GLU:CG   | 2.30                     | 0.54              |
| 1:D:819:ASN:H    | 2:E:90:GLY:HA3   | 1.72                     | 0.54              |
| 1:D:788:THR:HG22 | 3:F:81:GLN:NE2   | 2.22                     | 0.54              |
| 1:G:649:VAL:HA   | 1:G:649:VAL:HG23 | 1.83                     | 0.54              |
| 1:G:508:ILE:HG21 | 1:G:711:PHE:CZ   | 2.42                     | 0.54              |
| 1:J:290:GLN:NE2  | 1:J:334:THR:OG1  | 2.40                     | 0.54              |
| 1:J:292:MET:HE1  | 1:J:309:PRO:CD   | 2.37                     | 0.54              |
| 1:J:604:ASN:OD1  | 1:J:607:VAL:HG23 | 2.06                     | 0.54              |
| 1:J:649:VAL:CG1  | 1:J:649:VAL:HA   | 2.35                     | 0.54              |
| 4:Z:365:ALA:HB3  | 4:Z:369:ILE:HB   | 1.88                     | 0.54              |
| 4:8:365:ALA:HB3  | 4:8:369:ILE:HB   | 1.88                     | 0.54              |
| 1:A:305:ILE:HG22 | 1:A:312:TYR:CE2  | 2.43                     | 0.54              |
| 1:A:82:PRO:HD2   | 1:A:85:TYR:HD2   | 1.72                     | 0.54              |
| 3:C:123:VAL:O    | 3:C:127:MET:HG2  | 2.06                     | 0.54              |
| 1:A:797:PHE:CG   | 3:C:149:VAL:HG11 | 2.35                     | 0.54              |
| 1:D:470:PHE:O    | 1:D:473:ASN:ND2  | 2.40                     | 0.54              |
| 1:D:553:MLY:HG3  | 4:7:44:MET:O     | 2.07                     | 0.54              |
| 1:D:649:VAL:HA   | 1:D:649:VAL:CG1  | 2.35                     | 0.54              |
| 1:D:839:MLY:HH11 | 2:E:159:HIS:CG   | 2.30                     | 0.54              |
| 3:F:123:VAL:O    | 3:F:127:MET:HG2  | 2.07                     | 0.54              |
| 1:D:793:ARG:HE   | 3:F:147:MET:HG2  | 1.71                     | 0.54              |
| 1:G:32:PHE:CG    | 1:G:83:PRO:HD3   | 2.41                     | 0.54              |
| 1:G:126:VAL:HG13 | 1:G:675:ILE:HG22 | 1.89                     | 0.54              |
| 1:G:735:GLY:O    | 1:G:743:ALA:HA   | 1.94                     | 0.54              |
| 1:G:765:VAL:HG12 | 1:G:766:PHE:N    | 2.22                     | 0.54              |
| 1:G:78:PHE:HB3   | 1:G:98:HIS:NE2   | 2.23                     | 0.54              |
| 1:G:751:GLY:CA   | 3:I:114:LEU:CD1  | 2.84                     | 0.54              |
| 1:J:470:PHE:O    | 1:J:473:ASN:ND2  | 2.40                     | 0.54              |
| 1:J:546:THR:HG21 | 1:J:548:THR:HB   | 1.88                     | 0.54              |
| 1:J:797:PHE:CD2  | 3:L:126:LEU:CD2  | 2.91                     | 0.54              |
| 1:J:556:ASP:CA   | 4:V:49:GLN:O     | 2.51                     | 0.54              |
| 4:0:365:ALA:HB3  | 4:0:369:ILE:HB   | 1.88                     | 0.54              |
| 4:2:365:ALA:HB3  | 4:2:369:ILE:HB   | 1.88                     | 0.54              |
| 1:G:530:MET:CB   | 4:6:354:GLN:HG3  | 2.37                     | 0.54              |
| 1:A:126:VAL:HG13 | 1:A:675:ILE:HG22 | 1.90                     | 0.54              |
| 1:A:78:PHE:HB3   | 1:A:98:HIS:NE2   | 2.22                     | 0.54              |
| 1:D:22:LYS:O     | 1:D:26:GLU:HG3   | 2.07                     | 0.54              |
| 1:D:724:TYR:OH   | 1:D:778:MET:HB2  | 2.07                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:220:ASP:O    | 1:G:224:SER:N    | 2.27                     | 0.54              |
| 1:G:546:THR:HG21 | 1:G:548:THR:HB   | 1.88                     | 0.54              |
| 1:G:82:PRO:HD2   | 1:G:85:TYR:HD2   | 1.72                     | 0.54              |
| 3:I:123:VAL:O    | 3:I:127:MET:HG2  | 2.07                     | 0.54              |
| 1:J:756:THR:HB   | 1:J:776:GLU:CD   | 2.28                     | 0.54              |
| 4:4:288:ASP:CA   | 4:6:204:ALA:HB2  | 2.31                     | 0.54              |
| 1:A:579:PHE:HE1  | 1:A:581:LEU:HD13 | 1.71                     | 0.54              |
| 1:D:10:PHE:O     | 1:D:12:GLU:N     | 2.41                     | 0.54              |
| 1:D:290:GLN:NE2  | 1:D:334:THR:OG1  | 2.40                     | 0.54              |
| 1:D:126:VAL:HG13 | 1:D:675:ILE:HG22 | 1.90                     | 0.54              |
| 1:D:82:PRO:HD2   | 1:D:85:TYR:HD2   | 1.72                     | 0.54              |
| 1:G:305:ILE:HG22 | 1:G:312:TYR:CZ   | 2.42                     | 0.54              |
| 1:G:345:ALA:O    | 1:G:349:THR:N    | 2.40                     | 0.54              |
| 1:G:38:VAL:CB    | 1:G:52:ILE:HD11  | 2.38                     | 0.54              |
| 1:G:783:LEU:HA   | 1:G:786:ILE:HB   | 1.87                     | 0.54              |
| 1:J:305:ILE:HG22 | 1:J:312:TYR:CE2  | 2.43                     | 0.54              |
| 2:K:146:GLY:O    | 2:K:147:ASN:ND2  | 2.41                     | 0.54              |
| 4:4:365:ALA:HB3  | 4:4:369:ILE:HB   | 1.88                     | 0.54              |
| 1:G:529:PRO:CB   | 4:6:354:GLN:HA   | 2.37                     | 0.54              |
| 4:6:365:ALA:HB3  | 4:6:369:ILE:HB   | 1.88                     | 0.54              |
| 2:B:156:VAL:HA   | 2:B:159:HIS:O    | 2.07                     | 0.54              |
| 1:D:571:ALA:O    | 1:D:572:LYS:CB   | 2.56                     | 0.54              |
| 1:D:739:ASP:CB   | 1:D:742:LYS:CB   | 2.81                     | 0.54              |
| 1:G:305:ILE:HG22 | 1:G:312:TYR:CE2  | 2.42                     | 0.54              |
| 1:G:406:VAL:HG12 | 1:G:407:GLY:H    | 1.71                     | 0.54              |
| 1:J:305:ILE:HG22 | 1:J:312:TYR:CZ   | 2.42                     | 0.54              |
| 1:J:537:GLU:HB3  | 1:J:648:THR:CB   | 2.36                     | 0.54              |
| 1:J:126:VAL:HG13 | 1:J:675:ILE:HG22 | 1.90                     | 0.54              |
| 1:J:757:GLN:OE1  | 1:J:773:GLY:N    | 2.40                     | 0.54              |
| 1:J:538:GLU:CG   | 4:7:351:THR:C    | 2.73                     | 0.54              |
| 1:A:571:ALA:O    | 1:A:572:LYS:CB   | 2.56                     | 0.54              |
| 1:A:629:GLU:CB   | 1:A:643:GLY:C    | 2.75                     | 0.54              |
| 1:A:800:ARG:HH11 | 3:C:149:VAL:CB   | 2.20                     | 0.54              |
| 1:A:95:THR:OG1   | 1:A:769:ALA:CA   | 2.53                     | 0.54              |
| 1:D:292:MET:HE1  | 1:D:309:PRO:CD   | 2.37                     | 0.54              |
| 1:D:345:ALA:O    | 1:D:349:THR:N    | 2.40                     | 0.54              |
| 1:D:630:ALA:HA   | 4:5:25:ASP:OD2   | 2.07                     | 0.54              |
| 1:D:649:VAL:HA   | 1:D:649:VAL:HG23 | 1.82                     | 0.54              |
| 1:D:78:PHE:HB3   | 1:D:98:HIS:NE2   | 2.22                     | 0.54              |
| 1:G:836:PHE:CD2  | 2:H:160:GLY:N    | 2.75                     | 0.54              |
| 2:H:117:LEU:CG   | 2:H:147:ASN:OD1  | 2.52                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:10:PHE:O     | 1:J:12:GLU:N     | 2.40                     | 0.54              |
| 1:J:546:THR:HB   | 1:J:549:SER:H    | 1.71                     | 0.54              |
| 1:J:78:PHE:HB3   | 1:J:98:HIS:NE2   | 2.22                     | 0.54              |
| 1:J:831:TRP:CZ3  | 2:K:34:ILE:HG21  | 2.42                     | 0.54              |
| 1:A:642:LYS:HG2  | 4:4:22:ALA:C     | 2.28                     | 0.54              |
| 1:A:721:LYS:C    | 1:A:736:GLN:OE1  | 2.46                     | 0.54              |
| 1:D:38:VAL:CB    | 1:D:52:ILE:HD11  | 2.38                     | 0.54              |
| 1:D:640:LYS:C    | 4:5:23:GLY:CA    | 2.64                     | 0.54              |
| 1:D:792:ALA:O    | 3:F:40:ASN:HB3   | 2.06                     | 0.54              |
| 1:G:530:MET:HE3  | 4:6:354:GLN:CB   | 2.38                     | 0.54              |
| 1:G:725:ARG:HG3  | 1:G:733:PRO:CA   | 2.36                     | 0.54              |
| 1:G:791:GLN:O    | 1:G:794:CYS:HB2  | 2.08                     | 0.54              |
| 1:J:135:TYR:HD2  | 1:J:191:ARG:HG2  | 1.72                     | 0.54              |
| 1:J:22:LYS:O     | 1:J:26:GLU:HG3   | 2.07                     | 0.54              |
| 1:J:503:TYR:CE1  | 1:J:711:PHE:CE2  | 2.94                     | 0.54              |
| 1:J:791:GLN:O    | 1:J:794:CYS:HB2  | 2.08                     | 0.54              |
| 1:A:410:ASN:CG   | 4:4:334:GLU:C    | 2.65                     | 0.54              |
| 1:A:135:TYR:HD2  | 1:A:191:ARG:HG2  | 1.72                     | 0.54              |
| 1:A:649:VAL:CG1  | 1:A:649:VAL:HA   | 2.35                     | 0.54              |
| 1:D:218:LEU:CD2  | 1:D:222:ILE:CG1  | 2.86                     | 0.54              |
| 1:D:218:LEU:HA   | 1:D:221:GLN:HG3  | 1.71                     | 0.54              |
| 1:D:732:ILE:CG2  | 1:D:747:LEU:HD11 | 1.26                     | 0.54              |
| 1:D:721:LYS:C    | 1:D:736:GLN:OE1  | 2.46                     | 0.54              |
| 1:G:10:PHE:O     | 1:G:12:GLU:N     | 2.41                     | 0.54              |
| 1:G:292:MET:HE1  | 1:G:309:PRO:CD   | 2.37                     | 0.54              |
| 1:J:493:HIS:ND1  | 1:J:514:ASP:OD2  | 2.41                     | 0.54              |
| 1:J:638:GLY:HA2  | 4:7:345:ILE:H    | 1.72                     | 0.54              |
| 1:J:629:GLU:CB   | 1:J:643:GLY:C    | 2.76                     | 0.54              |
| 3:L:92:ARG:HA    | 3:L:139:TYR:OH   | 2.08                     | 0.54              |
| 1:A:305:ILE:HG22 | 1:A:312:TYR:CZ   | 2.43                     | 0.54              |
| 1:A:470:PHE:O    | 1:A:473:ASN:ND2  | 2.40                     | 0.54              |
| 1:D:305:ILE:HG22 | 1:D:312:TYR:CZ   | 2.43                     | 0.54              |
| 1:D:724:TYR:OH   | 1:D:778:MET:CB   | 2.56                     | 0.54              |
| 2:E:146:GLY:O    | 2:E:147:ASN:ND2  | 2.41                     | 0.54              |
| 1:G:404:PRO:CG   | 1:G:417:GLU:HG3  | 2.38                     | 0.54              |
| 1:G:470:PHE:O    | 1:G:473:ASN:ND2  | 2.40                     | 0.54              |
| 1:G:493:HIS:ND1  | 1:G:514:ASP:OD2  | 2.41                     | 0.54              |
| 1:G:629:GLU:CB   | 1:G:643:GLY:C    | 2.76                     | 0.54              |
| 1:A:38:VAL:CB    | 1:A:52:ILE:HD11  | 2.38                     | 0.54              |
| 1:A:538:GLU:HG3  | 4:4:352:PHE:CA   | 2.38                     | 0.54              |
| 2:B:146:GLY:O    | 2:B:147:ASN:ND2  | 2.41                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:546:THR:HB   | 1:D:549:SER:H    | 1.71                     | 0.54              |
| 1:D:507:GLY:CA   | 1:D:762:HIS:ND1  | 2.71                     | 0.54              |
| 1:D:765:VAL:HG12 | 1:D:766:PHE:N    | 2.22                     | 0.54              |
| 1:D:792:ALA:C    | 3:F:40:ASN:CB    | 2.69                     | 0.54              |
| 1:G:571:ALA:O    | 1:G:572:LYS:CB   | 2.56                     | 0.54              |
| 1:G:576:GLU:CG   | 1:G:577:ALA:N    | 2.43                     | 0.54              |
| 1:J:642:LYS:HG2  | 4:7:22:ALA:C     | 2.27                     | 0.53              |
| 1:J:630:ALA:HA   | 4:7:25:ASP:OD2   | 2.07                     | 0.53              |
| 1:D:98:HIS:HB3   | 1:D:100:PRO:CD   | 2.25                     | 0.53              |
| 1:D:793:ARG:HE   | 3:F:147:MET:CB   | 2.21                     | 0.53              |
| 1:G:539:GLU:OE2  | 4:8:45:VAL:C     | 2.47                     | 0.53              |
| 1:G:769:ALA:C    | 1:G:773:GLY:HA3  | 2.29                     | 0.53              |
| 3:I:92:ARG:HA    | 3:I:139:TYR:OH   | 2.08                     | 0.53              |
| 1:J:38:VAL:CB    | 1:J:52:ILE:HD11  | 2.38                     | 0.53              |
| 1:J:553:MLY:O    | 4:V:48:GLY:CA    | 2.56                     | 0.53              |
| 1:J:640:LYS:C    | 4:7:23:GLY:CA    | 2.64                     | 0.53              |
| 1:J:800:ARG:HB3  | 3:L:149:VAL:HG23 | 1.85                     | 0.53              |
| 1:D:529:PRO:HB2  | 4:5:354:GLN:HA   | 1.91                     | 0.53              |
| 1:A:218:LEU:N    | 1:A:221:GLN:HG2  | 2.24                     | 0.53              |
| 1:A:404:PRO:CG   | 1:A:417:GLU:HG3  | 2.38                     | 0.53              |
| 1:A:553:MLY:O    | 4:6:48:GLY:CA    | 2.56                     | 0.53              |
| 1:A:584:TYR:CD1  | 1:A:585:ALA:N    | 2.77                     | 0.53              |
| 1:A:836:PHE:CE2  | 2:B:160:GLY:C    | 2.82                     | 0.53              |
| 1:D:629:GLU:CB   | 1:D:643:GLY:C    | 2.76                     | 0.53              |
| 1:D:815:CYS:O    | 2:E:90:GLY:HA3   | 2.08                     | 0.53              |
| 1:G:135:TYR:HD2  | 1:G:191:ARG:HD3  | 1.73                     | 0.53              |
| 1:G:135:TYR:HD2  | 1:G:191:ARG:HG2  | 1.73                     | 0.53              |
| 1:G:538:GLU:HG3  | 4:6:352:PHE:CA   | 2.38                     | 0.53              |
| 1:G:640:LYS:C    | 4:6:23:GLY:CA    | 2.64                     | 0.53              |
| 1:G:795:ARG:HH22 | 3:I:43:ASN:HB2   | 1.73                     | 0.53              |
| 2:H:146:GLY:O    | 2:H:147:ASN:ND2  | 2.41                     | 0.53              |
| 1:J:135:TYR:HD2  | 1:J:191:ARG:HD3  | 1.73                     | 0.53              |
| 1:J:530:MET:HE3  | 4:7:355:MET:SD   | 2.48                     | 0.53              |
| 1:J:538:GLU:HG3  | 4:7:352:PHE:CA   | 2.38                     | 0.53              |
| 1:J:707:CYS:C    | 1:J:714:ARG:HH22 | 2.11                     | 0.53              |
| 4:X:185:LEU:HD23 | 4:X:306:TYR:OH   | 2.09                     | 0.53              |
| 1:D:508:ILE:HG23 | 1:D:766:PHE:CD1  | 2.44                     | 0.53              |
| 1:D:723:ARG:HH11 | 1:D:723:ARG:CG   | 2.20                     | 0.53              |
| 1:G:661:MET:O    | 1:G:665:ARG:HG3  | 2.08                     | 0.53              |
| 1:J:793:ARG:HG2  | 3:L:147:MET:HG2  | 1.89                     | 0.53              |
| 1:J:553:MLY:HG3  | 4:V:44:MET:O     | 2.07                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:135:TYR:HD2  | 1:A:191:ARG:HD3  | 1.73                     | 0.53              |
| 1:A:800:ARG:HH11 | 3:C:149:VAL:CA   | 2.21                     | 0.53              |
| 2:B:121:LEU:CA   | 2:B:128:PHE:CG   | 2.89                     | 0.53              |
| 1:D:553:MLY:O    | 4:7:48:GLY:CA    | 2.56                     | 0.53              |
| 1:D:579:PHE:HE1  | 1:D:581:LEU:HD13 | 1.72                     | 0.53              |
| 3:F:35:ARG:HA    | 3:F:39:GLN:O     | 2.07                     | 0.53              |
| 1:G:732:ILE:H    | 1:G:733:PRO:HD2  | 1.74                     | 0.53              |
| 1:J:109:ARG:O    | 1:J:114:MET:N    | 2.37                     | 0.53              |
| 1:J:721:LYS:C    | 1:J:736:GLN:OE1  | 2.46                     | 0.53              |
| 1:A:295:MLY:HE2  | 1:A:332:MET:HE1  | 1.91                     | 0.53              |
| 1:A:529:PRO:HB2  | 4:4:354:GLN:HA   | 1.91                     | 0.53              |
| 1:D:404:PRO:CG   | 1:D:417:GLU:HG3  | 2.38                     | 0.53              |
| 1:D:42:HIS:HB3   | 1:D:45:GLN:O     | 2.09                     | 0.53              |
| 1:D:584:TYR:CD1  | 1:D:585:ALA:N    | 2.77                     | 0.53              |
| 1:D:724:TYR:CA   | 1:D:782:MLY:HH21 | 2.38                     | 0.53              |
| 2:E:114:LYS:O    | 2:E:147:ASN:ND2  | 2.41                     | 0.53              |
| 1:G:730:SER:HB2  | 3:I:109:HIS:CE1  | 2.43                     | 0.53              |
| 1:G:818:TYR:CD1  | 2:H:127:ARG:CZ   | 2.79                     | 0.53              |
| 1:J:295:MLY:CG   | 1:J:332:MET:HE1  | 2.39                     | 0.53              |
| 1:J:404:PRO:CG   | 1:J:417:GLU:HG3  | 2.38                     | 0.53              |
| 1:J:765:VAL:HG12 | 1:J:766:PHE:N    | 2.22                     | 0.53              |
| 1:J:834:LEU:HD11 | 2:K:54:MET:HG3   | 1.90                     | 0.53              |
| 1:J:32:PHE:CD1   | 1:J:83:PRO:HD3   | 2.43                     | 0.53              |
| 2:E:162:ASP:O    | 2:K:21:GLU:HB3   | 2.08                     | 0.53              |
| 4:V:185:LEU:HD23 | 4:V:306:TYR:OH   | 2.09                     | 0.53              |
| 4:3:185:LEU:HD23 | 4:3:306:TYR:OH   | 2.09                     | 0.53              |
| 4:4:185:LEU:HD23 | 4:4:306:TYR:OH   | 2.09                     | 0.53              |
| 1:G:553:MLY:O    | 4:8:48:GLY:CA    | 2.56                     | 0.53              |
| 1:A:791:GLN:O    | 1:A:794:CYS:HB2  | 2.08                     | 0.53              |
| 1:D:135:TYR:CD2  | 1:D:191:ARG:HG2  | 2.44                     | 0.53              |
| 1:D:277:PHE:CG   | 1:D:278:GLN:N    | 2.76                     | 0.53              |
| 1:D:510:TRP:CZ3  | 1:D:711:PHE:HE2  | 2.26                     | 0.53              |
| 1:D:830:PRO:HD2  | 2:E:67:MET:HE2   | 1.90                     | 0.53              |
| 1:G:251:ARG:HB2  | 1:G:264:ASP:HB2  | 1.91                     | 0.53              |
| 1:G:32:PHE:CD1   | 1:G:83:PRO:HD3   | 2.44                     | 0.53              |
| 1:G:728:ASN:ND2  | 3:I:109:HIS:O    | 2.41                     | 0.53              |
| 1:J:571:ALA:O    | 1:J:572:LYS:CB   | 2.56                     | 0.53              |
| 1:J:584:TYR:CD1  | 1:J:585:ALA:N    | 2.77                     | 0.53              |
| 1:J:642:LYS:CG   | 4:7:22:ALA:CA    | 2.80                     | 0.53              |
| 1:J:599:ASN:CG   | 1:J:649:VAL:H    | 2.12                     | 0.53              |
| 1:J:661:MET:O    | 1:J:665:ARG:HG3  | 2.09                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:22:LYS:O     | 1:A:26:GLU:N     | 2.30                     | 0.53              |
| 1:A:42:HIS:HB3   | 1:A:45:GLN:O     | 2.09                     | 0.53              |
| 1:D:135:TYR:HD2  | 1:D:191:ARG:HD3  | 1.73                     | 0.53              |
| 1:G:277:PHE:CG   | 1:G:278:GLN:N    | 2.76                     | 0.53              |
| 1:G:149:GLN:OE1  | 1:G:762:HIS:HB3  | 2.09                     | 0.53              |
| 1:G:817:GLN:HB3  | 2:H:127:ARG:NH1  | 2.17                     | 0.53              |
| 1:J:218:LEU:N    | 1:J:221:GLN:HG2  | 2.24                     | 0.53              |
| 1:J:22:LYS:O     | 1:J:26:GLU:N     | 2.29                     | 0.53              |
| 2:K:121:LEU:CA   | 2:K:128:PHE:CG   | 2.89                     | 0.53              |
| 1:G:636:LYS:HB2  | 4:6:334:GLU:OE1  | 2.09                     | 0.53              |
| 1:A:539:GLU:OE2  | 4:6:45:VAL:C     | 2.48                     | 0.53              |
| 1:A:156:PHE:HD1  | 1:A:195:TYR:CD1  | 2.27                     | 0.53              |
| 1:A:217:THR:C    | 1:A:221:GLN:NE2  | 2.62                     | 0.53              |
| 1:A:493:HIS:ND1  | 1:A:514:ASP:OD2  | 2.41                     | 0.53              |
| 1:A:579:PHE:CD2  | 1:A:592:ILE:HD11 | 2.40                     | 0.53              |
| 1:A:739:ASP:CB   | 1:A:742:LYS:CB   | 2.81                     | 0.53              |
| 1:D:642:LYS:HG2  | 4:5:22:ALA:C     | 2.27                     | 0.53              |
| 1:D:661:MET:O    | 1:D:665:ARG:HG3  | 2.09                     | 0.53              |
| 1:D:793:ARG:NE   | 3:F:147:MET:HG2  | 2.23                     | 0.53              |
| 1:D:32:PHE:CD1   | 1:D:83:PRO:HD3   | 2.43                     | 0.53              |
| 1:G:292:MET:CE   | 1:G:309:PRO:HA   | 2.39                     | 0.53              |
| 2:H:114:LYS:O    | 2:H:147:ASN:ND2  | 2.41                     | 0.53              |
| 1:G:797:PHE:CE2  | 3:I:126:LEU:CD2  | 2.92                     | 0.53              |
| 1:G:798:LEU:HD21 | 3:I:126:LEU:HG   | 1.90                     | 0.53              |
| 1:J:295:MLY:HE2  | 1:J:332:MET:HE1  | 1.91                     | 0.53              |
| 1:J:404:PRO:HG3  | 1:J:417:GLU:HG3  | 1.91                     | 0.53              |
| 2:K:114:LYS:O    | 2:K:147:ASN:ND2  | 2.41                     | 0.53              |
| 3:L:53:PRO:HB2   | 3:L:55:LYS:HG3   | 1.91                     | 0.53              |
| 4:5:185:LEU:HD23 | 4:5:306:TYR:OH   | 2.09                     | 0.53              |
| 1:A:502:GLU:OE1  | 1:A:763:THR:CA   | 2.57                     | 0.53              |
| 1:D:599:ASN:CG   | 1:D:649:VAL:H    | 2.12                     | 0.53              |
| 2:E:114:LYS:N    | 2:E:146:GLY:O    | 2.40                     | 0.53              |
| 1:D:796:GLY:CA   | 3:F:40:ASN:OD1   | 2.52                     | 0.53              |
| 3:F:92:ARG:HA    | 3:F:139:TYR:OH   | 2.08                     | 0.53              |
| 1:G:218:LEU:N    | 1:G:221:GLN:HG2  | 2.24                     | 0.53              |
| 1:G:295:MLY:HE2  | 1:G:332:MET:HE1  | 1.91                     | 0.53              |
| 3:I:53:PRO:HB2   | 3:I:55:LYS:HG3   | 1.91                     | 0.53              |
| 1:J:251:ARG:HB2  | 1:J:264:ASP:HB2  | 1.91                     | 0.53              |
| 1:J:529:PRO:HB2  | 4:7:354:GLN:HA   | 1.91                     | 0.53              |
| 1:J:612:GLN:HE22 | 1:J:627:GLY:HA2  | 1.66                     | 0.53              |
| 2:K:129:THR:O    | 2:K:133:ILE:HG13 | 2.09                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:X:287:ILE:HG22 | 4:Z:204:ALA:HB3  | 1.91                     | 0.53              |
| 4:1:185:LEU:HD23 | 4:1:306:TYR:OH   | 2.09                     | 0.53              |
| 1:A:135:TYR:CD2  | 1:A:191:ARG:HG2  | 2.44                     | 0.53              |
| 1:A:732:ILE:H    | 1:A:733:PRO:HD2  | 1.74                     | 0.53              |
| 1:A:32:PHE:CD1   | 1:A:83:PRO:HD3   | 2.44                     | 0.53              |
| 1:D:493:HIS:ND1  | 1:D:514:ASP:OD2  | 2.41                     | 0.53              |
| 2:E:129:THR:O    | 2:E:133:ILE:HG13 | 2.09                     | 0.53              |
| 1:D:834:LEU:HD13 | 2:E:51:PHE:CD1   | 2.39                     | 0.53              |
| 1:G:534:SER:C    | 4:6:351:THR:CA   | 2.48                     | 0.53              |
| 1:G:642:LYS:HG2  | 4:6:22:ALA:C     | 2.27                     | 0.53              |
| 1:G:721:LYS:C    | 1:G:736:GLN:OE1  | 2.46                     | 0.53              |
| 1:J:418:THR:CB   | 1:J:421:GLU:HG3  | 2.37                     | 0.53              |
| 4:Z:185:LEU:HD23 | 4:Z:306:TYR:OH   | 2.09                     | 0.53              |
| 4:2:185:LEU:HD23 | 4:2:306:TYR:OH   | 2.09                     | 0.52              |
| 4:3:180:LEU:HD22 | 4:3:267:ILE:HD11 | 1.92                     | 0.52              |
| 1:D:642:LYS:CG   | 4:5:22:ALA:CA    | 2.80                     | 0.52              |
| 1:G:634:GLY:N    | 4:6:25:ASP:O     | 2.31                     | 0.52              |
| 1:A:599:ASN:CG   | 1:A:649:VAL:H    | 2.12                     | 0.52              |
| 1:A:661:MET:O    | 1:A:665:ARG:HG3  | 2.09                     | 0.52              |
| 1:D:154:HIS:CE1  | 1:D:156:PHE:HD2  | 2.27                     | 0.52              |
| 1:D:218:LEU:N    | 1:D:221:GLN:HG2  | 2.24                     | 0.52              |
| 1:D:404:PRO:HG3  | 1:D:417:GLU:HG3  | 1.91                     | 0.52              |
| 1:D:494:HIS:O    | 1:D:498:LEU:HB2  | 2.09                     | 0.52              |
| 1:D:556:ASP:HB3  | 4:7:43:VAL:HG12  | 1.91                     | 0.52              |
| 1:D:732:ILE:H    | 1:D:733:PRO:HD2  | 1.74                     | 0.52              |
| 1:D:800:ARG:CG   | 3:F:149:VAL:HG22 | 2.37                     | 0.52              |
| 1:G:579:PHE:CD2  | 1:G:592:ILE:HD11 | 2.39                     | 0.52              |
| 1:J:197:ALA:O    | 1:J:201:ALA:HB2  | 2.09                     | 0.52              |
| 1:J:510:TRP:CD2  | 1:J:768:MLY:CH1  | 2.92                     | 0.52              |
| 1:J:707:CYS:HG   | 1:J:714:ARG:HH12 | 1.45                     | 0.52              |
| 4:V:287:ILE:HG22 | 4:X:204:ALA:HB3  | 1.91                     | 0.52              |
| 4:0:287:ILE:HG22 | 4:2:204:ALA:HB3  | 1.91                     | 0.52              |
| 4:1:285:CYS:O    | 4:1:290:ARG:NH1  | 2.43                     | 0.52              |
| 4:2:180:LEU:HD22 | 4:2:267:ILE:HD11 | 1.92                     | 0.52              |
| 4:2:288:ASP:CA   | 4:4:204:ALA:HB2  | 2.31                     | 0.52              |
| 1:D:538:GLU:HG3  | 4:5:352:PHE:CA   | 2.38                     | 0.52              |
| 1:G:642:LYS:CG   | 4:6:22:ALA:HA    | 2.37                     | 0.52              |
| 4:6:185:LEU:HD23 | 4:6:306:TYR:OH   | 2.09                     | 0.52              |
| 4:8:185:LEU:HD23 | 4:8:306:TYR:OH   | 2.09                     | 0.52              |
| 1:A:555:TYR:N    | 4:6:48:GLY:N     | 2.58                     | 0.52              |
| 1:D:791:GLN:O    | 1:D:794:CYS:HB2  | 2.08                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:404:PRO:HG3  | 1:G:417:GLU:HG3  | 1.91                     | 0.52              |
| 1:G:584:TYR:CD1  | 1:G:585:ALA:N    | 2.77                     | 0.52              |
| 1:G:63:MLY:HG3   | 1:G:64:THR:H     | 1.75                     | 0.52              |
| 1:G:599:ASN:CG   | 1:G:649:VAL:H    | 2.12                     | 0.52              |
| 4:7:287:ILE:HG22 | 4:V:204:ALA:HB3  | 1.91                     | 0.52              |
| 4:W:185:LEU:HD23 | 4:W:306:TYR:OH   | 2.09                     | 0.52              |
| 4:6:180:LEU:HD22 | 4:6:267:ILE:HD11 | 1.92                     | 0.52              |
| 4:7:285:CYS:O    | 4:7:290:ARG:NH1  | 2.43                     | 0.52              |
| 1:A:277:PHE:CG   | 1:A:278:GLN:N    | 2.76                     | 0.52              |
| 1:A:732:ILE:HG23 | 1:A:747:LEU:CD1  | 1.04                     | 0.52              |
| 1:D:418:THR:CB   | 1:D:421:GLU:HG3  | 2.37                     | 0.52              |
| 1:D:636:LYS:HB2  | 4:5:334:GLU:OE1  | 2.09                     | 0.52              |
| 1:D:725:ARG:HG3  | 1:D:733:PRO:CA   | 2.36                     | 0.52              |
| 1:G:84:MLY:CH1   | 1:G:720:PHE:N    | 2.72                     | 0.52              |
| 1:J:135:TYR:CD2  | 1:J:191:ARG:HG2  | 2.44                     | 0.52              |
| 1:J:220:ASP:O    | 1:J:224:SER:N    | 2.27                     | 0.52              |
| 1:J:277:PHE:CG   | 1:J:278:GLN:N    | 2.76                     | 0.52              |
| 1:J:84:MLY:HH11  | 1:J:720:PHE:N    | 2.24                     | 0.52              |
| 1:J:732:ILE:HG23 | 1:J:747:LEU:CD1  | 1.05                     | 0.52              |
| 2:K:114:LYS:HA   | 2:K:147:ASN:HD22 | 1.74                     | 0.52              |
| 1:J:797:PHE:CG   | 3:L:149:VAL:CG1  | 2.80                     | 0.52              |
| 4:W:285:CYS:O    | 4:W:290:ARG:NH1  | 2.43                     | 0.52              |
| 4:X:285:CYS:O    | 4:X:290:ARG:NH1  | 2.43                     | 0.52              |
| 4:Y:285:CYS:O    | 4:Y:290:ARG:NH1  | 2.43                     | 0.52              |
| 4:Y:185:LEU:HD23 | 4:Y:306:TYR:OH   | 2.09                     | 0.52              |
| 4:Z:285:CYS:O    | 4:Z:290:ARG:NH1  | 2.43                     | 0.52              |
| 1:A:636:LYS:HB2  | 4:4:334:GLU:OE1  | 2.08                     | 0.52              |
| 4:5:180:LEU:HD22 | 4:5:267:ILE:HD11 | 1.92                     | 0.52              |
| 1:D:538:GLU:CG   | 4:5:351:THR:C    | 2.74                     | 0.52              |
| 4:6:285:CYS:O    | 4:6:290:ARG:NH1  | 2.43                     | 0.52              |
| 4:5:287:ILE:HG22 | 4:7:204:ALA:HB3  | 1.91                     | 0.52              |
| 1:J:642:LYS:CA   | 4:7:22:ALA:C     | 2.70                     | 0.52              |
| 4:7:185:LEU:HD23 | 4:7:306:TYR:OH   | 2.09                     | 0.52              |
| 1:A:504:MLY:HB2  | 1:A:762:HIS:NE2  | 2.24                     | 0.52              |
| 1:A:798:LEU:HD22 | 3:C:126:LEU:HD11 | 1.90                     | 0.52              |
| 3:C:104:GLY:HA2  | 3:C:137:ILE:HD11 | 1.91                     | 0.52              |
| 1:D:128:PRO:O    | 1:D:129:TYR:HB2  | 2.09                     | 0.52              |
| 1:J:156:PHE:HD1  | 1:J:195:TYR:CD1  | 2.27                     | 0.52              |
| 1:J:98:HIS:HB3   | 1:J:100:PRO:CD   | 2.25                     | 0.52              |
| 4:W:180:LEU:HD22 | 4:W:267:ILE:HD11 | 1.92                     | 0.52              |
| 4:5:285:CYS:O    | 4:5:290:ARG:NH1  | 2.43                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:109:ARG:HD3  | 1:A:117:THR:HB   | 1.92                     | 0.52              |
| 1:A:556:ASP:HB3  | 4:6:43:VAL:HG12  | 1.91                     | 0.52              |
| 1:A:63:MLY:HG3   | 1:A:64:THR:H     | 1.75                     | 0.52              |
| 1:D:732:ILE:H    | 1:D:733:PRO:CD   | 2.23                     | 0.52              |
| 1:G:217:THR:C    | 1:G:221:GLN:NE2  | 2.62                     | 0.52              |
| 1:G:530:MET:HG2  | 4:6:354:GLN:HB2  | 0.57                     | 0.52              |
| 1:J:759:ALA:O    | 1:J:766:PHE:N    | 2.32                     | 0.52              |
| 1:J:795:ARG:HD3  | 3:L:35:ARG:NH2   | 1.91                     | 0.52              |
| 2:K:112:ILE:C    | 2:K:147:ASN:O    | 2.42                     | 0.52              |
| 3:L:104:GLY:HA2  | 3:L:137:ILE:HD11 | 1.92                     | 0.52              |
| 3:L:110:VAL:HG13 | 3:L:114:LEU:HD12 | 1.92                     | 0.52              |
| 1:J:795:ARG:CB   | 3:L:35:ARG:NH2   | 2.73                     | 0.52              |
| 4:V:180:LEU:HD22 | 4:V:267:ILE:HD11 | 1.92                     | 0.52              |
| 4:Y:180:LEU:HD22 | 4:Y:267:ILE:HD11 | 1.92                     | 0.52              |
| 4:0:180:LEU:HD22 | 4:0:267:ILE:HD11 | 1.92                     | 0.52              |
| 4:1:180:LEU:HD22 | 4:1:267:ILE:HD11 | 1.92                     | 0.52              |
| 4:2:287:ILE:HG22 | 4:4:204:ALA:HB3  | 1.91                     | 0.52              |
| 4:4:180:LEU:HD22 | 4:4:267:ILE:HD11 | 1.92                     | 0.52              |
| 4:8:285:CYS:O    | 4:8:290:ARG:NH1  | 2.43                     | 0.52              |
| 1:A:154:HIS:CE1  | 1:A:156:PHE:HD2  | 2.27                     | 0.52              |
| 1:A:404:PRO:HG3  | 1:A:417:GLU:HG3  | 1.91                     | 0.52              |
| 1:A:494:HIS:O    | 1:A:498:LEU:HB2  | 2.09                     | 0.52              |
| 1:A:732:ILE:H    | 1:A:733:PRO:CD   | 2.23                     | 0.52              |
| 1:A:795:ARG:HG2  | 3:C:118:MET:HE3  | 1.90                     | 0.52              |
| 1:A:788:THR:CG2  | 3:C:42:THR:HG21  | 2.40                     | 0.52              |
| 3:F:104:GLY:HA2  | 3:F:137:ILE:HD11 | 1.92                     | 0.52              |
| 1:G:109:ARG:HD3  | 1:G:117:THR:HB   | 1.92                     | 0.52              |
| 1:G:42:HIS:HB3   | 1:G:45:GLN:O     | 2.09                     | 0.52              |
| 1:G:41:VAL:HG13  | 1:G:42:HIS:N     | 2.25                     | 0.52              |
| 1:G:732:ILE:HG23 | 1:G:747:LEU:CD1  | 1.04                     | 0.52              |
| 1:G:510:TRP:CH2  | 1:G:768:MLY:HH11 | 2.39                     | 0.52              |
| 2:H:114:LYS:HA   | 2:H:147:ASN:HD22 | 1.75                     | 0.52              |
| 1:J:556:ASP:HB3  | 4:V:43:VAL:HG12  | 1.91                     | 0.52              |
| 4:X:180:LEU:HD22 | 4:X:267:ILE:HD11 | 1.92                     | 0.52              |
| 4:0:185:LEU:HD23 | 4:0:306:TYR:OH   | 2.09                     | 0.52              |
| 4:2:285:CYS:O    | 4:2:290:ARG:NH1  | 2.43                     | 0.52              |
| 4:3:287:ILE:HG22 | 4:5:204:ALA:HB3  | 1.91                     | 0.52              |
| 1:A:212:GLY:O    | 1:A:213:LYS:HB2  | 2.10                     | 0.52              |
| 1:A:800:ARG:HB3  | 3:C:149:VAL:HG23 | 1.73                     | 0.52              |
| 3:C:92:ARG:HA    | 3:C:139:TYR:OH   | 2.09                     | 0.52              |
| 3:C:52:ASN:HB2   | 3:C:53:PRO:CD    | 2.28                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:53:PRO:HB2   | 3:C:55:LYS:HG3   | 1.91                     | 0.52              |
| 1:D:156:PHE:HD1  | 1:D:195:TYR:CD1  | 2.28                     | 0.52              |
| 1:D:41:VAL:HG13  | 1:D:42:HIS:N     | 2.25                     | 0.52              |
| 1:D:491:PHE:HD1  | 1:D:671:PHE:CE2  | 2.27                     | 0.52              |
| 1:D:538:GLU:HA   | 4:5:349:LEU:CB   | 2.40                     | 0.52              |
| 1:G:128:PRO:O    | 1:G:129:TYR:HB2  | 2.09                     | 0.52              |
| 1:G:135:TYR:CD2  | 1:G:191:ARG:HG2  | 2.44                     | 0.52              |
| 1:G:154:HIS:CE1  | 1:G:156:PHE:HD2  | 2.26                     | 0.52              |
| 1:G:40:VAL:HG13  | 1:G:41:VAL:O     | 2.10                     | 0.52              |
| 1:G:529:PRO:HB2  | 4:6:354:GLN:HA   | 1.92                     | 0.52              |
| 1:G:793:ARG:HH11 | 3:I:40:ASN:HD21  | 1.56                     | 0.52              |
| 1:J:42:HIS:HB3   | 1:J:45:GLN:O     | 2.09                     | 0.52              |
| 1:J:41:VAL:HG13  | 1:J:42:HIS:N     | 2.25                     | 0.52              |
| 1:J:530:MET:HG2  | 4:7:354:GLN:HB2  | 0.57                     | 0.52              |
| 1:J:817:GLN:HG3  | 2:K:128:PHE:CZ   | 2.45                     | 0.52              |
| 4:7:180:LEU:HD22 | 4:7:267:ILE:HD11 | 1.92                     | 0.52              |
| 1:A:218:LEU:CD2  | 1:A:222:ILE:CG1  | 2.85                     | 0.52              |
| 1:A:491:PHE:HD1  | 1:A:671:PHE:CE2  | 2.27                     | 0.52              |
| 1:A:795:ARG:CD   | 3:C:43:ASN:OD1   | 2.58                     | 0.52              |
| 1:A:798:LEU:HD11 | 3:C:126:LEU:HG   | 1.90                     | 0.52              |
| 1:D:839:MLY:HH11 | 2:E:159:HIS:HB3  | 1.87                     | 0.52              |
| 3:F:53:PRO:HB2   | 3:F:55:LYS:HG3   | 1.91                     | 0.52              |
| 1:G:156:PHE:HD1  | 1:G:195:TYR:CD1  | 2.27                     | 0.52              |
| 1:G:197:ALA:O    | 1:G:201:ALA:HB2  | 2.09                     | 0.52              |
| 1:G:491:PHE:HD1  | 1:G:671:PHE:CE2  | 2.27                     | 0.52              |
| 1:J:642:LYS:HG2  | 4:7:21:PHE:C     | 2.29                     | 0.52              |
| 4:V:285:CYS:O    | 4:V:290:ARG:NH1  | 2.43                     | 0.52              |
| 1:J:555:TYR:N    | 4:V:48:GLY:N     | 2.58                     | 0.52              |
| 4:8:287:ILE:HG22 | 4:W:204:ALA:HB3  | 1.91                     | 0.52              |
| 4:Z:180:LEU:HD22 | 4:Z:267:ILE:HD11 | 1.92                     | 0.52              |
| 4:0:285:CYS:O    | 4:0:290:ARG:NH1  | 2.43                     | 0.52              |
| 4:8:180:LEU:HD22 | 4:8:267:ILE:HD11 | 1.92                     | 0.52              |
| 1:A:251:ARG:HB2  | 1:A:264:ASP:HB2  | 1.91                     | 0.52              |
| 1:D:251:ARG:HB2  | 1:D:264:ASP:HB2  | 1.91                     | 0.52              |
| 1:D:63:MLY:HG3   | 1:D:64:THR:H     | 1.75                     | 0.52              |
| 1:D:830:PRO:CD   | 2:E:67:MET:HE2   | 2.38                     | 0.52              |
| 3:F:110:VAL:HG13 | 3:F:114:LEU:HD12 | 1.91                     | 0.52              |
| 1:J:128:PRO:O    | 1:J:129:TYR:HB2  | 2.09                     | 0.52              |
| 1:J:154:HIS:CE1  | 1:J:156:PHE:HD2  | 2.26                     | 0.52              |
| 4:W:287:ILE:HG22 | 4:Y:204:ALA:HB3  | 1.91                     | 0.52              |
| 1:J:636:LYS:HB2  | 4:7:334:GLU:OE1  | 2.09                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:556:ASP:HB3  | 4:8:43:VAL:HG12  | 1.92                     | 0.52              |
| 1:A:292:MET:CE   | 1:A:309:PRO:HA   | 2.39                     | 0.52              |
| 1:A:40:VAL:HG13  | 1:A:41:VAL:O     | 2.10                     | 0.52              |
| 2:B:129:THR:O    | 2:B:133:ILE:HG13 | 2.09                     | 0.52              |
| 1:A:797:PHE:CD1  | 3:C:149:VAL:HG12 | 2.20                     | 0.52              |
| 1:D:109:ARG:HD3  | 1:D:117:THR:HB   | 1.92                     | 0.52              |
| 1:D:195:TYR:CE2  | 1:D:199:ILE:CD1  | 2.93                     | 0.52              |
| 1:D:642:LYS:HG2  | 4:5:21:PHE:C     | 2.30                     | 0.52              |
| 1:D:733:PRO:O    | 1:D:737:PHE:CE1  | 2.53                     | 0.52              |
| 1:D:41:VAL:HG21  | 1:D:76:GLN:HG3   | 1.92                     | 0.52              |
| 1:G:481:ASN:ND2  | 1:G:481:ASN:N    | 2.51                     | 0.52              |
| 1:G:494:HIS:O    | 1:G:498:LEU:HB2  | 2.09                     | 0.52              |
| 1:J:135:TYR:HD2  | 1:J:191:ARG:CD   | 2.23                     | 0.52              |
| 1:J:232:PHE:CE1  | 1:J:287:ILE:HD13 | 2.44                     | 0.52              |
| 1:J:491:PHE:HD1  | 1:J:671:PHE:CE2  | 2.27                     | 0.52              |
| 1:J:510:TRP:CE2  | 1:J:768:MLY:HH13 | 2.45                     | 0.52              |
| 1:J:553:MLY:CE   | 4:V:45:VAL:CA    | 2.49                     | 0.52              |
| 1:J:642:LYS:HB2  | 4:7:24:ASP:O     | 1.89                     | 0.52              |
| 1:J:90:ASP:OD2   | 1:J:764:MLY:HH21 | 2.08                     | 0.52              |
| 3:L:100:GLY:O    | 3:L:138:ASN:HA   | 2.10                     | 0.52              |
| 1:A:642:LYS:CG   | 4:4:22:ALA:HA    | 2.38                     | 0.51              |
| 1:D:410:ASN:CG   | 4:5:334:GLU:C    | 2.65                     | 0.51              |
| 4:4:287:ILE:HG22 | 4:6:204:ALA:HB3  | 1.91                     | 0.51              |
| 1:D:555:TYR:N    | 4:7:48:GLY:N     | 2.58                     | 0.51              |
| 1:A:135:TYR:HD2  | 1:A:191:ARG:CD   | 2.23                     | 0.51              |
| 1:A:538:GLU:HA   | 4:4:349:LEU:CB   | 2.39                     | 0.51              |
| 1:A:578:HIS:O    | 1:A:579:PHE:HB3  | 2.11                     | 0.51              |
| 1:A:725:ARG:O    | 1:A:729:ALA:HA   | 2.10                     | 0.51              |
| 2:B:114:LYS:O    | 2:B:147:ASN:ND2  | 2.41                     | 0.51              |
| 1:D:40:VAL:HG13  | 1:D:41:VAL:O     | 2.10                     | 0.51              |
| 2:E:114:LYS:HA   | 2:E:147:ASN:HD22 | 1.74                     | 0.51              |
| 1:G:221:GLN:HB2  | 1:G:449:LEU:HD11 | 1.92                     | 0.51              |
| 2:H:129:THR:O    | 2:H:133:ILE:HG13 | 2.09                     | 0.51              |
| 3:I:110:VAL:HG13 | 3:I:114:LEU:HD12 | 1.91                     | 0.51              |
| 1:J:292:MET:CE   | 1:J:309:PRO:HA   | 2.40                     | 0.51              |
| 1:J:40:VAL:HG13  | 1:J:41:VAL:O     | 2.10                     | 0.51              |
| 1:J:221:GLN:HB2  | 1:J:449:LEU:HD11 | 1.92                     | 0.51              |
| 1:J:539:GLU:OE2  | 4:V:45:VAL:C     | 2.47                     | 0.51              |
| 1:D:221:GLN:HB2  | 1:D:449:LEU:HD11 | 1.92                     | 0.51              |
| 1:D:813:ILE:CB   | 2:E:127:ARG:NH1  | 2.73                     | 0.51              |
| 1:G:93:MET:CG    | 1:G:716:LEU:HD12 | 2.39                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:727:LEU:O    | 3:I:113:THR:CB   | 2.58                     | 0.51              |
| 1:J:494:HIS:O    | 1:J:498:LEU:HB2  | 2.09                     | 0.51              |
| 1:J:538:GLU:HA   | 4:7:349:LEU:CB   | 2.40                     | 0.51              |
| 1:J:63:MLY:HG3   | 1:J:64:THR:H     | 1.75                     | 0.51              |
| 1:A:408:VAL:CG1  | 4:4:332:PRO:HB3  | 2.40                     | 0.51              |
| 1:A:530:MET:CE   | 4:4:354:GLN:HG3  | 2.35                     | 0.51              |
| 1:A:530:MET:HG2  | 4:4:354:GLN:HB2  | 0.57                     | 0.51              |
| 1:A:501:GLU:C    | 1:A:762:HIS:CE1  | 2.84                     | 0.51              |
| 1:A:97:LEU:CD2   | 1:A:712:PRO:CB   | 2.88                     | 0.51              |
| 2:B:114:LYS:HA   | 2:B:147:ASN:HD22 | 1.74                     | 0.51              |
| 1:D:295:MLY:HE2  | 1:D:332:MET:HE1  | 1.91                     | 0.51              |
| 3:F:100:GLY:O    | 3:F:138:ASN:HA   | 2.11                     | 0.51              |
| 1:G:232:PHE:CE1  | 1:G:287:ILE:HD13 | 2.45                     | 0.51              |
| 1:G:559:LEU:HD23 | 1:G:559:LEU:C    | 2.31                     | 0.51              |
| 1:G:762:HIS:N    | 1:G:762:HIS:CD2  | 2.78                     | 0.51              |
| 1:J:195:TYR:CE2  | 1:J:199:ILE:CD1  | 2.93                     | 0.51              |
| 4:1:287:ILE:HG22 | 4:3:204:ALA:HB3  | 1.91                     | 0.51              |
| 4:3:285:CYS:O    | 4:3:290:ARG:NH1  | 2.43                     | 0.51              |
| 1:D:642:LYS:CA   | 4:5:22:ALA:C     | 2.71                     | 0.51              |
| 1:A:221:GLN:HB2  | 1:A:449:LEU:HD11 | 1.92                     | 0.51              |
| 1:A:232:PHE:CE1  | 1:A:287:ILE:HD13 | 2.45                     | 0.51              |
| 1:A:546:THR:CG2  | 1:A:548:THR:HB   | 2.41                     | 0.51              |
| 1:A:592:ILE:O    | 1:A:592:ILE:HG22 | 2.11                     | 0.51              |
| 1:D:248:MLY:N    | 1:D:463:ASP:O    | 2.44                     | 0.51              |
| 1:G:538:GLU:HA   | 4:6:349:LEU:CB   | 2.40                     | 0.51              |
| 1:G:546:THR:CG2  | 1:G:548:THR:HB   | 2.41                     | 0.51              |
| 1:J:248:MLY:N    | 1:J:463:ASP:O    | 2.44                     | 0.51              |
| 1:J:640:LYS:CA   | 1:J:645:SER:OG   | 2.58                     | 0.51              |
| 1:J:818:TYR:CD1  | 2:K:127:ARG:NH1  | 2.78                     | 0.51              |
| 4:4:285:CYS:O    | 4:4:290:ARG:NH1  | 2.43                     | 0.51              |
| 1:G:411:GLU:H    | 4:6:333:PRO:CG   | 2.24                     | 0.51              |
| 1:A:195:TYR:CE2  | 1:A:199:ILE:CD1  | 2.93                     | 0.51              |
| 1:D:232:PHE:CE1  | 1:D:287:ILE:HD13 | 2.45                     | 0.51              |
| 1:D:538:GLU:CD   | 4:5:355:MET:HE3  | 2.29                     | 0.51              |
| 1:G:195:TYR:CE2  | 1:G:199:ILE:CD1  | 2.93                     | 0.51              |
| 1:G:418:THR:O    | 1:G:422:VAL:HG23 | 2.11                     | 0.51              |
| 1:G:578:HIS:O    | 1:G:579:PHE:HB3  | 2.11                     | 0.51              |
| 3:I:100:GLY:O    | 3:I:138:ASN:HA   | 2.11                     | 0.51              |
| 3:I:104:GLY:HA2  | 3:I:137:ILE:HD11 | 1.92                     | 0.51              |
| 1:J:13:ALA:C     | 1:J:15:PRO:HD2   | 2.31                     | 0.51              |
| 1:J:212:GLY:O    | 1:J:213:LYS:HB2  | 2.11                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:418:THR:O    | 1:J:422:VAL:HG23 | 2.11                     | 0.51              |
| 1:J:578:HIS:O    | 1:J:579:PHE:HB3  | 2.11                     | 0.51              |
| 1:J:687:GLU:O    | 1:J:691:VAL:HG23 | 2.11                     | 0.51              |
| 4:6:287:ILE:HG22 | 4:8:204:ALA:HB3  | 1.91                     | 0.51              |
| 1:A:248:MLY:N    | 1:A:463:ASP:O    | 2.44                     | 0.51              |
| 1:A:38:VAL:CG1   | 1:A:39:PHE:N     | 2.74                     | 0.51              |
| 1:A:41:VAL:HG13  | 1:A:42:HIS:N     | 2.25                     | 0.51              |
| 1:A:559:LEU:HD23 | 1:A:559:LEU:C    | 2.31                     | 0.51              |
| 1:A:814:PHE:CA   | 2:B:127:ARG:NH2  | 2.67                     | 0.51              |
| 1:D:197:ALA:O    | 1:D:201:ALA:HB2  | 2.10                     | 0.51              |
| 2:E:112:ILE:HG23 | 2:E:147:ASN:HB3  | 1.93                     | 0.51              |
| 1:G:248:MLY:N    | 1:G:463:ASP:O    | 2.44                     | 0.51              |
| 1:G:675:ILE:CG2  | 1:G:676:ILE:N    | 2.74                     | 0.51              |
| 1:G:826:VAL:HG21 | 2:H:88:LEU:HD21  | 1.93                     | 0.51              |
| 1:A:418:THR:O    | 1:A:422:VAL:HG23 | 2.11                     | 0.51              |
| 1:A:757:GLN:HG3  | 1:A:771:LEU:CD1  | 2.30                     | 0.51              |
| 1:D:237:THR:O    | 1:D:240:ASN:O    | 2.29                     | 0.51              |
| 1:D:411:GLU:H    | 4:5:333:PRO:CG   | 2.24                     | 0.51              |
| 1:D:400:ALA:HB1  | 1:D:606:THR:HG22 | 1.92                     | 0.51              |
| 1:G:311:ASP:HB2  | 1:G:312:TYR:CE1  | 2.46                     | 0.51              |
| 1:G:38:VAL:CG1   | 1:G:39:PHE:N     | 2.74                     | 0.51              |
| 1:G:41:VAL:HG21  | 1:G:76:GLN:HG3   | 1.93                     | 0.51              |
| 1:J:202:SER:HB2  | 1:J:207:LYS:NZ   | 2.26                     | 0.51              |
| 1:J:592:ILE:HG22 | 1:J:592:ILE:O    | 2.10                     | 0.51              |
| 1:J:90:ASP:CG    | 1:J:764:MLY:CH2  | 2.79                     | 0.51              |
| 1:J:818:TYR:OH   | 2:K:127:ARG:NH2  | 2.35                     | 0.51              |
| 2:K:114:LYS:N    | 2:K:146:GLY:O    | 2.40                     | 0.51              |
| 1:A:400:ALA:HB1  | 1:A:606:THR:HG22 | 1.92                     | 0.51              |
| 1:A:631:GLU:C    | 4:4:25:ASP:HB2   | 2.31                     | 0.51              |
| 1:D:13:ALA:C     | 1:D:15:PRO:HD2   | 2.31                     | 0.51              |
| 1:D:135:TYR:HD2  | 1:D:191:ARG:CD   | 2.23                     | 0.51              |
| 1:D:217:THR:C    | 1:D:221:GLN:NE2  | 2.62                     | 0.51              |
| 1:D:553:MLY:CE   | 4:7:45:VAL:CA    | 2.49                     | 0.51              |
| 1:D:592:ILE:O    | 1:D:592:ILE:HG22 | 2.10                     | 0.51              |
| 1:G:13:ALA:C     | 1:G:15:PRO:HD2   | 2.31                     | 0.51              |
| 1:G:400:ALA:HB1  | 1:G:606:THR:HG22 | 1.93                     | 0.51              |
| 1:G:631:GLU:C    | 4:6:25:ASP:HB2   | 2.31                     | 0.51              |
| 1:G:725:ARG:O    | 1:G:729:ALA:HA   | 2.10                     | 0.51              |
| 1:J:742:LYS:O    | 1:J:745:GLU:HB2  | 2.10                     | 0.51              |
| 1:J:41:VAL:HG21  | 1:J:76:GLN:HG3   | 1.93                     | 0.51              |
| 1:A:506:GLU:OE1  | 1:A:761:GLY:N    | 2.41                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:110:VAL:HG13 | 3:C:114:LEU:HD12 | 1.92                     | 0.51              |
| 1:D:202:SER:HB2  | 1:D:207:LYS:NZ   | 2.26                     | 0.51              |
| 1:D:530:MET:HG2  | 4:5:354:GLN:HB2  | 0.57                     | 0.51              |
| 1:D:687:GLU:O    | 1:D:691:VAL:HG23 | 2.11                     | 0.51              |
| 2:E:121:LEU:HA   | 2:E:128:PHE:CD2  | 2.46                     | 0.51              |
| 1:D:815:CYS:O    | 2:E:90:GLY:CA    | 2.59                     | 0.51              |
| 1:G:267:THR:HG21 | 1:G:438:PHE:HE2  | 1.76                     | 0.51              |
| 1:J:649:VAL:HG23 | 1:J:649:VAL:HA   | 1.83                     | 0.51              |
| 4:7:288:ASP:CA   | 4:V:204:ALA:HB2  | 2.31                     | 0.51              |
| 1:A:128:PRO:O    | 1:A:129:TYR:HB2  | 2.09                     | 0.51              |
| 1:A:197:ALA:O    | 1:A:201:ALA:HB2  | 2.10                     | 0.51              |
| 1:A:311:ASP:HB2  | 1:A:312:TYR:CE1  | 2.46                     | 0.51              |
| 1:D:38:VAL:CG1   | 1:D:39:PHE:N     | 2.74                     | 0.51              |
| 1:D:632:GLY:HA3  | 1:D:643:GLY:N    | 2.17                     | 0.51              |
| 1:D:725:ARG:O    | 1:D:729:ALA:HA   | 2.10                     | 0.51              |
| 1:G:212:GLY:O    | 1:G:213:LYS:HB2  | 2.10                     | 0.51              |
| 2:H:114:LYS:N    | 2:H:146:GLY:O    | 2.40                     | 0.51              |
| 1:J:169:ASP:N    | 1:J:169:ASP:OD1  | 2.44                     | 0.51              |
| 1:J:768:MLY:HH21 | 1:J:772:LEU:HD13 | 1.93                     | 0.51              |
| 1:A:556:ASP:CA   | 4:6:49:GLN:O     | 2.52                     | 0.50              |
| 1:J:408:VAL:CG1  | 4:7:332:PRO:HB3  | 2.40                     | 0.50              |
| 1:A:640:LYS:CA   | 1:A:645:SER:OG   | 2.58                     | 0.50              |
| 1:A:646:PHE:CE2  | 1:A:652:LEU:CD2  | 2.87                     | 0.50              |
| 1:A:675:ILE:CG2  | 1:A:676:ILE:N    | 2.74                     | 0.50              |
| 1:A:822:SER:HB3  | 2:B:88:LEU:CD2   | 2.41                     | 0.50              |
| 1:D:212:GLY:O    | 1:D:213:LYS:HB2  | 2.11                     | 0.50              |
| 1:D:218:LEU:N    | 1:D:221:GLN:CG   | 2.74                     | 0.50              |
| 1:D:578:HIS:O    | 1:D:579:PHE:HB3  | 2.10                     | 0.50              |
| 1:G:429:LEU:O    | 1:G:433:VAL:HG23 | 2.11                     | 0.50              |
| 1:G:797:PHE:CD2  | 3:I:126:LEU:CD2  | 2.93                     | 0.50              |
| 1:J:109:ARG:HD3  | 1:J:117:THR:HB   | 1.92                     | 0.50              |
| 1:J:632:GLY:HA3  | 1:J:643:GLY:N    | 2.17                     | 0.50              |
| 1:J:733:PRO:O    | 1:J:737:PHE:CE1  | 2.53                     | 0.50              |
| 1:D:631:GLU:C    | 4:5:25:ASP:HB2   | 2.31                     | 0.50              |
| 1:A:41:VAL:HG21  | 1:A:76:GLN:HG3   | 1.92                     | 0.50              |
| 1:A:687:GLU:O    | 1:A:691:VAL:HG23 | 2.11                     | 0.50              |
| 1:D:546:THR:CG2  | 1:D:548:THR:HB   | 2.41                     | 0.50              |
| 1:D:559:LEU:C    | 1:D:559:LEU:HD23 | 2.31                     | 0.50              |
| 1:D:818:TYR:CG   | 2:E:89:LYS:CB    | 2.93                     | 0.50              |
| 1:D:818:TYR:HB3  | 2:E:90:GLY:N     | 2.26                     | 0.50              |
| 1:G:135:TYR:HD2  | 1:G:191:ARG:CD   | 2.23                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:218:LEU:N    | 1:G:221:GLN:CG   | 2.74                     | 0.50              |
| 1:G:730:SER:CB   | 3:I:109:HIS:CE1  | 2.94                     | 0.50              |
| 1:J:218:LEU:N    | 1:J:221:GLN:CG   | 2.74                     | 0.50              |
| 1:J:237:THR:O    | 1:J:240:ASN:O    | 2.29                     | 0.50              |
| 1:J:411:GLU:H    | 4:7:333:PRO:CG   | 2.25                     | 0.50              |
| 1:G:555:TYR:N    | 4:8:48:GLY:N     | 2.59                     | 0.50              |
| 1:A:629:GLU:CB   | 1:A:645:SER:N    | 2.74                     | 0.50              |
| 1:A:759:ALA:O    | 1:A:766:PHE:N    | 2.32                     | 0.50              |
| 1:D:169:ASP:OD1  | 1:D:169:ASP:N    | 2.44                     | 0.50              |
| 1:D:418:THR:O    | 1:D:422:VAL:HG23 | 2.11                     | 0.50              |
| 1:D:723:ARG:C    | 1:D:782:MLY:NZ   | 2.65                     | 0.50              |
| 1:D:742:LYS:O    | 1:D:745:GLU:HB2  | 2.10                     | 0.50              |
| 1:G:202:SER:HB2  | 1:G:207:LYS:NZ   | 2.26                     | 0.50              |
| 1:G:237:THR:O    | 1:G:240:ASN:O    | 2.29                     | 0.50              |
| 1:J:646:PHE:HE2  | 1:J:652:LEU:CG   | 2.25                     | 0.50              |
| 1:J:725:ARG:O    | 1:J:729:ALA:HA   | 2.10                     | 0.50              |
| 1:J:732:ILE:H    | 1:J:733:PRO:CD   | 2.23                     | 0.50              |
| 1:J:823:PHE:HE1  | 2:K:156:VAL:O    | 1.88                     | 0.50              |
| 1:G:538:GLU:OE1  | 4:6:351:THR:HB   | 2.12                     | 0.50              |
| 1:A:13:ALA:C     | 1:A:15:PRO:HD2   | 2.31                     | 0.50              |
| 1:A:169:ASP:OD1  | 1:A:169:ASP:N    | 2.44                     | 0.50              |
| 1:A:267:THR:HG21 | 1:A:438:PHE:HE2  | 1.76                     | 0.50              |
| 1:A:839:MLY:HD3  | 2:B:159:HIS:CB   | 2.40                     | 0.50              |
| 1:A:817:GLN:CG   | 2:B:127:ARG:HG2  | 2.41                     | 0.50              |
| 1:D:154:HIS:CD2  | 1:D:155:ILE:H    | 2.30                     | 0.50              |
| 1:G:732:ILE:H    | 1:G:733:PRO:CD   | 2.23                     | 0.50              |
| 1:G:797:PHE:CE2  | 3:I:126:LEU:HD23 | 2.45                     | 0.50              |
| 1:G:800:ARG:CZ   | 3:I:149:VAL:HG22 | 2.30                     | 0.50              |
| 1:J:154:HIS:CD2  | 1:J:155:ILE:H    | 2.30                     | 0.50              |
| 1:J:311:ASP:HB2  | 1:J:312:TYR:CE1  | 2.46                     | 0.50              |
| 1:J:278:GLN:HG3  | 1:J:318:GLY:H    | 1.75                     | 0.50              |
| 1:J:346:ASP:O    | 1:J:349:THR:HB   | 2.12                     | 0.50              |
| 1:J:629:GLU:CB   | 1:J:645:SER:N    | 2.73                     | 0.50              |
| 1:J:631:GLU:C    | 4:7:25:ASP:HB2   | 2.31                     | 0.50              |
| 1:J:733:PRO:CA   | 1:J:737:PHE:CE1  | 2.95                     | 0.50              |
| 3:C:100:GLY:O    | 3:C:138:ASN:HA   | 2.11                     | 0.50              |
| 1:D:311:ASP:HB2  | 1:D:312:TYR:CE1  | 2.46                     | 0.50              |
| 1:D:346:ASP:O    | 1:D:349:THR:HB   | 2.11                     | 0.50              |
| 1:D:429:LEU:O    | 1:D:433:VAL:HG23 | 2.11                     | 0.50              |
| 1:D:646:PHE:HE2  | 1:D:652:LEU:CG   | 2.25                     | 0.50              |
| 1:G:687:GLU:O    | 1:G:691:VAL:HG23 | 2.11                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:733:PRO:O    | 1:G:737:PHE:CE1  | 2.53                     | 0.50              |
| 1:G:742:LYS:O    | 1:G:745:GLU:HB2  | 2.10                     | 0.50              |
| 1:J:538:GLU:CD   | 4:7:355:MET:HE3  | 2.30                     | 0.50              |
| 1:A:732:ILE:O    | 1:A:736:GLN:HG3  | 2.12                     | 0.50              |
| 1:A:715:VAL:O    | 1:A:764:MLY:HB3  | 2.12                     | 0.50              |
| 1:D:507:GLY:O    | 1:D:761:GLY:C    | 2.49                     | 0.50              |
| 1:D:640:LYS:CA   | 1:D:645:SER:OG   | 2.58                     | 0.50              |
| 1:D:732:ILE:HG23 | 1:D:747:LEU:HD12 | 0.94                     | 0.50              |
| 1:D:715:VAL:O    | 1:D:764:MLY:HB3  | 2.12                     | 0.50              |
| 1:G:592:ILE:O    | 1:G:592:ILE:HG22 | 2.10                     | 0.50              |
| 1:G:640:LYS:CA   | 1:G:645:SER:OG   | 2.58                     | 0.50              |
| 1:G:715:VAL:O    | 1:G:764:MLY:HB3  | 2.12                     | 0.50              |
| 1:G:149:GLN:OE1  | 1:G:762:HIS:CB   | 2.59                     | 0.50              |
| 1:J:400:ALA:HB1  | 1:J:606:THR:HG22 | 1.93                     | 0.50              |
| 1:J:792:ALA:CB   | 3:L:40:ASN:CB    | 2.52                     | 0.50              |
| 2:K:112:ILE:HG23 | 2:K:147:ASN:HB3  | 1.93                     | 0.50              |
| 4:0:288:ASP:CA   | 4:2:204:ALA:HB2  | 2.31                     | 0.50              |
| 4:7:318:THR:HA   | 4:7:327:ILE:HG12 | 1.94                     | 0.50              |
| 1:A:218:LEU:N    | 1:A:221:GLN:CG   | 2.74                     | 0.50              |
| 1:A:237:THR:O    | 1:A:240:ASN:O    | 2.29                     | 0.50              |
| 1:A:601:ASP:N    | 1:A:602:PRO:CD   | 2.75                     | 0.50              |
| 1:A:742:LYS:O    | 1:A:745:GLU:HB2  | 2.10                     | 0.50              |
| 1:D:278:GLN:HG3  | 1:D:318:GLY:H    | 1.75                     | 0.50              |
| 1:D:629:GLU:CA   | 1:D:643:GLY:C    | 2.73                     | 0.50              |
| 1:D:795:ARG:HB3  | 3:F:35:ARG:HD3   | 1.91                     | 0.50              |
| 1:D:798:LEU:HD11 | 3:F:126:LEU:CD2  | 2.19                     | 0.50              |
| 1:G:218:LEU:CD2  | 1:G:222:ILE:CG1  | 2.85                     | 0.50              |
| 1:G:291:ILE:HA   | 1:G:331:LEU:CD1  | 2.39                     | 0.50              |
| 1:G:646:PHE:CE2  | 1:G:652:LEU:CD2  | 2.87                     | 0.50              |
| 1:J:429:LEU:O    | 1:J:433:VAL:HG23 | 2.12                     | 0.50              |
| 1:J:546:THR:CG2  | 1:J:548:THR:HB   | 2.41                     | 0.50              |
| 1:J:559:LEU:HD23 | 1:J:559:LEU:C    | 2.31                     | 0.50              |
| 1:J:839:MLY:HB2  | 1:J:840:PRO:HD3  | 1.94                     | 0.50              |
| 4:4:70:PRO:HG3   | 4:4:81:ASP:HB3   | 1.94                     | 0.50              |
| 1:D:408:VAL:CG1  | 4:5:332:PRO:HB3  | 2.41                     | 0.50              |
| 1:A:202:SER:HB2  | 1:A:207:LYS:NZ   | 2.26                     | 0.50              |
| 1:A:471:ASP:HB3  | 1:A:573:GLY:O    | 2.12                     | 0.50              |
| 1:A:576:GLU:CG   | 1:A:577:ALA:N    | 2.43                     | 0.50              |
| 1:A:733:PRO:CA   | 1:A:737:PHE:CE1  | 2.95                     | 0.50              |
| 1:A:769:ALA:N    | 1:A:771:LEU:CB   | 2.74                     | 0.50              |
| 1:D:109:ARG:O    | 1:D:114:MET:N    | 2.37                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:471:ASP:HB3  | 1:D:573:GLY:O    | 2.12                     | 0.50              |
| 1:G:346:ASP:O    | 1:G:349:THR:HB   | 2.11                     | 0.50              |
| 1:G:707:CYS:C    | 1:G:714:ARG:NH2  | 2.52                     | 0.50              |
| 1:G:733:PRO:CA   | 1:G:737:PHE:CE1  | 2.95                     | 0.50              |
| 1:G:795:ARG:HH21 | 3:I:116:GLU:HB3  | 1.77                     | 0.50              |
| 1:J:732:ILE:O    | 1:J:736:GLN:HG3  | 2.12                     | 0.50              |
| 2:K:117:LEU:HG   | 2:K:147:ASN:HB3  | 1.93                     | 0.50              |
| 1:A:553:MLY:HG3  | 4:6:44:MET:O     | 2.07                     | 0.50              |
| 4:8:318:THR:HA   | 4:8:327:ILE:HG12 | 1.94                     | 0.50              |
| 1:A:409:GLY:N    | 1:A:636:LYS:CD   | 2.70                     | 0.50              |
| 1:A:530:MET:HA   | 4:4:354:GLN:CD   | 2.11                     | 0.50              |
| 1:A:547:ASP:O    | 1:A:550:PHE:HB3  | 2.12                     | 0.50              |
| 1:A:95:THR:HG1   | 1:A:769:ALA:HA   | 1.76                     | 0.50              |
| 1:D:539:GLU:OE2  | 4:7:45:VAL:C     | 2.47                     | 0.50              |
| 1:D:733:PRO:CA   | 1:D:737:PHE:CE1  | 2.94                     | 0.50              |
| 1:G:471:ASP:HB3  | 1:G:573:GLY:O    | 2.12                     | 0.50              |
| 1:G:839:MLY:N    | 1:G:840:PRO:CD   | 2.75                     | 0.50              |
| 1:J:217:THR:C    | 1:J:221:GLN:NE2  | 2.62                     | 0.50              |
| 1:J:38:VAL:CG1   | 1:J:39:PHE:N     | 2.74                     | 0.50              |
| 4:3:318:THR:HA   | 4:3:327:ILE:HG12 | 1.94                     | 0.49              |
| 4:5:318:THR:HA   | 4:5:327:ILE:HG12 | 1.95                     | 0.49              |
| 4:6:318:THR:HA   | 4:6:327:ILE:HG12 | 1.94                     | 0.49              |
| 1:J:642:LYS:HA   | 4:7:22:ALA:C     | 2.33                     | 0.49              |
| 1:J:642:LYS:CG   | 4:7:22:ALA:HA    | 2.37                     | 0.49              |
| 1:A:411:GLU:H    | 4:4:333:PRO:CG   | 2.24                     | 0.49              |
| 1:A:505:MLY:HB2  | 1:A:761:GLY:CA   | 2.42                     | 0.49              |
| 1:D:291:ILE:HA   | 1:D:331:LEU:CD1  | 2.39                     | 0.49              |
| 1:D:538:GLU:OE1  | 4:5:351:THR:HB   | 2.12                     | 0.49              |
| 2:E:140:PHE:HB3  | 2:E:144:VAL:HG12 | 1.94                     | 0.49              |
| 2:H:137:TRP:CA   | 2:H:145:ALA:CB   | 2.82                     | 0.49              |
| 1:J:251:ARG:O    | 1:J:263:ALA:HA   | 2.12                     | 0.49              |
| 1:J:675:ILE:CG2  | 1:J:676:ILE:N    | 2.74                     | 0.49              |
| 1:A:51:THR:C     | 1:A:62:VAL:HG13  | 2.32                     | 0.49              |
| 1:A:756:THR:O    | 1:A:758:TYR:N    | 2.46                     | 0.49              |
| 1:A:818:TYR:HB2  | 2:B:89:LYS:C     | 2.31                     | 0.49              |
| 2:B:140:PHE:HB3  | 2:B:144:VAL:HG12 | 1.94                     | 0.49              |
| 2:B:117:LEU:CG   | 2:B:147:ASN:OD1  | 2.52                     | 0.49              |
| 1:D:769:ALA:C    | 1:D:770:GLY:C    | 2.69                     | 0.49              |
| 1:G:169:ASP:OD1  | 1:G:169:ASP:N    | 2.44                     | 0.49              |
| 1:G:278:GLN:HG3  | 1:G:318:GLY:H    | 1.75                     | 0.49              |
| 1:G:632:GLY:HA3  | 1:G:643:GLY:N    | 2.17                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:756:THR:O    | 1:G:758:TYR:N    | 2.45                     | 0.49              |
| 1:J:192:VAL:O    | 1:J:195:TYR:HB3  | 2.12                     | 0.49              |
| 1:J:538:GLU:OE1  | 4:7:351:THR:HB   | 2.12                     | 0.49              |
| 2:E:162:ASP:HB2  | 2:K:20:ASP:HA    | 1.94                     | 0.49              |
| 4:W:318:THR:HA   | 4:W:327:ILE:HG12 | 1.94                     | 0.49              |
| 4:Z:70:PRO:HG3   | 4:Z:81:ASP:HB3   | 1.94                     | 0.49              |
| 4:1:318:THR:HA   | 4:1:327:ILE:HG12 | 1.94                     | 0.49              |
| 4:4:318:THR:HA   | 4:4:327:ILE:HG12 | 1.94                     | 0.49              |
| 1:A:154:HIS:CD2  | 1:A:155:ILE:H    | 2.30                     | 0.49              |
| 1:A:715:VAL:HG12 | 1:A:716:LEU:O    | 2.13                     | 0.49              |
| 2:B:112:ILE:HG23 | 2:B:147:ASN:HB3  | 1.93                     | 0.49              |
| 1:D:192:VAL:O    | 1:D:195:TYR:HB3  | 2.13                     | 0.49              |
| 1:D:251:ARG:O    | 1:D:263:ALA:HA   | 2.12                     | 0.49              |
| 1:D:725:ARG:NE   | 1:D:733:PRO:CB   | 1.95                     | 0.49              |
| 1:D:732:ILE:O    | 1:D:736:GLN:HG3  | 2.12                     | 0.49              |
| 1:D:817:GLN:CD   | 2:E:127:ARG:CZ   | 2.70                     | 0.49              |
| 1:G:543:PRO:CD   | 4:6:146:GLY:O    | 2.60                     | 0.49              |
| 1:G:751:GLY:H    | 3:I:114:LEU:CD1  | 2.25                     | 0.49              |
| 1:G:757:GLN:CD   | 1:G:772:LEU:CG   | 2.75                     | 0.49              |
| 2:H:112:ILE:HG23 | 2:H:147:ASN:HB3  | 1.93                     | 0.49              |
| 1:J:214:MET:HA   | 1:J:340:ILE:CD1  | 2.41                     | 0.49              |
| 1:J:595:TRP:N    | 1:J:595:TRP:CD1  | 2.80                     | 0.49              |
| 1:J:739:ASP:OD1  | 1:J:740:SER:N    | 2.45                     | 0.49              |
| 1:J:756:THR:O    | 1:J:758:TYR:N    | 2.45                     | 0.49              |
| 1:J:768:MLY:CE   | 1:J:772:LEU:CD2  | 2.90                     | 0.49              |
| 1:J:795:ARG:NE   | 3:L:35:ARG:HH12  | 2.10                     | 0.49              |
| 4:V:318:THR:HA   | 4:V:327:ILE:HG12 | 1.94                     | 0.49              |
| 4:X:253:GLU:HA   | 4:X:256:ARG:CG   | 2.42                     | 0.49              |
| 4:0:70:PRO:HG3   | 4:0:81:ASP:HB3   | 1.94                     | 0.49              |
| 4:2:70:PRO:HG3   | 4:2:81:ASP:HB3   | 1.94                     | 0.49              |
| 4:6:70:PRO:HG3   | 4:6:81:ASP:HB3   | 1.94                     | 0.49              |
| 1:J:543:PRO:CD   | 4:7:146:GLY:O    | 2.61                     | 0.49              |
| 1:A:20:SER:HB3   | 1:A:23:GLU:OE1   | 2.13                     | 0.49              |
| 1:A:278:GLN:HG3  | 1:A:318:GLY:H    | 1.75                     | 0.49              |
| 1:A:291:ILE:HA   | 1:A:331:LEU:CD1  | 2.39                     | 0.49              |
| 1:A:786:ILE:HD13 | 3:C:90:GLY:HA2   | 1.93                     | 0.49              |
| 1:A:839:MLY:HB2  | 1:A:840:PRO:HD3  | 1.94                     | 0.49              |
| 2:B:114:LYS:N    | 2:B:146:GLY:O    | 2.40                     | 0.49              |
| 1:D:601:ASP:N    | 1:D:602:PRO:CD   | 2.75                     | 0.49              |
| 1:D:831:TRP:HZ3  | 2:E:50:THR:HG21  | 1.77                     | 0.49              |
| 2:E:93:PRO:O     | 2:E:97:ILE:HG13  | 2.13                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:84:MLY:HH11  | 1:G:715:VAL:HG12 | 1.76                     | 0.49              |
| 1:J:471:ASP:HB3  | 1:J:573:GLY:O    | 2.12                     | 0.49              |
| 1:J:601:ASP:N    | 1:J:602:PRO:CD   | 2.75                     | 0.49              |
| 1:J:128:PRO:O    | 1:J:683:PRO:HB3  | 2.12                     | 0.49              |
| 1:J:715:VAL:O    | 1:J:764:MLY:HB3  | 2.12                     | 0.49              |
| 4:Y:318:THR:HA   | 4:Y:327:ILE:HG12 | 1.94                     | 0.49              |
| 4:0:124:PHE:CZ   | 4:0:132:MET:HG3  | 2.48                     | 0.49              |
| 4:2:318:THR:HA   | 4:2:327:ILE:HG12 | 1.94                     | 0.49              |
| 4:4:124:PHE:CZ   | 4:4:132:MET:HG3  | 2.48                     | 0.49              |
| 1:A:543:PRO:CD   | 4:4:146:GLY:O    | 2.61                     | 0.49              |
| 1:G:642:LYS:CB   | 4:6:24:ASP:O     | 2.60                     | 0.49              |
| 4:8:124:PHE:CZ   | 4:8:132:MET:HG3  | 2.48                     | 0.49              |
| 1:A:795:ARG:CD   | 3:C:35:ARG:CZ    | 2.76                     | 0.49              |
| 1:D:543:PRO:CD   | 4:5:146:GLY:O    | 2.61                     | 0.49              |
| 1:D:715:VAL:HG12 | 1:D:716:LEU:O    | 2.12                     | 0.49              |
| 2:E:162:ASP:HB3  | 2:K:20:ASP:CB    | 2.37                     | 0.49              |
| 1:G:290:GLN:HG2  | 1:G:331:LEU:CA   | 2.43                     | 0.49              |
| 1:G:530:MET:HA   | 4:6:354:GLN:CD   | 2.11                     | 0.49              |
| 1:G:601:ASP:N    | 1:G:602:PRO:CD   | 2.75                     | 0.49              |
| 1:G:715:VAL:HG12 | 1:G:716:LEU:O    | 2.12                     | 0.49              |
| 2:H:93:PRO:O     | 2:H:97:ILE:HG13  | 2.12                     | 0.49              |
| 1:J:237:THR:HG22 | 1:J:238:VAL:N    | 2.28                     | 0.49              |
| 1:J:291:ILE:HA   | 1:J:331:LEU:CD1  | 2.39                     | 0.49              |
| 1:J:310:TYR:CE2  | 1:J:320:ILE:CD1  | 2.94                     | 0.49              |
| 1:J:97:LEU:HD13  | 1:J:97:LEU:N     | 2.28                     | 0.49              |
| 4:W:124:PHE:CZ   | 4:W:132:MET:HG3  | 2.48                     | 0.49              |
| 4:2:124:PHE:CZ   | 4:2:132:MET:HG3  | 2.48                     | 0.49              |
| 1:D:642:LYS:CG   | 4:5:22:ALA:HA    | 2.37                     | 0.49              |
| 4:6:124:PHE:CZ   | 4:6:132:MET:HG3  | 2.48                     | 0.49              |
| 1:A:312:TYR:N    | 1:A:312:TYR:CD1  | 2.80                     | 0.49              |
| 1:A:642:LYS:HG2  | 4:4:21:PHE:C     | 2.30                     | 0.49              |
| 2:B:121:LEU:HA   | 2:B:128:PHE:CD2  | 2.46                     | 0.49              |
| 1:D:173:GLN:OE1  | 1:D:668:HIS:HB3  | 2.13                     | 0.49              |
| 1:D:214:MET:HA   | 1:D:340:ILE:CD1  | 2.42                     | 0.49              |
| 1:D:251:ARG:HB2  | 1:D:264:ASP:HB3  | 1.95                     | 0.49              |
| 1:D:332:MET:O    | 1:D:336:SER:OG   | 2.27                     | 0.49              |
| 1:D:739:ASP:OD1  | 1:D:740:SER:N    | 2.45                     | 0.49              |
| 2:E:117:LEU:HG   | 2:E:147:ASN:HB3  | 1.93                     | 0.49              |
| 1:G:732:ILE:O    | 1:G:736:GLN:HG3  | 2.12                     | 0.49              |
| 3:I:50:LEU:O     | 3:I:55:LYS:HB2   | 2.13                     | 0.49              |
| 1:J:218:LEU:HA   | 1:J:221:GLN:HG3  | 1.71                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:544:LYS:HD2  | 4:7:147:ARG:CB   | 2.36                     | 0.49              |
| 1:J:715:VAL:HG12 | 1:J:716:LEU:O    | 2.12                     | 0.49              |
| 2:K:114:LYS:HG3  | 2:K:137:TRP:CZ2  | 2.48                     | 0.49              |
| 4:X:318:THR:HA   | 4:X:327:ILE:HG12 | 1.94                     | 0.49              |
| 4:Z:124:PHE:CZ   | 4:Z:132:MET:HG3  | 2.48                     | 0.49              |
| 4:O:253:GLU:HA   | 4:O:256:ARG:CG   | 2.42                     | 0.49              |
| 1:D:538:GLU:HA   | 4:5:351:THR:H    | 1.77                     | 0.49              |
| 1:G:642:LYS:HA   | 4:6:22:ALA:C     | 2.33                     | 0.49              |
| 4:7:124:PHE:CZ   | 4:7:132:MET:HG3  | 2.48                     | 0.49              |
| 4:8:198:TYR:CZ   | 4:8:248:ILE:HG13 | 2.48                     | 0.49              |
| 4:8:70:PRO:HG3   | 4:8:81:ASP:HB3   | 1.94                     | 0.49              |
| 1:A:173:GLN:OE1  | 1:A:668:HIS:HB3  | 2.13                     | 0.49              |
| 1:A:354:LEU:HA   | 1:A:354:LEU:HD12 | 1.56                     | 0.49              |
| 1:A:429:LEU:O    | 1:A:433:VAL:HG23 | 2.12                     | 0.49              |
| 1:A:538:GLU:OE1  | 4:4:351:THR:HB   | 2.12                     | 0.49              |
| 1:A:739:ASP:OD1  | 1:A:740:SER:N    | 2.45                     | 0.49              |
| 1:A:834:LEU:HD13 | 2:B:54:MET:HG3   | 1.86                     | 0.49              |
| 1:D:290:GLN:HG2  | 1:D:331:LEU:CA   | 2.43                     | 0.49              |
| 1:D:507:GLY:HA2  | 1:D:762:HIS:CD2  | 2.47                     | 0.49              |
| 1:D:128:PRO:O    | 1:D:683:PRO:HB3  | 2.12                     | 0.49              |
| 1:D:732:ILE:HG21 | 1:D:747:LEU:CD1  | 0.64                     | 0.49              |
| 1:D:822:SER:OG   | 2:E:88:LEU:HA    | 2.13                     | 0.49              |
| 2:E:114:LYS:HG3  | 2:E:137:TRP:CZ2  | 2.48                     | 0.49              |
| 1:G:154:HIS:CD2  | 1:G:155:ILE:H    | 2.30                     | 0.49              |
| 1:G:642:LYS:HG2  | 4:6:21:PHE:C     | 2.30                     | 0.49              |
| 1:J:20:SER:HB3   | 1:J:23:GLU:OE1   | 2.13                     | 0.49              |
| 2:K:121:LEU:O    | 2:K:128:PHE:CG   | 2.61                     | 0.49              |
| 4:W:198:TYR:CZ   | 4:W:248:ILE:HG13 | 2.48                     | 0.49              |
| 4:1:198:TYR:CZ   | 4:1:248:ILE:HG13 | 2.48                     | 0.49              |
| 1:A:720:PHE:CD2  | 1:A:744:SER:HB3  | 2.48                     | 0.49              |
| 1:D:237:THR:HG22 | 1:D:238:VAL:N    | 2.28                     | 0.49              |
| 1:D:292:MET:HE1  | 1:D:309:PRO:HD3  | 1.95                     | 0.49              |
| 1:D:310:TYR:CE2  | 1:D:320:ILE:CD1  | 2.94                     | 0.49              |
| 1:D:642:LYS:HA   | 4:5:22:ALA:C     | 2.33                     | 0.49              |
| 1:D:64:THR:CG2   | 1:D:65:GLU:N     | 2.75                     | 0.49              |
| 1:D:756:THR:O    | 1:D:758:TYR:N    | 2.45                     | 0.49              |
| 1:D:793:ARG:HH21 | 3:F:147:MET:HB3  | 1.77                     | 0.49              |
| 2:E:128:PHE:O    | 2:E:133:ILE:HD11 | 2.13                     | 0.49              |
| 1:G:20:SER:HB3   | 1:G:23:GLU:OE1   | 2.12                     | 0.49              |
| 1:G:51:THR:C     | 1:G:62:VAL:HG13  | 2.32                     | 0.49              |
| 1:G:768:MLY:HD3  | 1:G:772:LEU:HB2  | 1.94                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:312:TYR:N    | 1:J:312:TYR:CD1  | 2.81                     | 0.49              |
| 1:J:768:MLY:HH11 | 1:J:772:LEU:HD22 | 1.78                     | 0.49              |
| 1:J:753:VAL:CA   | 1:J:780:ASP:OD2  | 2.54                     | 0.49              |
| 4:X:70:PRO:HG3   | 4:X:81:ASP:HB3   | 1.94                     | 0.49              |
| 4:Y:124:PHE:CZ   | 4:Y:132:MET:HG3  | 2.48                     | 0.49              |
| 4:Z:318:THR:HA   | 4:Z:327:ILE:HG12 | 1.94                     | 0.49              |
| 4:0:318:THR:HA   | 4:0:327:ILE:HG12 | 1.94                     | 0.49              |
| 4:1:213:LYS:O    | 4:1:217:CYS:HB2  | 2.13                     | 0.49              |
| 4:3:70:PRO:HG3   | 4:3:81:ASP:HB3   | 1.94                     | 0.49              |
| 4:6:198:TYR:CZ   | 4:6:248:ILE:HG13 | 2.48                     | 0.49              |
| 1:A:103:LEU:HD12 | 1:A:103:LEU:C    | 2.33                     | 0.49              |
| 1:A:168:THR:HG22 | 1:A:169:ASP:OD1  | 2.12                     | 0.49              |
| 1:A:192:VAL:O    | 1:A:195:TYR:HB3  | 2.13                     | 0.49              |
| 1:A:251:ARG:O    | 1:A:263:ALA:HA   | 2.12                     | 0.49              |
| 1:A:346:ASP:O    | 1:A:349:THR:HB   | 2.11                     | 0.49              |
| 1:A:839:MLY:N    | 1:A:840:PRO:CD   | 2.75                     | 0.49              |
| 1:A:97:LEU:N     | 1:A:97:LEU:HD13  | 2.28                     | 0.49              |
| 1:D:51:THR:C     | 1:D:62:VAL:HG13  | 2.32                     | 0.49              |
| 1:D:831:TRP:CZ3  | 2:E:50:THR:CB    | 2.96                     | 0.49              |
| 1:G:192:VAL:O    | 1:G:195:TYR:HB3  | 2.13                     | 0.49              |
| 1:G:237:THR:HG22 | 1:G:238:VAL:N    | 2.28                     | 0.49              |
| 1:G:41:VAL:CG1   | 1:G:42:HIS:N     | 2.75                     | 0.49              |
| 2:H:114:LYS:HG3  | 2:H:137:TRP:CZ2  | 2.48                     | 0.49              |
| 1:J:251:ARG:HB2  | 1:J:264:ASP:HB3  | 1.95                     | 0.49              |
| 1:J:51:THR:C     | 1:J:62:VAL:HG13  | 2.32                     | 0.49              |
| 1:J:64:THR:CG2   | 1:J:65:GLU:N     | 2.75                     | 0.49              |
| 1:J:173:GLN:OE1  | 1:J:668:HIS:HB3  | 2.13                     | 0.49              |
| 3:L:50:LEU:O     | 3:L:55:LYS:HB2   | 2.13                     | 0.49              |
| 4:X:124:PHE:CZ   | 4:X:132:MET:HG3  | 2.48                     | 0.49              |
| 4:Y:198:TYR:CZ   | 4:Y:248:ILE:HG13 | 2.48                     | 0.49              |
| 4:5:124:PHE:CZ   | 4:5:132:MET:HG3  | 2.48                     | 0.49              |
| 4:5:70:PRO:HG3   | 4:5:81:ASP:HB3   | 1.94                     | 0.49              |
| 1:A:128:PRO:O    | 1:A:683:PRO:HB3  | 2.12                     | 0.49              |
| 1:A:218:LEU:HD22 | 1:A:222:ILE:HG13 | 1.95                     | 0.49              |
| 1:A:768:MLY:O    | 1:A:771:LEU:HB3  | 2.13                     | 0.49              |
| 2:B:114:LYS:HG3  | 2:B:137:TRP:CZ2  | 2.48                     | 0.49              |
| 3:C:50:LEU:O     | 3:C:55:LYS:HB2   | 2.13                     | 0.49              |
| 1:D:20:SER:HB3   | 1:D:23:GLU:OE1   | 2.13                     | 0.49              |
| 1:D:547:ASP:O    | 1:D:550:PHE:HB3  | 2.12                     | 0.49              |
| 1:D:769:ALA:CB   | 1:D:770:GLY:N    | 2.75                     | 0.49              |
| 1:D:839:MLY:N    | 1:D:840:PRO:CD   | 2.75                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:831:TRP:CE2  | 2:E:47:LEU:CB    | 2.93                     | 0.49              |
| 1:D:830:PRO:CB   | 2:E:67:MET:HE1   | 2.41                     | 0.49              |
| 3:F:50:LEU:O     | 3:F:55:LYS:HB2   | 2.13                     | 0.49              |
| 1:G:547:ASP:O    | 1:G:550:PHE:HB3  | 2.12                     | 0.49              |
| 1:G:95:THR:OG1   | 1:G:713:SER:CB   | 2.55                     | 0.49              |
| 1:J:290:GLN:HG2  | 1:J:331:LEU:CA   | 2.43                     | 0.49              |
| 1:J:405:ARG:HB2  | 1:J:414:THR:OG1  | 2.13                     | 0.49              |
| 1:J:720:PHE:CD2  | 1:J:744:SER:HB3  | 2.48                     | 0.49              |
| 1:J:798:LEU:HD21 | 3:L:122:GLU:O    | 2.12                     | 0.49              |
| 1:J:831:TRP:HH2  | 2:K:34:ILE:CG2   | 2.24                     | 0.49              |
| 2:K:93:PRO:O     | 2:K:97:ILE:HG13  | 2.12                     | 0.49              |
| 4:1:124:PHE:CZ   | 4:1:132:MET:HG3  | 2.48                     | 0.48              |
| 4:1:70:PRO:HG3   | 4:1:81:ASP:HB3   | 1.94                     | 0.48              |
| 4:3:124:PHE:CZ   | 4:3:132:MET:HG3  | 2.48                     | 0.48              |
| 4:3:198:TYR:CZ   | 4:3:248:ILE:HG13 | 2.48                     | 0.48              |
| 1:J:530:MET:HE3  | 4:7:354:GLN:CB   | 2.43                     | 0.48              |
| 1:A:732:ILE:HG23 | 1:A:747:LEU:HD12 | 0.95                     | 0.48              |
| 1:A:795:ARG:NE   | 3:C:43:ASN:OD1   | 2.10                     | 0.48              |
| 1:A:93:MET:HE2   | 1:A:715:VAL:HA   | 1.94                     | 0.48              |
| 1:A:813:ILE:HG22 | 2:B:127:ARG:HD2  | 1.25                     | 0.48              |
| 1:D:168:THR:HG22 | 1:D:169:ASP:OD1  | 2.12                     | 0.48              |
| 1:D:267:THR:HG21 | 1:D:438:PHE:HE2  | 1.76                     | 0.48              |
| 1:D:793:ARG:O    | 1:D:797:PHE:N    | 2.39                     | 0.48              |
| 1:D:839:MLY:HB2  | 1:D:840:PRO:HD3  | 1.94                     | 0.48              |
| 1:G:134:VAL:C    | 1:G:136:ASN:H    | 2.16                     | 0.48              |
| 1:G:168:THR:HG22 | 1:G:169:ASP:OD1  | 2.12                     | 0.48              |
| 1:G:248:MLY:HE2  | 1:G:250:ILE:HD11 | 1.95                     | 0.48              |
| 1:G:128:PRO:O    | 1:G:683:PRO:HB3  | 2.12                     | 0.48              |
| 1:G:739:ASP:OD1  | 1:G:740:SER:N    | 2.46                     | 0.48              |
| 1:G:839:MLY:HB2  | 1:G:840:PRO:HD3  | 1.94                     | 0.48              |
| 1:J:84:MLY:CH1   | 1:J:715:VAL:HG11 | 2.17                     | 0.48              |
| 4:V:124:PHE:CZ   | 4:V:132:MET:HG3  | 2.48                     | 0.48              |
| 1:A:542:PHE:CD2  | 4:4:143:TYR:CD1  | 3.02                     | 0.48              |
| 4:4:198:TYR:CZ   | 4:4:248:ILE:HG13 | 2.48                     | 0.48              |
| 1:A:530:MET:HE3  | 4:4:355:MET:SD   | 2.53                     | 0.48              |
| 4:5:198:TYR:CZ   | 4:5:248:ILE:HG13 | 2.48                     | 0.48              |
| 4:7:70:PRO:HG3   | 4:7:81:ASP:HB3   | 1.94                     | 0.48              |
| 1:G:556:ASP:CA   | 4:8:49:GLN:O     | 2.51                     | 0.48              |
| 1:A:237:THR:HG22 | 1:A:238:VAL:N    | 2.28                     | 0.48              |
| 1:A:310:TYR:CE2  | 1:A:320:ILE:CD1  | 2.94                     | 0.48              |
| 1:A:290:GLN:HG2  | 1:A:331:LEU:CA   | 2.43                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:130:PRO:O    | 2:B:131:GLU:C    | 2.52                     | 0.48              |
| 1:G:405:ARG:HB2  | 1:G:414:THR:OG1  | 2.13                     | 0.48              |
| 1:G:836:PHE:CE2  | 2:H:160:GLY:HA3  | 2.47                     | 0.48              |
| 2:H:117:LEU:HG   | 2:H:147:ASN:HB3  | 1.93                     | 0.48              |
| 1:J:215:GLN:H    | 1:J:340:ILE:CD1  | 2.20                     | 0.48              |
| 1:J:817:GLN:CD   | 2:K:127:ARG:CD   | 2.58                     | 0.48              |
| 2:K:128:PHE:O    | 2:K:133:ILE:HD11 | 2.13                     | 0.48              |
| 4:W:70:PRO:HG3   | 4:W:81:ASP:HB3   | 1.94                     | 0.48              |
| 1:G:530:MET:HE3  | 4:6:355:MET:SD   | 2.53                     | 0.48              |
| 1:J:538:GLU:HA   | 4:7:351:THR:H    | 1.77                     | 0.48              |
| 1:A:642:LYS:HA   | 4:4:22:ALA:C     | 2.34                     | 0.48              |
| 2:B:93:PRO:O     | 2:B:97:ILE:HG13  | 2.13                     | 0.48              |
| 1:D:292:MET:CE   | 1:D:309:PRO:HA   | 2.39                     | 0.48              |
| 1:D:404:PRO:HD2  | 1:D:415:MLY:O    | 2.13                     | 0.48              |
| 1:D:724:TYR:CZ   | 1:D:778:MET:CB   | 2.97                     | 0.48              |
| 1:G:93:MET:CE    | 1:G:763:THR:O    | 2.60                     | 0.48              |
| 1:G:757:GLN:HE22 | 1:G:772:LEU:CD2  | 2.27                     | 0.48              |
| 1:G:797:PHE:HB2  | 3:I:149:VAL:CG1  | 2.43                     | 0.48              |
| 1:J:404:PRO:HD2  | 1:J:415:MLY:O    | 2.13                     | 0.48              |
| 1:J:739:ASP:CB   | 1:J:742:LYS:CB   | 2.81                     | 0.48              |
| 1:J:839:MLY:N    | 1:J:840:PRO:CD   | 2.75                     | 0.48              |
| 1:J:87:MLY:HD3   | 1:J:87:MLY:HH12  | 1.61                     | 0.48              |
| 1:A:499:GLU:HA   | 1:A:499:GLU:OE1  | 2.13                     | 0.48              |
| 1:D:724:TYR:CA   | 1:D:782:MLY:CH1  | 2.90                     | 0.48              |
| 1:G:251:ARG:O    | 1:G:263:ALA:HA   | 2.12                     | 0.48              |
| 1:G:759:ALA:O    | 1:G:766:PHE:N    | 2.32                     | 0.48              |
| 2:H:128:PHE:O    | 2:H:133:ILE:HD11 | 2.13                     | 0.48              |
| 1:J:136:ASN:O    | 1:J:139:VAL:N    | 2.47                     | 0.48              |
| 1:J:168:THR:HG22 | 1:J:169:ASP:OD1  | 2.12                     | 0.48              |
| 1:J:410:ASN:HD22 | 4:7:336:LYS:HE2  | 1.78                     | 0.48              |
| 1:J:547:ASP:O    | 1:J:550:PHE:HB3  | 2.12                     | 0.48              |
| 1:J:732:ILE:HG21 | 1:J:747:LEU:CD1  | 0.63                     | 0.48              |
| 1:J:817:GLN:HG2  | 2:K:127:ARG:CD   | 2.42                     | 0.48              |
| 2:K:130:PRO:O    | 2:K:131:GLU:C    | 2.52                     | 0.48              |
| 4:V:70:PRO:HG3   | 4:V:81:ASP:HB3   | 1.94                     | 0.48              |
| 4:1:253:GLU:HA   | 4:1:256:ARG:CG   | 2.42                     | 0.48              |
| 4:2:120:THR:HG21 | 4:2:370:VAL:HG11 | 1.95                     | 0.48              |
| 1:D:530:MET:HE3  | 4:5:354:GLN:CG   | 2.32                     | 0.48              |
| 1:G:538:GLU:HA   | 4:6:351:THR:H    | 1.77                     | 0.48              |
| 4:8:213:LYS:O    | 4:8:217:CYS:HB2  | 2.13                     | 0.48              |
| 4:8:253:GLU:HA   | 4:8:256:ARG:CG   | 2.42                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:406:VAL:CG1  | 1:A:407:GLY:N    | 2.77                     | 0.48              |
| 2:B:117:LEU:HG   | 2:B:147:ASN:HB3  | 1.93                     | 0.48              |
| 1:D:405:ARG:HB2  | 1:D:414:THR:OG1  | 2.13                     | 0.48              |
| 1:D:436:MLY:HE3  | 1:D:626:TYR:HE1  | 1.77                     | 0.48              |
| 1:D:544:LYS:HD2  | 4:5:147:ARG:CB   | 2.36                     | 0.48              |
| 1:G:310:TYR:CE2  | 1:G:320:ILE:CD1  | 2.94                     | 0.48              |
| 1:G:409:GLY:N    | 1:G:636:LYS:CD   | 2.71                     | 0.48              |
| 1:G:617:MLY:O    | 1:G:620:ALA:HB3  | 2.14                     | 0.48              |
| 1:G:173:GLN:OE1  | 1:G:668:HIS:HB3  | 2.13                     | 0.48              |
| 1:G:723:ARG:HG3  | 1:G:723:ARG:HH11 | 1.78                     | 0.48              |
| 1:G:720:PHE:CD2  | 1:G:744:SER:HB3  | 2.48                     | 0.48              |
| 1:G:800:ARG:NH1  | 3:I:149:VAL:CG2  | 2.26                     | 0.48              |
| 1:J:289:TYR:OH   | 1:J:315:VAL:O    | 2.27                     | 0.48              |
| 4:2:198:TYR:CZ   | 4:2:248:ILE:HG13 | 2.48                     | 0.48              |
| 4:3:213:LYS:O    | 4:3:217:CYS:HB2  | 2.13                     | 0.48              |
| 1:D:642:LYS:CB   | 4:5:24:ASP:O     | 2.59                     | 0.48              |
| 4:6:120:THR:HG21 | 4:6:370:VAL:HG11 | 1.95                     | 0.48              |
| 4:7:213:LYS:O    | 4:7:217:CYS:HB2  | 2.13                     | 0.48              |
| 4:7:198:TYR:CZ   | 4:7:248:ILE:HG13 | 2.48                     | 0.48              |
| 1:A:10:PHE:CD2   | 1:A:17:LEU:HD23  | 2.49                     | 0.48              |
| 1:A:544:LYS:HD2  | 4:4:147:ARG:CB   | 2.36                     | 0.48              |
| 2:B:128:PHE:O    | 2:B:133:ILE:HD11 | 2.13                     | 0.48              |
| 2:B:112:ILE:CG2  | 2:B:147:ASN:O    | 2.62                     | 0.48              |
| 1:D:103:LEU:HD12 | 1:D:103:LEU:C    | 2.33                     | 0.48              |
| 1:D:314:TYR:CZ   | 1:D:362:GLY:HA2  | 2.48                     | 0.48              |
| 1:D:617:MLY:O    | 1:D:620:ALA:HB3  | 2.14                     | 0.48              |
| 1:D:838:ILE:C    | 1:D:840:PRO:HD2  | 2.34                     | 0.48              |
| 1:G:499:GLU:HA   | 1:G:499:GLU:OE1  | 2.13                     | 0.48              |
| 1:G:64:THR:CG2   | 1:G:65:GLU:N     | 2.75                     | 0.48              |
| 1:J:103:LEU:C    | 1:J:103:LEU:HD12 | 2.33                     | 0.48              |
| 1:J:267:THR:HG21 | 1:J:438:PHE:HE2  | 1.76                     | 0.48              |
| 1:J:314:TYR:CZ   | 1:J:362:GLY:HA2  | 2.48                     | 0.48              |
| 1:J:41:VAL:CG1   | 1:J:42:HIS:N     | 2.76                     | 0.48              |
| 4:V:250:ILE:HG23 | 4:V:253:GLU:HG2  | 1.96                     | 0.48              |
| 4:7:250:ILE:HG23 | 4:7:253:GLU:HG2  | 1.96                     | 0.48              |
| 1:A:405:ARG:HB2  | 1:A:414:THR:OG1  | 2.13                     | 0.48              |
| 1:A:506:GLU:OE2  | 1:A:760:PHE:HD2  | 1.97                     | 0.48              |
| 1:A:64:THR:CG2   | 1:A:65:GLU:N     | 2.75                     | 0.48              |
| 1:D:106:LEU:HD12 | 1:D:117:THR:HG21 | 1.96                     | 0.48              |
| 1:D:550:PHE:CE2  | 1:D:592:ILE:CG2  | 2.97                     | 0.48              |
| 1:D:689:GLU:O    | 1:D:689:GLU:HG2  | 2.14                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:720:PHE:CD2  | 1:D:744:SER:HB3  | 2.48                     | 0.48              |
| 1:G:103:LEU:HD12 | 1:G:103:LEU:C    | 2.33                     | 0.48              |
| 1:G:739:ASP:CB   | 1:G:742:LYS:CB   | 2.81                     | 0.48              |
| 1:G:728:ASN:ND2  | 3:I:110:VAL:HA   | 2.18                     | 0.48              |
| 1:J:10:PHE:CD2   | 1:J:17:LEU:HD23  | 2.49                     | 0.48              |
| 1:J:617:MLY:O    | 1:J:620:ALA:HB3  | 2.14                     | 0.48              |
| 1:J:707:CYS:CB   | 1:J:714:ARG:NH2  | 2.73                     | 0.48              |
| 4:V:213:LYS:O    | 4:V:217:CYS:HB2  | 2.13                     | 0.48              |
| 4:Y:253:GLU:HA   | 4:Y:256:ARG:CG   | 2.42                     | 0.48              |
| 4:O:198:TYR:CZ   | 4:O:248:ILE:HG13 | 2.48                     | 0.48              |
| 4:6:213:LYS:O    | 4:6:217:CYS:HB2  | 2.13                     | 0.48              |
| 1:D:790:THR:HA   | 3:F:87:PHE:CZ    | 2.47                     | 0.48              |
| 1:G:10:PHE:CD2   | 1:G:17:LEU:HD23  | 2.49                     | 0.48              |
| 1:G:312:TYR:CD1  | 1:G:312:TYR:N    | 2.81                     | 0.48              |
| 1:J:664:LEU:HD12 | 1:J:664:LEU:HA   | 1.52                     | 0.48              |
| 1:J:723:ARG:HH11 | 1:J:723:ARG:HG3  | 1.78                     | 0.48              |
| 2:K:137:TRP:CA   | 2:K:145:ALA:CB   | 2.82                     | 0.48              |
| 4:X:250:ILE:HG23 | 4:X:253:GLU:HG2  | 1.96                     | 0.48              |
| 4:Y:70:PRO:HG3   | 4:Y:81:ASP:HB3   | 1.94                     | 0.48              |
| 4:Z:198:TYR:CZ   | 4:Z:248:ILE:HG13 | 2.48                     | 0.48              |
| 4:O:250:ILE:HG23 | 4:O:253:GLU:HG2  | 1.96                     | 0.48              |
| 4:1:120:THR:HG21 | 4:1:370:VAL:HG11 | 1.95                     | 0.48              |
| 4:2:250:ILE:HG23 | 4:2:253:GLU:HG2  | 1.96                     | 0.48              |
| 4:4:120:THR:HG21 | 4:4:370:VAL:HG11 | 1.95                     | 0.48              |
| 4:6:250:ILE:HG23 | 4:6:253:GLU:HG2  | 1.96                     | 0.48              |
| 1:A:765:VAL:CG1  | 1:A:766:PHE:N    | 2.77                     | 0.48              |
| 1:D:723:ARG:HG3  | 1:D:723:ARG:HH11 | 1.79                     | 0.48              |
| 1:D:806:MET:SD   | 3:F:17:PHE:HE2   | 2.37                     | 0.48              |
| 1:D:818:TYR:CD2  | 2:E:89:LYS:O     | 2.63                     | 0.48              |
| 1:G:635:GLY:HA3  | 4:6:334:GLU:CG   | 2.30                     | 0.48              |
| 1:G:838:ILE:C    | 1:G:840:PRO:HD2  | 2.34                     | 0.48              |
| 1:G:97:LEU:N     | 1:G:97:LEU:HD13  | 2.28                     | 0.48              |
| 2:H:130:PRO:O    | 2:H:131:GLU:C    | 2.52                     | 0.48              |
| 2:H:140:PHE:HB3  | 2:H:144:VAL:HG12 | 1.95                     | 0.48              |
| 1:G:823:PHE:CZ   | 2:H:156:VAL:HG12 | 2.48                     | 0.48              |
| 1:J:768:MLY:HE2  | 1:J:772:LEU:HD23 | 1.95                     | 0.48              |
| 4:V:198:TYR:CZ   | 4:V:248:ILE:HG13 | 2.48                     | 0.48              |
| 4:X:198:TYR:CZ   | 4:X:248:ILE:HG13 | 2.48                     | 0.48              |
| 4:W:288:ASP:CA   | 4:Y:204:ALA:HB2  | 2.31                     | 0.48              |
| 4:Y:213:LYS:O    | 4:Y:217:CYS:HB2  | 2.13                     | 0.48              |
| 4:Z:250:ILE:HG23 | 4:Z:253:GLU:HG2  | 1.96                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:0:120:THR:HG21 | 4:0:370:VAL:HG11 | 1.95                     | 0.48              |
| 4:1:250:ILE:HG23 | 4:1:253:GLU:HG2  | 1.96                     | 0.48              |
| 4:4:250:ILE:HG23 | 4:4:253:GLU:HG2  | 1.96                     | 0.48              |
| 1:A:410:ASN:HD22 | 4:4:336:LYS:HE2  | 1.78                     | 0.48              |
| 4:5:250:ILE:HG23 | 4:5:253:GLU:HG2  | 1.96                     | 0.48              |
| 4:8:120:THR:HG21 | 4:8:370:VAL:HG11 | 1.95                     | 0.48              |
| 1:A:248:MLY:HE2  | 1:A:250:ILE:HD11 | 1.95                     | 0.48              |
| 1:A:546:THR:CG2  | 1:A:547:ASP:N    | 2.77                     | 0.48              |
| 1:A:550:PHE:CE2  | 1:A:592:ILE:CG2  | 2.97                     | 0.48              |
| 1:A:617:MLY:O    | 1:A:620:ALA:HB3  | 2.14                     | 0.48              |
| 1:A:664:LEU:HD12 | 1:A:664:LEU:HA   | 1.53                     | 0.48              |
| 1:A:689:GLU:O    | 1:A:689:GLU:HG2  | 2.14                     | 0.48              |
| 1:A:723:ARG:HH11 | 1:A:723:ARG:HG3  | 1.78                     | 0.48              |
| 1:D:312:TYR:CD1  | 1:D:312:TYR:N    | 2.81                     | 0.48              |
| 1:D:578:HIS:HB3  | 1:D:592:ILE:CD1  | 2.38                     | 0.48              |
| 1:D:830:PRO:HG2  | 2:E:67:MET:HE3   | 0.48                     | 0.48              |
| 1:D:792:ALA:HB2  | 3:F:40:ASN:O     | 2.10                     | 0.48              |
| 1:J:134:VAL:C    | 1:J:136:ASN:H    | 2.16                     | 0.48              |
| 1:J:757:GLN:OE1  | 1:J:773:GLY:HA2  | 2.14                     | 0.48              |
| 2:K:121:LEU:HA   | 2:K:128:PHE:CD2  | 2.46                     | 0.48              |
| 4:V:253:GLU:HA   | 4:V:256:ARG:CG   | 2.42                     | 0.48              |
| 4:3:250:ILE:HG23 | 4:3:253:GLU:HG2  | 1.96                     | 0.47              |
| 4:3:120:THR:HG21 | 4:3:370:VAL:HG11 | 1.95                     | 0.47              |
| 1:J:542:PHE:CD2  | 4:7:143:TYR:CD1  | 3.02                     | 0.47              |
| 1:J:636:LYS:O    | 4:7:144:ALA:HB1  | 2.14                     | 0.47              |
| 4:8:250:ILE:HG23 | 4:8:253:GLU:HG2  | 1.96                     | 0.47              |
| 1:A:602:PRO:O    | 1:A:603:LEU:HD12 | 2.14                     | 0.47              |
| 1:A:640:LYS:HD2  | 1:A:646:PHE:O    | 2.14                     | 0.47              |
| 1:D:10:PHE:CD2   | 1:D:17:LEU:HD23  | 2.49                     | 0.47              |
| 1:D:542:PHE:CD2  | 4:5:143:TYR:CD1  | 3.02                     | 0.47              |
| 1:D:546:THR:CG2  | 1:D:547:ASP:N    | 2.77                     | 0.47              |
| 1:D:568:PRO:HD3  | 1:D:579:PHE:HA   | 1.96                     | 0.47              |
| 2:E:137:TRP:CA   | 2:E:145:ALA:CB   | 2.82                     | 0.47              |
| 2:E:160:GLY:O    | 2:E:161:GLU:HG2  | 2.14                     | 0.47              |
| 1:G:530:MET:CE   | 4:6:354:GLN:HG3  | 2.34                     | 0.47              |
| 1:G:544:LYS:HD2  | 4:6:147:ARG:CB   | 2.36                     | 0.47              |
| 1:G:707:CYS:CB   | 1:G:714:ARG:NH1  | 2.45                     | 0.47              |
| 2:H:121:LEU:O    | 2:H:128:PHE:CG   | 2.61                     | 0.47              |
| 1:J:550:PHE:CE2  | 1:J:592:ILE:CG2  | 2.97                     | 0.47              |
| 1:J:768:MLY:CE   | 1:J:772:LEU:HD23 | 2.44                     | 0.47              |
| 1:J:84:MLY:HH12  | 1:J:715:VAL:HG12 | 1.84                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:112:ILE:CG2  | 2:K:147:ASN:O    | 2.62                     | 0.47              |
| 4:W:213:LYS:O    | 4:W:217:CYS:HB2  | 2.13                     | 0.47              |
| 4:W:250:ILE:HG23 | 4:W:253:GLU:HG2  | 1.96                     | 0.47              |
| 4:Y:250:ILE:HG23 | 4:Y:253:GLU:HG2  | 1.96                     | 0.47              |
| 4:5:120:THR:HG21 | 4:5:370:VAL:HG11 | 1.95                     | 0.47              |
| 1:A:218:LEU:HA   | 1:A:221:GLN:H    | 1.79                     | 0.47              |
| 1:A:501:GLU:CA   | 1:A:762:HIS:CE1  | 2.97                     | 0.47              |
| 1:A:783:LEU:HA   | 1:A:786:ILE:HB   | 1.96                     | 0.47              |
| 2:B:160:GLY:O    | 2:B:161:GLU:HG2  | 2.14                     | 0.47              |
| 1:D:154:HIS:CE1  | 1:D:156:PHE:CE2  | 3.02                     | 0.47              |
| 1:D:602:PRO:O    | 1:D:603:LEU:HD12 | 2.14                     | 0.47              |
| 1:D:97:LEU:N     | 1:D:97:LEU:HD13  | 2.28                     | 0.47              |
| 2:E:144:VAL:HG12 | 2:E:153:ILE:HD13 | 1.92                     | 0.47              |
| 1:G:410:ASN:HD22 | 4:6:336:LYS:HE2  | 1.79                     | 0.47              |
| 1:G:550:PHE:CE2  | 1:G:592:ILE:CG2  | 2.97                     | 0.47              |
| 1:G:564:ASN:HD22 | 1:G:582:VAL:HB   | 1.79                     | 0.47              |
| 1:G:629:GLU:CA   | 1:G:643:GLY:C    | 2.73                     | 0.47              |
| 1:G:640:LYS:HD2  | 1:G:646:PHE:O    | 2.14                     | 0.47              |
| 1:G:701:LEU:HD12 | 1:G:701:LEU:HA   | 1.55                     | 0.47              |
| 1:G:795:ARG:HB2  | 3:I:35:ARG:CZ    | 2.44                     | 0.47              |
| 1:G:826:VAL:HG21 | 2:H:88:LEU:CD2   | 2.43                     | 0.47              |
| 1:J:218:LEU:CD2  | 1:J:222:ILE:CG1  | 2.86                     | 0.47              |
| 1:J:765:VAL:CG1  | 1:J:766:PHE:N    | 2.77                     | 0.47              |
| 4:X:213:LYS:O    | 4:X:217:CYS:HB2  | 2.13                     | 0.47              |
| 4:Y:120:THR:HG21 | 4:Y:370:VAL:HG11 | 1.95                     | 0.47              |
| 4:X:287:ILE:CB   | 4:Z:204:ALA:H    | 2.13                     | 0.47              |
| 4:Z:120:THR:HG21 | 4:Z:370:VAL:HG11 | 1.95                     | 0.47              |
| 4:0:213:LYS:O    | 4:0:217:CYS:HB2  | 2.13                     | 0.47              |
| 1:A:538:GLU:HA   | 4:4:351:THR:H    | 1.78                     | 0.47              |
| 1:A:314:TYR:CZ   | 1:A:362:GLY:HA2  | 2.48                     | 0.47              |
| 1:G:314:TYR:CZ   | 1:G:362:GLY:HA2  | 2.48                     | 0.47              |
| 1:G:546:THR:CG2  | 1:G:547:ASP:N    | 2.77                     | 0.47              |
| 1:G:793:ARG:O    | 1:G:797:PHE:N    | 2.39                     | 0.47              |
| 1:J:546:THR:CG2  | 1:J:547:ASP:N    | 2.77                     | 0.47              |
| 1:J:564:ASN:HD22 | 1:J:582:VAL:HB   | 1.79                     | 0.47              |
| 4:Z:213:LYS:O    | 4:Z:217:CYS:HB2  | 2.13                     | 0.47              |
| 4:5:213:LYS:O    | 4:5:217:CYS:HB2  | 2.13                     | 0.47              |
| 1:D:410:ASN:HD22 | 4:5:336:LYS:HE2  | 1.78                     | 0.47              |
| 1:A:122:PHE:CE2  | 1:A:700:VAL:HA   | 2.49                     | 0.47              |
| 1:A:595:TRP:CD1  | 1:A:595:TRP:N    | 2.80                     | 0.47              |
| 1:D:188:ASN:ND2  | 1:D:674:CYS:SG   | 2.88                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:564:ASN:HD22 | 1:D:582:VAL:HB   | 1.79                     | 0.47              |
| 1:D:765:VAL:CG1  | 1:D:766:PHE:N    | 2.77                     | 0.47              |
| 1:D:834:LEU:CD2  | 2:E:50:THR:HG22  | 2.44                     | 0.47              |
| 1:G:154:HIS:CE1  | 1:G:156:PHE:CE2  | 3.02                     | 0.47              |
| 1:G:22:LYS:O     | 1:G:26:GLU:N     | 2.29                     | 0.47              |
| 1:G:408:VAL:HG22 | 1:G:636:LYS:HG2  | 1.51                     | 0.47              |
| 1:G:725:ARG:CG   | 1:G:733:PRO:HA   | 2.43                     | 0.47              |
| 1:G:93:MET:CE    | 1:G:764:MLY:CG   | 2.88                     | 0.47              |
| 1:G:798:LEU:CD1  | 3:I:126:LEU:HD23 | 2.12                     | 0.47              |
| 2:H:160:GLY:O    | 2:H:161:GLU:HG2  | 2.15                     | 0.47              |
| 1:J:214:MET:C    | 1:J:340:ILE:CD1  | 2.82                     | 0.47              |
| 1:J:436:MLY:HE3  | 1:J:626:TYR:HE1  | 1.77                     | 0.47              |
| 2:K:140:PHE:HB3  | 2:K:144:VAL:HG12 | 1.94                     | 0.47              |
| 3:L:53:PRO:O     | 3:L:55:LYS:HG3   | 2.15                     | 0.47              |
| 1:J:786:ILE:CD1  | 3:L:86:ASP:HB3   | 2.45                     | 0.47              |
| 4:V:162:ASN:OD1  | 4:V:277:THR:HG22 | 2.15                     | 0.47              |
| 4:2:213:LYS:O    | 4:2:217:CYS:HB2  | 2.13                     | 0.47              |
| 4:3:162:ASN:OD1  | 4:3:277:THR:HG22 | 2.15                     | 0.47              |
| 4:5:288:ASP:CA   | 4:7:204:ALA:HB2  | 2.31                     | 0.47              |
| 4:7:162:ASN:OD1  | 4:7:277:THR:HG22 | 2.15                     | 0.47              |
| 4:8:162:ASN:OD1  | 4:8:277:THR:HG22 | 2.15                     | 0.47              |
| 1:A:136:ASN:O    | 1:A:139:VAL:N    | 2.47                     | 0.47              |
| 1:A:154:HIS:CE1  | 1:A:156:PHE:CE2  | 3.02                     | 0.47              |
| 1:A:176:LEU:CD1  | 1:A:176:LEU:N    | 2.74                     | 0.47              |
| 1:A:404:PRO:HD2  | 1:A:415:MLY:O    | 2.13                     | 0.47              |
| 1:A:646:PHE:HE2  | 1:A:652:LEU:CG   | 2.24                     | 0.47              |
| 1:A:838:ILE:C    | 1:A:840:PRO:HD2  | 2.35                     | 0.47              |
| 2:B:139:ALA:C    | 2:B:141:PRO:HD3  | 2.33                     | 0.47              |
| 1:D:636:LYS:O    | 4:5:144:ALA:HB1  | 2.14                     | 0.47              |
| 1:G:106:LEU:HD12 | 1:G:117:THR:HG21 | 1.96                     | 0.47              |
| 1:G:295:MLY:HG3  | 1:G:332:MET:HE2  | 1.94                     | 0.47              |
| 1:G:602:PRO:O    | 1:G:603:LEU:HD12 | 2.14                     | 0.47              |
| 1:G:664:LEU:HD12 | 1:G:664:LEU:HA   | 1.53                     | 0.47              |
| 2:H:112:ILE:CG2  | 2:H:147:ASN:O    | 2.62                     | 0.47              |
| 1:G:819:ASN:CB   | 2:H:92:ASP:HB2   | 2.41                     | 0.47              |
| 1:J:629:GLU:CA   | 1:J:643:GLY:C    | 2.73                     | 0.47              |
| 4:4:213:LYS:O    | 4:4:217:CYS:HB2  | 2.13                     | 0.47              |
| 4:7:120:THR:HG21 | 4:7:370:VAL:HG11 | 1.95                     | 0.47              |
| 1:A:214:MET:C    | 1:A:340:ILE:CD1  | 2.82                     | 0.47              |
| 1:D:499:GLU:OE1  | 1:D:499:GLU:HA   | 2.13                     | 0.47              |
| 1:D:640:LYS:HD2  | 1:D:646:PHE:O    | 2.15                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:715:VAL:HG11 | 1:D:720:PHE:CD1  | 2.50                     | 0.47              |
| 2:E:130:PRO:O    | 2:E:131:GLU:C    | 2.52                     | 0.47              |
| 1:G:122:PHE:CE2  | 1:G:700:VAL:HA   | 2.50                     | 0.47              |
| 1:G:292:MET:HE1  | 1:G:309:PRO:HD3  | 1.97                     | 0.47              |
| 1:G:542:PHE:CD2  | 4:6:143:TYR:CD1  | 3.03                     | 0.47              |
| 1:J:188:ASN:ND2  | 1:J:674:CYS:SG   | 2.88                     | 0.47              |
| 1:J:406:VAL:CG1  | 1:J:407:GLY:N    | 2.77                     | 0.47              |
| 1:J:689:GLU:O    | 1:J:689:GLU:HG2  | 2.14                     | 0.47              |
| 1:J:838:ILE:C    | 1:J:840:PRO:HD2  | 2.35                     | 0.47              |
| 4:W:120:THR:HG21 | 4:W:370:VAL:HG11 | 1.95                     | 0.47              |
| 4:X:162:ASN:OD1  | 4:X:277:THR:HG22 | 2.15                     | 0.47              |
| 4:Y:162:ASN:OD1  | 4:Y:277:THR:HG22 | 2.15                     | 0.47              |
| 4:Z:162:ASN:OD1  | 4:Z:277:THR:HG22 | 2.15                     | 0.47              |
| 1:D:642:LYS:HB2  | 4:5:24:ASP:O     | 1.88                     | 0.47              |
| 4:5:162:ASN:OD1  | 4:5:277:THR:HG22 | 2.15                     | 0.47              |
| 4:6:253:GLU:HA   | 4:6:256:ARG:CG   | 2.42                     | 0.47              |
| 1:A:505:MLY:HB2  | 1:A:761:GLY:HA2  | 1.96                     | 0.47              |
| 1:D:524:GLU:HB3  | 1:D:528:MLY:HG2  | 1.97                     | 0.47              |
| 1:D:675:ILE:CG2  | 1:D:676:ILE:N    | 2.74                     | 0.47              |
| 1:D:724:TYR:HD1  | 1:D:727:LEU:CD1  | 2.27                     | 0.47              |
| 2:E:139:ALA:C    | 2:E:141:PRO:HD3  | 2.33                     | 0.47              |
| 1:G:214:MET:HA   | 1:G:340:ILE:CD1  | 2.41                     | 0.47              |
| 1:G:215:GLN:H    | 1:G:340:ILE:CD1  | 2.20                     | 0.47              |
| 1:G:418:THR:CB   | 1:G:421:GLU:HG3  | 2.37                     | 0.47              |
| 1:G:689:GLU:HG2  | 1:G:689:GLU:O    | 2.14                     | 0.47              |
| 1:G:695:LEU:HB3  | 1:G:701:LEU:HD22 | 1.97                     | 0.47              |
| 1:G:84:MLY:NZ    | 1:G:719:ASP:O    | 2.18                     | 0.47              |
| 1:J:154:HIS:CE1  | 1:J:156:PHE:CE2  | 3.02                     | 0.47              |
| 1:J:519:LEU:CD1  | 1:J:519:LEU:N    | 2.77                     | 0.47              |
| 1:J:524:GLU:HB3  | 1:J:528:MLY:HG2  | 1.97                     | 0.47              |
| 1:J:554:LEU:HA   | 1:J:554:LEU:HD12 | 1.77                     | 0.47              |
| 1:J:568:PRO:HD3  | 1:J:579:PHE:HA   | 1.96                     | 0.47              |
| 1:J:602:PRO:O    | 1:J:603:LEU:HD12 | 2.14                     | 0.47              |
| 1:J:749:GLY:O    | 3:L:114:LEU:HD22 | 2.12                     | 0.47              |
| 1:J:510:TRP:CD2  | 1:J:768:MLY:HH13 | 2.50                     | 0.47              |
| 4:X:120:THR:HG21 | 4:X:370:VAL:HG11 | 1.95                     | 0.47              |
| 4:0:162:ASN:OD1  | 4:0:277:THR:HG22 | 2.15                     | 0.47              |
| 1:A:400:ALA:HB1  | 1:A:606:THR:CG2  | 2.45                     | 0.47              |
| 1:A:732:ILE:CG2  | 1:A:747:LEU:CD1  | 0.65                     | 0.47              |
| 1:D:248:MLY:HE2  | 1:D:250:ILE:HD11 | 1.96                     | 0.47              |
| 1:D:311:ASP:CB   | 1:D:312:TYR:CE1  | 2.98                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:214:MET:C    | 1:D:340:ILE:CD1  | 2.82                     | 0.47              |
| 1:D:783:LEU:HA   | 1:D:786:ILE:HB   | 1.97                     | 0.47              |
| 3:F:53:PRO:O     | 3:F:55:LYS:HG3   | 2.14                     | 0.47              |
| 1:G:406:VAL:CG1  | 1:G:407:GLY:N    | 2.77                     | 0.47              |
| 1:G:595:TRP:N    | 1:G:595:TRP:CD1  | 2.80                     | 0.47              |
| 1:G:84:MLY:HH11  | 1:G:719:ASP:C    | 2.33                     | 0.47              |
| 1:G:765:VAL:CG1  | 1:G:766:PHE:N    | 2.77                     | 0.47              |
| 2:H:121:LEU:HA   | 2:H:128:PHE:CD2  | 2.47                     | 0.47              |
| 1:J:406:VAL:CG1  | 1:J:407:GLY:H    | 2.28                     | 0.47              |
| 2:K:139:ALA:C    | 2:K:141:PRO:HD3  | 2.33                     | 0.47              |
| 2:K:137:TRP:CZ3  | 2:K:145:ALA:N    | 2.81                     | 0.47              |
| 4:3:253:GLU:HA   | 4:3:256:ARG:CG   | 2.42                     | 0.47              |
| 1:A:538:GLU:OE1  | 4:4:355:MET:HE3  | 2.15                     | 0.47              |
| 1:A:406:VAL:CG1  | 1:A:407:GLY:H    | 2.28                     | 0.47              |
| 1:A:564:ASN:HD22 | 1:A:582:VAL:HB   | 1.79                     | 0.47              |
| 1:D:496:PHE:CE2  | 1:D:514:ASP:HA   | 2.50                     | 0.47              |
| 1:D:400:ALA:HB1  | 1:D:606:THR:CG2  | 2.45                     | 0.47              |
| 1:D:629:GLU:CB   | 1:D:645:SER:N    | 2.74                     | 0.47              |
| 1:D:732:ILE:CG2  | 1:D:747:LEU:CD1  | 0.65                     | 0.47              |
| 1:G:251:ARG:HB2  | 1:G:264:ASP:HB3  | 1.95                     | 0.47              |
| 1:G:404:PRO:HD2  | 1:G:415:MLY:O    | 2.13                     | 0.47              |
| 1:G:543:PRO:HD2  | 4:6:146:GLY:O    | 2.15                     | 0.47              |
| 1:J:499:GLU:OE1  | 1:J:499:GLU:HA   | 2.13                     | 0.47              |
| 1:J:496:PHE:CE2  | 1:J:514:ASP:HA   | 2.50                     | 0.47              |
| 1:J:725:ARG:NE   | 1:J:733:PRO:CB   | 1.95                     | 0.47              |
| 4:2:162:ASN:OD1  | 4:2:277:THR:HG22 | 2.15                     | 0.47              |
| 1:D:543:PRO:HD2  | 4:5:146:GLY:O    | 2.15                     | 0.47              |
| 1:G:538:GLU:CD   | 4:6:355:MET:HE1  | 2.25                     | 0.47              |
| 1:A:524:GLU:HB3  | 1:A:528:MLY:HG2  | 1.96                     | 0.47              |
| 1:A:732:ILE:HG21 | 1:A:747:LEU:CD1  | 0.64                     | 0.47              |
| 1:A:768:MLY:CA   | 1:A:771:LEU:HB2  | 2.43                     | 0.47              |
| 1:A:839:MLY:NZ   | 2:B:159:HIS:CB   | 2.62                     | 0.47              |
| 1:D:406:VAL:CG1  | 1:D:407:GLY:N    | 2.77                     | 0.47              |
| 1:D:695:LEU:HB3  | 1:D:701:LEU:HD22 | 1.97                     | 0.47              |
| 1:D:809:ARG:NH1  | 2:E:124:GLY:C    | 2.68                     | 0.47              |
| 2:E:112:ILE:CG2  | 2:E:147:ASN:O    | 2.62                     | 0.47              |
| 1:G:202:SER:HA   | 1:G:207:LYS:NZ   | 2.22                     | 0.47              |
| 1:G:406:VAL:CG1  | 1:G:407:GLY:H    | 2.28                     | 0.47              |
| 1:G:793:ARG:HB2  | 3:I:40:ASN:ND2   | 2.30                     | 0.47              |
| 1:G:831:TRP:CZ2  | 2:H:67:MET:CB    | 2.98                     | 0.47              |
| 1:J:311:ASP:CB   | 1:J:312:TYR:CE1  | 2.98                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:578:HIS:HB3  | 1:J:592:ILE:CD1  | 2.38                     | 0.47              |
| 1:J:400:ALA:HB1  | 1:J:606:THR:CG2  | 2.45                     | 0.47              |
| 1:J:84:MLY:HG2   | 1:J:719:ASP:OD2  | 2.14                     | 0.47              |
| 4:4:162:ASN:OD1  | 4:4:277:THR:HG22 | 2.15                     | 0.47              |
| 4:4:324:THR:O    | 4:6:244:ASP:HA   | 2.08                     | 0.47              |
| 4:4:299:MET:HE2  | 4:4:331:ALA:HB2  | 1.96                     | 0.47              |
| 1:A:144:ARG:HA   | 1:A:144:ARG:HD2  | 1.78                     | 0.47              |
| 1:A:202:SER:HA   | 1:A:207:LYS:NZ   | 2.22                     | 0.47              |
| 1:A:265:ILE:CG2  | 1:A:266:GLU:N    | 2.78                     | 0.47              |
| 1:A:292:MET:HE1  | 1:A:309:PRO:HD3  | 1.97                     | 0.47              |
| 1:A:636:LYS:O    | 4:4:144:ALA:HB1  | 2.15                     | 0.47              |
| 1:A:810:ARG:HG2  | 1:A:810:ARG:NH1  | 2.29                     | 0.47              |
| 1:D:221:GLN:H    | 1:D:221:GLN:HG2  | 1.47                     | 0.47              |
| 1:D:30:MLY:HB3   | 1:D:31:PRO:HD2   | 1.97                     | 0.47              |
| 1:G:188:ASN:ND2  | 1:G:674:CYS:SG   | 2.88                     | 0.47              |
| 1:J:106:LEU:HD12 | 1:J:117:THR:HG21 | 1.96                     | 0.47              |
| 1:J:640:LYS:HD2  | 1:J:646:PHE:O    | 2.15                     | 0.47              |
| 3:L:50:LEU:O     | 3:L:53:PRO:CD    | 2.63                     | 0.47              |
| 4:V:120:THR:HG21 | 4:V:370:VAL:HG11 | 1.95                     | 0.47              |
| 4:2:299:MET:HE2  | 4:2:331:ALA:HB2  | 1.97                     | 0.46              |
| 4:6:162:ASN:OD1  | 4:6:277:THR:HG22 | 2.15                     | 0.46              |
| 1:D:556:ASP:CA   | 4:7:49:GLN:O     | 2.52                     | 0.46              |
| 1:A:251:ARG:HB2  | 1:A:264:ASP:HB3  | 1.95                     | 0.46              |
| 2:B:88:LEU:HB3   | 2:B:91:ALA:HB2   | 1.97                     | 0.46              |
| 3:C:53:PRO:O     | 3:C:55:LYS:HG3   | 2.15                     | 0.46              |
| 1:D:406:VAL:CG1  | 1:D:407:GLY:H    | 2.28                     | 0.46              |
| 1:G:214:MET:C    | 1:G:340:ILE:CD1  | 2.82                     | 0.46              |
| 1:G:559:LEU:HD23 | 1:G:560:GLY:N    | 2.30                     | 0.46              |
| 1:G:568:PRO:HD3  | 1:G:579:PHE:HA   | 1.97                     | 0.46              |
| 1:G:640:LYS:HB3  | 1:G:645:SER:CB   | 2.42                     | 0.46              |
| 1:G:823:PHE:CD1  | 2:H:157:ILE:HA   | 2.50                     | 0.46              |
| 1:J:122:PHE:CE2  | 1:J:700:VAL:HA   | 2.50                     | 0.46              |
| 1:J:248:MLY:HE2  | 1:J:250:ILE:HD11 | 1.95                     | 0.46              |
| 1:J:374:GLN:NE2  | 1:J:403:TYR:CE1  | 2.84                     | 0.46              |
| 1:J:640:LYS:C    | 4:7:23:GLY:C     | 2.74                     | 0.46              |
| 1:J:800:ARG:HD2  | 3:L:149:VAL:CA   | 2.45                     | 0.46              |
| 1:J:839:MLY:HH21 | 2:K:158:THR:HG22 | 1.97                     | 0.46              |
| 4:1:162:ASN:OD1  | 4:1:277:THR:HG22 | 2.15                     | 0.46              |
| 4:1:299:MET:HE2  | 4:1:331:ALA:HB2  | 1.96                     | 0.46              |
| 4:6:299:MET:HE2  | 4:6:331:ALA:HB2  | 1.96                     | 0.46              |
| 4:8:299:MET:HE2  | 4:8:331:ALA:HB2  | 1.95                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:188:ASN:ND2  | 1:A:674:CYS:SG   | 2.88                     | 0.46              |
| 1:A:332:MET:O    | 1:A:336:SER:OG   | 2.27                     | 0.46              |
| 1:A:640:LYS:HB3  | 1:A:645:SER:CB   | 2.42                     | 0.46              |
| 2:B:121:LEU:O    | 2:B:128:PHE:CG   | 2.61                     | 0.46              |
| 1:A:836:PHE:CD2  | 2:B:160:GLY:C    | 2.88                     | 0.46              |
| 1:D:122:PHE:CE2  | 1:D:700:VAL:HA   | 2.50                     | 0.46              |
| 1:D:732:ILE:HG23 | 1:D:747:LEU:CD1  | 1.04                     | 0.46              |
| 1:D:809:ARG:CZ   | 2:E:124:GLY:HA2  | 2.35                     | 0.46              |
| 1:D:831:TRP:CE3  | 2:E:34:ILE:HD13  | 2.50                     | 0.46              |
| 1:G:646:PHE:HE2  | 1:G:652:LEU:CG   | 2.24                     | 0.46              |
| 1:G:715:VAL:HG11 | 1:G:720:PHE:CD1  | 2.49                     | 0.46              |
| 1:G:724:TYR:HD1  | 1:G:727:LEU:CD1  | 2.27                     | 0.46              |
| 1:J:206:LYS:HD2  | 1:J:217:THR:CG2  | 2.17                     | 0.46              |
| 1:J:42:HIS:O     | 1:J:45:GLN:O     | 2.33                     | 0.46              |
| 1:J:529:PRO:HB2  | 4:7:354:GLN:HB3  | 1.98                     | 0.46              |
| 1:J:629:GLU:HG2  | 1:J:643:GLY:C    | 2.35                     | 0.46              |
| 1:J:714:ARG:HD3  | 1:J:766:PHE:CE2  | 2.50                     | 0.46              |
| 4:Y:299:MET:HE2  | 4:Y:331:ALA:HB2  | 1.96                     | 0.46              |
| 4:5:6:THR:HG22   | 4:5:101:HIS:HA   | 1.97                     | 0.46              |
| 1:D:643:GLY:N    | 4:5:23:GLY:C     | 2.55                     | 0.46              |
| 1:D:530:MET:HE3  | 4:5:354:GLN:CB   | 2.44                     | 0.46              |
| 4:7:6:THR:HG22   | 4:7:101:HIS:HA   | 1.98                     | 0.46              |
| 1:A:106:LEU:HD12 | 1:A:117:THR:HG21 | 1.96                     | 0.46              |
| 1:A:292:MET:HE1  | 1:A:309:PRO:CG   | 2.46                     | 0.46              |
| 1:A:41:VAL:CG1   | 1:A:42:HIS:N     | 2.76                     | 0.46              |
| 1:A:42:HIS:O     | 1:A:45:GLN:O     | 2.33                     | 0.46              |
| 1:A:714:ARG:HD3  | 1:A:766:PHE:CE2  | 2.50                     | 0.46              |
| 1:A:800:ARG:CZ   | 3:C:149:VAL:O    | 2.63                     | 0.46              |
| 1:D:42:HIS:O     | 1:D:45:GLN:O     | 2.33                     | 0.46              |
| 1:D:540:CYS:N    | 4:5:349:LEU:HD11 | 2.31                     | 0.46              |
| 1:D:715:VAL:CG1  | 1:D:720:PHE:HB2  | 2.46                     | 0.46              |
| 1:D:809:ARG:NH1  | 2:E:124:GLY:O    | 2.48                     | 0.46              |
| 1:D:815:CYS:O    | 2:E:90:GLY:C     | 2.53                     | 0.46              |
| 1:D:831:TRP:CA   | 2:E:51:PHE:CZ    | 2.98                     | 0.46              |
| 1:G:218:LEU:HA   | 1:G:221:GLN:H    | 1.79                     | 0.46              |
| 1:G:715:VAL:CG1  | 1:G:720:PHE:HB2  | 2.45                     | 0.46              |
| 3:I:53:PRO:O     | 3:I:55:LYS:HG3   | 2.15                     | 0.46              |
| 1:J:559:LEU:HD23 | 1:J:560:GLY:N    | 2.30                     | 0.46              |
| 1:J:715:VAL:CG1  | 1:J:720:PHE:HB2  | 2.45                     | 0.46              |
| 1:J:800:ARG:CB   | 3:L:149:VAL:HG23 | 2.26                     | 0.46              |
| 2:K:160:GLY:O    | 2:K:161:GLU:HG2  | 2.15                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:163:ALA:O    | 2:K:21:GLU:N     | 2.47                     | 0.46              |
| 4:V:6:THR:HG22   | 4:V:101:HIS:HA   | 1.97                     | 0.46              |
| 1:D:543:PRO:CD   | 4:5:143:TYR:O    | 2.64                     | 0.46              |
| 4:4:287:ILE:CB   | 4:6:204:ALA:H    | 2.13                     | 0.46              |
| 1:J:540:CYS:N    | 4:7:349:LEU:HD11 | 2.31                     | 0.46              |
| 1:A:559:LEU:HD23 | 1:A:560:GLY:N    | 2.30                     | 0.46              |
| 1:A:715:VAL:CG1  | 1:A:720:PHE:HB2  | 2.45                     | 0.46              |
| 1:A:724:TYR:HD1  | 1:A:727:LEU:CD1  | 2.27                     | 0.46              |
| 1:D:218:LEU:HA   | 1:D:221:GLN:H    | 1.79                     | 0.46              |
| 1:D:374:GLN:NE2  | 1:D:403:TYR:CE1  | 2.84                     | 0.46              |
| 1:D:595:TRP:CD1  | 1:D:595:TRP:N    | 2.80                     | 0.46              |
| 1:D:640:LYS:HB3  | 1:D:645:SER:CB   | 2.42                     | 0.46              |
| 1:D:714:ARG:HD3  | 1:D:766:PHE:CE2  | 2.50                     | 0.46              |
| 1:D:769:ALA:C    | 1:D:771:LEU:HA   | 2.36                     | 0.46              |
| 1:G:139:VAL:HG12 | 1:G:143:TYR:HD2  | 1.81                     | 0.46              |
| 1:G:784:ALA:O    | 1:G:788:THR:CA   | 2.62                     | 0.46              |
| 1:J:797:PHE:CD2  | 3:L:126:LEU:HD22 | 2.50                     | 0.46              |
| 1:J:82:PRO:HG2   | 1:J:85:TYR:CE2   | 2.50                     | 0.46              |
| 1:J:797:PHE:CE2  | 3:L:126:LEU:CD2  | 2.99                     | 0.46              |
| 1:A:543:PRO:HD2  | 4:4:146:GLY:O    | 2.15                     | 0.46              |
| 1:D:529:PRO:HB2  | 4:5:354:GLN:HB3  | 1.98                     | 0.46              |
| 1:A:136:ASN:HA   | 1:A:137:PRO:HD3  | 1.50                     | 0.46              |
| 1:A:374:GLN:NE2  | 1:A:403:TYR:CE1  | 2.84                     | 0.46              |
| 1:A:568:PRO:HD3  | 1:A:579:PHE:HA   | 1.97                     | 0.46              |
| 1:A:834:LEU:CD1  | 2:B:54:MET:CG    | 2.49                     | 0.46              |
| 1:A:87:MLY:HH12  | 1:A:87:MLY:HD3   | 1.61                     | 0.46              |
| 1:A:836:PHE:CB   | 2:B:161:GLU:HG2  | 2.37                     | 0.46              |
| 1:D:322:VAL:HB   | 1:D:325:ILE:HG13 | 1.97                     | 0.46              |
| 1:D:332:MET:HG2  | 1:D:332:MET:H    | 1.52                     | 0.46              |
| 1:D:629:GLU:HG2  | 1:D:643:GLY:C    | 2.35                     | 0.46              |
| 1:D:797:PHE:CE2  | 3:F:126:LEU:HD22 | 2.50                     | 0.46              |
| 1:D:82:PRO:HG2   | 1:D:85:TYR:CE2   | 2.51                     | 0.46              |
| 1:G:311:ASP:CB   | 1:G:312:TYR:CE1  | 2.98                     | 0.46              |
| 1:G:659:MLY:HD2  | 1:G:659:MLY:HH22 | 1.42                     | 0.46              |
| 1:J:218:LEU:HA   | 1:J:221:GLN:H    | 1.79                     | 0.46              |
| 1:J:292:MET:HE1  | 1:J:309:PRO:CG   | 2.46                     | 0.46              |
| 1:J:84:MLY:HH11  | 1:J:720:PHE:CA   | 2.45                     | 0.46              |
| 1:J:793:ARG:O    | 1:J:797:PHE:N    | 2.39                     | 0.46              |
| 4:V:366:GLY:O    | 4:V:369:ILE:HG22 | 2.16                     | 0.46              |
| 4:W:253:GLU:HA   | 4:W:256:ARG:CG   | 2.42                     | 0.46              |
| 4:X:6:THR:HG22   | 4:X:101:HIS:HA   | 1.97                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:543:PRO:CD   | 4:4:143:TYR:O    | 2.63                     | 0.46              |
| 1:A:411:GLU:H    | 4:4:333:PRO:HB2  | 1.80                     | 0.46              |
| 4:7:366:GLY:O    | 4:7:369:ILE:HG22 | 2.16                     | 0.46              |
| 1:A:326:ASP:O    | 1:A:330:GLU:HG2  | 2.16                     | 0.46              |
| 1:A:783:LEU:N    | 1:A:783:LEU:CD1  | 2.79                     | 0.46              |
| 1:D:206:LYS:HD3  | 1:D:217:THR:OG1  | 2.16                     | 0.46              |
| 1:D:265:ILE:CG2  | 1:D:266:GLU:N    | 2.78                     | 0.46              |
| 1:D:448:GLN:C    | 1:D:450:ASP:H    | 2.19                     | 0.46              |
| 1:D:640:LYS:C    | 4:5:23:GLY:C     | 2.74                     | 0.46              |
| 1:G:374:GLN:NE2  | 1:G:403:TYR:CE1  | 2.84                     | 0.46              |
| 1:G:524:GLU:HB3  | 1:G:528:MLY:HG2  | 1.96                     | 0.46              |
| 1:G:400:ALA:HB1  | 1:G:606:THR:CG2  | 2.45                     | 0.46              |
| 1:G:636:LYS:O    | 4:6:144:ALA:HB1  | 2.14                     | 0.46              |
| 1:G:835:PHE:O    | 1:G:839:MLY:N    | 2.49                     | 0.46              |
| 1:A:642:LYS:CB   | 4:4:24:ASP:O     | 2.59                     | 0.46              |
| 1:G:642:LYS:HA   | 4:6:21:PHE:C     | 2.36                     | 0.46              |
| 1:J:543:PRO:HD2  | 4:7:146:GLY:O    | 2.16                     | 0.46              |
| 1:J:642:LYS:HA   | 4:7:21:PHE:C     | 2.36                     | 0.46              |
| 1:A:206:LYS:HD3  | 1:A:217:THR:OG1  | 2.16                     | 0.46              |
| 1:A:311:ASP:CB   | 1:A:312:TYR:CE1  | 2.98                     | 0.46              |
| 1:A:335:ASP:OD1  | 1:A:348:MLY:NZ   | 2.49                     | 0.46              |
| 1:A:361:TYR:O    | 1:A:364:LEU:HB2  | 2.16                     | 0.46              |
| 1:A:640:LYS:C    | 4:4:23:GLY:C     | 2.74                     | 0.46              |
| 1:A:93:MET:CE    | 1:A:715:VAL:HA   | 2.45                     | 0.46              |
| 1:A:817:GLN:NE2  | 2:B:127:ARG:HG2  | 2.30                     | 0.46              |
| 1:D:335:ASP:OD1  | 1:D:348:MLY:NZ   | 2.49                     | 0.46              |
| 2:E:114:LYS:CG   | 2:E:146:GLY:HA2  | 2.46                     | 0.46              |
| 1:G:136:ASN:HA   | 1:G:137:PRO:HD3  | 1.49                     | 0.46              |
| 1:G:335:ASP:OD1  | 1:G:348:MLY:NZ   | 2.49                     | 0.46              |
| 1:G:725:ARG:NE   | 1:G:733:PRO:CB   | 1.95                     | 0.46              |
| 1:G:714:ARG:HD3  | 1:G:766:PHE:CE2  | 2.51                     | 0.46              |
| 1:G:89:GLU:CD    | 1:G:153:PRO:HD2  | 2.36                     | 0.46              |
| 2:H:88:LEU:HB3   | 2:H:91:ALA:HB2   | 1.98                     | 0.46              |
| 1:J:194:GLN:HE21 | 1:J:194:GLN:HB3  | 1.43                     | 0.46              |
| 1:J:206:LYS:HD3  | 1:J:217:THR:OG1  | 2.16                     | 0.46              |
| 1:J:30:MLY:HB3   | 1:J:31:PRO:HD2   | 1.97                     | 0.46              |
| 1:J:503:TYR:CZ   | 1:J:711:PHE:CD2  | 3.03                     | 0.46              |
| 4:X:299:MET:HE2  | 4:X:331:ALA:HB2  | 1.98                     | 0.46              |
| 4:X:366:GLY:O    | 4:X:369:ILE:HG22 | 2.16                     | 0.46              |
| 4:Z:366:GLY:O    | 4:Z:369:ILE:HG22 | 2.16                     | 0.46              |
| 4:0:190:MET:O    | 4:0:194:THR:HG23 | 2.16                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:3:299:MET:HE2  | 4:3:331:ALA:HB2  | 1.97                     | 0.46              |
| 4:3:366:GLY:O    | 4:3:369:ILE:HG22 | 2.16                     | 0.46              |
| 4:3:6:THR:HG22   | 4:3:101:HIS:HA   | 1.98                     | 0.46              |
| 4:5:366:GLY:O    | 4:5:369:ILE:HG22 | 2.16                     | 0.46              |
| 1:A:629:GLU:CA   | 1:A:643:GLY:C    | 2.73                     | 0.46              |
| 1:A:642:LYS:HA   | 4:4:21:PHE:C     | 2.36                     | 0.46              |
| 1:A:695:LEU:HB3  | 1:A:701:LEU:HD22 | 1.97                     | 0.46              |
| 1:A:725:ARG:NE   | 1:A:733:PRO:CB   | 1.95                     | 0.46              |
| 1:A:793:ARG:HE   | 3:C:147:MET:CB   | 2.29                     | 0.46              |
| 2:B:149:ASP:CG   | 2:B:150:TYR:N    | 2.49                     | 0.46              |
| 1:D:443:ILE:HG22 | 1:D:444:ARG:N    | 2.29                     | 0.46              |
| 1:D:510:TRP:CZ3  | 1:D:711:PHE:CE2  | 3.04                     | 0.46              |
| 1:D:767:PHE:C    | 1:D:771:LEU:HD11 | 2.36                     | 0.46              |
| 1:D:831:TRP:CE2  | 2:E:47:LEU:HB3   | 2.50                     | 0.46              |
| 1:G:278:GLN:HB3  | 1:G:278:GLN:HE21 | 1.42                     | 0.46              |
| 1:G:361:TYR:O    | 1:G:364:LEU:HB2  | 2.16                     | 0.46              |
| 1:G:42:HIS:O     | 1:G:45:GLN:O     | 2.33                     | 0.46              |
| 1:J:322:VAL:HB   | 1:J:325:ILE:HG13 | 1.98                     | 0.46              |
| 1:J:695:LEU:HB3  | 1:J:701:LEU:HD22 | 1.97                     | 0.46              |
| 1:J:795:ARG:HH22 | 3:L:116:GLU:CD   | 2.19                     | 0.46              |
| 1:J:797:PHE:HE2  | 3:L:126:LEU:HD23 | 1.81                     | 0.46              |
| 2:K:88:LEU:HB3   | 2:K:91:ALA:HB2   | 1.98                     | 0.46              |
| 4:V:190:MET:O    | 4:V:194:THR:HG23 | 2.16                     | 0.46              |
| 4:W:162:ASN:OD1  | 4:W:277:THR:HG22 | 2.15                     | 0.46              |
| 1:D:642:LYS:HA   | 4:5:21:PHE:C     | 2.36                     | 0.46              |
| 4:3:324:THR:N    | 4:5:245:GLY:CA   | 2.69                     | 0.46              |
| 1:G:411:GLU:H    | 4:6:333:PRO:HB2  | 1.80                     | 0.46              |
| 1:A:464:ILE:CG2  | 1:A:465:ALA:N    | 2.79                     | 0.46              |
| 2:B:137:TRP:CA   | 2:B:145:ALA:HB2  | 2.37                     | 0.46              |
| 1:D:99:GLU:N     | 1:D:100:PRO:CD   | 2.79                     | 0.46              |
| 1:G:206:LYS:HD3  | 1:G:217:THR:OG1  | 2.16                     | 0.46              |
| 1:G:326:ASP:O    | 1:G:330:GLU:HG2  | 2.16                     | 0.46              |
| 1:J:769:ALA:HB2  | 1:J:770:GLY:N    | 2.30                     | 0.46              |
| 1:J:798:LEU:HD12 | 1:J:798:LEU:HA   | 1.36                     | 0.46              |
| 1:G:543:PRO:CD   | 4:6:143:TYR:O    | 2.64                     | 0.46              |
| 4:7:253:GLU:HA   | 4:7:256:ARG:CG   | 2.42                     | 0.46              |
| 1:A:214:MET:HA   | 1:A:340:ILE:CD1  | 2.42                     | 0.46              |
| 1:A:295:MLY:HG3  | 1:A:332:MET:HE2  | 1.95                     | 0.46              |
| 1:A:332:MET:HG2  | 1:A:332:MET:H    | 1.52                     | 0.46              |
| 1:A:418:THR:CG2  | 1:A:419:VAL:N    | 2.79                     | 0.46              |
| 1:A:418:THR:CB   | 1:A:421:GLU:HG3  | 2.37                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:502:GLU:OE2  | 1:A:764:MLY:O    | 2.34                     | 0.46              |
| 1:A:793:ARG:O    | 1:A:797:PHE:N    | 2.40                     | 0.46              |
| 1:A:798:LEU:HD13 | 3:C:126:LEU:HD11 | 1.98                     | 0.46              |
| 3:C:50:LEU:O     | 3:C:53:PRO:CD    | 2.63                     | 0.46              |
| 1:D:136:ASN:O    | 1:D:139:VAL:N    | 2.47                     | 0.46              |
| 1:D:89:GLU:CD    | 1:D:153:PRO:HD2  | 2.36                     | 0.46              |
| 1:D:559:LEU:HD23 | 1:D:560:GLY:N    | 2.30                     | 0.46              |
| 1:D:810:ARG:HG2  | 1:D:810:ARG:NH1  | 2.29                     | 0.46              |
| 1:D:822:SER:HB3  | 2:E:88:LEU:CD2   | 2.40                     | 0.46              |
| 3:F:50:LEU:O     | 3:F:53:PRO:CD    | 2.63                     | 0.46              |
| 1:G:206:LYS:HD2  | 1:G:217:THR:CG2  | 2.17                     | 0.46              |
| 1:G:354:LEU:HD12 | 1:G:354:LEU:HA   | 1.56                     | 0.46              |
| 1:G:821:ARG:NH2  | 2:H:127:ARG:CD   | 2.74                     | 0.46              |
| 1:G:82:PRO:HG2   | 1:G:85:TYR:CE2   | 2.51                     | 0.46              |
| 2:H:137:TRP:CZ3  | 2:H:145:ALA:N    | 2.81                     | 0.46              |
| 1:J:218:LEU:HD22 | 1:J:222:ILE:HG13 | 1.95                     | 0.46              |
| 1:J:361:TYR:O    | 1:J:364:LEU:HB2  | 2.16                     | 0.46              |
| 1:J:715:VAL:HG11 | 1:J:720:PHE:CD1  | 2.49                     | 0.46              |
| 2:K:112:ILE:O    | 2:K:148:VAL:HA   | 2.16                     | 0.46              |
| 4:V:223:PHE:CD2  | 4:V:259:GLU:HG3  | 2.51                     | 0.46              |
| 4:W:32:PRO:HB2   | 4:W:34:ILE:HD11  | 1.98                     | 0.46              |
| 4:1:190:MET:O    | 4:1:194:THR:HG23 | 2.16                     | 0.45              |
| 4:4:253:GLU:HA   | 4:4:256:ARG:CG   | 2.42                     | 0.45              |
| 4:7:223:PHE:CD2  | 4:7:259:GLU:HG3  | 2.51                     | 0.45              |
| 1:A:501:GLU:HG2  | 1:A:762:HIS:CE1  | 2.44                     | 0.45              |
| 1:D:664:LEU:HD12 | 1:D:664:LEU:HA   | 1.53                     | 0.45              |
| 1:D:818:TYR:HB3  | 2:E:89:LYS:HB2   | 1.99                     | 0.45              |
| 1:G:332:MET:O    | 1:G:336:SER:OG   | 2.27                     | 0.45              |
| 1:G:448:GLN:C    | 1:G:450:ASP:H    | 2.19                     | 0.45              |
| 1:G:464:ILE:CG2  | 1:G:465:ALA:N    | 2.79                     | 0.45              |
| 1:G:728:ASN:HD21 | 3:I:109:HIS:C    | 2.20                     | 0.45              |
| 1:J:292:MET:HE1  | 1:J:309:PRO:HD3  | 1.98                     | 0.45              |
| 1:J:330:GLU:O    | 1:J:333:ALA:HB3  | 2.16                     | 0.45              |
| 1:J:783:LEU:N    | 1:J:783:LEU:CD1  | 2.78                     | 0.45              |
| 3:L:52:ASN:CB    | 3:L:53:PRO:CD    | 2.92                     | 0.45              |
| 4:8:324:THR:N    | 4:W:245:GLY:CA   | 2.69                     | 0.45              |
| 4:V:288:ASP:CA   | 4:X:204:ALA:HB2  | 2.31                     | 0.45              |
| 4:Y:32:PRO:HB2   | 4:Y:34:ILE:HD11  | 1.98                     | 0.45              |
| 4:Z:6:THR:HG22   | 4:Z:101:HIS:HA   | 1.98                     | 0.45              |
| 4:0:6:THR:HG22   | 4:0:101:HIS:HA   | 1.97                     | 0.45              |
| 4:0:366:GLY:O    | 4:0:369:ILE:HG22 | 2.16                     | 0.45              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 4:2:190:MET:O   | 4:2:194:THR:HG23 | 2.16                     | 0.45              |
| 1:A:637:LYS:HD2 | 4:4:144:ALA:HB3  | 1.21                     | 0.45              |
| 4:7:190:MET:O   | 4:7:194:THR:HG23 | 2.16                     | 0.45              |
| 1:J:642:LYS:NZ  | 4:7:340:TRP:O    | 2.50                     | 0.45              |
| 1:A:30:MLY:HB3  | 1:A:31:PRO:HD2   | 1.97                     | 0.45              |
| 1:A:629:GLU:HG2 | 1:A:643:GLY:C    | 2.35                     | 0.45              |
| 1:A:82:PRO:HG2  | 1:A:85:TYR:CE2   | 2.51                     | 0.45              |
| 1:D:726:VAL:H   | 1:D:782:MLY:HH21 | 1.80                     | 0.45              |
| 1:D:724:TYR:N   | 1:D:782:MLY:CH2  | 2.80                     | 0.45              |
| 1:D:818:TYR:CD2 | 2:E:89:LYS:CB    | 2.99                     | 0.45              |
| 1:G:30:MLY:HB3  | 1:G:31:PRO:HD2   | 1.97                     | 0.45              |
| 1:G:436:MLY:HE3 | 1:G:626:TYR:HE1  | 1.77                     | 0.45              |
| 1:J:265:ILE:CG2 | 1:J:266:GLU:N    | 2.79                     | 0.45              |
| 1:J:335:ASP:OD1 | 1:J:348:MLY:NZ   | 2.49                     | 0.45              |
| 1:J:56:GLU:HB2  | 1:J:59:MLY:CB    | 2.30                     | 0.45              |
| 1:J:84:MLY:HH23 | 1:J:716:LEU:O    | 2.12                     | 0.45              |
| 1:J:815:CYS:SG  | 2:K:92:ASP:OD1   | 2.74                     | 0.45              |
| 4:X:190:MET:O   | 4:X:194:THR:HG23 | 2.16                     | 0.45              |
| 4:X:324:THR:N   | 4:Z:245:GLY:CA   | 2.69                     | 0.45              |
| 4:1:6:THR:HG22  | 4:1:101:HIS:HA   | 1.98                     | 0.45              |
| 1:G:637:LYS:HD2 | 4:6:144:ALA:HB3  | 1.20                     | 0.45              |
| 1:G:639:GLY:CA  | 4:6:344:SER:O    | 2.40                     | 0.45              |
| 1:A:17:LEU:HA   | 1:A:17:LEU:HD12  | 1.68                     | 0.45              |
| 1:A:476:GLU:OE2 | 1:A:598:MLY:HH13 | 2.17                     | 0.45              |
| 1:A:667:THR:O   | 1:A:669:PRO:HD3  | 2.16                     | 0.45              |
| 1:A:723:ARG:NH1 | 1:A:723:ARG:CG   | 2.79                     | 0.45              |
| 1:A:733:PRO:O   | 1:A:737:PHE:CE1  | 2.53                     | 0.45              |
| 1:D:136:ASN:HA  | 1:D:137:PRO:HD3  | 1.50                     | 0.45              |
| 1:D:410:ASN:HA  | 4:5:334:GLU:HB3  | 1.29                     | 0.45              |
| 1:D:476:GLU:OE2 | 1:D:598:MLY:HH13 | 2.16                     | 0.45              |
| 1:D:612:GLN:NE2 | 1:D:627:GLY:H    | 2.14                     | 0.45              |
| 1:G:144:ARG:HA  | 1:G:144:ARG:HD2  | 1.78                     | 0.45              |
| 1:G:17:LEU:HA   | 1:G:17:LEU:HD12  | 1.67                     | 0.45              |
| 1:G:186:THR:O   | 1:G:190:MLY:HG2  | 2.17                     | 0.45              |
| 1:G:322:VAL:HB  | 1:G:325:ILE:HG13 | 1.98                     | 0.45              |
| 1:G:55:MLY:HH23 | 1:G:60:VAL:HG22  | 1.99                     | 0.45              |
| 1:G:93:MET:SD   | 1:G:763:THR:CG2  | 2.94                     | 0.45              |
| 2:H:112:ILE:O   | 2:H:148:VAL:HA   | 2.16                     | 0.45              |
| 1:J:186:THR:O   | 1:J:190:MLY:HG2  | 2.17                     | 0.45              |
| 1:J:202:SER:HA  | 1:J:207:LYS:NZ   | 2.22                     | 0.45              |
| 1:J:332:MET:O   | 1:J:336:SER:OG   | 2.27                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:448:GLN:C    | 1:J:450:ASP:H    | 2.19                     | 0.45              |
| 1:J:732:ILE:CG2  | 1:J:747:LEU:CD1  | 0.65                     | 0.45              |
| 4:X:223:PHE:CD2  | 4:X:259:GLU:HG3  | 2.52                     | 0.45              |
| 4:X:288:ASP:CA   | 4:Z:204:ALA:HB2  | 2.31                     | 0.45              |
| 4:1:32:PRO:HB2   | 4:1:34:ILE:HD11  | 1.98                     | 0.45              |
| 4:1:366:GLY:O    | 4:1:369:ILE:HG22 | 2.16                     | 0.45              |
| 1:A:529:PRO:HB2  | 4:4:354:GLN:HB3  | 1.98                     | 0.45              |
| 4:5:299:MET:HE2  | 4:5:331:ALA:HB2  | 1.98                     | 0.45              |
| 4:6:32:PRO:HB2   | 4:6:34:ILE:HD11  | 1.98                     | 0.45              |
| 1:G:540:CYS:C    | 4:6:349:LEU:HD21 | 2.36                     | 0.45              |
| 1:J:534:SER:HB2  | 4:7:354:GLN:HE22 | 1.56                     | 0.45              |
| 4:8:6:THR:HG22   | 4:8:101:HIS:HA   | 1.98                     | 0.45              |
| 1:A:139:VAL:HG12 | 1:A:143:TYR:HD2  | 1.81                     | 0.45              |
| 1:A:206:LYS:CE   | 1:A:217:THR:HG23 | 2.29                     | 0.45              |
| 1:A:322:VAL:HB   | 1:A:325:ILE:HG13 | 1.98                     | 0.45              |
| 1:A:496:PHE:CE2  | 1:A:514:ASP:HA   | 2.50                     | 0.45              |
| 1:A:642:LYS:HB2  | 4:4:24:ASP:O     | 1.88                     | 0.45              |
| 1:D:330:GLU:O    | 1:D:333:ALA:HB3  | 2.17                     | 0.45              |
| 1:D:464:ILE:CG2  | 1:D:465:ALA:N    | 2.79                     | 0.45              |
| 1:D:818:TYR:CD2  | 2:E:89:LYS:HB3   | 2.52                     | 0.45              |
| 1:D:830:PRO:CB   | 2:E:51:PHE:CE2   | 2.95                     | 0.45              |
| 1:G:265:ILE:CG2  | 1:G:266:GLU:N    | 2.79                     | 0.45              |
| 1:G:540:CYS:N    | 4:6:349:LEU:HD11 | 2.31                     | 0.45              |
| 1:G:629:GLU:CB   | 1:G:645:SER:N    | 2.74                     | 0.45              |
| 2:H:114:LYS:CG   | 2:H:146:GLY:HA2  | 2.46                     | 0.45              |
| 1:G:823:PHE:HE1  | 2:H:156:VAL:O    | 1.89                     | 0.45              |
| 1:J:17:LEU:HA    | 1:J:17:LEU:HD12  | 1.67                     | 0.45              |
| 1:J:723:ARG:CG   | 1:J:723:ARG:NH1  | 2.79                     | 0.45              |
| 4:8:288:ASP:CA   | 4:W:204:ALA:HB2  | 2.31                     | 0.45              |
| 1:A:411:GLU:H    | 4:4:333:PRO:CB   | 2.30                     | 0.45              |
| 4:5:223:PHE:CD2  | 4:5:259:GLU:HG3  | 2.51                     | 0.45              |
| 1:D:411:GLU:H    | 4:5:333:PRO:CB   | 2.29                     | 0.45              |
| 4:8:32:PRO:HB2   | 4:8:34:ILE:HD11  | 1.98                     | 0.45              |
| 1:A:89:GLU:CD    | 1:A:153:PRO:HD2  | 2.36                     | 0.45              |
| 1:A:296:MLY:O    | 1:A:299:LEU:HB2  | 2.17                     | 0.45              |
| 1:D:449:LEU:HA   | 1:D:449:LEU:HD12 | 1.60                     | 0.45              |
| 1:D:97:LEU:HD12  | 1:D:97:LEU:HA    | 1.67                     | 0.45              |
| 2:E:112:ILE:O    | 2:E:148:VAL:HA   | 2.17                     | 0.45              |
| 1:G:757:GLN:HE22 | 1:G:772:LEU:HG   | 1.80                     | 0.45              |
| 1:G:757:GLN:NE2  | 1:G:772:LEU:CD2  | 2.80                     | 0.45              |
| 3:I:50:LEU:O     | 3:I:53:PRO:CD    | 2.63                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:476:GLU:OE2  | 1:J:598:MLY:HH13 | 2.16                     | 0.45              |
| 1:J:640:LYS:HB3  | 1:J:645:SER:CB   | 2.42                     | 0.45              |
| 1:J:724:TYR:HD1  | 1:J:727:LEU:CD1  | 2.27                     | 0.45              |
| 1:J:725:ARG:HA   | 1:J:732:ILE:HG22 | 1.99                     | 0.45              |
| 1:J:89:GLU:CD    | 1:J:153:PRO:HD2  | 2.37                     | 0.45              |
| 4:X:287:ILE:HA   | 4:Z:202:THR:HG21 | 1.59                     | 0.45              |
| 4:0:223:PHE:CD2  | 4:0:259:GLU:HG3  | 2.51                     | 0.45              |
| 4:0:287:ILE:HA   | 4:2:202:THR:HG21 | 1.59                     | 0.45              |
| 4:2:253:GLU:HA   | 4:2:256:ARG:CG   | 2.42                     | 0.45              |
| 4:2:366:GLY:O    | 4:2:369:ILE:HG22 | 2.16                     | 0.45              |
| 4:2:6:THR:HG22   | 4:2:101:HIS:HA   | 1.98                     | 0.45              |
| 4:3:190:MET:O    | 4:3:194:THR:HG23 | 2.16                     | 0.45              |
| 4:3:32:PRO:HB2   | 4:3:34:ILE:HD11  | 1.98                     | 0.45              |
| 1:D:642:LYS:NZ   | 4:5:340:TRP:O    | 2.50                     | 0.45              |
| 1:G:529:PRO:HB2  | 4:6:354:GLN:HB3  | 1.98                     | 0.45              |
| 4:6:6:THR:HG22   | 4:6:101:HIS:HA   | 1.97                     | 0.45              |
| 4:5:290:ARG:HH22 | 4:7:202:THR:CG2  | 2.17                     | 0.45              |
| 1:A:179:GLY:O    | 1:A:185:LYS:HE2  | 2.17                     | 0.45              |
| 1:A:443:ILE:HG22 | 1:A:444:ARG:N    | 2.29                     | 0.45              |
| 1:A:55:MLY:HH23  | 1:A:60:VAL:HG22  | 1.99                     | 0.45              |
| 1:D:179:GLY:O    | 1:D:185:LYS:HE2  | 2.17                     | 0.45              |
| 1:D:725:ARG:HH21 | 1:D:733:PRO:HB2  | 1.81                     | 0.45              |
| 1:D:783:LEU:CD1  | 1:D:783:LEU:N    | 2.78                     | 0.45              |
| 1:G:173:GLN:HG3  | 1:G:670:HIS:HD2  | 1.82                     | 0.45              |
| 1:G:725:ARG:HH21 | 1:G:733:PRO:HB2  | 1.81                     | 0.45              |
| 1:G:800:ARG:CD   | 3:I:149:VAL:HG22 | 2.41                     | 0.45              |
| 1:J:530:MET:CE   | 4:7:354:GLN:HG3  | 2.35                     | 0.45              |
| 1:J:173:GLN:HG3  | 1:J:670:HIS:HD2  | 1.82                     | 0.45              |
| 1:J:707:CYS:C    | 1:J:714:ARG:NH2  | 2.70                     | 0.45              |
| 1:J:797:PHE:HD2  | 3:L:126:LEU:CD2  | 2.27                     | 0.45              |
| 4:Z:223:PHE:CD2  | 4:Z:259:GLU:HG3  | 2.52                     | 0.45              |
| 1:A:540:CYS:N    | 4:4:349:LEU:HD11 | 2.31                     | 0.45              |
| 4:4:366:GLY:O    | 4:4:369:ILE:HG22 | 2.16                     | 0.45              |
| 1:G:642:LYS:NZ   | 4:6:340:TRP:O    | 2.50                     | 0.45              |
| 4:6:288:ASP:CA   | 4:8:204:ALA:HB2  | 2.31                     | 0.45              |
| 1:A:210:GLN:C    | 1:A:211:SER:HG   | 2.15                     | 0.45              |
| 1:A:448:GLN:C    | 1:A:450:ASP:H    | 2.19                     | 0.45              |
| 2:B:112:ILE:O    | 2:B:148:VAL:HA   | 2.17                     | 0.45              |
| 1:D:229:LEU:HD12 | 1:D:229:LEU:HA   | 1.75                     | 0.45              |
| 1:D:296:MLY:O    | 1:D:299:LEU:HB2  | 2.17                     | 0.45              |
| 1:D:326:ASP:O    | 1:D:330:GLU:HG2  | 2.16                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:295:MLY:CG   | 1:D:332:MET:HE1  | 2.46                     | 0.45              |
| 1:D:361:TYR:O    | 1:D:364:LEU:HB2  | 2.16                     | 0.45              |
| 1:D:103:LEU:HD22 | 1:D:692:LEU:HG   | 1.98                     | 0.45              |
| 1:D:822:SER:HB3  | 2:E:88:LEU:HD21  | 1.99                     | 0.45              |
| 1:D:835:PHE:O    | 1:D:839:MLY:N    | 2.49                     | 0.45              |
| 1:G:292:MET:HE1  | 1:G:309:PRO:CG   | 2.46                     | 0.45              |
| 1:G:418:THR:CG2  | 1:G:419:VAL:N    | 2.79                     | 0.45              |
| 1:G:496:PHE:CE2  | 1:G:514:ASP:HA   | 2.50                     | 0.45              |
| 1:G:612:GLN:NE2  | 1:G:627:GLY:H    | 2.14                     | 0.45              |
| 1:J:179:GLY:O    | 1:J:185:LYS:HE2  | 2.17                     | 0.45              |
| 1:J:326:ASP:O    | 1:J:330:GLU:HG2  | 2.16                     | 0.45              |
| 1:J:732:ILE:H    | 1:J:733:PRO:HD2  | 1.74                     | 0.45              |
| 4:W:6:THR:HG22   | 4:W:101:HIS:HA   | 1.98                     | 0.45              |
| 4:Y:366:GLY:O    | 4:Y:369:ILE:HG22 | 2.16                     | 0.45              |
| 4:0:287:ILE:CB   | 4:2:204:ALA:H    | 2.13                     | 0.45              |
| 4:2:287:ILE:HA   | 4:4:202:THR:HG21 | 1.59                     | 0.45              |
| 4:1:288:ASP:CA   | 4:3:204:ALA:HB2  | 2.32                     | 0.45              |
| 4:4:190:MET:O    | 4:4:194:THR:HG23 | 2.16                     | 0.45              |
| 1:G:410:ASN:HA   | 4:6:334:GLU:HB3  | 1.28                     | 0.45              |
| 1:A:206:LYS:HD2  | 1:A:217:THR:CG2  | 2.17                     | 0.45              |
| 1:A:278:GLN:HB3  | 1:A:278:GLN:HE21 | 1.42                     | 0.45              |
| 1:D:14:ALA:N     | 1:D:15:PRO:HD2   | 2.32                     | 0.45              |
| 1:D:202:SER:HA   | 1:D:207:LYS:NZ   | 2.23                     | 0.45              |
| 1:D:226:ASN:N    | 1:D:227:PRO:HD2  | 2.32                     | 0.45              |
| 1:D:37:SER:O     | 1:D:38:VAL:HG23  | 2.17                     | 0.45              |
| 1:D:725:ARG:CG   | 1:D:733:PRO:HA   | 2.43                     | 0.45              |
| 1:D:767:PHE:C    | 1:D:771:LEU:CD1  | 2.85                     | 0.45              |
| 1:G:476:GLU:OE2  | 1:G:598:MLY:HH13 | 2.17                     | 0.45              |
| 1:G:485:GLU:OE1  | 1:G:583:HIS:ND1  | 2.49                     | 0.45              |
| 1:G:597:GLU:O    | 1:G:600:MLY:N    | 2.50                     | 0.45              |
| 1:G:747:LEU:C    | 1:G:749:GLY:H    | 2.20                     | 0.45              |
| 1:G:99:GLU:N     | 1:G:100:PRO:CD   | 2.80                     | 0.45              |
| 2:K:137:TRP:CA   | 2:K:145:ALA:HB2  | 2.37                     | 0.45              |
| 4:0:32:PRO:HB2   | 4:0:34:ILE:HD11  | 1.98                     | 0.45              |
| 4:2:223:PHE:CD2  | 4:2:259:GLU:HG3  | 2.52                     | 0.45              |
| 4:4:6:THR:HG22   | 4:4:101:HIS:HA   | 1.98                     | 0.45              |
| 4:8:223:PHE:CD2  | 4:8:259:GLU:HG3  | 2.51                     | 0.45              |
| 1:D:186:THR:O    | 1:D:190:MLY:HG2  | 2.17                     | 0.45              |
| 1:D:597:GLU:O    | 1:D:600:MLY:N    | 2.50                     | 0.45              |
| 1:D:769:ALA:HB1  | 1:D:771:LEU:N    | 2.25                     | 0.45              |
| 1:G:176:LEU:N    | 1:G:176:LEU:CD1  | 2.75                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:642:LYS:HG3  | 4:6:23:GLY:CA    | 2.31                     | 0.45              |
| 1:G:725:ARG:CG   | 1:G:733:PRO:CA   | 2.95                     | 0.45              |
| 2:H:137:TRP:CA   | 2:H:145:ALA:HB2  | 2.37                     | 0.45              |
| 1:J:408:VAL:HG22 | 1:J:636:LYS:HG2  | 1.51                     | 0.45              |
| 1:J:794:CYS:O    | 1:J:797:PHE:HB3  | 2.17                     | 0.45              |
| 4:Y:6:THR:HG22   | 4:Y:101:HIS:HA   | 1.98                     | 0.45              |
| 4:4:223:PHE:CD2  | 4:4:259:GLU:HG3  | 2.51                     | 0.45              |
| 4:6:223:PHE:CD2  | 4:6:259:GLU:HG3  | 2.51                     | 0.45              |
| 4:6:324:THR:O    | 4:8:244:ASP:HA   | 2.09                     | 0.45              |
| 1:G:408:VAL:CG1  | 4:6:332:PRO:HB3  | 2.41                     | 0.45              |
| 1:J:642:LYS:CB   | 4:7:24:ASP:O     | 2.60                     | 0.45              |
| 4:8:366:GLY:O    | 4:8:369:ILE:HG22 | 2.16                     | 0.45              |
| 1:A:106:LEU:HA   | 1:A:106:LEU:HD12 | 1.79                     | 0.45              |
| 1:A:163:TYR:O    | 1:A:166:MET:HB3  | 2.16                     | 0.45              |
| 1:A:195:TYR:CE2  | 1:A:199:ILE:HD12 | 2.52                     | 0.45              |
| 1:A:224:SER:O    | 1:A:227:PRO:HD2  | 2.17                     | 0.45              |
| 1:A:322:VAL:CG1  | 1:A:325:ILE:HD11 | 2.47                     | 0.45              |
| 1:A:488:GLN:O    | 1:A:491:PHE:HB3  | 2.17                     | 0.45              |
| 1:A:519:LEU:CD1  | 1:A:519:LEU:N    | 2.77                     | 0.45              |
| 1:A:747:LEU:C    | 1:A:749:GLY:H    | 2.20                     | 0.45              |
| 1:A:839:MLY:CE   | 2:B:159:HIS:HB3  | 2.47                     | 0.45              |
| 1:D:106:LEU:HD12 | 1:D:106:LEU:HA   | 1.79                     | 0.45              |
| 1:D:64:THR:HB    | 1:D:68:GLU:N     | 2.33                     | 0.45              |
| 1:D:675:ILE:HG23 | 1:D:676:ILE:N    | 2.32                     | 0.45              |
| 1:G:14:ALA:N     | 1:G:15:PRO:HD2   | 2.32                     | 0.45              |
| 1:G:296:MLY:O    | 1:G:299:LEU:HB2  | 2.17                     | 0.45              |
| 1:G:640:LYS:C    | 4:6:23:GLY:C     | 2.75                     | 0.45              |
| 1:G:768:MLY:HD3  | 1:G:772:LEU:CB   | 2.47                     | 0.45              |
| 1:G:794:CYS:O    | 1:G:797:PHE:HB3  | 2.17                     | 0.45              |
| 1:J:14:ALA:N     | 1:J:15:PRO:HD2   | 2.32                     | 0.45              |
| 1:J:322:VAL:CG1  | 1:J:325:ILE:HD11 | 2.47                     | 0.45              |
| 1:J:37:SER:O     | 1:J:38:VAL:HG23  | 2.17                     | 0.45              |
| 1:J:553:MLY:NZ   | 4:V:45:VAL:CA    | 2.58                     | 0.45              |
| 1:J:597:GLU:O    | 1:J:600:MLY:N    | 2.50                     | 0.45              |
| 1:J:667:THR:O    | 1:J:669:PRO:HD3  | 2.16                     | 0.45              |
| 1:J:797:PHE:CE2  | 3:L:126:LEU:HD23 | 2.52                     | 0.45              |
| 1:J:831:TRP:CZ3  | 2:K:34:ILE:HD11  | 2.36                     | 0.45              |
| 4:W:223:PHE:CD2  | 4:W:259:GLU:HG3  | 2.51                     | 0.45              |
| 4:V:287:ILE:CB   | 4:X:204:ALA:H    | 2.13                     | 0.45              |
| 4:W:287:ILE:HA   | 4:Y:202:THR:HG21 | 1.59                     | 0.45              |
| 4:Z:32:PRO:HB2   | 4:Z:34:ILE:HD11  | 1.98                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:0:223:PHE:HB3  | 4:0:259:GLU:OE2  | 2.18                     | 0.44              |
| 4:0:299:MET:HE2  | 4:0:331:ALA:HB2  | 1.99                     | 0.44              |
| 4:2:223:PHE:HB3  | 4:2:259:GLU:OE2  | 2.18                     | 0.44              |
| 4:3:223:PHE:HB3  | 4:3:259:GLU:OE2  | 2.18                     | 0.44              |
| 4:4:32:PRO:HB2   | 4:4:34:ILE:HD11  | 1.98                     | 0.44              |
| 4:5:190:MET:O    | 4:5:194:THR:HG23 | 2.16                     | 0.44              |
| 4:5:223:PHE:HB3  | 4:5:259:GLU:OE2  | 2.18                     | 0.44              |
| 1:A:99:GLU:N     | 1:A:100:PRO:CD   | 2.80                     | 0.44              |
| 1:A:229:LEU:HA   | 1:A:229:LEU:HD12 | 1.75                     | 0.44              |
| 1:A:346:ASP:O    | 1:A:350:ALA:N    | 2.46                     | 0.44              |
| 1:A:37:SER:O     | 1:A:38:VAL:HG23  | 2.17                     | 0.44              |
| 1:A:597:GLU:O    | 1:A:600:MLY:N    | 2.50                     | 0.44              |
| 1:A:642:LYS:NZ   | 4:4:340:TRP:O    | 2.50                     | 0.44              |
| 1:D:139:VAL:HG12 | 1:D:143:TYR:HD2  | 1.81                     | 0.44              |
| 1:D:41:VAL:CG1   | 1:D:42:HIS:N     | 2.75                     | 0.44              |
| 1:D:486:MLY:HH22 | 1:D:527:GLU:CD   | 2.37                     | 0.44              |
| 1:D:568:PRO:CG   | 1:D:578:HIS:H    | 2.30                     | 0.44              |
| 2:E:137:TRP:CZ3  | 2:E:145:ALA:N    | 2.81                     | 0.44              |
| 1:G:64:THR:HB    | 1:G:68:GLU:N     | 2.32                     | 0.44              |
| 1:G:667:THR:O    | 1:G:669:PRO:HD3  | 2.16                     | 0.44              |
| 1:J:226:ASN:N    | 1:J:227:PRO:HD2  | 2.32                     | 0.44              |
| 1:J:464:ILE:CG2  | 1:J:465:ALA:N    | 2.80                     | 0.44              |
| 1:J:673:ARG:HD2  | 1:J:673:ARG:HA   | 1.79                     | 0.44              |
| 1:J:732:ILE:HG23 | 1:J:747:LEU:HD12 | 0.95                     | 0.44              |
| 1:J:829:TRP:HA   | 1:J:830:PRO:HD2  | 1.86                     | 0.44              |
| 4:X:32:PRO:HB2   | 4:X:34:ILE:HD11  | 1.98                     | 0.44              |
| 4:Z:223:PHE:HB3  | 4:Z:259:GLU:OE2  | 2.18                     | 0.44              |
| 4:1:223:PHE:HB3  | 4:1:259:GLU:OE2  | 2.18                     | 0.44              |
| 4:5:32:PRO:HB2   | 4:5:34:ILE:HD11  | 1.98                     | 0.44              |
| 4:4:324:THR:N    | 4:6:245:GLY:CA   | 2.69                     | 0.44              |
| 1:G:411:GLU:H    | 4:6:333:PRO:CB   | 2.29                     | 0.44              |
| 4:7:223:PHE:HB3  | 4:7:259:GLU:OE2  | 2.18                     | 0.44              |
| 4:7:32:PRO:HB2   | 4:7:34:ILE:HD11  | 1.98                     | 0.44              |
| 1:A:48:VAL:HA    | 1:A:104:TYR:OH   | 2.17                     | 0.44              |
| 1:A:186:THR:O    | 1:A:190:MLY:HG2  | 2.17                     | 0.44              |
| 1:A:64:THR:HB    | 1:A:68:GLU:N     | 2.33                     | 0.44              |
| 1:A:711:PHE:HB3  | 1:A:766:PHE:HB3  | 1.99                     | 0.44              |
| 1:A:794:CYS:O    | 1:A:797:PHE:HB3  | 2.17                     | 0.44              |
| 1:D:163:TYR:O    | 1:D:166:MET:HB3  | 2.17                     | 0.44              |
| 1:D:278:GLN:HB3  | 1:D:278:GLN:HE21 | 1.42                     | 0.44              |
| 1:D:640:LYS:C    | 1:D:645:SER:HG   | 2.09                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:121:LEU:O    | 2:E:128:PHE:CG   | 2.61                     | 0.44              |
| 1:G:155:ILE:HG22 | 1:G:156:PHE:N    | 2.33                     | 0.44              |
| 1:G:485:GLU:HA   | 1:G:584:TYR:HE2  | 1.83                     | 0.44              |
| 1:G:488:GLN:O    | 1:G:491:PHE:HB3  | 2.17                     | 0.44              |
| 1:G:519:LEU:CD1  | 1:G:519:LEU:N    | 2.77                     | 0.44              |
| 1:G:823:PHE:CE2  | 2:H:140:PHE:CZ   | 3.05                     | 0.44              |
| 1:J:64:THR:HB    | 1:J:68:GLU:N     | 2.33                     | 0.44              |
| 1:J:689:GLU:HA   | 1:J:692:LEU:HB2  | 2.00                     | 0.44              |
| 4:W:366:GLY:O    | 4:W:369:ILE:HG22 | 2.16                     | 0.44              |
| 4:V:287:ILE:HA   | 4:X:202:THR:HG21 | 1.59                     | 0.44              |
| 4:X:223:PHE:HB3  | 4:X:259:GLU:OE2  | 2.18                     | 0.44              |
| 4:Z:190:MET:O    | 4:Z:194:THR:HG23 | 2.16                     | 0.44              |
| 4:1:223:PHE:CD2  | 4:1:259:GLU:HG3  | 2.52                     | 0.44              |
| 4:3:288:ASP:CA   | 4:5:204:ALA:HB2  | 2.31                     | 0.44              |
| 4:6:190:MET:O    | 4:6:194:THR:HG23 | 2.16                     | 0.44              |
| 1:G:530:MET:CB   | 4:6:354:GLN:CB   | 2.96                     | 0.44              |
| 1:J:543:PRO:CD   | 4:7:143:TYR:O    | 2.64                     | 0.44              |
| 1:J:639:GLY:H    | 4:7:344:SER:HB3  | 1.83                     | 0.44              |
| 1:A:725:ARG:HH21 | 1:A:733:PRO:HB2  | 1.81                     | 0.44              |
| 1:A:97:LEU:HA    | 1:A:97:LEU:HD12  | 1.67                     | 0.44              |
| 1:D:488:GLN:O    | 1:D:491:PHE:HB3  | 2.17                     | 0.44              |
| 1:D:689:GLU:HA   | 1:D:692:LEU:HB2  | 1.99                     | 0.44              |
| 1:D:708:ARG:O    | 1:D:710:GLY:N    | 2.50                     | 0.44              |
| 1:D:723:ARG:O    | 1:D:782:MLY:HD2  | 1.99                     | 0.44              |
| 1:D:794:CYS:O    | 1:D:797:PHE:HB3  | 2.16                     | 0.44              |
| 2:E:129:THR:HG23 | 2:E:132:GLU:OE1  | 2.17                     | 0.44              |
| 1:G:179:GLY:O    | 1:G:185:LYS:HE2  | 2.17                     | 0.44              |
| 1:G:629:GLU:HG2  | 1:G:643:GLY:C    | 2.35                     | 0.44              |
| 2:H:112:ILE:O    | 2:H:148:VAL:N    | 2.50                     | 0.44              |
| 1:J:408:VAL:HA   | 1:J:636:LYS:HG3  | 1.03                     | 0.44              |
| 1:J:488:GLN:O    | 1:J:491:PHE:HB3  | 2.17                     | 0.44              |
| 1:J:486:MLY:HH22 | 1:J:527:GLU:CD   | 2.37                     | 0.44              |
| 1:J:725:ARG:HH21 | 1:J:733:PRO:HB2  | 1.82                     | 0.44              |
| 1:J:817:GLN:CB   | 2:K:127:ARG:HD2  | 2.47                     | 0.44              |
| 4:V:223:PHE:HB3  | 4:V:259:GLU:OE2  | 2.18                     | 0.44              |
| 4:V:32:PRO:HB2   | 4:V:34:ILE:HD11  | 1.98                     | 0.44              |
| 4:Y:223:PHE:CD2  | 4:Y:259:GLU:HG3  | 2.52                     | 0.44              |
| 4:3:223:PHE:CD2  | 4:3:259:GLU:HG3  | 2.52                     | 0.44              |
| 4:4:223:PHE:HB3  | 4:4:259:GLU:OE2  | 2.18                     | 0.44              |
| 4:6:223:PHE:HB3  | 4:6:259:GLU:OE2  | 2.18                     | 0.44              |
| 1:A:502:GLU:CD   | 1:A:763:THR:N    | 2.56                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:793:ARG:HH21 | 3:C:147:MET:CE   | 2.28                     | 0.44              |
| 1:D:292:MET:HE3  | 1:D:309:PRO:CA   | 2.44                     | 0.44              |
| 1:D:809:ARG:NH2  | 2:E:124:GLY:HA3  | 2.33                     | 0.44              |
| 1:G:768:MLY:CD   | 1:G:772:LEU:HB2  | 2.47                     | 0.44              |
| 1:J:296:MLY:O    | 1:J:299:LEU:HB2  | 2.17                     | 0.44              |
| 1:J:410:ASN:HA   | 4:7:334:GLU:HB3  | 1.29                     | 0.44              |
| 4:W:287:ILE:CB   | 4:Y:204:ALA:H    | 2.13                     | 0.44              |
| 4:O:290:ARG:HH22 | 4:2:202:THR:CG2  | 2.17                     | 0.44              |
| 1:J:540:CYS:C    | 4:7:349:LEU:HD21 | 2.36                     | 0.44              |
| 1:A:193:ILE:HD11 | 1:A:250:ILE:CD1  | 2.48                     | 0.44              |
| 1:A:485:GLU:HA   | 1:A:584:TYR:HE2  | 1.83                     | 0.44              |
| 1:A:103:LEU:HD22 | 1:A:692:LEU:HG   | 1.98                     | 0.44              |
| 1:A:701:LEU:HA   | 1:A:701:LEU:HD12 | 1.55                     | 0.44              |
| 1:D:292:MET:HE1  | 1:D:309:PRO:CG   | 2.48                     | 0.44              |
| 1:D:322:VAL:CG1  | 1:D:325:ILE:HD11 | 2.47                     | 0.44              |
| 1:D:725:ARG:CG   | 1:D:733:PRO:CA   | 2.95                     | 0.44              |
| 1:D:747:LEU:C    | 1:D:749:GLY:H    | 2.21                     | 0.44              |
| 1:G:136:ASN:O    | 1:G:139:VAL:N    | 2.47                     | 0.44              |
| 1:G:320:ILE:O    | 1:G:320:ILE:HG22 | 2.18                     | 0.44              |
| 1:G:214:MET:CA   | 1:G:340:ILE:HD11 | 2.45                     | 0.44              |
| 1:G:37:SER:O     | 1:G:38:VAL:HG23  | 2.17                     | 0.44              |
| 1:G:103:LEU:HD22 | 1:G:692:LEU:HG   | 1.98                     | 0.44              |
| 1:G:723:ARG:NH1  | 1:G:723:ARG:CG   | 2.79                     | 0.44              |
| 2:H:129:THR:HG23 | 2:H:132:GLU:OE1  | 2.17                     | 0.44              |
| 1:J:99:GLU:N     | 1:J:100:PRO:CD   | 2.80                     | 0.44              |
| 1:J:155:ILE:HG22 | 1:J:156:PHE:N    | 2.33                     | 0.44              |
| 1:J:195:TYR:CE2  | 1:J:199:ILE:HD12 | 2.52                     | 0.44              |
| 1:J:443:ILE:HG22 | 1:J:444:ARG:N    | 2.29                     | 0.44              |
| 1:J:568:PRO:CG   | 1:J:578:HIS:H    | 2.30                     | 0.44              |
| 1:J:692:LEU:O    | 1:J:696:ARG:HG3  | 2.18                     | 0.44              |
| 1:J:725:ARG:CG   | 1:J:733:PRO:CA   | 2.95                     | 0.44              |
| 1:J:795:ARG:HH22 | 3:L:43:ASN:HB2   | 1.82                     | 0.44              |
| 2:K:129:THR:HG23 | 2:K:132:GLU:OE1  | 2.17                     | 0.44              |
| 4:Y:223:PHE:HB3  | 4:Y:259:GLU:OE2  | 2.18                     | 0.44              |
| 4:Z:299:MET:HE2  | 4:Z:331:ALA:HB2  | 2.00                     | 0.44              |
| 4:1:193:LEU:O    | 4:1:198:TYR:HD2  | 2.01                     | 0.44              |
| 4:2:32:PRO:HB2   | 4:2:34:ILE:HD11  | 1.98                     | 0.44              |
| 4:4:287:ILE:HA   | 4:6:202:THR:HG21 | 1.59                     | 0.44              |
| 4:7:299:MET:HE2  | 4:7:331:ALA:HB2  | 2.00                     | 0.44              |
| 4:6:290:ARG:HH22 | 4:8:202:THR:CG2  | 2.17                     | 0.44              |
| 4:8:223:PHE:HB3  | 4:8:259:GLU:OE2  | 2.18                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:14:ALA:N     | 1:A:15:PRO:HD2   | 2.32                     | 0.44              |
| 1:A:123:CYS:CB   | 1:A:158:ILE:HD13 | 2.48                     | 0.44              |
| 1:A:485:GLU:OE2  | 1:A:584:TYR:N    | 2.50                     | 0.44              |
| 1:A:516:GLY:O    | 1:A:518:ASP:N    | 2.51                     | 0.44              |
| 1:A:641:LYS:CE   | 1:A:647:GLN:CB   | 2.74                     | 0.44              |
| 1:A:173:GLN:HG3  | 1:A:670:HIS:HD2  | 1.82                     | 0.44              |
| 1:A:692:LEU:O    | 1:A:696:ARG:HG3  | 2.18                     | 0.44              |
| 1:A:835:PHE:O    | 1:A:839:MLY:N    | 2.49                     | 0.44              |
| 1:D:541:MET:HB3  | 4:5:345:ILE:HG22 | 2.00                     | 0.44              |
| 1:D:692:LEU:O    | 1:D:696:ARG:HG3  | 2.18                     | 0.44              |
| 1:D:725:ARG:CZ   | 1:D:733:PRO:CB   | 2.83                     | 0.44              |
| 1:D:768:MLY:O    | 1:D:771:LEU:HD12 | 0.62                     | 0.44              |
| 1:G:195:TYR:CE2  | 1:G:199:ILE:HD12 | 2.52                     | 0.44              |
| 1:G:692:LEU:O    | 1:G:696:ARG:HG3  | 2.18                     | 0.44              |
| 1:G:725:ARG:CZ   | 1:G:733:PRO:CB   | 2.83                     | 0.44              |
| 3:I:119:THR:O    | 3:I:123:VAL:HG23 | 2.18                     | 0.44              |
| 1:J:163:TYR:O    | 1:J:166:MET:HB3  | 2.17                     | 0.44              |
| 1:J:485:GLU:OE1  | 1:J:583:HIS:ND1  | 2.49                     | 0.44              |
| 1:J:516:GLY:O    | 1:J:518:ASP:N    | 2.51                     | 0.44              |
| 2:K:114:LYS:CG   | 2:K:146:GLY:HA2  | 2.46                     | 0.44              |
| 3:L:122:GLU:HA   | 3:L:125:GLU:OE1  | 2.18                     | 0.44              |
| 4:Y:190:MET:O    | 4:Y:194:THR:HG23 | 2.16                     | 0.44              |
| 4:4:193:LEU:O    | 4:4:198:TYR:HD2  | 2.01                     | 0.44              |
| 4:6:366:GLY:O    | 4:6:369:ILE:HG22 | 2.16                     | 0.44              |
| 4:8:190:MET:O    | 4:8:194:THR:HG23 | 2.16                     | 0.44              |
| 1:A:226:ASN:N    | 1:A:227:PRO:HD2  | 2.32                     | 0.44              |
| 1:A:439:LEU:CD1  | 1:A:439:LEU:N    | 2.81                     | 0.44              |
| 1:A:632:GLY:HA3  | 1:A:643:GLY:N    | 2.17                     | 0.44              |
| 1:A:725:ARG:CG   | 1:A:733:PRO:CA   | 2.95                     | 0.44              |
| 1:D:418:THR:CG2  | 1:D:419:VAL:N    | 2.79                     | 0.44              |
| 1:D:642:LYS:HG3  | 4:5:23:GLY:CA    | 2.31                     | 0.44              |
| 1:G:175:ILE:C    | 1:G:176:LEU:HD12 | 2.38                     | 0.44              |
| 1:G:224:SER:O    | 1:G:227:PRO:HD2  | 2.17                     | 0.44              |
| 1:G:322:VAL:CG1  | 1:G:325:ILE:HD11 | 2.47                     | 0.44              |
| 1:G:493:HIS:O    | 1:G:496:PHE:HB3  | 2.18                     | 0.44              |
| 1:G:675:ILE:HG23 | 1:G:676:ILE:N    | 2.32                     | 0.44              |
| 1:G:732:ILE:HG21 | 1:G:747:LEU:CD1  | 0.64                     | 0.44              |
| 1:G:728:ASN:ND2  | 3:I:109:HIS:C    | 2.71                     | 0.44              |
| 3:I:122:GLU:HA   | 3:I:125:GLU:OE1  | 2.18                     | 0.44              |
| 3:I:69:LEU:HB3   | 3:I:70:PRO:HD3   | 1.99                     | 0.44              |
| 1:J:139:VAL:HG12 | 1:J:143:TYR:HD2  | 1.81                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:439:LEU:CD1  | 1:J:439:LEU:N    | 2.81                     | 0.44              |
| 1:J:476:GLU:CD   | 1:J:476:GLU:H    | 2.21                     | 0.44              |
| 1:J:725:ARG:CG   | 1:J:733:PRO:HA   | 2.43                     | 0.44              |
| 1:J:747:LEU:C    | 1:J:749:GLY:H    | 2.20                     | 0.44              |
| 1:J:91:MET:CE    | 1:J:119:SER:HB2  | 2.48                     | 0.44              |
| 1:J:818:TYR:CB   | 2:K:90:GLY:HA3   | 2.37                     | 0.44              |
| 3:L:50:LEU:O     | 3:L:53:PRO:HG2   | 2.18                     | 0.44              |
| 4:W:190:MET:O    | 4:W:194:THR:HG23 | 2.16                     | 0.44              |
| 4:W:223:PHE:HB3  | 4:W:259:GLU:OE2  | 2.18                     | 0.44              |
| 4:2:287:ILE:N    | 4:4:202:THR:CG2  | 2.77                     | 0.44              |
| 1:A:530:MET:CB   | 4:4:354:GLN:CB   | 2.95                     | 0.44              |
| 4:6:220:ALA:HB3  | 4:6:223:PHE:CD1  | 2.53                     | 0.44              |
| 4:6:287:ILE:HA   | 4:8:202:THR:HG21 | 1.59                     | 0.44              |
| 1:A:675:ILE:HG23 | 1:A:676:ILE:N    | 2.32                     | 0.44              |
| 1:A:715:VAL:HG12 | 1:A:720:PHE:HB2  | 2.00                     | 0.44              |
| 1:A:504:MLY:CB   | 1:A:762:HIS:NE2  | 2.80                     | 0.44              |
| 1:A:793:ARG:HH21 | 3:C:147:MET:CG   | 2.31                     | 0.44              |
| 1:D:123:CYS:CB   | 1:D:158:ILE:HD13 | 2.48                     | 0.44              |
| 1:D:266:GLU:OE1  | 1:D:659:MLY:NZ   | 2.51                     | 0.44              |
| 1:D:485:GLU:OE1  | 1:D:583:HIS:ND1  | 2.49                     | 0.44              |
| 1:D:541:MET:HG2  | 4:5:345:ILE:HG22 | 2.00                     | 0.44              |
| 1:D:667:THR:O    | 1:D:669:PRO:HD3  | 2.16                     | 0.44              |
| 1:D:508:ILE:HG12 | 1:D:766:PHE:HE1  | 1.33                     | 0.44              |
| 1:D:788:THR:HG22 | 3:F:81:GLN:HE22  | 1.83                     | 0.44              |
| 1:D:813:ILE:CG2  | 2:E:127:ARG:NH1  | 2.76                     | 0.44              |
| 1:G:163:TYR:O    | 1:G:166:MET:HB3  | 2.17                     | 0.44              |
| 1:G:330:GLU:O    | 1:G:333:ALA:HB3  | 2.17                     | 0.44              |
| 2:H:139:ALA:C    | 2:H:141:PRO:HD3  | 2.33                     | 0.44              |
| 3:I:101:THR:HA   | 3:I:137:ILE:O    | 2.18                     | 0.44              |
| 3:I:50:LEU:O     | 3:I:53:PRO:HG2   | 2.18                     | 0.44              |
| 1:J:123:CYS:CB   | 1:J:158:ILE:HD13 | 2.48                     | 0.44              |
| 1:J:136:ASN:HA   | 1:J:137:PRO:HD3  | 1.50                     | 0.44              |
| 1:J:411:GLU:H    | 4:7:333:PRO:CB   | 2.30                     | 0.44              |
| 1:J:103:LEU:HD22 | 1:J:692:LEU:HG   | 1.98                     | 0.44              |
| 1:J:810:ARG:NH1  | 1:J:810:ARG:HG2  | 2.29                     | 0.44              |
| 3:L:101:THR:HA   | 3:L:137:ILE:O    | 2.18                     | 0.44              |
| 4:Z:253:GLU:HA   | 4:Z:256:ARG:CG   | 2.42                     | 0.44              |
| 4:7:205:GLU:O    | 4:7:208:ILE:HG22 | 2.18                     | 0.44              |
| 4:8:220:ALA:HB3  | 4:8:223:PHE:CD1  | 2.53                     | 0.44              |
| 1:A:123:CYS:HB2  | 1:A:158:ILE:HD13 | 2.00                     | 0.44              |
| 1:A:174:SER:OG   | 1:A:669:PRO:HA   | 2.18                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:175:ILE:C    | 1:A:176:LEU:HD12 | 2.38                     | 0.44              |
| 1:A:639:GLY:H    | 4:4:344:SER:HB3  | 1.82                     | 0.44              |
| 1:A:753:VAL:HG12 | 1:A:775:LEU:CD1  | 2.47                     | 0.44              |
| 1:A:831:TRP:CG   | 2:B:51:PHE:CZ    | 3.03                     | 0.44              |
| 1:D:195:TYR:CE2  | 1:D:199:ILE:HD12 | 2.52                     | 0.44              |
| 1:D:206:LYS:CE   | 1:D:217:THR:HG23 | 2.29                     | 0.44              |
| 1:D:218:LEU:HD22 | 1:D:222:ILE:HG13 | 1.95                     | 0.44              |
| 1:D:346:ASP:O    | 1:D:350:ALA:N    | 2.46                     | 0.44              |
| 1:D:439:LEU:CD1  | 1:D:439:LEU:N    | 2.81                     | 0.44              |
| 1:D:485:GLU:OE2  | 1:D:584:TYR:N    | 2.50                     | 0.44              |
| 1:D:711:PHE:HB3  | 1:D:766:PHE:HB3  | 1.99                     | 0.44              |
| 1:D:798:LEU:HA   | 1:D:798:LEU:HD12 | 1.36                     | 0.44              |
| 2:E:137:TRP:CA   | 2:E:145:ALA:HB2  | 2.37                     | 0.44              |
| 3:F:122:GLU:HA   | 3:F:125:GLU:OE1  | 2.18                     | 0.44              |
| 1:G:14:ALA:N     | 1:G:15:PRO:CD    | 2.81                     | 0.44              |
| 1:G:193:ILE:HD11 | 1:G:250:ILE:CD1  | 2.48                     | 0.44              |
| 1:G:226:ASN:HB2  | 1:G:227:PRO:CD   | 2.48                     | 0.44              |
| 1:G:439:LEU:N    | 1:G:439:LEU:CD1  | 2.81                     | 0.44              |
| 1:G:798:LEU:HD22 | 3:I:126:LEU:CD1  | 2.41                     | 0.44              |
| 1:J:144:ARG:HD2  | 1:J:144:ARG:HA   | 1.78                     | 0.44              |
| 1:J:206:LYS:CE   | 1:J:217:THR:HG23 | 2.29                     | 0.44              |
| 1:J:193:ILE:HD11 | 1:J:250:ILE:CD1  | 2.48                     | 0.44              |
| 1:J:308:ASN:HA   | 1:J:309:PRO:HD2  | 1.88                     | 0.44              |
| 1:J:493:HIS:O    | 1:J:496:PHE:HB3  | 2.18                     | 0.44              |
| 1:J:55:MLY:HH23  | 1:J:60:VAL:HG22  | 1.99                     | 0.44              |
| 1:J:599:ASN:CG   | 1:J:649:VAL:CB   | 2.80                     | 0.44              |
| 1:J:675:ILE:HG23 | 1:J:676:ILE:N    | 2.33                     | 0.44              |
| 1:J:84:MLY:HH11  | 1:J:719:ASP:C    | 2.39                     | 0.44              |
| 1:J:836:PHE:CD2  | 2:K:160:GLY:C    | 2.87                     | 0.44              |
| 4:8:287:ILE:HA   | 4:W:202:THR:HG21 | 1.59                     | 0.44              |
| 4:W:220:ALA:HB3  | 4:W:223:PHE:CD1  | 2.53                     | 0.44              |
| 4:X:205:GLU:O    | 4:X:208:ILE:HG22 | 2.18                     | 0.44              |
| 4:Y:171:LEU:HA   | 4:Y:172:PRO:HD2  | 1.84                     | 0.44              |
| 4:2:193:LEU:O    | 4:2:198:TYR:HD2  | 2.01                     | 0.43              |
| 1:D:540:CYS:C    | 4:5:349:LEU:HD21 | 2.36                     | 0.43              |
| 1:D:530:MET:CB   | 4:5:354:GLN:CB   | 2.95                     | 0.43              |
| 1:G:639:GLY:H    | 4:6:344:SER:HB3  | 1.83                     | 0.43              |
| 1:A:217:THR:HG22 | 1:A:218:LEU:N    | 2.33                     | 0.43              |
| 1:A:391:GLY:HA3  | 1:A:616:VAL:HG23 | 2.00                     | 0.43              |
| 1:A:787:ILE:HG23 | 1:A:791:GLN:HG3  | 2.00                     | 0.43              |
| 2:B:137:TRP:CZ3  | 2:B:145:ALA:N    | 2.81                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:48:VAL:HA    | 1:D:104:TYR:OH   | 2.17                     | 0.43              |
| 1:D:134:VAL:C    | 1:D:136:ASN:H    | 2.16                     | 0.43              |
| 1:D:485:GLU:HA   | 1:D:584:TYR:HE2  | 1.83                     | 0.43              |
| 1:D:516:GLY:O    | 1:D:518:ASP:N    | 2.51                     | 0.43              |
| 1:D:724:TYR:C    | 1:D:782:MLY:CH1  | 2.79                     | 0.43              |
| 1:D:40:VAL:HG23  | 1:D:76:GLN:O     | 2.18                     | 0.43              |
| 1:G:123:CYS:CB   | 1:G:158:ILE:HD13 | 2.48                     | 0.43              |
| 1:G:309:PRO:C    | 1:G:311:ASP:H    | 2.22                     | 0.43              |
| 1:G:578:HIS:HB3  | 1:G:592:ILE:CD1  | 2.38                     | 0.43              |
| 1:G:107:MLY:CB   | 1:G:686:MET:HE2  | 2.37                     | 0.43              |
| 1:J:129:TYR:HD1  | 1:J:129:TYR:HA   | 1.65                     | 0.43              |
| 1:J:576:GLU:CG   | 1:J:577:ALA:N    | 2.44                     | 0.43              |
| 3:L:69:LEU:HB3   | 3:L:70:PRO:HD3   | 1.99                     | 0.43              |
| 4:V:299:MET:HE2  | 4:V:331:ALA:HB2  | 2.00                     | 0.43              |
| 4:W:193:LEU:O    | 4:W:198:TYR:HD2  | 2.01                     | 0.43              |
| 4:3:193:LEU:O    | 4:3:198:TYR:HD2  | 2.01                     | 0.43              |
| 4:4:220:ALA:HB3  | 4:4:223:PHE:CD1  | 2.53                     | 0.43              |
| 1:A:534:SER:CB   | 4:4:351:THR:HA   | 2.48                     | 0.43              |
| 4:3:287:ILE:CB   | 4:5:204:ALA:H    | 2.13                     | 0.43              |
| 4:5:253:GLU:HA   | 4:5:256:ARG:CG   | 2.42                     | 0.43              |
| 1:D:639:GLY:H    | 4:5:344:SER:HB3  | 1.83                     | 0.43              |
| 1:J:541:MET:HB3  | 4:7:345:ILE:HG22 | 2.01                     | 0.43              |
| 1:A:201:ALA:O    | 1:A:202:SER:OG   | 2.36                     | 0.43              |
| 1:A:753:VAL:HG12 | 1:A:775:LEU:CG   | 2.47                     | 0.43              |
| 1:D:123:CYS:HB2  | 1:D:158:ILE:HD13 | 2.00                     | 0.43              |
| 1:D:55:MLY:HH23  | 1:D:60:VAL:HG22  | 1.99                     | 0.43              |
| 1:D:400:ALA:CB   | 1:D:606:THR:HG22 | 2.48                     | 0.43              |
| 1:D:64:THR:CG2   | 1:D:65:GLU:H     | 2.32                     | 0.43              |
| 1:D:173:GLN:HG3  | 1:D:670:HIS:HD2  | 1.82                     | 0.43              |
| 2:E:88:LEU:HB3   | 2:E:91:ALA:HB2   | 1.98                     | 0.43              |
| 1:G:322:VAL:CG1  | 1:G:325:ILE:HG13 | 2.48                     | 0.43              |
| 1:J:174:SER:OG   | 1:J:669:PRO:HA   | 2.18                     | 0.43              |
| 1:J:246:PHE:HB3  | 1:J:270:LEU:HD12 | 2.01                     | 0.43              |
| 1:J:391:GLY:HA3  | 1:J:616:VAL:HG23 | 2.00                     | 0.43              |
| 1:J:835:PHE:O    | 1:J:839:MLY:N    | 2.49                     | 0.43              |
| 4:0:205:GLU:O    | 4:0:208:ILE:HG22 | 2.18                     | 0.43              |
| 4:6:193:LEU:O    | 4:6:198:TYR:HD2  | 2.01                     | 0.43              |
| 1:A:549:SER:C    | 4:6:45:VAL:O     | 2.56                     | 0.43              |
| 1:A:348:MLY:HH12 | 1:A:348:MLY:HD2  | 1.82                     | 0.43              |
| 1:A:436:MLY:HE3  | 1:A:626:TYR:HE1  | 1.77                     | 0.43              |
| 1:A:496:PHE:HB2  | 1:A:515:PHE:CD2  | 2.53                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:747:LEU:C    | 1:A:749:GLY:N    | 2.71                     | 0.43              |
| 2:B:129:THR:HG23 | 2:B:132:GLU:OE1  | 2.18                     | 0.43              |
| 3:C:122:GLU:HA   | 3:C:125:GLU:OE1  | 2.18                     | 0.43              |
| 3:C:119:THR:O    | 3:C:123:VAL:HG23 | 2.18                     | 0.43              |
| 3:C:50:LEU:O     | 3:C:53:PRO:HG2   | 2.18                     | 0.43              |
| 1:D:193:ILE:HD11 | 1:D:250:ILE:CD1  | 2.48                     | 0.43              |
| 1:D:322:VAL:CG1  | 1:D:325:ILE:HG13 | 2.48                     | 0.43              |
| 1:D:747:LEU:C    | 1:D:749:GLY:N    | 2.72                     | 0.43              |
| 2:E:112:ILE:O    | 2:E:148:VAL:N    | 2.50                     | 0.43              |
| 3:F:101:THR:HA   | 3:F:137:ILE:O    | 2.18                     | 0.43              |
| 1:G:48:VAL:HA    | 1:G:104:TYR:OH   | 2.18                     | 0.43              |
| 1:G:266:GLU:OE1  | 1:G:659:MLY:NZ   | 2.51                     | 0.43              |
| 1:G:486:MLY:HH22 | 1:G:527:GLU:CD   | 2.37                     | 0.43              |
| 1:G:391:GLY:HA3  | 1:G:616:VAL:HG23 | 2.01                     | 0.43              |
| 1:G:692:LEU:HA   | 1:G:692:LEU:HD23 | 1.84                     | 0.43              |
| 1:G:725:ARG:CZ   | 1:G:737:PHE:CZ   | 3.01                     | 0.43              |
| 1:G:787:ILE:HG23 | 1:G:791:GLN:HG3  | 2.00                     | 0.43              |
| 1:G:834:LEU:HD11 | 2:H:51:PHE:CD1   | 2.52                     | 0.43              |
| 1:J:322:VAL:HA   | 1:J:323:PRO:HD3  | 1.87                     | 0.43              |
| 1:J:409:GLY:N    | 1:J:636:LYS:CD   | 2.70                     | 0.43              |
| 1:J:48:VAL:HA    | 1:J:104:TYR:OH   | 2.18                     | 0.43              |
| 1:J:496:PHE:HB2  | 1:J:515:PHE:CD2  | 2.53                     | 0.43              |
| 1:J:711:PHE:HB3  | 1:J:766:PHE:HB3  | 2.00                     | 0.43              |
| 1:J:813:ILE:HG23 | 2:K:128:PHE:CZ   | 2.53                     | 0.43              |
| 4:V:193:LEU:O    | 4:V:198:TYR:HD2  | 2.01                     | 0.43              |
| 4:Y:220:ALA:HB3  | 4:Y:223:PHE:CD1  | 2.53                     | 0.43              |
| 4:2:220:ALA:HB3  | 4:2:223:PHE:CD1  | 2.53                     | 0.43              |
| 4:3:149:THR:HA   | 4:3:165:ILE:O    | 2.19                     | 0.43              |
| 4:4:149:THR:HA   | 4:4:165:ILE:O    | 2.19                     | 0.43              |
| 1:D:530:MET:CE   | 4:5:354:GLN:HG3  | 2.35                     | 0.43              |
| 4:7:149:THR:HA   | 4:7:165:ILE:O    | 2.19                     | 0.43              |
| 1:J:541:MET:HG2  | 4:7:345:ILE:HG22 | 2.00                     | 0.43              |
| 1:A:109:ARG:CD   | 1:A:117:THR:HB   | 2.48                     | 0.43              |
| 1:A:14:ALA:N     | 1:A:15:PRO:CD    | 2.81                     | 0.43              |
| 1:A:322:VAL:CG1  | 1:A:325:ILE:HG13 | 2.49                     | 0.43              |
| 1:A:642:LYS:HG3  | 4:4:23:GLY:CA    | 2.32                     | 0.43              |
| 1:A:725:ARG:CZ   | 1:A:737:PHE:CZ   | 3.01                     | 0.43              |
| 1:D:166:MET:CE   | 1:D:254:PHE:CD2  | 3.01                     | 0.43              |
| 1:D:292:MET:CE   | 1:D:309:PRO:CA   | 2.97                     | 0.43              |
| 1:D:726:VAL:CA   | 1:D:782:MLY:HH13 | 2.45                     | 0.43              |
| 1:D:793:ARG:HE   | 3:F:147:MET:CG   | 2.31                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:201:ALA:O    | 1:G:202:SER:OG   | 2.36                     | 0.43              |
| 1:G:568:PRO:CG   | 1:G:578:HIS:H    | 2.29                     | 0.43              |
| 1:G:783:LEU:CD1  | 1:G:783:LEU:N    | 2.78                     | 0.43              |
| 1:G:795:ARG:HE   | 3:I:118:MET:CE   | 2.31                     | 0.43              |
| 1:J:266:GLU:OE1  | 1:J:659:MLY:NZ   | 2.51                     | 0.43              |
| 1:J:790:THR:N    | 3:L:87:PHE:HE2   | 2.12                     | 0.43              |
| 4:0:149:THR:HA   | 4:0:165:ILE:O    | 2.19                     | 0.43              |
| 4:2:149:THR:HA   | 4:2:165:ILE:O    | 2.19                     | 0.43              |
| 4:2:205:GLU:O    | 4:2:208:ILE:HG22 | 2.18                     | 0.43              |
| 4:3:205:GLU:O    | 4:3:208:ILE:HG22 | 2.18                     | 0.43              |
| 1:A:540:CYS:C    | 4:4:349:LEU:HD21 | 2.36                     | 0.43              |
| 1:A:529:PRO:HB3  | 4:4:354:GLN:HA   | 1.99                     | 0.43              |
| 1:D:541:MET:CE   | 4:5:346:LEU:HD12 | 2.48                     | 0.43              |
| 1:D:530:MET:HA   | 4:5:354:GLN:CD   | 2.11                     | 0.43              |
| 1:J:541:MET:CE   | 4:7:346:LEU:HD12 | 2.47                     | 0.43              |
| 1:J:529:PRO:HB3  | 4:7:354:GLN:HA   | 2.00                     | 0.43              |
| 1:A:129:TYR:HA   | 1:A:129:TYR:HD1  | 1.65                     | 0.43              |
| 1:A:295:MLY:CE   | 1:A:332:MET:CE   | 2.96                     | 0.43              |
| 1:A:320:ILE:O    | 1:A:320:ILE:HG22 | 2.18                     | 0.43              |
| 1:A:40:VAL:HG23  | 1:A:76:GLN:O     | 2.19                     | 0.43              |
| 1:A:476:GLU:H    | 1:A:476:GLU:CD   | 2.22                     | 0.43              |
| 1:A:486:MLY:HH22 | 1:A:527:GLU:CD   | 2.37                     | 0.43              |
| 1:A:537:GLU:OE1  | 4:4:350:SER:HA   | 2.19                     | 0.43              |
| 1:A:568:PRO:CG   | 1:A:578:HIS:H    | 2.30                     | 0.43              |
| 1:A:86:ASP:OD2   | 1:A:87:MLY:HH22  | 2.19                     | 0.43              |
| 3:C:101:THR:HA   | 3:C:137:ILE:O    | 2.18                     | 0.43              |
| 1:D:155:ILE:HG22 | 1:D:156:PHE:N    | 2.33                     | 0.43              |
| 1:D:224:SER:O    | 1:D:227:PRO:HD2  | 2.17                     | 0.43              |
| 1:D:493:HIS:O    | 1:D:496:PHE:HB3  | 2.18                     | 0.43              |
| 1:D:508:ILE:CG2  | 1:D:766:PHE:CD1  | 3.01                     | 0.43              |
| 1:G:174:SER:OG   | 1:G:669:PRO:HA   | 2.18                     | 0.43              |
| 1:G:217:THR:HG22 | 1:G:218:LEU:N    | 2.34                     | 0.43              |
| 1:G:218:LEU:HD22 | 1:G:222:ILE:HG13 | 1.95                     | 0.43              |
| 1:G:226:ASN:N    | 1:G:227:PRO:HD2  | 2.32                     | 0.43              |
| 1:G:292:MET:CE   | 1:G:309:PRO:CA   | 2.97                     | 0.43              |
| 1:G:295:MLY:CE   | 1:G:332:MET:CE   | 2.97                     | 0.43              |
| 1:G:496:PHE:HB2  | 1:G:515:PHE:CD2  | 2.53                     | 0.43              |
| 1:G:643:GLY:CA   | 4:6:24:ASP:OD1   | 2.62                     | 0.43              |
| 1:G:689:GLU:HA   | 1:G:692:LEU:HB2  | 1.99                     | 0.43              |
| 1:G:708:ARG:HA   | 1:G:714:ARG:NH2  | 2.33                     | 0.43              |
| 1:G:92:ALA:HB3   | 1:G:764:MLY:HH13 | 1.31                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:I:49:ILE:CA    | 3:I:52:ASN:ND2   | 2.53                     | 0.43              |
| 1:J:217:THR:HG22 | 1:J:218:LEU:N    | 2.34                     | 0.43              |
| 1:J:166:MET:CE   | 1:J:254:PHE:HB2  | 2.47                     | 0.43              |
| 1:J:322:VAL:CG1  | 1:J:325:ILE:HG13 | 2.49                     | 0.43              |
| 1:J:503:TYR:CZ   | 1:J:711:PHE:CE2  | 3.05                     | 0.43              |
| 1:J:757:GLN:OE1  | 1:J:773:GLY:CA   | 2.66                     | 0.43              |
| 4:Z:205:GLU:O    | 4:Z:208:ILE:HG22 | 2.18                     | 0.43              |
| 1:A:639:GLY:CA   | 4:4:344:SER:O    | 2.40                     | 0.43              |
| 4:6:149:THR:HA   | 4:6:165:ILE:O    | 2.19                     | 0.43              |
| 1:J:530:MET:HA   | 4:7:354:GLN:CD   | 2.11                     | 0.43              |
| 1:G:549:SER:C    | 4:8:45:VAL:O     | 2.57                     | 0.43              |
| 1:A:151:ALA:HB1  | 1:A:152:PRO:HD2  | 2.01                     | 0.43              |
| 1:A:449:LEU:HD12 | 1:A:449:LEU:HA   | 1.60                     | 0.43              |
| 1:A:612:GLN:NE2  | 1:A:627:GLY:H    | 2.14                     | 0.43              |
| 1:A:266:GLU:OE1  | 1:A:659:MLY:NZ   | 2.51                     | 0.43              |
| 1:D:226:ASN:HB2  | 1:D:227:PRO:CD   | 2.47                     | 0.43              |
| 1:D:246:PHE:HB3  | 1:D:270:LEU:HD12 | 2.01                     | 0.43              |
| 1:D:391:GLY:HA3  | 1:D:616:VAL:HG23 | 2.00                     | 0.43              |
| 1:D:723:ARG:NH1  | 1:D:723:ARG:CG   | 2.80                     | 0.43              |
| 1:D:789:ALA:C    | 3:F:87:PHE:HE2   | 2.11                     | 0.43              |
| 1:G:332:MET:H    | 1:G:332:MET:HG2  | 1.52                     | 0.43              |
| 1:G:40:VAL:HG23  | 1:G:76:GLN:O     | 2.19                     | 0.43              |
| 1:G:516:GLY:O    | 1:G:518:ASP:N    | 2.51                     | 0.43              |
| 1:G:711:PHE:HB3  | 1:G:766:PHE:HB3  | 2.00                     | 0.43              |
| 1:J:14:ALA:N     | 1:J:15:PRO:CD    | 2.81                     | 0.43              |
| 1:J:400:ALA:CB   | 1:J:606:THR:HG22 | 2.49                     | 0.43              |
| 1:J:537:GLU:OE1  | 4:7:350:SER:HA   | 2.19                     | 0.43              |
| 1:J:725:ARG:CZ   | 1:J:737:PHE:CZ   | 3.01                     | 0.43              |
| 1:J:747:LEU:C    | 1:J:749:GLY:N    | 2.71                     | 0.43              |
| 2:E:163:ALA:CA   | 2:K:21:GLU:HB3   | 2.37                     | 0.43              |
| 3:L:119:THR:O    | 3:L:123:VAL:HG23 | 2.18                     | 0.43              |
| 4:V:205:GLU:O    | 4:V:208:ILE:HG22 | 2.18                     | 0.43              |
| 4:X:149:THR:HA   | 4:X:165:ILE:O    | 2.19                     | 0.43              |
| 4:X:193:LEU:O    | 4:X:198:TYR:HD2  | 2.01                     | 0.43              |
| 4:Z:149:THR:HA   | 4:Z:165:ILE:O    | 2.19                     | 0.43              |
| 4:3:217:CYS:C    | 4:3:218:TYR:HD1  | 2.22                     | 0.43              |
| 1:A:541:MET:HB3  | 4:4:345:ILE:HG22 | 2.00                     | 0.43              |
| 1:G:541:MET:HG2  | 4:6:345:ILE:HG22 | 2.00                     | 0.43              |
| 4:7:220:ALA:HB3  | 4:7:223:PHE:CD1  | 2.53                     | 0.43              |
| 4:8:149:THR:HA   | 4:8:165:ILE:O    | 2.19                     | 0.43              |
| 1:A:155:ILE:HG22 | 1:A:156:PHE:N    | 2.33                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:369:MLY:HD3  | 1:A:369:MLY:HH22 | 1.79                     | 0.43              |
| 1:A:442:VAL:O    | 1:A:445:ILE:HB   | 2.19                     | 0.43              |
| 1:A:400:ALA:CB   | 1:A:606:THR:HG22 | 2.48                     | 0.43              |
| 1:A:715:VAL:HG11 | 1:A:720:PHE:CD1  | 2.50                     | 0.43              |
| 1:D:295:MLY:HG3  | 1:D:332:MET:HE2  | 2.00                     | 0.43              |
| 1:D:541:MET:HG2  | 4:5:345:ILE:HG23 | 2.01                     | 0.43              |
| 1:D:712:PRO:HB2  | 1:D:713:SER:H    | 1.61                     | 0.43              |
| 1:D:725:ARG:CZ   | 1:D:737:PHE:CE1  | 3.01                     | 0.43              |
| 1:D:789:ALA:O    | 3:F:87:PHE:HZ    | 1.98                     | 0.43              |
| 1:D:822:SER:OG   | 2:E:87:LYS:O     | 2.20                     | 0.43              |
| 1:D:818:TYR:CB   | 2:E:89:LYS:HB2   | 2.48                     | 0.43              |
| 1:G:294:ASN:OD1  | 1:G:307:THR:HG21 | 2.19                     | 0.43              |
| 1:G:725:ARG:CZ   | 1:G:737:PHE:CE1  | 3.02                     | 0.43              |
| 1:G:86:ASP:OD2   | 1:G:87:MLY:HH22  | 2.19                     | 0.43              |
| 1:J:123:CYS:HB2  | 1:J:158:ILE:HD13 | 2.00                     | 0.43              |
| 1:J:224:SER:O    | 1:J:227:PRO:HD2  | 2.17                     | 0.43              |
| 1:J:485:GLU:OE2  | 1:J:584:TYR:N    | 2.50                     | 0.43              |
| 1:J:64:THR:CG2   | 1:J:65:GLU:H     | 2.32                     | 0.43              |
| 1:J:724:TYR:HB3  | 1:J:727:LEU:CD1  | 2.48                     | 0.43              |
| 1:J:725:ARG:CZ   | 1:J:737:PHE:CE1  | 3.02                     | 0.43              |
| 4:7:287:ILE:CB   | 4:V:204:ALA:H    | 2.13                     | 0.43              |
| 1:A:551:MLY:C    | 4:6:47:MET:HA    | 2.48                     | 0.43              |
| 4:8:193:LEU:O    | 4:8:198:TYR:HD2  | 2.01                     | 0.43              |
| 1:A:330:GLU:H    | 1:A:330:GLU:HG2  | 1.55                     | 0.43              |
| 1:A:500:GLN:HB2  | 1:A:512:PHE:CZ   | 2.54                     | 0.43              |
| 1:A:533:PHE:HA   | 1:A:533:PHE:HD1  | 1.79                     | 0.43              |
| 1:D:144:ARG:HA   | 1:D:144:ARG:HD2  | 1.78                     | 0.43              |
| 1:D:14:ALA:N     | 1:D:15:PRO:CD    | 2.81                     | 0.43              |
| 1:D:17:LEU:HD12  | 1:D:17:LEU:HA    | 1.68                     | 0.43              |
| 1:D:725:ARG:HA   | 1:D:732:ILE:HG22 | 1.99                     | 0.43              |
| 3:F:119:THR:O    | 3:F:123:VAL:HG23 | 2.18                     | 0.43              |
| 3:F:69:LEU:HB3   | 3:F:70:PRO:HD3   | 1.99                     | 0.43              |
| 1:G:500:GLN:HB2  | 1:G:512:PHE:CZ   | 2.54                     | 0.43              |
| 1:J:169:ASP:O    | 1:J:170:ARG:HB2  | 2.19                     | 0.43              |
| 1:J:195:TYR:CD2  | 1:J:199:ILE:HD13 | 2.54                     | 0.43              |
| 1:J:201:ALA:O    | 1:J:202:SER:OG   | 2.36                     | 0.43              |
| 1:J:292:MET:CE   | 1:J:309:PRO:CA   | 2.97                     | 0.43              |
| 1:J:309:PRO:C    | 1:J:311:ASP:H    | 2.22                     | 0.43              |
| 2:K:140:PHE:HA   | 2:K:141:PRO:HD2  | 1.57                     | 0.43              |
| 4:V:220:ALA:HB3  | 4:V:223:PHE:CD1  | 2.53                     | 0.43              |
| 4:Y:193:LEU:O    | 4:Y:198:TYR:HD2  | 2.01                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:1:220:ALA:HB3  | 4:1:223:PHE:CD1  | 2.53                     | 0.43              |
| 4:1:180:LEU:HD11 | 4:1:261:LEU:HD23 | 2.01                     | 0.43              |
| 1:D:529:PRO:HB3  | 4:5:354:GLN:HA   | 2.00                     | 0.43              |
| 4:7:193:LEU:O    | 4:7:198:TYR:HD2  | 2.01                     | 0.43              |
| 1:A:294:ASN:OD1  | 1:A:307:THR:HG21 | 2.19                     | 0.43              |
| 1:A:330:GLU:O    | 1:A:333:ALA:HB3  | 2.17                     | 0.43              |
| 1:A:485:GLU:OE1  | 1:A:583:HIS:ND1  | 2.49                     | 0.43              |
| 1:A:578:HIS:HB3  | 1:A:592:ILE:CD1  | 2.38                     | 0.43              |
| 1:A:408:VAL:HG22 | 1:A:636:LYS:HG2  | 1.51                     | 0.43              |
| 1:A:502:GLU:HG2  | 1:A:766:PHE:CE1  | 2.54                     | 0.43              |
| 3:C:69:LEU:HB3   | 3:C:70:PRO:HD3   | 1.99                     | 0.43              |
| 1:D:174:SER:OG   | 1:D:669:PRO:HA   | 2.18                     | 0.43              |
| 1:G:109:ARG:CD   | 1:G:117:THR:HB   | 2.48                     | 0.43              |
| 1:G:151:ALA:HB1  | 1:G:152:PRO:HD2  | 2.01                     | 0.43              |
| 1:G:206:LYS:CE   | 1:G:217:THR:HG23 | 2.30                     | 0.43              |
| 1:G:442:VAL:O    | 1:G:445:ILE:HB   | 2.19                     | 0.43              |
| 1:G:445:ILE:HG22 | 1:G:449:LEU:HD22 | 2.01                     | 0.43              |
| 1:G:725:ARG:HA   | 1:G:732:ILE:HG22 | 1.99                     | 0.43              |
| 3:I:11:LYS:HE2   | 3:I:11:LYS:HB3   | 1.83                     | 0.43              |
| 1:J:109:ARG:CD   | 1:J:117:THR:HB   | 2.49                     | 0.43              |
| 1:J:320:ILE:O    | 1:J:320:ILE:HG22 | 2.18                     | 0.43              |
| 1:J:549:SER:C    | 4:V:45:VAL:O     | 2.56                     | 0.43              |
| 1:J:783:LEU:HA   | 1:J:786:ILE:HB   | 2.00                     | 0.43              |
| 1:J:97:LEU:HD12  | 1:J:97:LEU:HA    | 1.67                     | 0.43              |
| 4:V:287:ILE:HD11 | 4:X:202:THR:HA   | 1.66                     | 0.43              |
| 4:W:149:THR:HA   | 4:W:165:ILE:O    | 2.19                     | 0.43              |
| 4:X:290:ARG:HH22 | 4:Z:202:THR:CG2  | 2.17                     | 0.43              |
| 4:0:193:LEU:O    | 4:0:198:TYR:HD2  | 2.01                     | 0.43              |
| 4:1:217:CYS:C    | 4:1:218:TYR:HD1  | 2.22                     | 0.43              |
| 1:D:550:PHE:C    | 4:7:46:GLY:CA    | 2.87                     | 0.43              |
| 4:8:324:THR:O    | 4:W:244:ASP:HA   | 2.08                     | 0.43              |
| 1:A:91:MET:CE    | 1:A:119:SER:HB2  | 2.47                     | 0.43              |
| 1:A:309:PRO:C    | 1:A:311:ASP:H    | 2.22                     | 0.43              |
| 1:A:493:HIS:O    | 1:A:496:PHE:HB3  | 2.18                     | 0.43              |
| 1:A:636:LYS:CB   | 4:4:334:GLU:OE1  | 2.67                     | 0.43              |
| 1:A:725:ARG:HA   | 1:A:732:ILE:HG22 | 1.99                     | 0.43              |
| 2:B:140:PHE:CD2  | 2:B:144:VAL:HG11 | 2.54                     | 0.43              |
| 1:D:169:ASP:O    | 1:D:170:ARG:HB2  | 2.19                     | 0.43              |
| 1:D:599:ASN:CG   | 1:D:649:VAL:CB   | 2.80                     | 0.43              |
| 1:D:715:VAL:HG12 | 1:D:720:PHE:HB2  | 2.00                     | 0.43              |
| 1:D:829:TRP:O    | 1:D:832:MET:N    | 2.50                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:195:TYR:CD2  | 1:G:199:ILE:HD13 | 2.54                     | 0.43              |
| 1:G:213:LYS:HA   | 1:G:220:ASP:OD2  | 2.19                     | 0.43              |
| 1:G:246:PHE:HB3  | 1:G:270:LEU:HD12 | 2.01                     | 0.43              |
| 1:G:476:GLU:H    | 1:G:476:GLU:CD   | 2.21                     | 0.43              |
| 1:G:747:LEU:C    | 1:G:749:GLY:N    | 2.71                     | 0.43              |
| 1:J:442:VAL:O    | 1:J:445:ILE:HB   | 2.19                     | 0.43              |
| 1:J:568:PRO:O    | 1:J:570:PRO:HD3  | 2.19                     | 0.43              |
| 4:W:222:ASP:OD1  | 4:W:224:GLU:HB3  | 2.19                     | 0.43              |
| 4:Y:149:THR:HA   | 4:Y:165:ILE:O    | 2.19                     | 0.43              |
| 4:Y:217:CYS:C    | 4:Y:218:TYR:HD1  | 2.23                     | 0.43              |
| 4:Z:180:LEU:HD11 | 4:Z:261:LEU:HD23 | 2.01                     | 0.43              |
| 4:0:220:ALA:HB3  | 4:0:223:PHE:CD1  | 2.53                     | 0.42              |
| 4:0:180:LEU:HD11 | 4:0:261:LEU:HD23 | 2.02                     | 0.42              |
| 4:2:180:LEU:HD11 | 4:2:261:LEU:HD23 | 2.01                     | 0.42              |
| 4:4:180:LEU:HD11 | 4:4:261:LEU:HD23 | 2.01                     | 0.42              |
| 4:4:205:GLU:O    | 4:4:208:ILE:HG22 | 2.18                     | 0.42              |
| 4:5:180:LEU:HD11 | 4:5:261:LEU:HD23 | 2.01                     | 0.42              |
| 4:5:220:ALA:HB3  | 4:5:223:PHE:CD1  | 2.53                     | 0.42              |
| 1:J:530:MET:CB   | 4:7:354:GLN:CB   | 2.95                     | 0.42              |
| 1:D:549:SER:C    | 4:7:45:VAL:O     | 2.57                     | 0.42              |
| 1:A:195:TYR:CD2  | 1:A:199:ILE:HD13 | 2.54                     | 0.42              |
| 1:A:246:PHE:HB3  | 1:A:270:LEU:HD12 | 2.01                     | 0.42              |
| 1:A:292:MET:CE   | 1:A:309:PRO:CA   | 2.97                     | 0.42              |
| 1:A:64:THR:CG2   | 1:A:65:GLU:H     | 2.32                     | 0.42              |
| 1:A:689:GLU:HA   | 1:A:692:LEU:HB2  | 2.00                     | 0.42              |
| 1:D:195:TYR:CD2  | 1:D:199:ILE:HD13 | 2.54                     | 0.42              |
| 1:D:217:THR:HG22 | 1:D:218:LEU:N    | 2.34                     | 0.42              |
| 1:D:442:VAL:O    | 1:D:445:ILE:HB   | 2.19                     | 0.42              |
| 1:D:725:ARG:CZ   | 1:D:737:PHE:CZ   | 3.01                     | 0.42              |
| 1:D:787:ILE:HG23 | 1:D:791:GLN:HG3  | 2.00                     | 0.42              |
| 1:G:129:TYR:HD1  | 1:G:129:TYR:HA   | 1.65                     | 0.42              |
| 1:G:289:TYR:OH   | 1:G:315:VAL:O    | 2.27                     | 0.42              |
| 1:G:443:ILE:HG22 | 1:G:444:ARG:N    | 2.29                     | 0.42              |
| 1:G:568:PRO:O    | 1:G:570:PRO:HD3  | 2.19                     | 0.42              |
| 1:G:715:VAL:HG12 | 1:G:720:PHE:HB2  | 2.00                     | 0.42              |
| 1:G:829:TRP:O    | 1:G:832:MET:N    | 2.50                     | 0.42              |
| 3:I:63:ILE:CG2   | 3:I:64:THR:H     | 2.32                     | 0.42              |
| 1:J:294:ASN:OD1  | 1:J:307:THR:HG21 | 2.19                     | 0.42              |
| 1:J:406:VAL:O    | 1:J:412:ALA:HA   | 2.19                     | 0.42              |
| 1:J:541:MET:HG2  | 4:7:345:ILE:HG23 | 2.01                     | 0.42              |
| 1:J:787:ILE:HG23 | 1:J:791:GLN:HG3  | 2.00                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:X:220:ALA:HB3  | 4:X:223:PHE:CD1  | 2.53                     | 0.42              |
| 4:Z:220:ALA:HB3  | 4:Z:223:PHE:CD1  | 2.53                     | 0.42              |
| 4:1:149:THR:HA   | 4:1:165:ILE:O    | 2.19                     | 0.42              |
| 4:2:315:LYS:HD2  | 4:2:315:LYS:HA   | 1.92                     | 0.42              |
| 4:3:180:LEU:HD11 | 4:3:261:LEU:HD23 | 2.02                     | 0.42              |
| 4:5:217:CYS:C    | 4:5:218:TYR:HD1  | 2.22                     | 0.42              |
| 4:6:287:ILE:CB   | 4:8:204:ALA:H    | 2.13                     | 0.42              |
| 1:A:445:ILE:HG22 | 1:A:449:LEU:HD22 | 2.01                     | 0.42              |
| 1:A:62:VAL:O     | 1:A:69:THR:HA    | 2.19                     | 0.42              |
| 1:A:692:LEU:HA   | 1:A:692:LEU:HD23 | 1.84                     | 0.42              |
| 1:D:206:LYS:HD2  | 1:D:217:THR:CG2  | 2.17                     | 0.42              |
| 1:D:496:PHE:HB2  | 1:D:515:PHE:CD2  | 2.54                     | 0.42              |
| 1:D:673:ARG:HA   | 1:D:673:ARG:HD2  | 1.79                     | 0.42              |
| 1:D:692:LEU:HD23 | 1:D:692:LEU:HA   | 1.84                     | 0.42              |
| 1:D:701:LEU:HA   | 1:D:701:LEU:HD12 | 1.55                     | 0.42              |
| 1:D:834:LEU:HD21 | 2:E:54:MET:HG2   | 1.96                     | 0.42              |
| 2:E:149:ASP:CG   | 2:E:150:TYR:N    | 2.49                     | 0.42              |
| 3:F:50:LEU:O     | 3:F:53:PRO:HG2   | 2.18                     | 0.42              |
| 1:G:141:LEU:N    | 1:G:141:LEU:HD12 | 2.32                     | 0.42              |
| 1:G:64:THR:CG2   | 1:G:65:GLU:H     | 2.32                     | 0.42              |
| 1:J:40:VAL:HG23  | 1:J:76:GLN:O     | 2.19                     | 0.42              |
| 1:J:62:VAL:HG12  | 1:J:63:MLY:N     | 2.34                     | 0.42              |
| 1:J:747:LEU:O    | 1:J:749:GLY:N    | 2.52                     | 0.42              |
| 1:J:84:MLY:CG    | 1:J:719:ASP:OD2  | 2.66                     | 0.42              |
| 2:K:112:ILE:O    | 2:K:148:VAL:N    | 2.50                     | 0.42              |
| 4:7:287:ILE:HA   | 4:V:202:THR:HG21 | 1.59                     | 0.42              |
| 4:W:217:CYS:C    | 4:W:218:TYR:HD1  | 2.22                     | 0.42              |
| 4:Y:222:ASP:OD1  | 4:Y:224:GLU:HB3  | 2.19                     | 0.42              |
| 4:Z:193:LEU:O    | 4:Z:198:TYR:HD2  | 2.01                     | 0.42              |
| 4:0:217:CYS:C    | 4:0:218:TYR:HD1  | 2.22                     | 0.42              |
| 4:4:206:ARG:O    | 4:4:209:VAL:HG12 | 2.20                     | 0.42              |
| 4:6:205:GLU:O    | 4:6:208:ILE:HG22 | 2.18                     | 0.42              |
| 1:G:529:PRO:HB3  | 4:6:354:GLN:HA   | 2.00                     | 0.42              |
| 4:5:324:THR:N    | 4:7:245:GLY:CA   | 2.69                     | 0.42              |
| 1:A:402:CYS:C    | 1:A:404:PRO:HD3  | 2.39                     | 0.42              |
| 1:A:724:TYR:HB3  | 1:A:727:LEU:CD1  | 2.48                     | 0.42              |
| 1:A:829:TRP:O    | 1:A:832:MET:N    | 2.50                     | 0.42              |
| 3:C:96:LYS:HG3   | 3:C:96:LYS:H     | 1.66                     | 0.42              |
| 1:D:109:ARG:CD   | 1:D:117:THR:HB   | 2.49                     | 0.42              |
| 1:D:449:LEU:CD1  | 1:D:449:LEU:N    | 2.82                     | 0.42              |
| 1:D:62:VAL:HG12  | 1:D:63:MLY:N     | 2.35                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:741:LYS:HG2  | 1:D:742:LYS:N    | 2.35                     | 0.42              |
| 1:D:829:TRP:HE1  | 2:E:67:MET:CB    | 2.26                     | 0.42              |
| 2:E:140:PHE:CD2  | 2:E:144:VAL:HG11 | 2.54                     | 0.42              |
| 1:G:406:VAL:O    | 1:G:412:ALA:HA   | 2.19                     | 0.42              |
| 1:G:747:LEU:O    | 1:G:749:GLY:N    | 2.52                     | 0.42              |
| 1:G:798:LEU:HD12 | 1:G:798:LEU:HA   | 1.36                     | 0.42              |
| 2:H:144:VAL:HG12 | 2:H:153:ILE:HD13 | 1.92                     | 0.42              |
| 1:J:278:GLN:HE21 | 1:J:278:GLN:HB3  | 1.42                     | 0.42              |
| 1:J:445:ILE:HG22 | 1:J:449:LEU:HD22 | 2.01                     | 0.42              |
| 1:J:449:LEU:CD1  | 1:J:449:LEU:N    | 2.81                     | 0.42              |
| 4:W:315:LYS:HD2  | 4:W:315:LYS:HA   | 1.92                     | 0.42              |
| 4:X:180:LEU:HD11 | 4:X:261:LEU:HD23 | 2.01                     | 0.42              |
| 4:Y:180:LEU:HD11 | 4:Y:261:LEU:HD23 | 2.01                     | 0.42              |
| 4:1:205:GLU:O    | 4:1:208:ILE:HG22 | 2.18                     | 0.42              |
| 4:4:217:CYS:C    | 4:4:218:TYR:HD1  | 2.22                     | 0.42              |
| 4:8:205:GLU:O    | 4:8:208:ILE:HG22 | 2.18                     | 0.42              |
| 1:G:551:MLY:C    | 4:8:47:MET:HA    | 2.48                     | 0.42              |
| 1:A:214:MET:CA   | 1:A:340:ILE:HD11 | 2.46                     | 0.42              |
| 1:A:625:THR:H    | 1:A:625:THR:HG22 | 1.48                     | 0.42              |
| 1:A:797:PHE:HE2  | 3:C:126:LEU:CD2  | 1.91                     | 0.42              |
| 2:B:114:LYS:CG   | 2:B:146:GLY:HA2  | 2.46                     | 0.42              |
| 1:A:831:TRP:CZ2  | 2:B:51:PHE:CE1   | 3.07                     | 0.42              |
| 1:D:175:ILE:C    | 1:D:176:LEU:HD12 | 2.38                     | 0.42              |
| 1:D:295:MLY:CE   | 1:D:332:MET:CE   | 2.97                     | 0.42              |
| 1:D:320:ILE:O    | 1:D:320:ILE:HG22 | 2.17                     | 0.42              |
| 1:D:445:ILE:HG22 | 1:D:449:LEU:HD22 | 2.01                     | 0.42              |
| 1:D:733:PRO:CB   | 1:D:737:PHE:CE1  | 3.02                     | 0.42              |
| 1:D:793:ARG:HG2  | 3:F:147:MET:HG2  | 2.01                     | 0.42              |
| 1:G:123:CYS:HB2  | 1:G:158:ILE:HD13 | 2.00                     | 0.42              |
| 1:G:62:VAL:O     | 1:G:69:THR:HA    | 2.19                     | 0.42              |
| 1:G:173:GLN:HG3  | 1:G:670:HIS:CD2  | 2.55                     | 0.42              |
| 1:G:741:LYS:HG2  | 1:G:742:LYS:N    | 2.35                     | 0.42              |
| 1:J:485:GLU:HA   | 1:J:584:TYR:HE2  | 1.83                     | 0.42              |
| 1:J:533:PHE:HD1  | 1:J:533:PHE:HA   | 1.79                     | 0.42              |
| 1:J:173:GLN:HG3  | 1:J:670:HIS:CD2  | 2.54                     | 0.42              |
| 1:J:831:TRP:CH2  | 2:K:34:ILE:CG2   | 2.95                     | 0.42              |
| 1:J:86:ASP:OD2   | 1:J:87:MLY:HH22  | 2.19                     | 0.42              |
| 3:L:63:ILE:CG2   | 3:L:64:THR:H     | 2.33                     | 0.42              |
| 4:V:149:THR:HA   | 4:V:165:ILE:O    | 2.19                     | 0.42              |
| 4:V:222:ASP:OD1  | 4:V:224:GLU:HB3  | 2.19                     | 0.42              |
| 4:8:287:ILE:CB   | 4:W:204:ALA:H    | 2.13                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:W:196:ARG:HH21 | 4:W:249:THR:HG23 | 1.85                     | 0.42              |
| 4:Z:217:CYS:C    | 4:Z:218:TYR:HD1  | 2.22                     | 0.42              |
| 4:1:196:ARG:HH21 | 4:1:249:THR:HG23 | 1.85                     | 0.42              |
| 4:4:222:ASP:OD1  | 4:4:224:GLU:HB3  | 2.20                     | 0.42              |
| 4:4:196:ARG:HH21 | 4:4:249:THR:HG23 | 1.85                     | 0.42              |
| 1:A:541:MET:CE   | 4:4:346:LEU:HD12 | 2.48                     | 0.42              |
| 4:5:193:LEU:O    | 4:5:198:TYR:HD2  | 2.01                     | 0.42              |
| 4:5:205:GLU:O    | 4:5:208:ILE:HG22 | 2.18                     | 0.42              |
| 1:D:534:SER:CB   | 4:5:351:THR:HA   | 2.49                     | 0.42              |
| 4:6:217:CYS:C    | 4:6:218:TYR:HD1  | 2.22                     | 0.42              |
| 1:G:534:SER:CB   | 4:6:351:THR:HA   | 2.50                     | 0.42              |
| 4:7:180:LEU:HD11 | 4:7:261:LEU:HD23 | 2.01                     | 0.42              |
| 1:J:534:SER:CB   | 4:7:351:THR:HA   | 2.49                     | 0.42              |
| 4:8:217:CYS:C    | 4:8:218:TYR:HD1  | 2.22                     | 0.42              |
| 1:A:38:VAL:HG13  | 1:A:39:PHE:N     | 2.35                     | 0.42              |
| 1:A:501:GLU:HA   | 1:A:762:HIS:CE1  | 2.54                     | 0.42              |
| 1:A:712:PRO:HB2  | 1:A:713:SER:H    | 1.61                     | 0.42              |
| 1:A:744:SER:O    | 1:A:748:LEU:HD12 | 2.20                     | 0.42              |
| 1:A:747:LEU:O    | 1:A:749:GLY:N    | 2.52                     | 0.42              |
| 1:D:14:ALA:HB3   | 1:D:15:PRO:CD    | 2.45                     | 0.42              |
| 1:D:354:LEU:HA   | 1:D:354:LEU:HD12 | 1.56                     | 0.42              |
| 1:D:476:GLU:H    | 1:D:476:GLU:CD   | 2.22                     | 0.42              |
| 1:D:519:LEU:H    | 1:D:519:LEU:HD12 | 1.83                     | 0.42              |
| 1:D:723:ARG:HE   | 1:D:779:ARG:HA   | 1.84                     | 0.42              |
| 2:E:140:PHE:HA   | 2:E:141:PRO:HD2  | 1.57                     | 0.42              |
| 1:G:346:ASP:O    | 1:G:350:ALA:N    | 2.46                     | 0.42              |
| 1:G:578:HIS:CD2  | 1:G:592:ILE:H    | 2.38                     | 0.42              |
| 1:G:842:LEU:N    | 1:G:842:LEU:CD1  | 2.82                     | 0.42              |
| 1:J:175:ILE:C    | 1:J:176:LEU:HD12 | 2.39                     | 0.42              |
| 1:J:226:ASN:HB2  | 1:J:227:PRO:CD   | 2.47                     | 0.42              |
| 1:J:271:GLU:OE1  | 1:J:274:ARG:NH1  | 2.53                     | 0.42              |
| 1:J:295:MLY:CE   | 1:J:332:MET:CE   | 2.97                     | 0.42              |
| 1:J:354:LEU:HA   | 1:J:354:LEU:HD12 | 1.56                     | 0.42              |
| 1:J:578:HIS:CD2  | 1:J:592:ILE:H    | 2.38                     | 0.42              |
| 1:J:93:MET:CA    | 1:J:714:ARG:HG3  | 2.44                     | 0.42              |
| 4:V:206:ARG:O    | 4:V:209:VAL:HG12 | 2.20                     | 0.42              |
| 4:W:206:ARG:O    | 4:W:209:VAL:HG12 | 2.20                     | 0.42              |
| 4:W:205:GLU:O    | 4:W:208:ILE:HG22 | 2.18                     | 0.42              |
| 4:X:222:ASP:OD1  | 4:X:224:GLU:HB3  | 2.19                     | 0.42              |
| 4:Y:205:GLU:O    | 4:Y:208:ILE:HG22 | 2.18                     | 0.42              |
| 4:2:222:ASP:OD1  | 4:2:224:GLU:HB3  | 2.20                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:2:324:THR:HG23 | 4:4:245:GLY:HA2  | 1.09                     | 0.42              |
| 4:6:180:LEU:HD11 | 4:6:261:LEU:HD23 | 2.01                     | 0.42              |
| 4:7:222:ASP:OD1  | 4:7:224:GLU:HB3  | 2.20                     | 0.42              |
| 4:8:222:ASP:OD1  | 4:8:224:GLU:HB3  | 2.19                     | 0.42              |
| 1:A:169:ASP:O    | 1:A:170:ARG:HB2  | 2.19                     | 0.42              |
| 1:A:166:MET:CE   | 1:A:254:PHE:HB2  | 2.46                     | 0.42              |
| 2:B:113:LYS:O    | 2:B:147:ASN:HB2  | 2.20                     | 0.42              |
| 1:A:791:GLN:OE1  | 3:C:116:GLU:HB2  | 2.20                     | 0.42              |
| 1:D:402:CYS:C    | 1:D:404:PRO:HD3  | 2.40                     | 0.42              |
| 1:D:409:GLY:N    | 1:D:636:LYS:CD   | 2.71                     | 0.42              |
| 1:D:725:ARG:HA   | 1:D:732:ILE:CG2  | 2.50                     | 0.42              |
| 1:D:842:LEU:CD1  | 1:D:842:LEU:N    | 2.83                     | 0.42              |
| 1:D:822:SER:HG   | 2:E:88:LEU:HA    | 1.84                     | 0.42              |
| 1:J:151:ALA:HB1  | 1:J:152:PRO:HD2  | 2.01                     | 0.42              |
| 1:J:174:SER:HA   | 1:J:460:GLY:O    | 2.20                     | 0.42              |
| 1:J:462:LEU:HD11 | 1:J:464:ILE:CD1  | 2.50                     | 0.42              |
| 1:J:62:VAL:O     | 1:J:69:THR:HA    | 2.20                     | 0.42              |
| 4:X:206:ARG:O    | 4:X:209:VAL:HG12 | 2.20                     | 0.42              |
| 4:Z:196:ARG:HH21 | 4:Z:249:THR:HG23 | 1.85                     | 0.42              |
| 4:3:220:ALA:HB3  | 4:3:223:PHE:CD1  | 2.53                     | 0.42              |
| 4:5:149:THR:HA   | 4:5:165:ILE:O    | 2.19                     | 0.42              |
| 1:D:636:LYS:CB   | 4:5:334:GLU:OE1  | 2.68                     | 0.42              |
| 4:7:217:CYS:C    | 4:7:218:TYR:HD1  | 2.22                     | 0.42              |
| 4:8:369:ILE:HG23 | 4:8:370:VAL:N    | 2.35                     | 0.42              |
| 1:A:141:LEU:N    | 1:A:141:LEU:HD12 | 2.32                     | 0.42              |
| 1:A:213:LYS:HA   | 1:A:220:ASP:OD2  | 2.19                     | 0.42              |
| 1:A:568:PRO:O    | 1:A:570:PRO:HD3  | 2.19                     | 0.42              |
| 1:A:60:VAL:O     | 1:A:72:VAL:N     | 2.51                     | 0.42              |
| 1:A:642:LYS:HB3  | 4:4:24:ASP:HB2   | 1.37                     | 0.42              |
| 1:A:501:GLU:CB   | 1:A:762:HIS:ND1  | 2.82                     | 0.42              |
| 1:D:204:GLU:N    | 1:D:207:LYS:HE3  | 2.23                     | 0.42              |
| 1:D:279:LEU:CB   | 1:D:280:PRO:HD2  | 2.49                     | 0.42              |
| 1:D:406:VAL:O    | 1:D:412:ALA:HA   | 2.20                     | 0.42              |
| 1:D:537:GLU:OE1  | 4:5:350:SER:HA   | 2.19                     | 0.42              |
| 1:D:659:MLY:HD2  | 1:D:659:MLY:HH22 | 1.42                     | 0.42              |
| 1:D:759:ALA:O    | 1:D:766:PHE:N    | 2.32                     | 0.42              |
| 1:G:166:MET:CE   | 1:G:254:PHE:HB2  | 2.46                     | 0.42              |
| 1:G:400:ALA:CB   | 1:G:606:THR:HG22 | 2.49                     | 0.42              |
| 2:H:140:PHE:CD2  | 2:H:144:VAL:HG11 | 2.55                     | 0.42              |
| 1:J:214:MET:CA   | 1:J:340:ILE:HD11 | 2.45                     | 0.42              |
| 1:J:418:THR:CG2  | 1:J:419:VAL:N    | 2.79                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:795:ARG:HH21 | 3:L:116:GLU:HB3  | 1.84                     | 0.42              |
| 1:J:826:VAL:O    | 1:J:828:HIS:N    | 2.53                     | 0.42              |
| 4:V:217:CYS:C    | 4:V:218:TYR:HD1  | 2.23                     | 0.42              |
| 4:V:180:LEU:HD11 | 4:V:261:LEU:HD23 | 2.02                     | 0.42              |
| 4:Z:222:ASP:OD1  | 4:Z:224:GLU:HB3  | 2.19                     | 0.42              |
| 4:1:171:LEU:HA   | 4:1:172:PRO:HD2  | 1.84                     | 0.42              |
| 4:1:206:ARG:O    | 4:1:209:VAL:HG12 | 2.20                     | 0.42              |
| 4:1:369:ILE:HG23 | 4:1:370:VAL:N    | 2.35                     | 0.42              |
| 4:2:193:LEU:HD11 | 4:2:250:ILE:HG13 | 2.02                     | 0.42              |
| 4:5:222:ASP:OD1  | 4:5:224:GLU:HB3  | 2.19                     | 0.42              |
| 4:6:222:ASP:OD1  | 4:6:224:GLU:HB3  | 2.19                     | 0.42              |
| 1:G:633:GLY:HA2  | 4:6:25:ASP:HA    | 1.26                     | 0.42              |
| 1:A:195:TYR:CE2  | 1:A:199:ILE:HD13 | 2.55                     | 0.42              |
| 1:A:553:MLY:HE2  | 4:6:45:VAL:CA    | 2.38                     | 0.42              |
| 1:A:173:GLN:HG3  | 1:A:670:HIS:CD2  | 2.54                     | 0.42              |
| 1:A:757:GLN:CD   | 1:A:771:LEU:CD1  | 2.86                     | 0.42              |
| 1:D:294:ASN:OD1  | 1:D:307:THR:HG21 | 2.19                     | 0.42              |
| 1:D:174:SER:HA   | 1:D:460:GLY:O    | 2.20                     | 0.42              |
| 1:D:839:MLY:N    | 1:D:840:PRO:HD2  | 2.35                     | 0.42              |
| 1:G:38:VAL:HG13  | 1:G:39:PHE:N     | 2.35                     | 0.42              |
| 1:G:733:PRO:CB   | 1:G:737:PHE:CE1  | 3.02                     | 0.42              |
| 1:J:11:GLY:O     | 1:J:14:ALA:HB3   | 2.20                     | 0.42              |
| 1:J:332:MET:HG2  | 1:J:332:MET:H    | 1.52                     | 0.42              |
| 1:J:500:GLN:HB2  | 1:J:512:PHE:CZ   | 2.54                     | 0.42              |
| 1:J:715:VAL:HG12 | 1:J:720:PHE:HB2  | 2.00                     | 0.42              |
| 2:K:140:PHE:CD2  | 2:K:144:VAL:HG11 | 2.54                     | 0.42              |
| 4:W:180:LEU:HD11 | 4:W:261:LEU:HD23 | 2.02                     | 0.42              |
| 4:W:369:ILE:HG23 | 4:W:370:VAL:N    | 2.35                     | 0.42              |
| 4:Y:369:ILE:HG23 | 4:Y:370:VAL:N    | 2.35                     | 0.42              |
| 4:0:206:ARG:O    | 4:0:209:VAL:HG12 | 2.20                     | 0.42              |
| 4:0:222:ASP:OD1  | 4:0:224:GLU:HB3  | 2.19                     | 0.42              |
| 4:0:196:ARG:HH21 | 4:0:249:THR:HG23 | 1.85                     | 0.42              |
| 4:3:369:ILE:HG23 | 4:3:370:VAL:N    | 2.35                     | 0.42              |
| 4:5:221:LEU:HA   | 4:5:312:ARG:HG2  | 2.02                     | 0.42              |
| 1:D:541:MET:CG   | 4:5:345:ILE:C    | 2.87                     | 0.42              |
| 4:8:180:LEU:HD11 | 4:8:261:LEU:HD23 | 2.01                     | 0.42              |
| 1:A:406:VAL:O    | 1:A:412:ALA:HA   | 2.19                     | 0.42              |
| 1:A:797:PHE:CD2  | 1:A:798:LEU:HD12 | 2.55                     | 0.42              |
| 1:D:215:GLN:H    | 1:D:340:ILE:CD1  | 2.21                     | 0.42              |
| 1:D:271:GLU:OE1  | 1:D:274:ARG:NH1  | 2.53                     | 0.42              |
| 1:D:462:LEU:HD11 | 1:D:464:ILE:CD1  | 2.50                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:471:ASP:CB   | 1:D:573:GLY:O    | 2.68                     | 0.42              |
| 1:D:578:HIS:CD2  | 1:D:592:ILE:H    | 2.38                     | 0.42              |
| 1:D:690:LEU:O    | 1:D:694:GLN:HG3  | 2.20                     | 0.42              |
| 1:D:744:SER:O    | 1:D:748:LEU:HD12 | 2.20                     | 0.42              |
| 1:G:732:ILE:HG23 | 1:G:747:LEU:HD12 | 0.95                     | 0.42              |
| 1:G:97:LEU:HD12  | 1:G:97:LEU:HA    | 1.67                     | 0.42              |
| 1:J:195:TYR:CE2  | 1:J:199:ILE:HD13 | 2.55                     | 0.42              |
| 4:X:193:LEU:HD11 | 4:X:250:ILE:HG13 | 2.02                     | 0.42              |
| 4:X:324:THR:HG23 | 4:Z:245:GLY:HA2  | 1.09                     | 0.42              |
| 4:Y:193:LEU:HD11 | 4:Y:250:ILE:HG13 | 2.02                     | 0.42              |
| 4:O:193:LEU:HD11 | 4:O:250:ILE:HG13 | 2.02                     | 0.42              |
| 4:3:221:LEU:HA   | 4:3:312:ARG:HG2  | 2.02                     | 0.42              |
| 4:5:369:ILE:HG23 | 4:5:370:VAL:N    | 2.35                     | 0.42              |
| 4:6:206:ARG:O    | 4:6:209:VAL:HG12 | 2.20                     | 0.42              |
| 4:6:196:ARG:HH21 | 4:6:249:THR:HG23 | 1.85                     | 0.42              |
| 4:7:206:ARG:O    | 4:7:209:VAL:HG12 | 2.20                     | 0.42              |
| 4:7:221:LEU:HA   | 4:7:312:ARG:HG2  | 2.02                     | 0.42              |
| 4:7:369:ILE:HG23 | 4:7:370:VAL:N    | 2.35                     | 0.42              |
| 4:8:206:ARG:O    | 4:8:209:VAL:HG12 | 2.20                     | 0.42              |
| 1:A:110:TYR:O    | 1:A:113:TRP:N    | 2.42                     | 0.42              |
| 1:A:322:VAL:HA   | 1:A:323:PRO:HD3  | 1.87                     | 0.42              |
| 1:A:578:HIS:CD2  | 1:A:592:ILE:H    | 2.38                     | 0.42              |
| 1:A:725:ARG:CZ   | 1:A:737:PHE:CE1  | 3.02                     | 0.42              |
| 1:D:747:LEU:O    | 1:D:749:GLY:N    | 2.52                     | 0.42              |
| 1:D:507:GLY:C    | 1:D:761:GLY:HA3  | 2.37                     | 0.42              |
| 1:D:86:ASP:OD2   | 1:D:87:MLY:HH22  | 2.19                     | 0.42              |
| 3:F:63:ILE:CG2   | 3:F:64:THR:H     | 2.32                     | 0.42              |
| 1:G:568:PRO:CG   | 1:G:578:HIS:N    | 2.83                     | 0.42              |
| 1:G:62:VAL:HG12  | 1:G:63:MLY:N     | 2.35                     | 0.42              |
| 1:G:732:ILE:CG2  | 1:G:747:LEU:CD1  | 0.65                     | 0.42              |
| 1:J:84:MLY:HH13  | 1:J:715:VAL:CG1  | 2.06                     | 0.42              |
| 1:J:754:ASP:HB3  | 1:J:776:GLU:HG3  | 1.72                     | 0.42              |
| 4:2:217:CYS:C    | 4:2:218:TYR:HD1  | 2.23                     | 0.41              |
| 4:3:193:LEU:HD11 | 4:3:250:ILE:HG13 | 2.02                     | 0.41              |
| 4:4:315:LYS:HA   | 4:4:315:LYS:HD2  | 1.92                     | 0.41              |
| 4:4:324:THR:HG23 | 4:6:245:GLY:HA2  | 1.09                     | 0.41              |
| 4:4:369:ILE:HG23 | 4:4:370:VAL:N    | 2.35                     | 0.41              |
| 4:7:193:LEU:HD11 | 4:7:250:ILE:HG13 | 2.02                     | 0.41              |
| 4:8:226:GLU:HG3  | 4:8:255:PHE:CE2  | 2.55                     | 0.41              |
| 1:A:11:GLY:O     | 1:A:14:ALA:HB3   | 2.20                     | 0.41              |
| 1:A:462:LEU:HD11 | 1:A:464:ILE:CD1  | 2.50                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:659:MLY:HH22 | 1:A:659:MLY:HD2  | 1.42                     | 0.41              |
| 1:A:826:VAL:O    | 1:A:828:HIS:N    | 2.53                     | 0.41              |
| 1:A:842:LEU:N    | 1:A:842:LEU:CD1  | 2.83                     | 0.41              |
| 1:D:151:ALA:HB1  | 1:D:152:PRO:HD2  | 2.01                     | 0.41              |
| 1:D:466:GLY:CA   | 1:D:484:ASN:HD21 | 2.32                     | 0.41              |
| 1:D:625:THR:H    | 1:D:625:THR:HG22 | 1.48                     | 0.41              |
| 1:G:11:GLY:O     | 1:G:14:ALA:HB3   | 2.20                     | 0.41              |
| 1:G:169:ASP:O    | 1:G:170:ARG:HB2  | 2.19                     | 0.41              |
| 1:G:166:MET:CE   | 1:G:254:PHE:CD2  | 3.01                     | 0.41              |
| 1:G:369:MLY:HD3  | 1:G:369:MLY:HH22 | 1.79                     | 0.41              |
| 1:G:60:VAL:O     | 1:G:72:VAL:N     | 2.51                     | 0.41              |
| 1:G:725:ARG:HA   | 1:G:732:ILE:CG2  | 2.50                     | 0.41              |
| 1:J:725:ARG:HA   | 1:J:732:ILE:CG2  | 2.50                     | 0.41              |
| 4:V:221:LEU:HA   | 4:V:312:ARG:HG2  | 2.02                     | 0.41              |
| 4:X:369:ILE:HG23 | 4:X:370:VAL:N    | 2.35                     | 0.41              |
| 4:Y:206:ARG:O    | 4:Y:209:VAL:HG12 | 2.20                     | 0.41              |
| 4:2:226:GLU:HG3  | 4:2:255:PHE:CE2  | 2.56                     | 0.41              |
| 4:3:222:ASP:OD1  | 4:3:224:GLU:HB3  | 2.20                     | 0.41              |
| 4:3:287:ILE:N    | 4:5:202:THR:CG2  | 2.77                     | 0.41              |
| 4:4:193:LEU:HD11 | 4:4:250:ILE:HG13 | 2.02                     | 0.41              |
| 4:6:193:LEU:HD11 | 4:6:250:ILE:HG13 | 2.02                     | 0.41              |
| 4:6:315:LYS:HA   | 4:6:315:LYS:HD2  | 1.92                     | 0.41              |
| 4:6:369:ILE:HG23 | 4:6:370:VAL:N    | 2.35                     | 0.41              |
| 1:J:541:MET:CG   | 4:7:345:ILE:C    | 2.87                     | 0.41              |
| 4:8:193:LEU:HD11 | 4:8:250:ILE:HG13 | 2.02                     | 0.41              |
| 4:8:287:ILE:HD11 | 4:W:202:THR:HA   | 1.66                     | 0.41              |
| 1:A:221:GLN:HG2  | 1:A:221:GLN:H    | 1.47                     | 0.41              |
| 1:A:330:GLU:OE1  | 1:A:330:GLU:HA   | 2.20                     | 0.41              |
| 1:A:541:MET:HG2  | 4:4:345:ILE:HG23 | 2.01                     | 0.41              |
| 1:A:568:PRO:CG   | 1:A:578:HIS:N    | 2.84                     | 0.41              |
| 1:A:725:ARG:HA   | 1:A:732:ILE:CG2  | 2.50                     | 0.41              |
| 2:B:140:PHE:HA   | 2:B:141:PRO:HD2  | 1.56                     | 0.41              |
| 3:C:95:ASP:OD1   | 3:C:139:TYR:HE1  | 2.03                     | 0.41              |
| 1:D:356:GLY:HA2  | 1:D:359:MET:HG3  | 2.02                     | 0.41              |
| 1:D:500:GLN:HB2  | 1:D:512:PHE:CZ   | 2.54                     | 0.41              |
| 1:D:568:PRO:CG   | 1:D:578:HIS:N    | 2.83                     | 0.41              |
| 1:D:787:ILE:HG21 | 1:D:787:ILE:HD13 | 1.67                     | 0.41              |
| 1:G:462:LEU:HD11 | 1:G:464:ILE:CD1  | 2.50                     | 0.41              |
| 1:G:730:SER:OG   | 3:I:109:HIS:ND1  | 2.49                     | 0.41              |
| 1:G:797:PHE:CD2  | 1:G:798:LEU:HD12 | 2.55                     | 0.41              |
| 1:G:826:VAL:O    | 1:G:828:HIS:N    | 2.53                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:I:25:ILE:O     | 3:I:63:ILE:CB    | 2.66                     | 0.41              |
| 3:I:95:ASP:OD1   | 3:I:139:TYR:HE1  | 2.03                     | 0.41              |
| 1:J:402:CYS:C    | 1:J:404:PRO:HD3  | 2.40                     | 0.41              |
| 1:J:568:PRO:CG   | 1:J:578:HIS:N    | 2.83                     | 0.41              |
| 1:J:636:LYS:CB   | 4:7:334:GLU:OE1  | 2.68                     | 0.41              |
| 1:J:690:LEU:O    | 1:J:694:GLN:HG3  | 2.20                     | 0.41              |
| 4:V:369:ILE:HG23 | 4:V:370:VAL:N    | 2.35                     | 0.41              |
| 4:W:299:MET:HE2  | 4:W:331:ALA:HB2  | 2.01                     | 0.41              |
| 4:Y:196:ARG:HH21 | 4:Y:249:THR:HG23 | 1.85                     | 0.41              |
| 4:Z:193:LEU:HD11 | 4:Z:250:ILE:HG13 | 2.02                     | 0.41              |
| 4:0:226:GLU:HG3  | 4:0:255:PHE:CE2  | 2.55                     | 0.41              |
| 4:0:369:ILE:HG23 | 4:0:370:VAL:N    | 2.35                     | 0.41              |
| 4:1:193:LEU:HD11 | 4:1:250:ILE:HG13 | 2.02                     | 0.41              |
| 4:1:221:LEU:HA   | 4:1:312:ARG:HG2  | 2.03                     | 0.41              |
| 4:2:206:ARG:O    | 4:2:209:VAL:HG12 | 2.20                     | 0.41              |
| 4:2:369:ILE:HG23 | 4:2:370:VAL:N    | 2.35                     | 0.41              |
| 4:3:206:ARG:O    | 4:3:209:VAL:HG12 | 2.20                     | 0.41              |
| 4:3:287:ILE:HA   | 4:5:202:THR:HG21 | 1.59                     | 0.41              |
| 4:5:226:GLU:HG3  | 4:5:255:PHE:CE2  | 2.55                     | 0.41              |
| 1:G:541:MET:HB3  | 4:6:345:ILE:HG22 | 2.01                     | 0.41              |
| 4:5:287:ILE:CB   | 4:7:204:ALA:H    | 2.13                     | 0.41              |
| 4:7:324:THR:HG23 | 4:V:245:GLY:HA2  | 1.09                     | 0.41              |
| 4:8:315:LYS:HA   | 4:8:315:LYS:HD2  | 1.92                     | 0.41              |
| 1:A:166:MET:CE   | 1:A:254:PHE:CD2  | 3.01                     | 0.41              |
| 1:A:25:ILE:HG23  | 1:A:29:ASN:HD22  | 1.85                     | 0.41              |
| 1:A:690:LEU:O    | 1:A:694:GLN:HG3  | 2.20                     | 0.41              |
| 1:A:795:ARG:CG   | 3:C:118:MET:HE1  | 2.50                     | 0.41              |
| 1:A:831:TRP:HZ2  | 2:B:47:LEU:HA    | 1.85                     | 0.41              |
| 1:D:129:TYR:HA   | 1:D:129:TYR:HD1  | 1.65                     | 0.41              |
| 1:D:135:TYR:CD2  | 1:D:191:ARG:HD3  | 2.55                     | 0.41              |
| 1:D:554:LEU:HA   | 1:D:554:LEU:HD12 | 1.77                     | 0.41              |
| 1:D:568:PRO:O    | 1:D:570:PRO:HD3  | 2.19                     | 0.41              |
| 1:D:641:LYS:CE   | 1:D:647:GLN:CB   | 2.75                     | 0.41              |
| 1:D:795:ARG:NE   | 3:F:43:ASN:OD1   | 2.53                     | 0.41              |
| 1:D:799:MET:CE   | 3:F:32:ASP:CB    | 2.83                     | 0.41              |
| 1:D:87:MLY:HD3   | 1:D:87:MLY:HH12  | 1.61                     | 0.41              |
| 1:G:136:ASN:O    | 1:G:138:MLY:N    | 2.54                     | 0.41              |
| 1:G:185:LYS:HG3  | 1:G:185:LYS:H    | 1.63                     | 0.41              |
| 1:G:641:LYS:CE   | 1:G:647:GLN:CB   | 2.75                     | 0.41              |
| 1:G:775:LEU:HA   | 1:G:775:LEU:HD12 | 1.71                     | 0.41              |
| 1:J:136:ASN:O    | 1:J:138:MLY:N    | 2.54                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:556:ASP:OD1  | 4:V:50:LYS:CG    | 2.69                     | 0.41              |
| 1:J:797:PHE:CD2  | 1:J:798:LEU:HD12 | 2.55                     | 0.41              |
| 1:J:821:ARG:CZ   | 2:K:127:ARG:HD3  | 2.51                     | 0.41              |
| 4:V:196:ARG:HH21 | 4:V:249:THR:HG23 | 1.85                     | 0.41              |
| 4:V:324:THR:HG23 | 4:X:245:GLY:HA2  | 1.09                     | 0.41              |
| 4:W:226:GLU:HG3  | 4:W:255:PHE:CE2  | 2.55                     | 0.41              |
| 4:W:193:LEU:HD11 | 4:W:250:ILE:HG13 | 2.02                     | 0.41              |
| 4:X:217:CYS:C    | 4:X:218:TYR:HD1  | 2.23                     | 0.41              |
| 4:X:221:LEU:HA   | 4:X:312:ARG:HG2  | 2.02                     | 0.41              |
| 4:Z:369:ILE:HG23 | 4:Z:370:VAL:N    | 2.35                     | 0.41              |
| 4:3:226:GLU:HG3  | 4:3:255:PHE:CE2  | 2.55                     | 0.41              |
| 4:5:196:ARG:HH21 | 4:5:249:THR:HG23 | 1.85                     | 0.41              |
| 1:G:541:MET:CE   | 4:6:346:LEU:HD12 | 2.48                     | 0.41              |
| 1:A:62:VAL:HG12  | 1:A:63:MLY:N     | 2.35                     | 0.41              |
| 1:A:741:LYS:HG2  | 1:A:742:LYS:N    | 2.35                     | 0.41              |
| 1:D:11:GLY:O     | 1:D:14:ALA:HB3   | 2.20                     | 0.41              |
| 1:D:812:SER:O    | 1:D:816:ILE:HG13 | 2.21                     | 0.41              |
| 1:D:822:SER:CB   | 2:E:88:LEU:HD21  | 2.47                     | 0.41              |
| 1:D:831:TRP:CE2  | 2:E:51:PHE:CZ    | 3.09                     | 0.41              |
| 2:E:113:LYS:O    | 2:E:147:ASN:HB2  | 2.20                     | 0.41              |
| 1:G:330:GLU:HA   | 1:G:330:GLU:OE1  | 2.20                     | 0.41              |
| 1:G:402:CYS:C    | 1:G:404:PRO:HD3  | 2.40                     | 0.41              |
| 1:G:541:MET:HG2  | 4:6:345:ILE:HG23 | 2.01                     | 0.41              |
| 1:G:471:ASP:CB   | 1:G:573:GLY:O    | 2.68                     | 0.41              |
| 1:G:744:SER:O    | 1:G:748:LEU:HD12 | 2.20                     | 0.41              |
| 1:J:229:LEU:HA   | 1:J:229:LEU:HD12 | 1.76                     | 0.41              |
| 1:J:335:ASP:O    | 1:J:338:ILE:HB   | 2.20                     | 0.41              |
| 1:J:471:ASP:CB   | 1:J:573:GLY:O    | 2.68                     | 0.41              |
| 4:Y:221:LEU:HA   | 4:Y:312:ARG:HG2  | 2.02                     | 0.41              |
| 4:0:32:PRO:HB2   | 4:0:34:ILE:CD1   | 2.51                     | 0.41              |
| 4:4:227:MET:O    | 4:4:230:ALA:HB3  | 2.21                     | 0.41              |
| 4:5:206:ARG:O    | 4:5:209:VAL:HG12 | 2.20                     | 0.41              |
| 1:G:642:LYS:HE2  | 4:6:344:SER:HA   | 1.56                     | 0.41              |
| 4:7:226:GLU:HG3  | 4:7:255:PHE:CE2  | 2.55                     | 0.41              |
| 4:8:196:ARG:HH21 | 4:8:249:THR:HG23 | 1.85                     | 0.41              |
| 1:A:135:TYR:HD2  | 1:A:191:ARG:CG   | 2.33                     | 0.41              |
| 1:A:839:MLY:N    | 1:A:840:PRO:HD2  | 2.35                     | 0.41              |
| 2:B:140:PHE:HB3  | 2:B:144:VAL:HG11 | 2.03                     | 0.41              |
| 2:B:150:TYR:HB3  | 2:B:151:LYS:HG3  | 2.03                     | 0.41              |
| 1:D:296:MLY:HH11 | 1:D:348:MLY:CH2  | 2.48                     | 0.41              |
| 1:D:25:ILE:HG23  | 1:D:29:ASN:HD22  | 1.85                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:507:GLY:HA3  | 1:D:762:HIS:N    | 2.36                     | 0.41              |
| 1:D:173:GLN:HG3  | 1:D:670:HIS:CD2  | 2.55                     | 0.41              |
| 2:E:141:PRO:CB   | 2:E:142:PRO:HD3  | 2.48                     | 0.41              |
| 1:G:135:TYR:HD2  | 1:G:191:ARG:CG   | 2.33                     | 0.41              |
| 1:G:195:TYR:CE2  | 1:G:199:ILE:HD13 | 2.55                     | 0.41              |
| 1:G:217:THR:CA   | 1:G:221:GLN:HE21 | 2.33                     | 0.41              |
| 1:G:174:SER:HA   | 1:G:460:GLY:O    | 2.20                     | 0.41              |
| 1:G:556:ASP:OD1  | 4:8:50:LYS:CG    | 2.68                     | 0.41              |
| 1:G:690:LEU:O    | 1:G:694:GLN:HG3  | 2.20                     | 0.41              |
| 1:G:810:ARG:HG2  | 1:G:810:ARG:NH1  | 2.28                     | 0.41              |
| 1:J:14:ALA:HB3   | 1:J:15:PRO:CD    | 2.46                     | 0.41              |
| 1:J:296:MLY:HH11 | 1:J:348:MLY:CH2  | 2.48                     | 0.41              |
| 1:J:320:ILE:O    | 1:J:320:ILE:CG2  | 2.68                     | 0.41              |
| 1:J:295:MLY:CE   | 1:J:332:MET:HE1  | 2.51                     | 0.41              |
| 1:J:346:ASP:O    | 1:J:350:ALA:N    | 2.46                     | 0.41              |
| 1:J:464:ILE:HD13 | 1:J:464:ILE:HG21 | 1.69                     | 0.41              |
| 1:J:612:GLN:NE2  | 1:J:627:GLY:H    | 2.14                     | 0.41              |
| 1:J:829:TRP:O    | 1:J:832:MET:N    | 2.50                     | 0.41              |
| 1:J:817:GLN:CB   | 2:K:127:ARG:HH11 | 2.24                     | 0.41              |
| 2:K:144:VAL:HG12 | 2:K:153:ILE:HD13 | 1.92                     | 0.41              |
| 4:V:193:LEU:HD11 | 4:V:250:ILE:HG13 | 2.02                     | 0.41              |
| 4:X:226:GLU:HG3  | 4:X:255:PHE:CE2  | 2.55                     | 0.41              |
| 4:Z:206:ARG:O    | 4:Z:209:VAL:HG12 | 2.20                     | 0.41              |
| 4:Z:226:GLU:HG3  | 4:Z:255:PHE:CE2  | 2.55                     | 0.41              |
| 4:Z:144:ALA:HB2  | 4:Z:342:GLY:CA   | 2.51                     | 0.41              |
| 4:0:144:ALA:HB2  | 4:0:342:GLY:CA   | 2.51                     | 0.41              |
| 4:1:222:ASP:OD1  | 4:1:224:GLU:HB3  | 2.19                     | 0.41              |
| 4:2:144:ALA:HB2  | 4:2:342:GLY:CA   | 2.51                     | 0.41              |
| 4:4:288:ASP:OD1  | 4:6:204:ALA:HA   | 2.21                     | 0.41              |
| 4:3:290:ARG:HH22 | 4:5:202:THR:CG2  | 2.17                     | 0.41              |
| 4:5:193:LEU:HD11 | 4:5:250:ILE:HG13 | 2.02                     | 0.41              |
| 1:G:636:LYS:CB   | 4:6:334:GLU:OE1  | 2.68                     | 0.41              |
| 4:7:227:MET:O    | 4:7:230:ALA:HB3  | 2.21                     | 0.41              |
| 1:G:550:PHE:C    | 4:8:46:GLY:CA    | 2.88                     | 0.41              |
| 1:A:134:VAL:C    | 1:A:136:ASN:H    | 2.16                     | 0.41              |
| 2:B:144:VAL:HG12 | 2:B:153:ILE:HD11 | 1.75                     | 0.41              |
| 1:D:408:VAL:HG22 | 1:D:636:LYS:HG2  | 1.51                     | 0.41              |
| 1:D:62:VAL:O     | 1:D:69:THR:HA    | 2.19                     | 0.41              |
| 1:D:723:ARG:HH21 | 1:D:783:LEU:CD1  | 2.33                     | 0.41              |
| 1:D:797:PHE:CD2  | 1:D:798:LEU:HD12 | 2.55                     | 0.41              |
| 1:D:826:VAL:O    | 1:D:828:HIS:N    | 2.53                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:839:MLY:N    | 1:G:840:PRO:HD2  | 2.35                     | 0.41              |
| 1:J:204:GLU:N    | 1:J:207:LYS:HE3  | 2.23                     | 0.41              |
| 1:J:797:PHE:HB2  | 3:L:149:VAL:HG13 | 1.96                     | 0.41              |
| 4:0:288:ASP:OD1  | 4:2:204:ALA:HA   | 2.21                     | 0.41              |
| 4:1:32:PRO:HB2   | 4:1:34:ILE:CD1   | 2.51                     | 0.41              |
| 4:2:288:ASP:OD1  | 4:4:204:ALA:HA   | 2.21                     | 0.41              |
| 4:3:196:ARG:HH21 | 4:3:249:THR:HG23 | 1.85                     | 0.41              |
| 4:3:32:PRO:HB2   | 4:3:34:ILE:CD1   | 2.51                     | 0.41              |
| 4:4:226:GLU:HG3  | 4:4:255:PHE:CE2  | 2.55                     | 0.41              |
| 1:D:534:SER:HB2  | 4:5:354:GLN:HE22 | 1.56                     | 0.41              |
| 4:6:226:GLU:HG3  | 4:6:255:PHE:CE2  | 2.55                     | 0.41              |
| 4:8:144:ALA:HB2  | 4:8:342:GLY:CA   | 2.51                     | 0.41              |
| 1:A:174:SER:HA   | 1:A:460:GLY:O    | 2.20                     | 0.41              |
| 1:A:49:MLY:HH23  | 1:A:80:MET:CE    | 2.51                     | 0.41              |
| 1:A:541:MET:HG2  | 4:4:345:ILE:HG22 | 2.00                     | 0.41              |
| 2:B:149:ASP:OD2  | 2:B:150:TYR:CA   | 2.64                     | 0.41              |
| 1:D:136:ASN:O    | 1:D:138:MLY:N    | 2.54                     | 0.41              |
| 1:D:330:GLU:HA   | 1:D:330:GLU:OE1  | 2.21                     | 0.41              |
| 2:E:150:TYR:HB3  | 2:E:151:LYS:HG3  | 2.03                     | 0.41              |
| 3:F:48:LYS:HA    | 3:F:48:LYS:HD3   | 1.17                     | 0.41              |
| 1:G:449:LEU:CD1  | 1:G:449:LEU:N    | 2.82                     | 0.41              |
| 1:G:56:GLU:HB2   | 1:G:59:MLY:CB    | 2.30                     | 0.41              |
| 1:G:831:TRP:CE2  | 2:H:67:MET:CB    | 3.01                     | 0.41              |
| 1:J:25:ILE:HG23  | 1:J:29:ASN:HD22  | 1.85                     | 0.41              |
| 1:J:610:LEU:CD1  | 1:J:610:LEU:N    | 2.84                     | 0.41              |
| 1:J:90:ASP:CB    | 1:J:764:MLY:HH11 | 2.42                     | 0.41              |
| 1:J:821:ARG:HH12 | 2:K:127:ARG:CZ   | 2.33                     | 0.41              |
| 1:J:838:ILE:CD1  | 2:K:54:MET:HE1   | 2.42                     | 0.41              |
| 4:V:226:GLU:HG3  | 4:V:255:PHE:CE2  | 2.55                     | 0.41              |
| 4:V:144:ALA:HB2  | 4:V:342:GLY:CA   | 2.51                     | 0.41              |
| 4:W:324:THR:O    | 4:Y:244:ASP:HA   | 2.09                     | 0.41              |
| 4:W:144:ALA:HB2  | 4:W:342:GLY:CA   | 2.51                     | 0.41              |
| 4:X:144:ALA:HB2  | 4:X:342:GLY:CA   | 2.51                     | 0.41              |
| 4:Z:221:LEU:HA   | 4:Z:312:ARG:HG2  | 2.02                     | 0.41              |
| 4:1:226:GLU:HG3  | 4:1:255:PHE:CE2  | 2.56                     | 0.41              |
| 4:1:288:ASP:OD1  | 4:3:204:ALA:HA   | 2.21                     | 0.41              |
| 4:6:144:ALA:HB2  | 4:6:342:GLY:CA   | 2.51                     | 0.41              |
| 4:5:287:ILE:N    | 4:7:202:THR:CG2  | 2.77                     | 0.41              |
| 1:A:136:ASN:O    | 1:A:138:MLY:N    | 2.54                     | 0.41              |
| 1:A:193:ILE:HD11 | 1:A:250:ILE:HD12 | 2.03                     | 0.41              |
| 1:A:107:MLY:CB   | 1:A:686:MET:HE2  | 2.40                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:711:PHE:O    | 1:A:714:ARG:NH2  | 2.54                     | 0.41              |
| 1:A:812:SER:O    | 1:A:816:ILE:HG13 | 2.21                     | 0.41              |
| 3:C:63:ILE:CG2   | 3:C:64:THR:H     | 2.33                     | 0.41              |
| 1:D:91:MET:CE    | 1:D:119:SER:HB2  | 2.48                     | 0.41              |
| 1:D:308:ASN:HA   | 1:D:309:PRO:HD2  | 1.88                     | 0.41              |
| 1:D:322:VAL:HG12 | 1:D:325:ILE:HG13 | 2.03                     | 0.41              |
| 1:D:38:VAL:HG13  | 1:D:39:PHE:N     | 2.34                     | 0.41              |
| 1:D:629:GLU:HB3  | 1:D:643:GLY:C    | 2.41                     | 0.41              |
| 1:D:799:MET:SD   | 3:F:32:ASP:HA    | 2.51                     | 0.41              |
| 1:G:193:ILE:CD1  | 1:G:250:ILE:HD13 | 2.51                     | 0.41              |
| 1:G:665:ARG:C    | 1:G:667:THR:N    | 2.74                     | 0.41              |
| 1:G:797:PHE:CD1  | 3:I:149:VAL:CB   | 2.85                     | 0.41              |
| 1:J:135:TYR:CD2  | 1:J:191:ARG:HD3  | 2.55                     | 0.41              |
| 1:J:193:ILE:HD11 | 1:J:250:ILE:HD12 | 2.03                     | 0.41              |
| 1:J:356:GLY:HA2  | 1:J:359:MET:HG3  | 2.02                     | 0.41              |
| 1:J:629:GLU:HB3  | 1:J:643:GLY:C    | 2.41                     | 0.41              |
| 1:J:657:LEU:HD12 | 1:J:657:LEU:O    | 2.21                     | 0.41              |
| 1:J:741:LYS:HG2  | 1:J:742:LYS:N    | 2.35                     | 0.41              |
| 1:J:744:SER:O    | 1:J:748:LEU:HD12 | 2.20                     | 0.41              |
| 1:J:812:SER:O    | 1:J:816:ILE:HG13 | 2.21                     | 0.41              |
| 4:W:221:LEU:HA   | 4:W:312:ARG:HG2  | 2.02                     | 0.41              |
| 4:Y:32:PRO:HB2   | 4:Y:34:ILE:CD1   | 2.51                     | 0.41              |
| 4:2:196:ARG:HH21 | 4:2:249:THR:HG23 | 1.85                     | 0.41              |
| 4:2:227:MET:O    | 4:2:230:ALA:HB3  | 2.21                     | 0.41              |
| 4:2:32:PRO:HB2   | 4:2:34:ILE:CD1   | 2.51                     | 0.41              |
| 4:4:144:ALA:HB2  | 4:4:342:GLY:CA   | 2.51                     | 0.41              |
| 4:5:32:PRO:HB2   | 4:5:34:ILE:CD1   | 2.51                     | 0.41              |
| 1:G:534:SER:HB2  | 4:6:354:GLN:HE22 | 1.56                     | 0.41              |
| 4:7:144:ALA:HB2  | 4:7:342:GLY:CA   | 2.51                     | 0.41              |
| 1:A:193:ILE:CD1  | 1:A:250:ILE:HD13 | 2.51                     | 0.41              |
| 1:A:194:GLN:HB3  | 1:A:194:GLN:HE21 | 1.43                     | 0.41              |
| 1:A:732:ILE:HG23 | 1:A:747:LEU:HD13 | 1.37                     | 0.41              |
| 1:A:72:VAL:O     | 1:A:73:LYS:O     | 2.39                     | 0.41              |
| 1:A:800:ARG:HD3  | 3:C:149:VAL:C    | 2.35                     | 0.41              |
| 1:D:195:TYR:CE2  | 1:D:199:ILE:HD13 | 2.55                     | 0.41              |
| 1:D:322:VAL:HB   | 1:D:325:ILE:HD12 | 2.03                     | 0.41              |
| 1:D:407:GLY:HA2  | 1:D:411:GLU:O    | 2.21                     | 0.41              |
| 1:D:493:HIS:O    | 1:D:496:PHE:N    | 2.54                     | 0.41              |
| 1:G:14:ALA:HB3   | 1:G:15:PRO:CD    | 2.46                     | 0.41              |
| 1:G:322:VAL:HA   | 1:G:323:PRO:HD3  | 1.87                     | 0.41              |
| 1:G:335:ASP:O    | 1:G:338:ILE:HB   | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:384:ASP:HA   | 1:G:394:SER:OG   | 2.21                     | 0.41              |
| 1:G:485:GLU:OE2  | 1:G:584:TYR:N    | 2.50                     | 0.41              |
| 1:G:717:TYR:OH   | 1:G:760:PHE:HB3  | 2.21                     | 0.41              |
| 1:G:832:MET:SD   | 2:H:84:PHE:CE2   | 3.06                     | 0.41              |
| 2:H:140:PHE:HA   | 2:H:141:PRO:HD2  | 1.57                     | 0.41              |
| 1:J:322:VAL:HG12 | 1:J:325:ILE:HG13 | 2.03                     | 0.41              |
| 1:J:330:GLU:HG2  | 1:J:330:GLU:H    | 1.54                     | 0.41              |
| 4:W:32:PRO:HB2   | 4:W:34:ILE:CD1   | 2.51                     | 0.41              |
| 4:Y:144:ALA:HB2  | 4:Y:342:GLY:CA   | 2.51                     | 0.41              |
| 4:Z:227:MET:O    | 4:Z:230:ALA:HB3  | 2.21                     | 0.41              |
| 4:O:221:LEU:HA   | 4:O:312:ARG:HG2  | 2.02                     | 0.41              |
| 4:5:227:MET:O    | 4:5:230:ALA:HB3  | 2.21                     | 0.41              |
| 4:5:144:ALA:HB2  | 4:5:342:GLY:CA   | 2.51                     | 0.41              |
| 4:6:227:MET:O    | 4:6:230:ALA:HB3  | 2.21                     | 0.41              |
| 4:6:288:ASP:OD1  | 4:8:204:ALA:HA   | 2.21                     | 0.41              |
| 1:A:217:THR:CA   | 1:A:221:GLN:HE21 | 2.33                     | 0.41              |
| 1:A:226:ASN:HB2  | 1:A:227:PRO:CD   | 2.47                     | 0.41              |
| 1:A:303:LEU:O    | 1:A:304:LEU:HB2  | 2.21                     | 0.41              |
| 1:A:356:GLY:HA2  | 1:A:359:MET:HG3  | 2.02                     | 0.41              |
| 1:A:172:ASN:OD1  | 1:A:457:TYR:HA   | 2.21                     | 0.41              |
| 1:A:471:ASP:CB   | 1:A:573:GLY:O    | 2.68                     | 0.41              |
| 2:B:111:SER:OG   | 2:B:148:VAL:CA   | 2.69                     | 0.41              |
| 1:A:793:ARG:HH21 | 3:C:147:MET:HE2  | 1.84                     | 0.41              |
| 1:A:800:ARG:NE   | 3:C:149:VAL:C    | 2.73                     | 0.41              |
| 3:C:56:GLU:OE1   | 3:C:59:ASN:ND2   | 2.54                     | 0.41              |
| 1:D:242:ASN:OD1  | 1:D:286:HIS:NE2  | 2.49                     | 0.41              |
| 1:D:309:PRO:C    | 1:D:311:ASP:H    | 2.22                     | 0.41              |
| 1:D:398:LEU:HA   | 1:D:398:LEU:HD12 | 1.84                     | 0.41              |
| 1:G:356:GLY:HA2  | 1:G:359:MET:HG3  | 2.02                     | 0.41              |
| 1:G:537:GLU:OE1  | 4:6:350:SER:HA   | 2.20                     | 0.41              |
| 1:G:768:MLY:HG2  | 1:G:772:LEU:HD23 | 2.03                     | 0.41              |
| 1:G:812:SER:O    | 1:G:816:ILE:HG13 | 2.21                     | 0.41              |
| 1:G:791:GLN:HB3  | 3:I:118:MET:CE   | 2.51                     | 0.41              |
| 1:J:107:MLY:N    | 1:J:686:MET:HE1  | 2.35                     | 0.41              |
| 1:J:839:MLY:N    | 1:J:840:PRO:HD2  | 2.35                     | 0.41              |
| 2:K:149:ASP:CG   | 2:K:150:TYR:N    | 2.49                     | 0.41              |
| 4:V:227:MET:O    | 4:V:230:ALA:HB3  | 2.21                     | 0.41              |
| 1:J:550:PHE:C    | 4:V:46:GLY:CA    | 2.88                     | 0.41              |
| 4:1:287:ILE:N    | 4:3:202:THR:CG2  | 2.77                     | 0.41              |
| 4:3:227:MET:O    | 4:3:230:ALA:HB3  | 2.21                     | 0.41              |
| 4:4:219:VAL:HG22 | 4:4:258:PRO:CB   | 2.52                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:6:219:VAL:HG22 | 4:6:258:PRO:CB   | 2.51                     | 0.41              |
| 4:7:32:PRO:HB2   | 4:7:34:ILE:CD1   | 2.51                     | 0.41              |
| 1:J:642:LYS:HE2  | 4:7:344:SER:HA   | 1.56                     | 0.41              |
| 4:8:221:LEU:HA   | 4:8:312:ARG:HG2  | 2.02                     | 0.41              |
| 1:A:502:GLU:HG2  | 1:A:766:PHE:HE1  | 1.85                     | 0.41              |
| 1:A:817:GLN:HG3  | 2:B:127:ARG:HD3  | 1.03                     | 0.41              |
| 1:D:217:THR:CA   | 1:D:221:GLN:HE21 | 2.33                     | 0.41              |
| 1:D:335:ASP:O    | 1:D:338:ILE:HB   | 2.20                     | 0.41              |
| 1:D:47:PHE:HE1   | 1:D:78:PHE:CE1   | 2.40                     | 0.41              |
| 1:D:723:ARG:C    | 1:D:782:MLY:CH2  | 2.89                     | 0.41              |
| 1:D:724:TYR:CA   | 1:D:782:MLY:HH11 | 2.48                     | 0.41              |
| 1:G:91:MET:CE    | 1:G:119:SER:HB2  | 2.47                     | 0.41              |
| 1:G:193:ILE:HD11 | 1:G:250:ILE:HD12 | 2.03                     | 0.41              |
| 1:G:172:ASN:OD1  | 1:G:457:TYR:HA   | 2.21                     | 0.41              |
| 1:G:657:LEU:O    | 1:G:657:LEU:HD12 | 2.21                     | 0.41              |
| 1:G:712:PRO:HB2  | 1:G:713:SER:H    | 1.61                     | 0.41              |
| 2:H:113:LYS:O    | 2:H:147:ASN:HB2  | 2.20                     | 0.41              |
| 1:G:798:LEU:CD2  | 3:I:126:LEU:HD11 | 2.44                     | 0.41              |
| 1:G:795:ARG:HH22 | 3:I:43:ASN:CB    | 2.33                     | 0.41              |
| 3:I:56:GLU:OE1   | 3:I:59:ASN:ND2   | 2.54                     | 0.41              |
| 1:J:193:ILE:CD1  | 1:J:250:ILE:HD13 | 2.51                     | 0.41              |
| 1:J:322:VAL:HB   | 1:J:325:ILE:HD12 | 2.03                     | 0.41              |
| 1:J:493:HIS:O    | 1:J:496:PHE:N    | 2.54                     | 0.41              |
| 1:J:519:LEU:H    | 1:J:519:LEU:HD12 | 1.83                     | 0.41              |
| 1:J:701:LEU:HA   | 1:J:701:LEU:HD12 | 1.55                     | 0.41              |
| 1:J:733:PRO:CB   | 1:J:737:PHE:CE1  | 3.02                     | 0.41              |
| 1:J:776:GLU:O    | 1:J:780:ASP:N    | 2.45                     | 0.41              |
| 1:J:842:LEU:N    | 1:J:842:LEU:CD1  | 2.83                     | 0.41              |
| 1:J:793:ARG:HD2  | 3:L:146:ILE:O    | 2.21                     | 0.41              |
| 4:X:288:ASP:OD1  | 4:Z:204:ALA:HA   | 2.21                     | 0.41              |
| 4:0:227:MET:O    | 4:0:230:ALA:HB3  | 2.21                     | 0.40              |
| 4:1:219:VAL:HG22 | 4:1:258:PRO:CB   | 2.52                     | 0.40              |
| 4:1:144:ALA:HB2  | 4:1:342:GLY:CA   | 2.51                     | 0.40              |
| 4:3:144:ALA:HB2  | 4:3:342:GLY:CA   | 2.51                     | 0.40              |
| 4:5:288:ASP:OD1  | 4:7:204:ALA:HA   | 2.21                     | 0.40              |
| 4:6:32:PRO:HB2   | 4:6:34:ILE:CD1   | 2.51                     | 0.40              |
| 4:5:287:ILE:HA   | 4:7:202:THR:HG21 | 1.59                     | 0.40              |
| 1:D:556:ASP:OD1  | 4:7:50:LYS:CG    | 2.69                     | 0.40              |
| 4:8:32:PRO:HB2   | 4:8:34:ILE:CD1   | 2.51                     | 0.40              |
| 1:A:295:MLY:CG   | 1:A:332:MET:HE1  | 2.50                     | 0.40              |
| 1:A:335:ASP:O    | 1:A:338:ILE:HB   | 2.20                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:410:ASN:HA   | 4:4:334:GLU:HB3  | 1.30                     | 0.40              |
| 1:A:757:GLN:OE1  | 1:A:771:LEU:CD1  | 2.69                     | 0.40              |
| 2:B:139:ALA:O    | 2:B:141:PRO:CD   | 2.51                     | 0.40              |
| 1:D:135:TYR:HD2  | 1:D:191:ARG:CG   | 2.33                     | 0.40              |
| 1:D:193:ILE:HD11 | 1:D:250:ILE:HD12 | 2.03                     | 0.40              |
| 1:D:48:VAL:CG2   | 1:D:49:MLY:N     | 2.84                     | 0.40              |
| 1:G:528:MLY:HB2  | 1:G:529:PRO:HD2  | 2.03                     | 0.40              |
| 1:G:835:PHE:CZ   | 2:H:27:PHE:CE1   | 3.09                     | 0.40              |
| 1:G:817:GLN:CG   | 2:H:128:PHE:CE1  | 3.01                     | 0.40              |
| 1:J:330:GLU:OE1  | 1:J:330:GLU:HA   | 2.20                     | 0.40              |
| 1:J:384:ASP:HA   | 1:J:394:SER:OG   | 2.21                     | 0.40              |
| 1:J:508:ILE:HD13 | 1:J:759:ALA:HB2  | 1.79                     | 0.40              |
| 2:K:113:LYS:O    | 2:K:147:ASN:HB2  | 2.20                     | 0.40              |
| 3:L:48:LYS:HA    | 3:L:48:LYS:HD3   | 1.17                     | 0.40              |
| 3:L:56:GLU:OE1   | 3:L:59:ASN:ND2   | 2.54                     | 0.40              |
| 4:W:219:VAL:HG22 | 4:W:258:PRO:CB   | 2.52                     | 0.40              |
| 4:X:250:ILE:HG22 | 4:X:254:ARG:HB2  | 2.04                     | 0.40              |
| 4:Z:219:VAL:HG22 | 4:Z:258:PRO:CB   | 2.51                     | 0.40              |
| 4:1:120:THR:HG21 | 4:1:370:VAL:CG1  | 2.52                     | 0.40              |
| 4:2:219:VAL:HG22 | 4:2:258:PRO:CB   | 2.51                     | 0.40              |
| 4:4:221:LEU:HA   | 4:4:312:ARG:HG2  | 2.02                     | 0.40              |
| 4:5:120:THR:HG21 | 4:5:370:VAL:CG1  | 2.52                     | 0.40              |
| 1:A:384:ASP:HA   | 1:A:394:SER:OG   | 2.21                     | 0.40              |
| 2:B:63:GLU:O     | 2:B:67:MET:HG3   | 2.22                     | 0.40              |
| 1:A:795:ARG:HH22 | 3:C:43:ASN:HB2   | 1.86                     | 0.40              |
| 1:D:193:ILE:CD1  | 1:D:250:ILE:HD13 | 2.51                     | 0.40              |
| 1:D:213:LYS:HA   | 1:D:220:ASP:OD2  | 2.19                     | 0.40              |
| 1:D:320:ILE:O    | 1:D:320:ILE:CG2  | 2.68                     | 0.40              |
| 1:D:348:MLY:HD2  | 1:D:348:MLY:HH12 | 1.82                     | 0.40              |
| 1:D:528:MLY:HB2  | 1:D:529:PRO:HD2  | 2.03                     | 0.40              |
| 3:F:56:GLU:OE1   | 3:F:59:ASN:ND2   | 2.54                     | 0.40              |
| 1:G:110:TYR:O    | 1:G:113:TRP:N    | 2.42                     | 0.40              |
| 1:G:25:ILE:HG23  | 1:G:29:ASN:HD22  | 1.85                     | 0.40              |
| 1:G:464:ILE:HG22 | 1:G:465:ALA:H    | 1.87                     | 0.40              |
| 1:G:493:HIS:O    | 1:G:496:PHE:N    | 2.54                     | 0.40              |
| 1:G:739:ASP:OD1  | 1:G:739:ASP:C    | 2.58                     | 0.40              |
| 1:G:795:ARG:NH2  | 3:I:116:GLU:HB3  | 2.36                     | 0.40              |
| 1:G:795:ARG:NH2  | 3:I:43:ASN:OD1   | 1.62                     | 0.40              |
| 1:J:303:LEU:O    | 1:J:304:LEU:HB2  | 2.21                     | 0.40              |
| 1:J:172:ASN:OD1  | 1:J:457:TYR:HA   | 2.21                     | 0.40              |
| 1:J:88:ILE:HG22  | 1:J:90:ASP:C     | 2.42                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:V:120:THR:HG21 | 4:V:370:VAL:CG1  | 2.52                     | 0.40              |
| 4:W:120:THR:HG21 | 4:W:370:VAL:CG1  | 2.51                     | 0.40              |
| 4:Y:219:VAL:HG22 | 4:Y:258:PRO:CB   | 2.52                     | 0.40              |
| 4:Y:227:MET:O    | 4:Y:230:ALA:HB3  | 2.21                     | 0.40              |
| 4:Y:226:GLU:HG3  | 4:Y:255:PHE:CE2  | 2.55                     | 0.40              |
| 4:2:221:LEU:HA   | 4:2:312:ARG:HG2  | 2.02                     | 0.40              |
| 4:3:219:VAL:HG22 | 4:3:258:PRO:CB   | 2.51                     | 0.40              |
| 4:6:221:LEU:HA   | 4:6:312:ARG:HG2  | 2.02                     | 0.40              |
| 4:6:324:THR:HG23 | 4:8:245:GLY:HA2  | 1.09                     | 0.40              |
| 1:J:544:LYS:N    | 4:7:146:GLY:O    | 2.55                     | 0.40              |
| 4:7:196:ARG:HH21 | 4:7:249:THR:HG23 | 1.85                     | 0.40              |
| 4:8:287:ILE:N    | 4:W:202:THR:CG2  | 2.77                     | 0.40              |
| 1:A:464:ILE:HG22 | 1:A:465:ALA:H    | 1.87                     | 0.40              |
| 1:A:798:LEU:HA   | 1:A:798:LEU:HD12 | 1.37                     | 0.40              |
| 2:B:112:ILE:O    | 2:B:148:VAL:N    | 2.50                     | 0.40              |
| 1:D:201:ALA:O    | 1:D:202:SER:OG   | 2.36                     | 0.40              |
| 1:D:237:THR:CG2  | 1:D:238:VAL:N    | 2.85                     | 0.40              |
| 1:D:60:VAL:O     | 1:D:72:VAL:N     | 2.51                     | 0.40              |
| 1:D:657:LEU:HD12 | 1:D:657:LEU:O    | 2.21                     | 0.40              |
| 1:G:303:LEU:O    | 1:G:304:LEU:HB2  | 2.21                     | 0.40              |
| 1:G:407:GLY:HA2  | 1:G:411:GLU:O    | 2.21                     | 0.40              |
| 1:G:768:MLY:HD3  | 1:G:772:LEU:HD23 | 1.87                     | 0.40              |
| 1:J:38:VAL:HG13  | 1:J:39:PHE:N     | 2.35                     | 0.40              |
| 1:J:528:MLY:HB2  | 1:J:529:PRO:HD2  | 2.03                     | 0.40              |
| 1:J:659:MLY:HH22 | 1:J:659:MLY:HD2  | 1.42                     | 0.40              |
| 3:L:95:ASP:OD1   | 3:L:139:TYR:HE1  | 2.04                     | 0.40              |
| 4:X:196:ARG:HH21 | 4:X:249:THR:HG23 | 1.85                     | 0.40              |
| 4:X:287:ILE:N    | 4:Z:202:THR:CG2  | 2.77                     | 0.40              |
| 4:1:227:MET:O    | 4:1:230:ALA:HB3  | 2.21                     | 0.40              |
| 4:6:120:THR:HG21 | 4:6:370:VAL:CG1  | 2.52                     | 0.40              |
| 4:8:227:MET:O    | 4:8:230:ALA:HB3  | 2.21                     | 0.40              |
| 4:8:250:ILE:HG22 | 4:8:254:ARG:HB2  | 2.04                     | 0.40              |
| 4:8:219:VAL:HG22 | 4:8:258:PRO:CB   | 2.52                     | 0.40              |
| 1:A:817:GLN:CB   | 2:B:127:ARG:CZ   | 2.69                     | 0.40              |
| 3:C:84:PHE:HB3   | 3:C:147:MET:HE1  | 2.04                     | 0.40              |
| 1:D:176:LEU:CD1  | 1:D:176:LEU:N    | 2.75                     | 0.40              |
| 1:D:303:LEU:O    | 1:D:304:LEU:HB2  | 2.21                     | 0.40              |
| 1:D:172:ASN:OD1  | 1:D:457:TYR:HA   | 2.21                     | 0.40              |
| 1:D:507:GLY:HA2  | 1:D:762:HIS:NE2  | 2.36                     | 0.40              |
| 1:D:610:LEU:N    | 1:D:610:LEU:CD1  | 2.84                     | 0.40              |
| 1:D:64:THR:OG1   | 1:D:68:GLU:HB3   | 2.22                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:717:TYR:OH   | 1:D:760:PHE:HB3  | 2.21                     | 0.40              |
| 1:D:88:ILE:HG22  | 1:D:90:ASP:C     | 2.42                     | 0.40              |
| 1:D:813:ILE:HG22 | 2:E:127:ARG:NH1  | 2.08                     | 0.40              |
| 1:G:305:ILE:HG22 | 1:G:312:TYR:OH   | 2.22                     | 0.40              |
| 1:G:93:MET:SD    | 1:G:764:MLY:HH23 | 2.61                     | 0.40              |
| 1:J:47:PHE:HE1   | 1:J:78:PHE:CE1   | 2.40                     | 0.40              |
| 1:J:648:THR:CG2  | 1:J:651:ALA:CB   | 2.92                     | 0.40              |
| 1:J:717:TYR:OH   | 1:J:760:PHE:HB3  | 2.21                     | 0.40              |
| 3:L:62:ALA:O     | 3:L:63:ILE:CB    | 2.63                     | 0.40              |
| 4:8:288:ASP:OD1  | 4:W:204:ALA:HA   | 2.21                     | 0.40              |
| 4:W:250:ILE:HG22 | 4:W:254:ARG:HB2  | 2.04                     | 0.40              |
| 4:X:32:PRO:HB2   | 4:X:34:ILE:CD1   | 2.51                     | 0.40              |
| 4:1:250:ILE:HG22 | 4:1:254:ARG:HB2  | 2.04                     | 0.40              |
| 4:4:287:ILE:N    | 4:6:202:THR:CG2  | 2.77                     | 0.40              |
| 4:4:32:PRO:HB2   | 4:4:34:ILE:CD1   | 2.51                     | 0.40              |
| 1:A:556:ASP:OD1  | 4:6:50:LYS:CG    | 2.69                     | 0.40              |
| 4:8:88:HIS:HA    | 4:8:92:ASN:OD1   | 2.22                     | 0.40              |
| 1:A:237:THR:CG2  | 1:A:238:VAL:N    | 2.84                     | 0.40              |
| 1:A:292:MET:CE   | 1:A:309:PRO:HD3  | 2.52                     | 0.40              |
| 2:B:137:TRP:CA   | 2:B:145:ALA:CB   | 2.82                     | 0.40              |
| 1:D:89:GLU:HB3   | 1:D:153:PRO:HG3  | 2.03                     | 0.40              |
| 1:D:400:ALA:CB   | 1:D:606:THR:CG2  | 3.00                     | 0.40              |
| 2:E:163:ALA:O    | 2:K:20:ASP:OD2   | 2.39                     | 0.40              |
| 1:G:193:ILE:HD13 | 1:G:252:ILE:HD11 | 2.04                     | 0.40              |
| 2:H:63:GLU:O     | 2:H:67:MET:HG3   | 2.22                     | 0.40              |
| 1:J:63:MLY:HH23  | 1:J:63:MLY:HD3   | 1.76                     | 0.40              |
| 4:V:32:PRO:HB2   | 4:V:34:ILE:CD1   | 2.51                     | 0.40              |
| 4:W:193:LEU:HD12 | 4:W:193:LEU:HA   | 1.96                     | 0.40              |
| 4:W:288:ASP:OD1  | 4:Y:204:ALA:HA   | 2.21                     | 0.40              |
| 4:X:227:MET:O    | 4:X:230:ALA:HB3  | 2.21                     | 0.40              |
| 4:V:324:THR:N    | 4:X:245:GLY:CA   | 2.69                     | 0.40              |
| 4:Y:120:THR:HG21 | 4:Y:370:VAL:CG1  | 2.52                     | 0.40              |

All (10902) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1          | Atom-2                | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------------|--------------------------|-------------------|
| 4:2:206:ARG:CG  | 4:Z:200:PHE:CA[1_556] | 0.14                     | 2.06              |
| 4:0:206:ARG:CG  | 4:X:200:PHE:CA[1_556] | 0.14                     | 2.06              |
| 4:0:186:THR:OG1 | 4:X:189:LEU:O[1_556]  | 0.15                     | 2.05              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:186:THR:OG1 | 4:Z:189:LEU:O[1_556]   | 0.16                     | 2.04              |
| 4:1:32:PRO:CD   | 4:Y:211:ASP:CG[1_556]  | 0.17                     | 2.03              |
| 4:1:180:LEU:CG  | 4:Y:267:ILE:CG1[1_556] | 0.21                     | 1.99              |
| 4:2:180:LEU:CG  | 4:Z:267:ILE:CG1[1_556] | 0.22                     | 1.98              |
| 4:1:206:ARG:CG  | 4:Y:200:PHE:CA[1_556]  | 0.22                     | 1.98              |
| 4:0:180:LEU:CG  | 4:X:267:ILE:CG1[1_556] | 0.24                     | 1.96              |
| 4:2:32:PRO:CD   | 4:Z:211:ASP:CG[1_556]  | 0.24                     | 1.96              |
| 4:1:186:THR:OG1 | 4:Y:189:LEU:O[1_556]   | 0.24                     | 1.96              |
| 4:0:32:PRO:CD   | 4:X:211:ASP:CG[1_556]  | 0.25                     | 1.95              |
| 4:1:164:PRO:N   | 4:Y:278:THR:CB[1_556]  | 0.25                     | 1.95              |
| 4:2:253:GLU:OE1 | 4:Y:112:PRO:C[1_556]   | 0.26                     | 1.94              |
| 4:1:336:LYS:NZ  | 4:Y:254:ARG:NH2[1_556] | 0.27                     | 1.93              |
| 4:0:253:GLU:OE1 | 4:W:112:PRO:C[1_556]   | 0.28                     | 1.92              |
| 4:1:162:ASN:CG  | 4:Y:273:GLY:C[1_556]   | 0.28                     | 1.92              |
| 4:0:136:ILE:CA  | 4:X:299:MET:C[1_556]   | 0.28                     | 1.92              |
| 4:2:336:LYS:NZ  | 4:Z:254:ARG:NH2[1_556] | 0.30                     | 1.90              |
| 4:1:77:THR:OG1  | 4:Y:14:SER:C[1_556]    | 0.30                     | 1.90              |
| 4:0:336:LYS:NZ  | 4:X:254:ARG:NH2[1_556] | 0.30                     | 1.90              |
| 4:2:136:ILE:CA  | 4:Z:299:MET:C[1_556]   | 0.30                     | 1.90              |
| 4:2:297:ASN:CG  | 4:Z:316:GLU:OE1[1_556] | 0.30                     | 1.90              |
| 4:0:171:LEU:CA  | 4:X:151:ILE:CD1[1_556] | 0.31                     | 1.89              |
| 4:0:152:VAL:CG2 | 4:X:313:MET:CB[1_556]  | 0.31                     | 1.89              |
| 4:1:186:THR:C   | 4:Y:191:LYS:CA[1_556]  | 0.31                     | 1.89              |
| 4:0:164:PRO:N   | 4:X:278:THR:CB[1_556]  | 0.32                     | 1.88              |
| 4:0:297:ASN:CG  | 4:X:316:GLU:OE1[1_556] | 0.32                     | 1.88              |
| 4:2:164:PRO:N   | 4:Z:278:THR:CB[1_556]  | 0.32                     | 1.88              |
| 4:1:171:LEU:CA  | 4:Y:151:ILE:CD1[1_556] | 0.32                     | 1.88              |
| 4:2:152:VAL:CG2 | 4:Z:313:MET:CB[1_556]  | 0.32                     | 1.88              |
| 4:2:171:LEU:CA  | 4:Z:151:ILE:CD1[1_556] | 0.32                     | 1.88              |
| 4:1:122:ILE:CD1 | 4:Y:19:ALA:N[1_556]    | 0.32                     | 1.88              |
| 4:1:136:ILE:CA  | 4:Y:299:MET:C[1_556]   | 0.32                     | 1.88              |
| 4:1:62:ARG:NE   | 4:Y:205:GLU:N[1_556]   | 0.34                     | 1.86              |
| 4:3:63:GLY:C    | 4:Y:289:ILE:N[1_556]   | 0.34                     | 1.86              |
| 4:0:63:GLY:C    | 4:V:289:ILE:N[1_556]   | 0.35                     | 1.85              |
| 4:1:253:GLU:OE1 | 4:X:112:PRO:C[1_556]   | 0.35                     | 1.85              |
| 4:1:63:GLY:C    | 4:W:289:ILE:N[1_556]   | 0.36                     | 1.84              |
| 4:2:63:GLY:C    | 4:X:289:ILE:N[1_556]   | 0.36                     | 1.84              |
| 4:3:253:GLU:OE1 | 4:Z:112:PRO:C[1_556]   | 0.36                     | 1.84              |
| 4:2:196:ARG:CD  | 4:Y:115:ASN:CG[1_556]  | 0.36                     | 1.84              |
| 4:2:272:ALA:CB  | 4:Z:270:GLU:O[1_556]   | 0.36                     | 1.84              |
| 4:0:186:THR:C   | 4:X:191:LYS:CA[1_556]  | 0.36                     | 1.84              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:305:MET:C   | 4:Y:255:PHE:CD1[1_556] | 0.37                     | 1.83              |
| 4:2:152:VAL:CB  | 4:Z:313:MET:CG[1_556]  | 0.37                     | 1.83              |
| 4:0:77:THR:OG1  | 4:X:14:SER:C[1_556]    | 0.37                     | 1.83              |
| 4:4:63:GLY:C    | 4:Z:289:ILE:N[1_556]   | 0.37                     | 1.83              |
| 4:0:272:ALA:CB  | 4:X:270:GLU:O[1_556]   | 0.37                     | 1.83              |
| 4:0:196:ARG:CD  | 4:W:115:ASN:CG[1_556]  | 0.37                     | 1.83              |
| 4:2:162:ASN:CG  | 4:Z:273:GLY:C[1_556]   | 0.37                     | 1.83              |
| 4:0:162:ASN:CG  | 4:X:273:GLY:C[1_556]   | 0.38                     | 1.82              |
| 4:2:305:MET:C   | 4:Z:255:PHE:CD1[1_556] | 0.38                     | 1.82              |
| 4:2:186:THR:C   | 4:Z:191:LYS:CA[1_556]  | 0.38                     | 1.82              |
| 4:1:297:ASN:CG  | 4:Y:316:GLU:OE1[1_556] | 0.38                     | 1.82              |
| 4:1:285:CYS:SG  | 4:Y:279:TYR:O[1_556]   | 0.38                     | 1.82              |
| 4:0:337:TYR:CA  | 4:X:307:PRO:CB[1_556]  | 0.38                     | 1.82              |
| 4:0:152:VAL:CB  | 4:X:313:MET:CG[1_556]  | 0.38                     | 1.82              |
| 4:2:77:THR:OG1  | 4:Z:14:SER:C[1_556]    | 0.38                     | 1.82              |
| 4:2:337:TYR:CA  | 4:Z:307:PRO:CB[1_556]  | 0.38                     | 1.82              |
| 4:1:62:ARG:O    | 4:W:288:ASP:CB[1_556]  | 0.39                     | 1.81              |
| 4:0:305:MET:C   | 4:X:255:PHE:CD1[1_556] | 0.39                     | 1.81              |
| 4:3:270:GLU:OE1 | 4:Z:286:ASP:CB[1_556]  | 0.39                     | 1.81              |
| 4:1:209:VAL:C   | 4:Y:193:LEU:O[1_556]   | 0.39                     | 1.81              |
| 4:1:152:VAL:CG2 | 4:Y:313:MET:CB[1_556]  | 0.39                     | 1.81              |
| 4:1:270:GLU:OE1 | 4:X:286:ASP:CB[1_556]  | 0.39                     | 1.81              |
| 4:1:369:ILE:CG2 | 4:Y:345:ILE:C[1_556]   | 0.40                     | 1.80              |
| 4:1:272:ALA:CB  | 4:Y:270:GLU:O[1_556]   | 0.40                     | 1.80              |
| 4:0:372:ARG:NH2 | 4:X:145:SER:N[1_556]   | 0.40                     | 1.80              |
| 4:2:369:ILE:CG2 | 4:Z:345:ILE:C[1_556]   | 0.40                     | 1.80              |
| 4:3:62:ARG:O    | 4:Y:288:ASP:CB[1_556]  | 0.41                     | 1.79              |
| 4:2:62:ARG:NE   | 4:Z:205:GLU:N[1_556]   | 0.41                     | 1.79              |
| 4:2:122:ILE:CD1 | 4:Z:19:ALA:N[1_556]    | 0.41                     | 1.79              |
| 4:0:122:ILE:CD1 | 4:X:19:ALA:N[1_556]    | 0.41                     | 1.79              |
| 4:0:62:ARG:NE   | 4:X:205:GLU:N[1_556]   | 0.41                     | 1.79              |
| 4:2:16:LEU:CA   | 4:Z:214:GLU:CB[1_556]  | 0.41                     | 1.79              |
| 4:2:372:ARG:NH2 | 4:Z:145:SER:N[1_556]   | 0.42                     | 1.78              |
| 4:2:147:ARG:CG  | 4:Z:314:GLN:OE1[1_556] | 0.42                     | 1.78              |
| 4:1:152:VAL:CB  | 4:Y:313:MET:CG[1_556]  | 0.42                     | 1.78              |
| 4:0:147:ARG:CG  | 4:X:314:GLN:OE1[1_556] | 0.42                     | 1.78              |
| 4:0:16:LEU:CA   | 4:X:214:GLU:CB[1_556]  | 0.43                     | 1.77              |
| 4:0:369:ILE:CG2 | 4:X:345:ILE:C[1_556]   | 0.43                     | 1.77              |
| 4:1:140:LEU:CD2 | 4:Y:331:ALA:C[1_556]   | 0.43                     | 1.77              |
| 4:0:209:VAL:C   | 4:X:193:LEU:O[1_556]   | 0.43                     | 1.77              |
| 4:4:62:ARG:O    | 4:Z:288:ASP:CB[1_556]  | 0.43                     | 1.77              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:41:GLN:N    | 4:V:167:GLU:OE2[1_556] | 0.43                     | 1.77              |
| 4:2:41:GLN:N    | 4:X:167:GLU:OE2[1_556] | 0.43                     | 1.77              |
| 4:1:175:ILE:CB  | 4:Y:162:ASN:OD1[1_556] | 0.44                     | 1.76              |
| 4:1:40:HIS:ND1  | 4:W:166:TYR:CG[1_556]  | 0.44                     | 1.76              |
| 4:4:41:GLN:N    | 4:Z:167:GLU:OE2[1_556] | 0.44                     | 1.76              |
| 4:2:209:VAL:C   | 4:Z:193:LEU:O[1_556]   | 0.44                     | 1.76              |
| 4:1:196:ARG:CD  | 4:X:115:ASN:CG[1_556]  | 0.45                     | 1.75              |
| 4:2:169:TYR:CE1 | 4:Z:150:GLY:O[1_556]   | 0.45                     | 1.75              |
| 4:3:40:HIS:ND1  | 4:Y:166:TYR:CG[1_556]  | 0.45                     | 1.75              |
| 4:1:369:ILE:O   | 4:Y:143:TYR:CE2[1_556] | 0.45                     | 1.75              |
| 4:0:285:CYS:SG  | 4:X:279:TYR:O[1_556]   | 0.45                     | 1.75              |
| 4:2:62:ARG:O    | 4:X:288:ASP:CB[1_556]  | 0.45                     | 1.75              |
| 4:2:285:CYS:SG  | 4:Z:279:TYR:O[1_556]   | 0.45                     | 1.75              |
| 4:3:196:ARG:CD  | 4:Z:115:ASN:CG[1_556]  | 0.45                     | 1.75              |
| 4:1:337:TYR:CA  | 4:Y:307:PRO:CB[1_556]  | 0.45                     | 1.75              |
| 4:1:79:TRP:CE3  | 4:Y:18:LYS:N[1_556]    | 0.45                     | 1.75              |
| 4:1:331:ALA:O   | 4:Y:221:LEU:O[1_556]   | 0.45                     | 1.75              |
| 4:0:169:TYR:CE1 | 4:X:150:GLY:O[1_556]   | 0.46                     | 1.74              |
| 4:0:62:ARG:O    | 4:V:288:ASP:CB[1_556]  | 0.46                     | 1.74              |
| 4:1:164:PRO:CD  | 4:Y:278:THR:CA[1_556]  | 0.47                     | 1.73              |
| 4:1:177:ARG:NH1 | 4:Y:159:VAL:CA[1_556]  | 0.47                     | 1.73              |
| 4:1:209:VAL:CG2 | 4:Y:194:THR:C[1_556]   | 0.47                     | 1.73              |
| 4:1:338:SER:OG  | 4:Y:308:GLY:CA[1_556]  | 0.47                     | 1.73              |
| 4:0:270:GLU:OE1 | 4:W:286:ASP:CB[1_556]  | 0.47                     | 1.73              |
| 4:2:338:SER:OG  | 4:Z:308:GLY:CA[1_556]  | 0.48                     | 1.72              |
| 4:0:166:TYR:C   | 4:X:294:TYR:C[1_556]   | 0.48                     | 1.72              |
| 4:2:166:TYR:C   | 4:Z:294:TYR:C[1_556]   | 0.48                     | 1.72              |
| 4:0:137:GLN:OE1 | 4:X:304:THR:N[1_556]   | 0.48                     | 1.72              |
| 4:2:270:GLU:OE1 | 4:Y:286:ASP:CB[1_556]  | 0.48                     | 1.72              |
| 4:0:209:VAL:CG2 | 4:X:194:THR:C[1_556]   | 0.48                     | 1.72              |
| 4:1:185:LEU:CG  | 4:Y:188:TYR:CE1[1_556] | 0.48                     | 1.72              |
| 4:1:86:TRP:NE1  | 4:Y:337:TYR:OH[1_556]  | 0.48                     | 1.72              |
| 4:1:372:ARG:NH2 | 4:Y:145:SER:N[1_556]   | 0.48                     | 1.72              |
| 4:0:338:SER:OG  | 4:X:308:GLY:CA[1_556]  | 0.49                     | 1.71              |
| 4:1:362:TYR:CA  | 4:Y:348:SER:OG[1_556]  | 0.49                     | 1.71              |
| 4:1:147:ARG:CG  | 4:Y:314:GLN:OE1[1_556] | 0.49                     | 1.71              |
| 4:0:278:THR:O   | 4:X:276:GLU:CG[1_556]  | 0.50                     | 1.70              |
| 4:1:366:GLY:O   | 4:Y:347:ALA:N[1_556]   | 0.50                     | 1.70              |
| 4:0:33:SER:C    | 4:X:210:ARG:NH2[1_556] | 0.50                     | 1.70              |
| 4:2:137:GLN:OE1 | 4:Z:304:THR:N[1_556]   | 0.50                     | 1.70              |
| 4:1:16:LEU:CB   | 4:Y:214:GLU:CA[1_556]  | 0.50                     | 1.70              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:209:VAL:CG2 | 4:Z:194:THR:C[1_556]   | 0.50                     | 1.70              |
| 4:2:140:LEU:CD2 | 4:Z:331:ALA:C[1_556]   | 0.50                     | 1.70              |
| 4:2:33:SER:C    | 4:Z:210:ARG:NH2[1_556] | 0.50                     | 1.70              |
| 4:2:278:THR:O   | 4:Z:276:GLU:CG[1_556]  | 0.50                     | 1.70              |
| 4:2:169:TYR:CD1 | 4:Z:150:GLY:C[1_556]   | 0.50                     | 1.70              |
| 4:1:278:THR:O   | 4:Y:276:GLU:CG[1_556]  | 0.50                     | 1.70              |
| 4:0:164:PRO:CD  | 4:X:278:THR:CA[1_556]  | 0.50                     | 1.70              |
| 4:1:277:THR:CG2 | 4:Y:272:ALA:C[1_556]   | 0.51                     | 1.69              |
| 4:1:185:LEU:CD2 | 4:Y:188:TYR:CZ[1_556]  | 0.51                     | 1.69              |
| 4:2:164:PRO:CD  | 4:Z:278:THR:CA[1_556]  | 0.51                     | 1.69              |
| 4:0:169:TYR:CD1 | 4:X:150:GLY:C[1_556]   | 0.51                     | 1.69              |
| 4:1:16:LEU:CA   | 4:Y:214:GLU:CB[1_556]  | 0.51                     | 1.69              |
| 4:0:140:LEU:CD2 | 4:X:331:ALA:C[1_556]   | 0.51                     | 1.69              |
| 4:2:79:TRP:CE3  | 4:Z:18:LYS:N[1_556]    | 0.51                     | 1.69              |
| 4:1:169:TYR:CE1 | 4:Y:150:GLY:O[1_556]   | 0.52                     | 1.68              |
| 4:2:210:ARG:C   | 4:Z:193:LEU:CD1[1_556] | 0.52                     | 1.68              |
| 4:3:41:GLN:N    | 4:Y:167:GLU:OE2[1_556] | 0.52                     | 1.68              |
| 4:0:79:TRP:CE3  | 4:X:18:LYS:N[1_556]    | 0.52                     | 1.68              |
| 4:1:137:GLN:OE1 | 4:Y:304:THR:N[1_556]   | 0.52                     | 1.68              |
| 4:1:301:GLY:N   | 4:Y:219:VAL:CG2[1_556] | 0.52                     | 1.68              |
| 4:1:169:TYR:CD1 | 4:Y:150:GLY:C[1_556]   | 0.52                     | 1.68              |
| 4:1:41:GLN:N    | 4:W:167:GLU:OE2[1_556] | 0.52                     | 1.68              |
| 4:1:208:ILE:CG1 | 4:Y:198:TYR:CE1[1_556] | 0.52                     | 1.68              |
| 4:0:175:ILE:CB  | 4:X:162:ASN:OD1[1_556] | 0.52                     | 1.68              |
| 4:0:277:THR:CG2 | 4:X:272:ALA:C[1_556]   | 0.52                     | 1.68              |
| 4:0:331:ALA:O   | 4:X:221:LEU:O[1_556]   | 0.53                     | 1.67              |
| 4:1:268:GLY:O   | 4:X:284:LYS:O[1_556]   | 0.53                     | 1.67              |
| 4:3:268:GLY:O   | 4:Z:284:LYS:O[1_556]   | 0.53                     | 1.67              |
| 4:2:277:THR:CG2 | 4:Z:272:ALA:C[1_556]   | 0.53                     | 1.67              |
| 4:4:40:HIS:ND1  | 4:Z:166:TYR:CG[1_556]  | 0.53                     | 1.67              |
| 4:2:331:ALA:O   | 4:Z:221:LEU:O[1_556]   | 0.53                     | 1.67              |
| 4:0:369:ILE:O   | 4:X:143:TYR:CE2[1_556] | 0.53                     | 1.67              |
| 4:2:175:ILE:CB  | 4:Z:162:ASN:OD1[1_556] | 0.53                     | 1.67              |
| 4:2:369:ILE:O   | 4:Z:143:TYR:CE2[1_556] | 0.53                     | 1.67              |
| 4:2:303:THR:CB  | 4:Z:257:CYS:C[1_556]   | 0.54                     | 1.66              |
| 4:0:210:ARG:C   | 4:X:193:LEU:CD1[1_556] | 0.54                     | 1.66              |
| 4:0:40:HIS:ND1  | 4:V:166:TYR:CG[1_556]  | 0.54                     | 1.66              |
| 4:2:40:HIS:ND1  | 4:X:166:TYR:CG[1_556]  | 0.54                     | 1.66              |
| 4:0:208:ILE:CG1 | 4:X:198:TYR:CE1[1_556] | 0.54                     | 1.66              |
| 4:0:16:LEU:CB   | 4:X:214:GLU:CA[1_556]  | 0.55                     | 1.65              |
| 4:1:215:LYS:O   | 4:Y:252:ASN:OD1[1_556] | 0.55                     | 1.65              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:208:ILE:CG1 | 4:Z:198:TYR:CE1[1_556] | 0.55                     | 1.65              |
| 4:2:233:SER:C   | 4:Y:367:PRO:CD[1_556]  | 0.55                     | 1.65              |
| 4:0:185:LEU:CD2 | 4:X:188:TYR:CZ[1_556]  | 0.55                     | 1.65              |
| 4:1:189:LEU:CG  | 4:Y:195:GLU:CB[1_556]  | 0.55                     | 1.65              |
| 4:2:137:GLN:NE2 | 4:Z:301:GLY:O[1_556]   | 0.55                     | 1.65              |
| 4:1:62:ARG:CG   | 4:Y:204:ALA:CA[1_556]  | 0.55                     | 1.65              |
| 4:2:86:TRP:NE1  | 4:Z:337:TYR:OH[1_556]  | 0.55                     | 1.65              |
| 4:0:86:TRP:NE1  | 4:X:337:TYR:OH[1_556]  | 0.55                     | 1.65              |
| 4:0:303:THR:CB  | 4:X:257:CYS:C[1_556]   | 0.56                     | 1.64              |
| 4:0:304:THR:O   | 4:X:223:PHE:CD1[1_556] | 0.56                     | 1.64              |
| 4:1:210:ARG:C   | 4:Y:193:LEU:CD1[1_556] | 0.56                     | 1.64              |
| 4:2:304:THR:O   | 4:Z:223:PHE:CD1[1_556] | 0.56                     | 1.64              |
| 4:1:33:SER:C    | 4:Y:210:ARG:NH2[1_556] | 0.56                     | 1.64              |
| 4:2:16:LEU:CB   | 4:Z:214:GLU:CA[1_556]  | 0.56                     | 1.64              |
| 4:1:303:THR:CB  | 4:Y:257:CYS:C[1_556]   | 0.56                     | 1.64              |
| 4:1:285:CYS:C   | 4:Y:283:MET:CB[1_556]  | 0.56                     | 1.64              |
| 4:0:177:ARG:NH1 | 4:X:159:VAL:CA[1_556]  | 0.56                     | 1.64              |
| 4:2:118:LYS:O   | 4:Z:340:TRP:NE1[1_556] | 0.56                     | 1.64              |
| 4:2:296:ASN:CG  | 4:Z:318:THR:OG1[1_556] | 0.56                     | 1.64              |
| 4:0:185:LEU:CG  | 4:X:188:TYR:CE1[1_556] | 0.56                     | 1.64              |
| 4:2:185:LEU:CD2 | 4:Z:188:TYR:CZ[1_556]  | 0.56                     | 1.64              |
| 4:2:177:ARG:NH1 | 4:Z:159:VAL:CA[1_556]  | 0.57                     | 1.63              |
| 4:0:137:GLN:NE2 | 4:X:301:GLY:O[1_556]   | 0.57                     | 1.63              |
| 4:0:233:SER:C   | 4:W:367:PRO:CD[1_556]  | 0.57                     | 1.63              |
| 4:1:72:GLU:CA   | 4:Y:157:ASP:OD2[1_556] | 0.57                     | 1.63              |
| 4:0:296:ASN:CG  | 4:X:318:THR:OG1[1_556] | 0.57                     | 1.63              |
| 4:0:118:LYS:O   | 4:X:340:TRP:NE1[1_556] | 0.57                     | 1.63              |
| 4:2:185:LEU:CG  | 4:Z:188:TYR:CE1[1_556] | 0.57                     | 1.63              |
| 4:1:296:ASN:CG  | 4:Y:318:THR:OG1[1_556] | 0.57                     | 1.63              |
| 4:1:233:SER:CA  | 4:X:367:PRO:CA[1_556]  | 0.57                     | 1.63              |
| 4:2:301:GLY:N   | 4:Z:219:VAL:CG2[1_556] | 0.57                     | 1.63              |
| 4:3:267:ILE:CA  | 4:Z:173:HIS:CA[1_556]  | 0.57                     | 1.63              |
| 4:2:184:ASP:N   | 4:Z:188:TYR:N[1_556]   | 0.58                     | 1.62              |
| 4:2:362:TYR:CA  | 4:Z:348:SER:OG[1_556]  | 0.58                     | 1.62              |
| 4:1:166:TYR:C   | 4:Y:294:TYR:C[1_556]   | 0.58                     | 1.62              |
| 4:0:301:GLY:N   | 4:X:219:VAL:CG2[1_556] | 0.58                     | 1.62              |
| 4:0:267:ILE:CA  | 4:W:173:HIS:CA[1_556]  | 0.58                     | 1.62              |
| 4:0:362:TYR:CA  | 4:X:348:SER:OG[1_556]  | 0.58                     | 1.62              |
| 4:0:191:LYS:CE  | 4:W:110:LEU:CD2[1_556] | 0.58                     | 1.62              |
| 4:3:233:SER:CA  | 4:Z:367:PRO:CA[1_556]  | 0.58                     | 1.62              |
| 4:1:107:GLU:O   | 4:Y:300:SER:C[1_556]   | 0.58                     | 1.62              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:184:ASP:N   | 4:X:188:TYR:N[1_556]   | 0.58                     | 1.62              |
| 4:0:114:ALA:CA  | 4:X:106:THR:CB[1_556]  | 0.59                     | 1.61              |
| 4:2:191:LYS:CE  | 4:Y:110:LEU:CD2[1_556] | 0.59                     | 1.61              |
| 4:1:267:ILE:CA  | 4:X:173:HIS:CA[1_556]  | 0.59                     | 1.61              |
| 4:2:267:ILE:CA  | 4:Y:173:HIS:CA[1_556]  | 0.59                     | 1.61              |
| 4:2:366:GLY:O   | 4:Z:347:ALA:N[1_556]   | 0.59                     | 1.61              |
| 4:0:366:GLY:O   | 4:X:347:ALA:N[1_556]   | 0.59                     | 1.61              |
| 4:2:365:ALA:CB  | 4:Z:349:LEU:CB[1_556]  | 0.59                     | 1.61              |
| 4:0:285:CYS:C   | 4:X:283:MET:CB[1_556]  | 0.60                     | 1.60              |
| 4:2:114:ALA:CA  | 4:Z:106:THR:CB[1_556]  | 0.60                     | 1.60              |
| 4:2:191:LYS:CD  | 4:Y:110:LEU:CD1[1_556] | 0.60                     | 1.60              |
| 4:0:365:ALA:CB  | 4:X:349:LEU:CB[1_556]  | 0.60                     | 1.60              |
| 4:1:362:TYR:O   | 4:Y:348:SER:CA[1_556]  | 0.60                     | 1.60              |
| 4:2:212:ILE:CA  | 4:Z:196:ARG:CG[1_556]  | 0.60                     | 1.60              |
| 4:1:116:ARG:CZ  | 4:Y:141:SER:CA[1_556]  | 0.61                     | 1.59              |
| 4:0:212:ILE:CA  | 4:X:196:ARG:CG[1_556]  | 0.61                     | 1.59              |
| 4:0:281:SER:OG  | 4:X:277:THR:N[1_556]   | 0.61                     | 1.59              |
| 4:2:285:CYS:C   | 4:Z:283:MET:CB[1_556]  | 0.61                     | 1.59              |
| 4:1:162:ASN:CA  | 4:Y:274:ILE:CA[1_556]  | 0.61                     | 1.59              |
| 4:2:62:ARG:CG   | 4:Z:204:ALA:CA[1_556]  | 0.61                     | 1.59              |
| 4:1:194:THR:OG1 | 4:X:177:ARG:NH1[1_556] | 0.61                     | 1.59              |
| 4:1:114:ALA:CA  | 4:Y:106:THR:CB[1_556]  | 0.61                     | 1.59              |
| 4:0:208:ILE:C   | 4:X:198:TYR:CG[1_556]  | 0.61                     | 1.59              |
| 4:2:215:LYS:O   | 4:Z:252:ASN:OD1[1_556] | 0.61                     | 1.59              |
| 4:2:208:ILE:C   | 4:Z:198:TYR:CG[1_556]  | 0.61                     | 1.59              |
| 4:3:227:MET:CB  | 4:Z:372:ARG:C[1_556]   | 0.61                     | 1.59              |
| 4:0:157:ASP:O   | 4:X:185:LEU:C[1_556]   | 0.61                     | 1.59              |
| 4:0:191:LYS:CD  | 4:W:110:LEU:CD1[1_556] | 0.62                     | 1.58              |
| 4:1:233:SER:C   | 4:X:367:PRO:CD[1_556]  | 0.62                     | 1.58              |
| 4:0:62:ARG:CG   | 4:X:204:ALA:CA[1_556]  | 0.62                     | 1.58              |
| 4:1:208:ILE:O   | 4:Y:198:TYR:CD2[1_556] | 0.62                     | 1.58              |
| 4:2:281:SER:OG  | 4:Z:277:THR:N[1_556]   | 0.62                     | 1.58              |
| 4:1:307:PRO:CB  | 4:Y:227:MET:CA[1_556]  | 0.62                     | 1.58              |
| 4:1:11:ASP:OD1  | 4:Y:305:MET:CG[1_556]  | 0.62                     | 1.58              |
| 4:1:299:MET:SD  | 4:Y:312:ARG:CZ[1_556]  | 0.62                     | 1.58              |
| 4:3:194:THR:OG1 | 4:Z:177:ARG:NH1[1_556] | 0.62                     | 1.58              |
| 4:0:268:GLY:O   | 4:W:284:LYS:O[1_556]   | 0.62                     | 1.58              |
| 4:0:215:LYS:O   | 4:X:252:ASN:OD1[1_556] | 0.62                     | 1.58              |
| 4:2:72:GLU:CA   | 4:Z:157:ASP:OD2[1_556] | 0.62                     | 1.58              |
| 4:1:227:MET:CB  | 4:X:372:ARG:C[1_556]   | 0.62                     | 1.58              |
| 4:2:268:GLY:O   | 4:Y:284:LYS:O[1_556]   | 0.63                     | 1.57              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:134:VAL:CG1 | 4:X:338:SER:CB[1_556]  | 0.63                     | 1.57              |
| 4:1:208:ILE:C   | 4:Y:198:TYR:CG[1_556]  | 0.63                     | 1.57              |
| 4:2:189:LEU:CG  | 4:Z:195:GLU:CB[1_556]  | 0.63                     | 1.57              |
| 4:0:137:GLN:CG  | 4:X:304:THR:OG1[1_556] | 0.63                     | 1.57              |
| 4:3:233:SER:C   | 4:Z:367:PRO:CD[1_556]  | 0.63                     | 1.57              |
| 4:2:107:GLU:O   | 4:Z:300:SER:C[1_556]   | 0.63                     | 1.57              |
| 4:1:140:LEU:CB  | 4:Y:331:ALA:CB[1_556]  | 0.63                     | 1.57              |
| 4:2:157:ASP:O   | 4:Z:185:LEU:C[1_556]   | 0.63                     | 1.57              |
| 4:0:189:LEU:CG  | 4:X:195:GLU:CB[1_556]  | 0.63                     | 1.57              |
| 4:2:137:GLN:CG  | 4:Z:304:THR:OG1[1_556] | 0.63                     | 1.57              |
| 4:1:251:GLY:N   | 4:X:114:ALA:CB[1_556]  | 0.63                     | 1.57              |
| 4:1:304:THR:O   | 4:Y:223:PHE:CD1[1_556] | 0.63                     | 1.57              |
| 4:1:272:ALA:CA  | 4:Y:270:GLU:CA[1_556]  | 0.64                     | 1.56              |
| 4:2:153:LEU:CD1 | 4:Z:262:PHE:CA[1_556]  | 0.64                     | 1.56              |
| 4:1:137:GLN:NE2 | 4:Y:301:GLY:O[1_556]   | 0.64                     | 1.56              |
| 4:2:208:ILE:O   | 4:Z:198:TYR:CD2[1_556] | 0.64                     | 1.56              |
| 4:0:72:GLU:CA   | 4:X:157:ASP:OD2[1_556] | 0.64                     | 1.56              |
| 4:2:134:VAL:CG1 | 4:Z:338:SER:CB[1_556]  | 0.64                     | 1.56              |
| 4:2:162:ASN:CA  | 4:Z:274:ILE:CA[1_556]  | 0.64                     | 1.56              |
| 4:1:362:TYR:C   | 4:Y:348:SER:CB[1_556]  | 0.64                     | 1.56              |
| 4:1:212:ILE:CA  | 4:Y:196:ARG:CG[1_556]  | 0.64                     | 1.56              |
| 4:0:367:PRO:CA  | 4:X:343:GLY:O[1_556]   | 0.64                     | 1.56              |
| 4:0:307:PRO:CB  | 4:X:227:MET:CA[1_556]  | 0.64                     | 1.56              |
| 4:3:191:LYS:CE  | 4:Z:110:LEU:CD2[1_556] | 0.64                     | 1.56              |
| 4:2:307:PRO:CB  | 4:Z:227:MET:CA[1_556]  | 0.64                     | 1.56              |
| 4:0:162:ASN:CA  | 4:X:274:ILE:CA[1_556]  | 0.64                     | 1.56              |
| 4:2:11:ASP:OD1  | 4:Z:305:MET:CG[1_556]  | 0.64                     | 1.56              |
| 4:1:157:ASP:O   | 4:Y:185:LEU:C[1_556]   | 0.64                     | 1.56              |
| 4:2:299:MET:SD  | 4:Z:312:ARG:CZ[1_556]  | 0.64                     | 1.56              |
| 4:0:107:GLU:O   | 4:X:300:SER:C[1_556]   | 0.64                     | 1.56              |
| 4:3:251:GLY:N   | 4:Z:114:ALA:CB[1_556]  | 0.64                     | 1.56              |
| 4:0:62:ARG:CD   | 4:X:204:ALA:C[1_556]   | 0.65                     | 1.55              |
| 4:0:153:LEU:CD1 | 4:X:262:PHE:CA[1_556]  | 0.65                     | 1.55              |
| 4:1:365:ALA:CB  | 4:Y:349:LEU:CB[1_556]  | 0.65                     | 1.55              |
| 4:0:227:MET:CB  | 4:W:372:ARG:C[1_556]   | 0.65                     | 1.55              |
| 4:2:194:THR:OG1 | 4:Y:177:ARG:NH1[1_556] | 0.65                     | 1.55              |
| 4:2:107:GLU:C   | 4:Z:301:GLY:N[1_556]   | 0.65                     | 1.55              |
| 4:1:309:ILE:CB  | 4:Y:259:GLU:OE2[1_556] | 0.65                     | 1.55              |
| 4:1:137:GLN:CB  | 4:Y:304:THR:CB[1_556]  | 0.65                     | 1.55              |
| 4:0:231:ALA:CB  | 4:W:370:VAL:N[1_556]   | 0.65                     | 1.55              |
| 4:1:191:LYS:CD  | 4:X:110:LEU:CD1[1_556] | 0.65                     | 1.55              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:288:ASP:O   | 4:X:322:PRO:CG[1_556]  | 0.65                     | 1.55              |
| 4:2:288:ASP:O   | 4:Z:322:PRO:CG[1_556]  | 0.65                     | 1.55              |
| 4:2:62:ARG:CD   | 4:Z:204:ALA:C[1_556]   | 0.65                     | 1.55              |
| 4:1:141:SER:C   | 4:Y:310:ALA:CA[1_556]  | 0.65                     | 1.55              |
| 4:1:191:LYS:CE  | 4:X:110:LEU:CD2[1_556] | 0.65                     | 1.55              |
| 4:2:367:PRO:CA  | 4:Z:343:GLY:O[1_556]   | 0.65                     | 1.55              |
| 4:0:194:THR:OG1 | 4:W:177:ARG:NH1[1_556] | 0.65                     | 1.55              |
| 4:1:37:ARG:CB   | 4:Y:60:SER:CB[1_556]   | 0.66                     | 1.54              |
| 4:0:107:GLU:C   | 4:X:301:GLY:N[1_556]   | 0.66                     | 1.54              |
| 4:2:231:ALA:CB  | 4:Y:370:VAL:N[1_556]   | 0.66                     | 1.54              |
| 4:1:137:GLN:CG  | 4:Y:304:THR:OG1[1_556] | 0.66                     | 1.54              |
| 4:2:227:MET:CB  | 4:Y:372:ARG:C[1_556]   | 0.66                     | 1.54              |
| 4:0:208:ILE:O   | 4:X:198:TYR:CD2[1_556] | 0.66                     | 1.54              |
| 4:1:118:LYS:O   | 4:Y:340:TRP:NE1[1_556] | 0.66                     | 1.54              |
| 4:0:11:ASP:OD1  | 4:X:305:MET:CG[1_556]  | 0.66                     | 1.54              |
| 4:0:37:ARG:CB   | 4:X:60:SER:CB[1_556]   | 0.66                     | 1.54              |
| 4:1:161:HIS:CA  | 4:Y:274:ILE:CD1[1_556] | 0.66                     | 1.54              |
| 4:1:336:LYS:CG  | 4:Y:218:TYR:CD1[1_556] | 0.66                     | 1.54              |
| 4:2:366:GLY:CA  | 4:Z:347:ALA:C[1_556]   | 0.66                     | 1.54              |
| 4:3:191:LYS:CD  | 4:Z:110:LEU:CD1[1_556] | 0.66                     | 1.54              |
| 4:0:299:MET:SD  | 4:X:312:ARG:CZ[1_556]  | 0.67                     | 1.53              |
| 4:2:251:GLY:N   | 4:Y:114:ALA:CB[1_556]  | 0.67                     | 1.53              |
| 4:2:206:ARG:CA  | 4:Z:199:SER:C[1_556]   | 0.67                     | 1.53              |
| 4:2:37:ARG:CB   | 4:Z:60:SER:CB[1_556]   | 0.67                     | 1.53              |
| 4:1:281:SER:OG  | 4:Y:277:THR:N[1_556]   | 0.67                     | 1.53              |
| 4:2:233:SER:CA  | 4:Y:367:PRO:CA[1_556]  | 0.67                     | 1.53              |
| 4:0:140:LEU:CB  | 4:X:331:ALA:CB[1_556]  | 0.67                     | 1.53              |
| 4:0:214:GLU:N   | 4:X:253:GLU:CD[1_556]  | 0.67                     | 1.53              |
| 4:2:140:LEU:CB  | 4:Z:331:ALA:CB[1_556]  | 0.67                     | 1.53              |
| 4:1:184:ASP:N   | 4:Y:188:TYR:N[1_556]   | 0.67                     | 1.53              |
| 4:0:233:SER:CA  | 4:W:367:PRO:CA[1_556]  | 0.67                     | 1.53              |
| 4:2:368:SER:C   | 4:Z:346:LEU:CB[1_556]  | 0.67                     | 1.53              |
| 4:0:366:GLY:CA  | 4:X:347:ALA:C[1_556]   | 0.67                     | 1.53              |
| 4:0:251:GLY:N   | 4:W:114:ALA:CB[1_556]  | 0.68                     | 1.52              |
| 4:1:134:VAL:CG1 | 4:Y:338:SER:CB[1_556]  | 0.68                     | 1.52              |
| 4:2:114:ALA:CB  | 4:Z:106:THR:CA[1_556]  | 0.68                     | 1.52              |
| 4:1:265:SER:C   | 4:X:173:HIS:CE1[1_556] | 0.68                     | 1.52              |
| 4:2:336:LYS:CG  | 4:Z:218:TYR:CD1[1_556] | 0.68                     | 1.52              |
| 4:2:214:GLU:N   | 4:Z:253:GLU:CD[1_556]  | 0.68                     | 1.52              |
| 4:1:166:TYR:OH  | 4:Y:325:MET:SD[1_556]  | 0.68                     | 1.52              |
| 4:1:153:LEU:CD1 | 4:Y:262:PHE:CA[1_556]  | 0.68                     | 1.52              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:304:THR:OG1 | 4:Y:223:PHE:CZ[1_556]  | 0.68                     | 1.52              |
| 4:2:285:CYS:O   | 4:Z:283:MET:CB[1_556]  | 0.69                     | 1.51              |
| 4:0:206:ARG:CA  | 4:X:199:SER:C[1_556]   | 0.69                     | 1.51              |
| 4:2:195:GLU:CD  | 4:Y:110:LEU:N[1_556]   | 0.69                     | 1.51              |
| 4:1:266:PHE:O   | 4:X:172:PRO:C[1_556]   | 0.69                     | 1.51              |
| 4:1:163:VAL:CG2 | 4:Y:153:LEU:CD1[1_556] | 0.69                     | 1.51              |
| 4:3:266:PHE:O   | 4:Z:172:PRO:C[1_556]   | 0.69                     | 1.51              |
| 4:2:161:HIS:CA  | 4:Z:274:ILE:CD1[1_556] | 0.69                     | 1.51              |
| 4:2:215:LYS:NZ  | 4:Z:249:THR:OG1[1_556] | 0.69                     | 1.51              |
| 4:0:362:TYR:O   | 4:X:348:SER:CA[1_556]  | 0.69                     | 1.51              |
| 4:0:114:ALA:CB  | 4:X:106:THR:CA[1_556]  | 0.69                     | 1.51              |
| 4:2:272:ALA:CA  | 4:Z:270:GLU:CA[1_556]  | 0.70                     | 1.50              |
| 4:0:304:THR:OG1 | 4:X:223:PHE:CZ[1_556]  | 0.70                     | 1.50              |
| 4:0:368:SER:C   | 4:X:346:LEU:CB[1_556]  | 0.70                     | 1.50              |
| 4:1:206:ARG:CA  | 4:Y:199:SER:C[1_556]   | 0.70                     | 1.50              |
| 4:1:212:ILE:CG1 | 4:Y:196:ARG:O[1_556]   | 0.70                     | 1.50              |
| 4:2:362:TYR:O   | 4:Z:348:SER:CA[1_556]  | 0.70                     | 1.50              |
| 4:1:171:LEU:CD1 | 4:Y:282:ILE:CG1[1_556] | 0.70                     | 1.50              |
| 4:3:265:SER:C   | 4:Z:173:HIS:CE1[1_556] | 0.70                     | 1.50              |
| 4:0:336:LYS:CG  | 4:X:218:TYR:CD1[1_556] | 0.70                     | 1.50              |
| 4:1:288:ASP:O   | 4:Y:322:PRO:CG[1_556]  | 0.70                     | 1.50              |
| 4:2:116:ARG:CZ  | 4:Z:141:SER:CA[1_556]  | 0.70                     | 1.50              |
| 4:0:215:LYS:NZ  | 4:X:249:THR:OG1[1_556] | 0.70                     | 1.50              |
| 4:1:112:PRO:O   | 4:Y:137:GLN:CG[1_556]  | 0.70                     | 1.50              |
| 4:0:161:HIS:CA  | 4:X:274:ILE:CD1[1_556] | 0.70                     | 1.50              |
| 4:0:272:ALA:CA  | 4:X:270:GLU:CA[1_556]  | 0.70                     | 1.50              |
| 4:0:116:ARG:CZ  | 4:X:141:SER:CA[1_556]  | 0.70                     | 1.50              |
| 4:0:285:CYS:O   | 4:X:283:MET:CB[1_556]  | 0.71                     | 1.49              |
| 4:1:165:ILE:CG1 | 4:Y:297:ASN:CG[1_556]  | 0.71                     | 1.49              |
| 4:1:298:VAL:CA  | 4:Y:312:ARG:O[1_556]   | 0.71                     | 1.49              |
| 4:0:195:GLU:CD  | 4:W:110:LEU:N[1_556]   | 0.71                     | 1.49              |
| 4:0:303:THR:OG1 | 4:X:257:CYS:CA[1_556]  | 0.71                     | 1.49              |
| 4:0:137:GLN:CB  | 4:X:304:THR:CB[1_556]  | 0.71                     | 1.49              |
| 4:2:304:THR:OG1 | 4:Z:223:PHE:CZ[1_556]  | 0.71                     | 1.49              |
| 4:1:106:THR:C   | 4:Y:335:ARG:O[1_556]   | 0.71                     | 1.49              |
| 4:0:166:TYR:OH  | 4:X:325:MET:SD[1_556]  | 0.72                     | 1.48              |
| 4:2:165:ILE:CG1 | 4:Z:297:ASN:CG[1_556]  | 0.72                     | 1.48              |
| 4:2:362:TYR:CE2 | 4:Z:22:ALA:C[1_556]    | 0.72                     | 1.48              |
| 4:1:279:TYR:N   | 4:Y:276:GLU:OE2[1_556] | 0.72                     | 1.48              |
| 4:0:362:TYR:C   | 4:X:348:SER:CB[1_556]  | 0.72                     | 1.48              |
| 4:2:298:VAL:CA  | 4:Z:312:ARG:O[1_556]   | 0.72                     | 1.48              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:153:LEU:O   | 4:Z:262:PHE:CZ[1_556]  | 0.72                     | 1.48              |
| 4:2:137:GLN:CB  | 4:Z:304:THR:CB[1_556]  | 0.72                     | 1.48              |
| 4:1:197:GLY:CA  | 4:X:75:ILE:CA[1_556]   | 0.72                     | 1.48              |
| 4:1:195:GLU:CD  | 4:X:110:LEU:N[1_556]   | 0.72                     | 1.48              |
| 4:1:368:SER:C   | 4:Y:346:LEU:CB[1_556]  | 0.73                     | 1.47              |
| 4:2:362:TYR:C   | 4:Z:348:SER:CB[1_556]  | 0.73                     | 1.47              |
| 4:1:182:GLY:O   | 4:Y:189:LEU:N[1_556]   | 0.73                     | 1.47              |
| 4:2:106:THR:C   | 4:Z:335:ARG:O[1_556]   | 0.73                     | 1.47              |
| 4:1:62:ARG:CD   | 4:Y:204:ALA:C[1_556]   | 0.73                     | 1.47              |
| 4:1:107:GLU:C   | 4:Y:301:GLY:N[1_556]   | 0.73                     | 1.47              |
| 4:2:112:PRO:C   | 4:Z:137:GLN:CG[1_556]  | 0.73                     | 1.47              |
| 4:0:165:ILE:CG1 | 4:X:297:ASN:CG[1_556]  | 0.73                     | 1.47              |
| 4:0:153:LEU:O   | 4:X:262:PHE:CZ[1_556]  | 0.73                     | 1.47              |
| 4:1:335:ARG:CG  | 4:Y:220:ALA:N[1_556]   | 0.73                     | 1.47              |
| 4:3:231:ALA:CB  | 4:Z:370:VAL:N[1_556]   | 0.73                     | 1.47              |
| 4:2:303:THR:OG1 | 4:Z:257:CYS:CA[1_556]  | 0.73                     | 1.47              |
| 4:0:261:LEU:CG  | 4:X:266:PHE:CG[1_556]  | 0.73                     | 1.47              |
| 4:2:309:ILE:CB  | 4:Z:259:GLU:OE2[1_556] | 0.73                     | 1.47              |
| 4:1:114:ALA:CB  | 4:Y:106:THR:CA[1_556]  | 0.73                     | 1.47              |
| 4:1:367:PRO:CA  | 4:Y:343:GLY:O[1_556]   | 0.73                     | 1.47              |
| 4:0:112:PRO:C   | 4:X:137:GLN:CG[1_556]  | 0.73                     | 1.47              |
| 4:0:362:TYR:CE2 | 4:X:22:ALA:C[1_556]    | 0.73                     | 1.47              |
| 4:2:166:TYR:OH  | 4:Z:325:MET:SD[1_556]  | 0.73                     | 1.47              |
| 4:1:81:ASP:N    | 4:Y:31:PHE:CB[1_556]   | 0.73                     | 1.47              |
| 4:0:141:SER:C   | 4:X:310:ALA:CA[1_556]  | 0.73                     | 1.47              |
| 4:0:212:ILE:CG1 | 4:X:196:ARG:O[1_556]   | 0.74                     | 1.46              |
| 4:1:167:GLU:C   | 4:Y:295:ALA:C[1_556]   | 0.74                     | 1.46              |
| 4:2:141:SER:C   | 4:Z:310:ALA:CA[1_556]  | 0.74                     | 1.46              |
| 4:0:298:VAL:CA  | 4:X:312:ARG:O[1_556]   | 0.74                     | 1.46              |
| 4:0:309:ILE:CB  | 4:X:259:GLU:OE2[1_556] | 0.74                     | 1.46              |
| 4:1:110:LEU:CB  | 4:Y:161:HIS:CB[1_556]  | 0.74                     | 1.46              |
| 4:0:274:ILE:CG1 | 4:X:263:GLN:CA[1_556]  | 0.74                     | 1.46              |
| 4:0:110:LEU:CB  | 4:X:161:HIS:CB[1_556]  | 0.74                     | 1.46              |
| 4:2:265:SER:C   | 4:Y:173:HIS:CE1[1_556] | 0.74                     | 1.46              |
| 4:0:86:TRP:CZ2  | 4:X:337:TYR:CE1[1_556] | 0.74                     | 1.46              |
| 4:1:231:ALA:CB  | 4:X:370:VAL:N[1_556]   | 0.74                     | 1.46              |
| 4:2:157:ASP:CB  | 4:Z:213:LYS:CD[1_556]  | 0.74                     | 1.46              |
| 4:2:105:LEU:N   | 4:Z:334:GLU:CB[1_556]  | 0.74                     | 1.46              |
| 4:3:195:GLU:CD  | 4:Z:110:LEU:N[1_556]   | 0.74                     | 1.46              |
| 4:2:167:GLU:C   | 4:Z:295:ALA:C[1_556]   | 0.75                     | 1.45              |
| 4:1:285:CYS:O   | 4:Y:283:MET:CB[1_556]  | 0.75                     | 1.45              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:197:GLY:CA  | 4:Z:75:ILE:CA[1_556]   | 0.75                     | 1.45              |
| 4:0:279:TYR:N   | 4:X:276:GLU:OE2[1_556] | 0.75                     | 1.45              |
| 4:2:279:TYR:N   | 4:Z:276:GLU:OE2[1_556] | 0.75                     | 1.45              |
| 4:0:106:THR:C   | 4:X:335:ARG:O[1_556]   | 0.75                     | 1.45              |
| 4:1:286:ASP:CG  | 4:Y:290:ARG:NE[1_556]  | 0.75                     | 1.45              |
| 4:1:112:PRO:C   | 4:Y:137:GLN:CG[1_556]  | 0.75                     | 1.45              |
| 4:2:206:ARG:NH2 | 4:Z:190:MET:SD[1_556]  | 0.75                     | 1.45              |
| 4:1:332:PRO:CB  | 4:Y:221:LEU:CD2[1_556] | 0.75                     | 1.45              |
| 4:1:78:ASN:O    | 4:Y:31:PHE:O[1_556]    | 0.75                     | 1.45              |
| 4:0:266:PHE:O   | 4:W:172:PRO:C[1_556]   | 0.75                     | 1.45              |
| 4:2:266:PHE:O   | 4:Y:172:PRO:C[1_556]   | 0.75                     | 1.45              |
| 4:2:261:LEU:CG  | 4:Z:266:PHE:CG[1_556]  | 0.75                     | 1.45              |
| 4:0:147:ARG:C   | 4:X:314:GLN:NE2[1_556] | 0.75                     | 1.45              |
| 4:1:305:MET:CB  | 4:Y:255:PHE:CB[1_556]  | 0.75                     | 1.45              |
| 4:2:212:ILE:CG1 | 4:Z:196:ARG:O[1_556]   | 0.75                     | 1.45              |
| 4:0:116:ARG:NE  | 4:X:141:SER:CA[1_556]  | 0.75                     | 1.45              |
| 4:2:196:ARG:NH1 | 4:Y:115:ASN:N[1_556]   | 0.75                     | 1.45              |
| 4:1:173:HIS:CA  | 4:Y:174:ALA:O[1_556]   | 0.76                     | 1.44              |
| 4:1:366:GLY:CA  | 4:Y:347:ALA:C[1_556]   | 0.76                     | 1.44              |
| 4:0:206:ARG:NH2 | 4:X:190:MET:SD[1_556]  | 0.76                     | 1.44              |
| 4:0:265:SER:C   | 4:W:173:HIS:CE1[1_556] | 0.76                     | 1.44              |
| 4:2:67:LEU:CD2  | 4:Z:207:GLU:OE1[1_556] | 0.76                     | 1.44              |
| 4:2:116:ARG:NE  | 4:Z:141:SER:CA[1_556]  | 0.76                     | 1.44              |
| 4:2:86:TRP:CZ2  | 4:Z:337:TYR:CE1[1_556] | 0.76                     | 1.44              |
| 4:1:78:ASN:CB   | 4:Y:32:PRO:C[1_556]    | 0.76                     | 1.44              |
| 4:2:197:GLY:CA  | 4:Y:75:ILE:CA[1_556]   | 0.76                     | 1.44              |
| 4:0:157:ASP:CB  | 4:X:213:LYS:CD[1_556]  | 0.76                     | 1.44              |
| 4:1:214:GLU:N   | 4:Y:253:GLU:CD[1_556]  | 0.76                     | 1.44              |
| 4:2:335:ARG:CD  | 4:Z:220:ALA:CA[1_556]  | 0.76                     | 1.44              |
| 4:0:288:ASP:OD2 | 4:Z:205:GLU:OE2[1_556] | 0.76                     | 1.44              |
| 4:0:67:LEU:CD2  | 4:X:207:GLU:OE1[1_556] | 0.76                     | 1.44              |
| 4:3:252:ASN:C   | 4:Z:113:LYS:CB[1_556]  | 0.76                     | 1.44              |
| 4:2:274:ILE:CG1 | 4:Z:263:GLN:CA[1_556]  | 0.76                     | 1.44              |
| 4:1:369:ILE:N   | 4:Y:346:LEU:CB[1_556]  | 0.76                     | 1.44              |
| 4:2:110:LEU:CB  | 4:Z:161:HIS:CB[1_556]  | 0.76                     | 1.44              |
| 4:0:167:GLU:C   | 4:X:295:ALA:C[1_556]   | 0.76                     | 1.44              |
| 4:1:83:GLU:OE1  | 4:Y:29:ALA:CB[1_556]   | 0.76                     | 1.44              |
| 4:0:196:ARG:NH1 | 4:W:115:ASN:N[1_556]   | 0.77                     | 1.43              |
| 4:2:126:THR:CB  | 4:Z:28:ARG:CG[1_556]   | 0.77                     | 1.43              |
| 4:1:161:HIS:CD2 | 4:Y:160:THR:CG2[1_556] | 0.77                     | 1.43              |
| 4:0:105:LEU:N   | 4:X:334:GLU:CB[1_556]  | 0.77                     | 1.43              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:147:ARG:C   | 4:Z:314:GLN:NE2[1_556] | 0.77                     | 1.43              |
| 4:1:62:ARG:C    | 4:W:288:ASP:CA[1_556]  | 0.77                     | 1.43              |
| 4:2:81:ASP:N    | 4:Z:31:PHE:CB[1_556]   | 0.77                     | 1.43              |
| 4:0:335:ARG:CD  | 4:X:220:ALA:CA[1_556]  | 0.77                     | 1.43              |
| 4:1:252:ASN:C   | 4:X:113:LYS:CB[1_556]  | 0.77                     | 1.43              |
| 4:0:132:MET:CE  | 4:X:341:ILE:CG1[1_556] | 0.77                     | 1.43              |
| 4:3:62:ARG:C    | 4:Y:288:ASP:CA[1_556]  | 0.77                     | 1.43              |
| 4:1:261:LEU:CG  | 4:Y:266:PHE:CG[1_556]  | 0.77                     | 1.43              |
| 4:0:112:PRO:O   | 4:X:137:GLN:CG[1_556]  | 0.77                     | 1.43              |
| 4:1:183:ARG:CB  | 4:Y:187:ASP:N[1_556]   | 0.77                     | 1.43              |
| 4:1:303:THR:OG1 | 4:Y:257:CYS:CA[1_556]  | 0.77                     | 1.43              |
| 4:0:116:ARG:N   | 4:X:339:VAL:CG1[1_556] | 0.77                     | 1.43              |
| 4:2:171:LEU:CD1 | 4:Z:282:ILE:CG1[1_556] | 0.77                     | 1.43              |
| 4:0:175:ILE:CG1 | 4:X:162:ASN:ND2[1_556] | 0.77                     | 1.43              |
| 4:0:126:THR:CB  | 4:X:28:ARG:CG[1_556]   | 0.77                     | 1.43              |
| 4:1:274:ILE:CG1 | 4:Y:263:GLN:CA[1_556]  | 0.77                     | 1.43              |
| 4:1:67:LEU:CD2  | 4:Y:207:GLU:OE1[1_556] | 0.77                     | 1.43              |
| 4:1:183:ARG:C   | 4:Y:187:ASP:C[1_556]   | 0.78                     | 1.42              |
| 4:2:278:THR:C   | 4:Z:276:GLU:CG[1_556]  | 0.78                     | 1.42              |
| 4:1:78:ASN:CG   | 4:Y:32:PRO:O[1_556]    | 0.78                     | 1.42              |
| 4:0:336:LYS:CG  | 4:X:218:TYR:CG[1_556]  | 0.78                     | 1.42              |
| 4:1:147:ARG:C   | 4:Y:314:GLN:NE2[1_556] | 0.78                     | 1.42              |
| 4:2:167:GLU:CA  | 4:Z:295:ALA:CA[1_556]  | 0.78                     | 1.42              |
| 4:2:183:ARG:CB  | 4:Z:186:THR:C[1_556]   | 0.78                     | 1.42              |
| 4:1:177:ARG:N   | 4:Y:178:LEU:CB[1_556]  | 0.78                     | 1.42              |
| 4:0:167:GLU:C   | 4:X:295:ALA:CA[1_556]  | 0.78                     | 1.42              |
| 4:2:109:PRO:CA  | 4:Z:154:ASP:N[1_556]   | 0.78                     | 1.42              |
| 4:1:126:THR:CB  | 4:Y:28:ARG:CG[1_556]   | 0.78                     | 1.42              |
| 4:0:171:LEU:CD1 | 4:X:282:ILE:CG1[1_556] | 0.78                     | 1.42              |
| 4:1:153:LEU:O   | 4:Y:262:PHE:CZ[1_556]  | 0.78                     | 1.42              |
| 4:0:197:GLY:CA  | 4:W:75:ILE:CA[1_556]   | 0.78                     | 1.42              |
| 4:0:81:ASP:N    | 4:X:31:PHE:CB[1_556]   | 0.78                     | 1.42              |
| 4:2:163:VAL:CG2 | 4:Z:153:LEU:CD1[1_556] | 0.78                     | 1.42              |
| 4:1:362:TYR:CE2 | 4:Y:22:ALA:C[1_556]    | 0.78                     | 1.42              |
| 4:2:182:GLY:O   | 4:Z:189:LEU:N[1_556]   | 0.78                     | 1.42              |
| 4:1:261:LEU:CD1 | 4:Y:266:PHE:CD2[1_556] | 0.78                     | 1.42              |
| 4:2:112:PRO:O   | 4:Z:137:GLN:CG[1_556]  | 0.78                     | 1.42              |
| 4:1:167:GLU:CA  | 4:Y:295:ALA:CA[1_556]  | 0.78                     | 1.42              |
| 4:1:136:ILE:N   | 4:Y:299:MET:O[1_556]   | 0.79                     | 1.41              |
| 4:1:167:GLU:N   | 4:Y:294:TYR:C[1_556]   | 0.79                     | 1.41              |
| 4:2:305:MET:CB  | 4:Z:255:PHE:CB[1_556]  | 0.79                     | 1.41              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:109:PRO:CA  | 4:X:154:ASP:N[1_556]   | 0.79                     | 1.41              |
| 4:0:171:LEU:CD1 | 4:X:282:ILE:CD1[1_556] | 0.79                     | 1.41              |
| 4:1:215:LYS:NZ  | 4:Y:249:THR:OG1[1_556] | 0.79                     | 1.41              |
| 4:0:163:VAL:CG2 | 4:X:153:LEU:CD1[1_556] | 0.79                     | 1.41              |
| 4:2:171:LEU:CD1 | 4:Z:282:ILE:CD1[1_556] | 0.79                     | 1.41              |
| 4:2:132:MET:CE  | 4:Z:341:ILE:CG1[1_556] | 0.79                     | 1.41              |
| 4:2:175:ILE:CG1 | 4:Z:162:ASN:ND2[1_556] | 0.79                     | 1.41              |
| 4:0:278:THR:C   | 4:X:276:GLU:CG[1_556]  | 0.79                     | 1.41              |
| 4:2:116:ARG:N   | 4:Z:339:VAL:CG1[1_556] | 0.79                     | 1.41              |
| 4:2:336:LYS:CG  | 4:Z:218:TYR:CG[1_556]  | 0.79                     | 1.41              |
| 4:0:136:ILE:N   | 4:X:299:MET:O[1_556]   | 0.79                     | 1.41              |
| 4:1:336:LYS:CG  | 4:Y:218:TYR:CG[1_556]  | 0.79                     | 1.41              |
| 4:0:183:ARG:CB  | 4:X:186:THR:C[1_556]   | 0.79                     | 1.41              |
| 4:1:163:VAL:C   | 4:Y:278:THR:OG1[1_556] | 0.79                     | 1.41              |
| 4:0:307:PRO:C   | 4:X:227:MET:CB[1_556]  | 0.80                     | 1.40              |
| 4:2:167:GLU:C   | 4:Z:295:ALA:CA[1_556]  | 0.80                     | 1.40              |
| 4:1:105:LEU:CA  | 4:Y:334:GLU:O[1_556]   | 0.80                     | 1.40              |
| 4:2:175:ILE:CB  | 4:Z:162:ASN:CG[1_556]  | 0.80                     | 1.40              |
| 4:0:305:MET:CB  | 4:X:255:PHE:CB[1_556]  | 0.80                     | 1.40              |
| 4:2:72:GLU:CA   | 4:Z:157:ASP:CG[1_556]  | 0.80                     | 1.40              |
| 4:1:132:MET:CE  | 4:Y:341:ILE:CG1[1_556] | 0.80                     | 1.40              |
| 4:0:182:GLY:O   | 4:X:189:LEU:N[1_556]   | 0.80                     | 1.40              |
| 4:1:158:GLY:C   | 4:Y:181:ALA:O[1_556]   | 0.80                     | 1.40              |
| 4:2:173:HIS:CA  | 4:Z:174:ALA:O[1_556]   | 0.80                     | 1.40              |
| 4:2:173:HIS:CB  | 4:Z:174:ALA:O[1_556]   | 0.80                     | 1.40              |
| 4:0:167:GLU:CA  | 4:X:295:ALA:CA[1_556]  | 0.80                     | 1.40              |
| 4:2:136:ILE:N   | 4:Z:299:MET:O[1_556]   | 0.80                     | 1.40              |
| 4:1:109:PRO:CA  | 4:Y:154:ASP:N[1_556]   | 0.80                     | 1.40              |
| 4:1:105:LEU:N   | 4:Y:334:GLU:CB[1_556]  | 0.80                     | 1.40              |
| 4:1:80:ASP:N    | 4:Y:31:PHE:CG[1_556]   | 0.80                     | 1.40              |
| 4:2:286:ASP:CG  | 4:Z:290:ARG:NE[1_556]  | 0.80                     | 1.40              |
| 4:0:72:GLU:CA   | 4:X:157:ASP:CG[1_556]  | 0.80                     | 1.40              |
| 4:1:86:TRP:CZ2  | 4:Y:337:TYR:CE1[1_556] | 0.80                     | 1.40              |
| 4:2:124:PHE:O   | 4:Z:24:ASP:OD1[1_556]  | 0.80                     | 1.40              |
| 4:0:173:HIS:CB  | 4:X:174:ALA:O[1_556]   | 0.80                     | 1.40              |
| 4:0:173:HIS:CA  | 4:X:174:ALA:O[1_556]   | 0.80                     | 1.40              |
| 4:1:138:ALA:C   | 4:Y:299:MET:SD[1_556]  | 0.81                     | 1.39              |
| 4:0:175:ILE:CB  | 4:X:162:ASN:CG[1_556]  | 0.81                     | 1.39              |
| 4:1:213:LYS:CD  | 4:Y:192:ILE:CG1[1_556] | 0.81                     | 1.39              |
| 4:1:175:ILE:CG1 | 4:Y:162:ASN:CG[1_556]  | 0.81                     | 1.39              |
| 4:1:279:TYR:N   | 4:Y:276:GLU:CD[1_556]  | 0.81                     | 1.39              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:307:PRO:C   | 4:Z:227:MET:CB[1_556]  | 0.81                     | 1.39              |
| 4:1:157:ASP:CB  | 4:Y:213:LYS:CD[1_556]  | 0.81                     | 1.39              |
| 4:0:261:LEU:CD1 | 4:X:266:PHE:CD2[1_556] | 0.81                     | 1.39              |
| 4:1:172:PRO:CG  | 4:Y:164:PRO:CD[1_556]  | 0.81                     | 1.39              |
| 4:0:309:ILE:CG1 | 4:X:259:GLU:OE2[1_556] | 0.81                     | 1.39              |
| 4:1:206:ARG:NH2 | 4:Y:190:MET:SD[1_556]  | 0.81                     | 1.39              |
| 4:1:116:ARG:NE  | 4:Y:141:SER:CA[1_556]  | 0.81                     | 1.39              |
| 4:1:167:GLU:C   | 4:Y:295:ALA:CA[1_556]  | 0.81                     | 1.39              |
| 4:2:172:PRO:CG  | 4:Z:164:PRO:N[1_556]   | 0.81                     | 1.39              |
| 4:2:161:HIS:CD2 | 4:Z:160:THR:CG2[1_556] | 0.81                     | 1.39              |
| 4:2:261:LEU:CD1 | 4:Z:266:PHE:CD2[1_556] | 0.82                     | 1.38              |
| 4:1:278:THR:C   | 4:Y:276:GLU:CG[1_556]  | 0.82                     | 1.38              |
| 4:2:123:MET:SD  | 4:Z:26:ALA:CB[1_556]   | 0.82                     | 1.38              |
| 4:1:195:GLU:CD  | 4:X:109:PRO:C[1_556]   | 0.82                     | 1.38              |
| 4:0:335:ARG:CG  | 4:X:220:ALA:N[1_556]   | 0.82                     | 1.38              |
| 4:1:164:PRO:C   | 4:Y:278:THR:CG2[1_556] | 0.82                     | 1.38              |
| 4:0:80:ASP:N    | 4:X:31:PHE:CG[1_556]   | 0.82                     | 1.38              |
| 4:3:195:GLU:CD  | 4:Z:109:PRO:C[1_556]   | 0.82                     | 1.38              |
| 4:1:124:PHE:O   | 4:Y:24:ASP:OD1[1_556]  | 0.82                     | 1.38              |
| 4:0:124:PHE:O   | 4:X:24:ASP:OD1[1_556]  | 0.82                     | 1.38              |
| 4:2:80:ASP:N    | 4:Z:31:PHE:CG[1_556]   | 0.82                     | 1.38              |
| 4:0:286:ASP:CG  | 4:X:290:ARG:NE[1_556]  | 0.82                     | 1.38              |
| 4:2:153:LEU:CB  | 4:Z:262:PHE:CD1[1_556] | 0.82                     | 1.38              |
| 4:2:274:ILE:CB  | 4:Z:263:GLN:CA[1_556]  | 0.82                     | 1.38              |
| 4:2:78:ASN:O    | 4:Z:31:PHE:O[1_556]    | 0.82                     | 1.38              |
| 4:2:335:ARG:CG  | 4:Z:220:ALA:N[1_556]   | 0.82                     | 1.38              |
| 4:2:290:ARG:CG  | 4:Z:279:TYR:OH[1_556]  | 0.82                     | 1.38              |
| 4:2:309:ILE:CG1 | 4:Z:259:GLU:OE2[1_556] | 0.82                     | 1.38              |
| 4:3:230:ALA:O   | 4:Z:367:PRO:O[1_556]   | 0.82                     | 1.38              |
| 4:1:173:HIS:CB  | 4:Y:174:ALA:O[1_556]   | 0.82                     | 1.38              |
| 4:0:210:ARG:CB  | 4:X:193:LEU:CG[1_556]  | 0.82                     | 1.38              |
| 4:2:279:TYR:N   | 4:Z:276:GLU:CD[1_556]  | 0.82                     | 1.38              |
| 4:2:158:GLY:C   | 4:Z:181:ALA:O[1_556]   | 0.82                     | 1.38              |
| 4:0:206:ARG:CB  | 4:X:200:PHE:N[1_556]   | 0.83                     | 1.37              |
| 4:0:161:HIS:CD2 | 4:X:160:THR:CG2[1_556] | 0.83                     | 1.37              |
| 4:1:366:GLY:C   | 4:Y:347:ALA:CA[1_556]  | 0.83                     | 1.37              |
| 4:1:116:ARG:N   | 4:Y:339:VAL:CG1[1_556] | 0.83                     | 1.37              |
| 4:0:78:ASN:CB   | 4:X:32:PRO:C[1_556]    | 0.83                     | 1.37              |
| 4:0:123:MET:SD  | 4:X:26:ALA:CB[1_556]   | 0.83                     | 1.37              |
| 4:4:62:ARG:C    | 4:Z:288:ASP:CA[1_556]  | 0.83                     | 1.37              |
| 4:0:78:ASN:O    | 4:X:31:PHE:O[1_556]    | 0.83                     | 1.37              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:207:GLU:OE1 | 4:Y:242:LEU:CD2[1_556] | 0.83                     | 1.37              |
| 4:0:153:LEU:CA  | 4:X:262:PHE:CD1[1_556] | 0.83                     | 1.37              |
| 4:1:183:ARG:O   | 4:Y:187:ASP:O[1_556]   | 0.83                     | 1.37              |
| 4:2:281:SER:CB  | 4:Z:276:GLU:C[1_556]   | 0.83                     | 1.37              |
| 4:2:78:ASN:CB   | 4:Z:32:PRO:C[1_556]    | 0.83                     | 1.37              |
| 4:1:126:THR:OG1 | 4:Y:28:ARG:CA[1_556]   | 0.83                     | 1.37              |
| 4:1:357:ILE:CG2 | 4:Y:345:ILE:CG1[1_556] | 0.83                     | 1.37              |
| 4:0:172:PRO:CG  | 4:X:164:PRO:N[1_556]   | 0.83                     | 1.37              |
| 4:2:206:ARG:CB  | 4:Z:200:PHE:N[1_556]   | 0.83                     | 1.37              |
| 4:1:119:MET:C   | 4:Y:340:TRP:CG[1_556]  | 0.83                     | 1.37              |
| 4:2:178:LEU:C   | 4:Z:180:LEU:CB[1_556]  | 0.83                     | 1.37              |
| 4:2:332:PRO:CB  | 4:Z:221:LEU:CD2[1_556] | 0.83                     | 1.37              |
| 4:0:158:GLY:C   | 4:X:181:ALA:O[1_556]   | 0.83                     | 1.37              |
| 4:2:62:ARG:C    | 4:X:288:ASP:CA[1_556]  | 0.83                     | 1.37              |
| 4:0:195:GLU:OE2 | 4:W:109:PRO:C[1_556]   | 0.83                     | 1.37              |
| 4:1:183:ARG:CB  | 4:Y:186:THR:C[1_556]   | 0.84                     | 1.36              |
| 4:0:290:ARG:CG  | 4:X:279:TYR:OH[1_556]  | 0.84                     | 1.36              |
| 4:0:62:ARG:C    | 4:V:288:ASP:CA[1_556]  | 0.84                     | 1.36              |
| 4:1:71:ILE:O    | 4:Y:157:ASP:OD1[1_556] | 0.84                     | 1.36              |
| 4:0:281:SER:CB  | 4:X:276:GLU:C[1_556]   | 0.84                     | 1.36              |
| 4:0:274:ILE:CB  | 4:X:263:GLN:CA[1_556]  | 0.84                     | 1.36              |
| 4:0:153:LEU:CB  | 4:X:262:PHE:CD1[1_556] | 0.84                     | 1.36              |
| 4:0:126:THR:OG1 | 4:X:28:ARG:CA[1_556]   | 0.84                     | 1.36              |
| 4:1:120:THR:CB  | 4:Y:340:TRP:O[1_556]   | 0.84                     | 1.36              |
| 4:2:210:ARG:CB  | 4:Z:193:LEU:CG[1_556]  | 0.84                     | 1.36              |
| 4:0:252:ASN:C   | 4:W:113:LYS:CB[1_556]  | 0.84                     | 1.36              |
| 4:0:207:GLU:OE1 | 4:X:242:LEU:CD2[1_556] | 0.84                     | 1.36              |
| 4:1:230:ALA:O   | 4:X:367:PRO:O[1_556]   | 0.84                     | 1.36              |
| 4:1:41:GLN:N    | 4:W:167:GLU:CD[1_556]  | 0.84                     | 1.36              |
| 4:1:215:LYS:CG  | 4:Y:196:ARG:NH2[1_556] | 0.84                     | 1.36              |
| 4:1:371:HIS:CB  | 4:Y:140:LEU:CD2[1_556] | 0.84                     | 1.36              |
| 4:0:362:TYR:CD2 | 4:X:23:GLY:N[1_556]    | 0.84                     | 1.36              |
| 4:1:175:ILE:CG1 | 4:Y:162:ASN:ND2[1_556] | 0.84                     | 1.36              |
| 4:0:332:PRO:CB  | 4:X:221:LEU:CD2[1_556] | 0.84                     | 1.36              |
| 4:0:279:TYR:N   | 4:X:276:GLU:CD[1_556]  | 0.84                     | 1.36              |
| 4:0:369:ILE:N   | 4:X:346:LEU:CB[1_556]  | 0.85                     | 1.35              |
| 4:1:79:TRP:CZ2  | 4:Y:11:ASP:O[1_556]    | 0.85                     | 1.35              |
| 4:2:177:ARG:N   | 4:Z:178:LEU:CB[1_556]  | 0.85                     | 1.35              |
| 4:1:307:PRO:C   | 4:Y:227:MET:CB[1_556]  | 0.85                     | 1.35              |
| 4:1:106:THR:CA  | 4:Y:335:ARG:C[1_556]   | 0.85                     | 1.35              |
| 4:1:126:THR:C   | 4:Y:28:ARG:NE[1_556]   | 0.85                     | 1.35              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:83:GLU:OE1  | 4:X:29:ALA:CB[1_556]   | 0.85                     | 1.35              |
| 4:2:153:LEU:CA  | 4:Z:262:PHE:CD1[1_556] | 0.85                     | 1.35              |
| 4:2:362:TYR:CD2 | 4:Z:23:GLY:N[1_556]    | 0.85                     | 1.35              |
| 4:2:252:ASN:C   | 4:Y:113:LYS:CB[1_556]  | 0.85                     | 1.35              |
| 4:1:335:ARG:CB  | 4:Y:219:VAL:O[1_556]   | 0.85                     | 1.35              |
| 4:2:207:GLU:OE1 | 4:Z:242:LEU:CD2[1_556] | 0.85                     | 1.35              |
| 4:3:195:GLU:OE2 | 4:Z:109:PRO:C[1_556]   | 0.85                     | 1.35              |
| 4:2:292:ASP:N   | 4:Z:321:ALA:O[1_556]   | 0.85                     | 1.35              |
| 4:1:196:ARG:NH1 | 4:X:115:ASN:N[1_556]   | 0.85                     | 1.35              |
| 4:2:105:LEU:C   | 4:Z:334:GLU:C[1_556]   | 0.85                     | 1.35              |
| 4:2:213:LYS:CD  | 4:Z:192:ILE:CG1[1_556] | 0.85                     | 1.35              |
| 4:3:41:GLN:N    | 4:Y:167:GLU:CD[1_556]  | 0.85                     | 1.35              |
| 4:0:153:LEU:O   | 4:X:262:PHE:CE2[1_556] | 0.85                     | 1.35              |
| 4:4:40:HIS:CE1  | 4:Z:166:TYR:CG[1_556]  | 0.85                     | 1.35              |
| 4:1:181:ALA:O   | 4:Y:188:TYR:CB[1_556]  | 0.85                     | 1.35              |
| 4:2:210:ARG:CG  | 4:Z:193:LEU:CD2[1_556] | 0.85                     | 1.35              |
| 4:0:292:ASP:N   | 4:X:321:ALA:O[1_556]   | 0.85                     | 1.35              |
| 4:0:213:LYS:CD  | 4:X:192:ILE:CG1[1_556] | 0.85                     | 1.35              |
| 4:2:369:ILE:N   | 4:Z:346:LEU:CB[1_556]  | 0.85                     | 1.35              |
| 4:0:178:LEU:C   | 4:X:180:LEU:CB[1_556]  | 0.85                     | 1.35              |
| 4:2:195:GLU:OE2 | 4:Y:109:PRO:C[1_556]   | 0.86                     | 1.34              |
| 4:3:196:ARG:NH1 | 4:Z:115:ASN:N[1_556]   | 0.86                     | 1.34              |
| 4:2:83:GLU:OE1  | 4:Z:29:ALA:CB[1_556]   | 0.86                     | 1.34              |
| 4:1:172:PRO:CG  | 4:Y:164:PRO:N[1_556]   | 0.86                     | 1.34              |
| 4:1:74:GLY:CA   | 4:Y:156:GLY:C[1_556]   | 0.86                     | 1.34              |
| 4:1:175:ILE:CB  | 4:Y:162:ASN:CG[1_556]  | 0.86                     | 1.34              |
| 4:0:210:ARG:CG  | 4:X:193:LEU:CD2[1_556] | 0.86                     | 1.34              |
| 4:1:206:ARG:CB  | 4:Y:200:PHE:N[1_556]   | 0.86                     | 1.34              |
| 4:0:177:ARG:N   | 4:X:178:LEU:CB[1_556]  | 0.86                     | 1.34              |
| 4:0:230:ALA:O   | 4:W:367:PRO:O[1_556]   | 0.86                     | 1.34              |
| 4:1:335:ARG:CD  | 4:Y:220:ALA:CA[1_556]  | 0.86                     | 1.34              |
| 4:2:40:HIS:CE1  | 4:X:166:TYR:CG[1_556]  | 0.86                     | 1.34              |
| 4:2:303:THR:N   | 4:Z:258:PRO:CD[1_556]  | 0.86                     | 1.34              |
| 4:1:118:LYS:CB  | 4:Y:11:ASP:N[1_556]    | 0.86                     | 1.34              |
| 4:2:126:THR:OG1 | 4:Z:28:ARG:CA[1_556]   | 0.86                     | 1.34              |
| 4:0:105:LEU:C   | 4:X:334:GLU:C[1_556]   | 0.86                     | 1.34              |
| 4:0:78:ASN:CG   | 4:X:32:PRO:O[1_556]    | 0.86                     | 1.34              |
| 4:1:110:LEU:CG  | 4:Y:161:HIS:CB[1_556]  | 0.87                     | 1.33              |
| 4:1:178:LEU:C   | 4:Y:180:LEU:CB[1_556]  | 0.87                     | 1.33              |
| 4:2:153:LEU:O   | 4:Z:262:PHE:CE2[1_556] | 0.87                     | 1.33              |
| 4:1:305:MET:O   | 4:Y:255:PHE:CE1[1_556] | 0.87                     | 1.33              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:170:ALA:O   | 4:X:151:ILE:CB[1_556]  | 0.87                     | 1.33              |
| 4:1:215:LYS:NZ  | 4:Y:249:THR:CB[1_556]  | 0.87                     | 1.33              |
| 4:2:183:ARG:CB  | 4:Z:187:ASP:N[1_556]   | 0.87                     | 1.33              |
| 4:2:183:ARG:C   | 4:Z:187:ASP:C[1_556]   | 0.87                     | 1.33              |
| 4:1:195:GLU:OE2 | 4:X:109:PRO:C[1_556]   | 0.87                     | 1.33              |
| 4:2:78:ASN:CG   | 4:Z:32:PRO:O[1_556]    | 0.87                     | 1.33              |
| 4:0:183:ARG:CB  | 4:X:187:ASP:N[1_556]   | 0.87                     | 1.33              |
| 4:0:141:SER:CB  | 4:X:310:ALA:N[1_556]   | 0.87                     | 1.33              |
| 4:1:205:GLU:O   | 4:Y:199:SER:N[1_556]   | 0.87                     | 1.33              |
| 4:0:183:ARG:C   | 4:X:187:ASP:C[1_556]   | 0.87                     | 1.33              |
| 4:0:362:TYR:CD1 | 4:X:344:SER:O[1_556]   | 0.87                     | 1.33              |
| 4:2:138:ALA:C   | 4:Z:299:MET:SD[1_556]  | 0.88                     | 1.32              |
| 4:0:40:HIS:CE1  | 4:V:166:TYR:CG[1_556]  | 0.88                     | 1.32              |
| 4:2:362:TYR:CZ  | 4:Z:22:ALA:CA[1_556]   | 0.88                     | 1.32              |
| 4:1:153:LEU:CB  | 4:Y:262:PHE:CD1[1_556] | 0.88                     | 1.32              |
| 4:2:167:GLU:N   | 4:Z:294:TYR:C[1_556]   | 0.88                     | 1.32              |
| 4:2:366:GLY:C   | 4:Z:347:ALA:CA[1_556]  | 0.88                     | 1.32              |
| 4:1:126:THR:CB  | 4:Y:28:ARG:CB[1_556]   | 0.88                     | 1.32              |
| 4:1:290:ARG:CG  | 4:Y:279:TYR:OH[1_556]  | 0.88                     | 1.32              |
| 4:0:105:LEU:CA  | 4:X:334:GLU:C[1_556]   | 0.88                     | 1.32              |
| 4:1:168:GLY:C   | 4:Y:296:ASN:C[1_556]   | 0.88                     | 1.32              |
| 4:0:40:HIS:ND1  | 4:V:166:TYR:CD1[1_556] | 0.88                     | 1.32              |
| 4:0:208:ILE:C   | 4:X:198:TYR:CD2[1_556] | 0.88                     | 1.32              |
| 4:2:170:ALA:O   | 4:Z:151:ILE:CB[1_556]  | 0.88                     | 1.32              |
| 4:1:331:ALA:C   | 4:Y:221:LEU:C[1_556]   | 0.88                     | 1.32              |
| 4:2:141:SER:CB  | 4:Z:310:ALA:N[1_556]   | 0.88                     | 1.32              |
| 4:2:230:ALA:O   | 4:Y:367:PRO:O[1_556]   | 0.88                     | 1.32              |
| 4:0:164:PRO:C   | 4:X:278:THR:CG2[1_556] | 0.88                     | 1.32              |
| 4:1:362:TYR:CE2 | 4:Y:22:ALA:CA[1_556]   | 0.88                     | 1.32              |
| 4:2:185:LEU:CD2 | 4:Z:188:TYR:CE2[1_556] | 0.88                     | 1.32              |
| 4:2:297:ASN:ND2 | 4:Z:316:GLU:OE2[1_556] | 0.88                     | 1.32              |
| 4:1:274:ILE:CB  | 4:Y:263:GLN:CA[1_556]  | 0.88                     | 1.32              |
| 4:0:303:THR:N   | 4:X:258:PRO:CD[1_556]  | 0.88                     | 1.32              |
| 4:0:167:GLU:N   | 4:X:294:TYR:C[1_556]   | 0.88                     | 1.32              |
| 4:1:297:ASN:ND2 | 4:Y:316:GLU:OE2[1_556] | 0.88                     | 1.32              |
| 4:2:335:ARG:CB  | 4:Z:219:VAL:O[1_556]   | 0.88                     | 1.32              |
| 4:2:290:ARG:O   | 4:Z:320:LEU:O[1_556]   | 0.88                     | 1.32              |
| 4:1:309:ILE:CG1 | 4:Y:259:GLU:OE2[1_556] | 0.88                     | 1.32              |
| 4:2:208:ILE:C   | 4:Z:198:TYR:CD2[1_556] | 0.88                     | 1.32              |
| 4:1:208:ILE:CB  | 4:Y:198:TYR:CD1[1_556] | 0.88                     | 1.32              |
| 4:0:162:ASN:N   | 4:X:274:ILE:CA[1_556]  | 0.89                     | 1.31              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:196:ARG:CZ  | 4:Z:115:ASN:N[1_556]   | 0.89                     | 1.31              |
| 4:2:164:PRO:C   | 4:Z:278:THR:CG2[1_556] | 0.89                     | 1.31              |
| 4:1:171:LEU:CD1 | 4:Y:282:ILE:CD1[1_556] | 0.89                     | 1.31              |
| 4:1:126:THR:OG1 | 4:Y:28:ARG:CB[1_556]   | 0.89                     | 1.31              |
| 4:2:362:TYR:CD1 | 4:Z:344:SER:O[1_556]   | 0.89                     | 1.31              |
| 4:1:113:LYS:CG  | 4:Y:136:ILE:CA[1_556]  | 0.89                     | 1.31              |
| 4:1:153:LEU:CA  | 4:Y:262:PHE:CD1[1_556] | 0.89                     | 1.31              |
| 4:3:253:GLU:CD  | 4:Z:112:PRO:C[1_556]   | 0.89                     | 1.31              |
| 4:2:126:THR:C   | 4:Z:28:ARG:NE[1_556]   | 0.89                     | 1.31              |
| 4:1:362:TYR:CD2 | 4:Y:23:GLY:N[1_556]    | 0.89                     | 1.31              |
| 4:2:163:VAL:C   | 4:Z:278:THR:OG1[1_556] | 0.89                     | 1.31              |
| 4:2:40:HIS:ND1  | 4:X:166:TYR:CD1[1_556] | 0.89                     | 1.31              |
| 4:0:138:ALA:C   | 4:X:299:MET:SD[1_556]  | 0.89                     | 1.31              |
| 4:1:303:THR:N   | 4:Y:258:PRO:CD[1_556]  | 0.89                     | 1.31              |
| 4:0:362:TYR:CZ  | 4:X:22:ALA:CA[1_556]   | 0.89                     | 1.31              |
| 4:0:366:GLY:C   | 4:X:347:ALA:CA[1_556]  | 0.89                     | 1.31              |
| 4:0:297:ASN:ND2 | 4:X:316:GLU:OE2[1_556] | 0.89                     | 1.31              |
| 4:0:120:THR:CB  | 4:X:340:TRP:O[1_556]   | 0.89                     | 1.31              |
| 4:1:253:GLU:CD  | 4:X:112:PRO:C[1_556]   | 0.89                     | 1.31              |
| 4:0:105:LEU:CA  | 4:X:334:GLU:O[1_556]   | 0.89                     | 1.31              |
| 4:0:181:ALA:O   | 4:X:188:TYR:CB[1_556]  | 0.89                     | 1.31              |
| 4:1:290:ARG:O   | 4:Y:320:LEU:O[1_556]   | 0.89                     | 1.31              |
| 4:1:116:ARG:NH1 | 4:Y:141:SER:C[1_556]   | 0.89                     | 1.31              |
| 4:0:163:VAL:C   | 4:X:278:THR:OG1[1_556] | 0.89                     | 1.31              |
| 4:1:166:TYR:CD1 | 4:Y:294:TYR:CD2[1_556] | 0.89                     | 1.31              |
| 4:2:181:ALA:O   | 4:Z:188:TYR:CB[1_556]  | 0.89                     | 1.31              |
| 4:1:196:ARG:CZ  | 4:X:115:ASN:N[1_556]   | 0.89                     | 1.31              |
| 4:0:196:ARG:CZ  | 4:W:115:ASN:N[1_556]   | 0.90                     | 1.30              |
| 4:0:175:ILE:CG1 | 4:X:162:ASN:CG[1_556]  | 0.90                     | 1.30              |
| 4:2:369:ILE:N   | 4:Z:346:LEU:CA[1_556]  | 0.90                     | 1.30              |
| 4:1:72:GLU:CA   | 4:Y:157:ASP:CG[1_556]  | 0.90                     | 1.30              |
| 4:1:177:ARG:NH2 | 4:Y:158:GLY:O[1_556]   | 0.90                     | 1.30              |
| 4:0:208:ILE:CB  | 4:X:198:TYR:CD1[1_556] | 0.90                     | 1.30              |
| 4:2:105:LEU:CA  | 4:Z:334:GLU:O[1_556]   | 0.90                     | 1.30              |
| 4:0:162:ASN:OD1 | 4:X:273:GLY:C[1_556]   | 0.90                     | 1.30              |
| 4:1:148:THR:OG1 | 4:Y:327:ILE:O[1_556]   | 0.90                     | 1.30              |
| 4:2:105:LEU:CA  | 4:Z:334:GLU:C[1_556]   | 0.90                     | 1.30              |
| 4:2:178:LEU:O   | 4:Z:180:LEU:CG[1_556]  | 0.90                     | 1.30              |
| 4:2:162:ASN:N   | 4:Z:274:ILE:CA[1_556]  | 0.90                     | 1.30              |
| 4:2:306:TYR:CD1 | 4:Z:256:ARG:CG[1_556]  | 0.90                     | 1.30              |
| 4:0:195:GLU:CD  | 4:W:109:PRO:C[1_556]   | 0.90                     | 1.30              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:335:ARG:CB  | 4:X:219:VAL:O[1_556]   | 0.90                     | 1.30              |
| 4:0:162:ASN:C   | 4:X:274:ILE:O[1_556]   | 0.90                     | 1.30              |
| 4:2:110:LEU:CG  | 4:Z:161:HIS:CB[1_556]  | 0.90                     | 1.30              |
| 4:0:178:LEU:O   | 4:X:180:LEU:CG[1_556]  | 0.90                     | 1.30              |
| 4:2:215:LYS:NZ  | 4:Z:249:THR:CB[1_556]  | 0.90                     | 1.30              |
| 4:2:106:THR:CA  | 4:Z:335:ARG:C[1_556]   | 0.90                     | 1.30              |
| 4:2:162:ASN:OD1 | 4:Z:273:GLY:C[1_556]   | 0.90                     | 1.30              |
| 4:0:185:LEU:CD2 | 4:X:188:TYR:CE2[1_556] | 0.90                     | 1.30              |
| 4:0:162:ASN:CA  | 4:X:274:ILE:C[1_556]   | 0.90                     | 1.30              |
| 4:0:357:ILE:CG2 | 4:X:345:ILE:CG1[1_556] | 0.90                     | 1.30              |
| 4:1:264:PRO:CB  | 4:Y:268:GLY:C[1_556]   | 0.90                     | 1.30              |
| 4:1:210:ARG:CG  | 4:Y:193:LEU:CD2[1_556] | 0.90                     | 1.30              |
| 4:1:210:ARG:CB  | 4:Y:193:LEU:CG[1_556]  | 0.90                     | 1.30              |
| 4:2:162:ASN:CA  | 4:Z:274:ILE:C[1_556]   | 0.90                     | 1.30              |
| 4:1:123:MET:SD  | 4:Y:26:ALA:CB[1_556]   | 0.90                     | 1.30              |
| 4:2:195:GLU:CD  | 4:Y:109:PRO:C[1_556]   | 0.90                     | 1.30              |
| 4:1:170:ALA:O   | 4:Y:151:ILE:CB[1_556]  | 0.90                     | 1.30              |
| 4:2:175:ILE:CG1 | 4:Z:162:ASN:CG[1_556]  | 0.90                     | 1.30              |
| 4:1:105:LEU:CA  | 4:Y:334:GLU:C[1_556]   | 0.90                     | 1.30              |
| 4:2:79:TRP:CZ2  | 4:Z:11:ASP:O[1_556]    | 0.91                     | 1.29              |
| 4:0:116:ARG:NH1 | 4:X:141:SER:C[1_556]   | 0.91                     | 1.29              |
| 4:0:172:PRO:CG  | 4:X:164:PRO:CD[1_556]  | 0.91                     | 1.29              |
| 4:0:290:ARG:O   | 4:X:320:LEU:O[1_556]   | 0.91                     | 1.29              |
| 4:4:40:HIS:ND1  | 4:Z:166:TYR:CD1[1_556] | 0.91                     | 1.29              |
| 4:0:215:LYS:NZ  | 4:X:249:THR:CB[1_556]  | 0.91                     | 1.29              |
| 4:2:196:ARG:CZ  | 4:Y:115:ASN:N[1_556]   | 0.91                     | 1.29              |
| 4:0:126:THR:CB  | 4:X:28:ARG:CB[1_556]   | 0.91                     | 1.29              |
| 4:0:126:THR:C   | 4:X:28:ARG:NE[1_556]   | 0.91                     | 1.29              |
| 4:1:362:TYR:CZ  | 4:Y:22:ALA:CA[1_556]   | 0.91                     | 1.29              |
| 4:2:172:PRO:CG  | 4:Z:164:PRO:CD[1_556]  | 0.91                     | 1.29              |
| 4:1:162:ASN:C   | 4:Y:274:ILE:O[1_556]   | 0.91                     | 1.29              |
| 4:2:120:THR:CB  | 4:Z:340:TRP:O[1_556]   | 0.91                     | 1.29              |
| 4:1:153:LEU:O   | 4:Y:262:PHE:CE2[1_556] | 0.91                     | 1.29              |
| 4:0:71:ILE:O    | 4:X:157:ASP:OD1[1_556] | 0.91                     | 1.29              |
| 4:2:148:THR:O   | 4:Z:328:LYS:N[1_556]   | 0.91                     | 1.29              |
| 4:1:11:ASP:CG   | 4:Y:305:MET:CB[1_556]  | 0.91                     | 1.29              |
| 4:0:177:ARG:NH2 | 4:X:158:GLY:O[1_556]   | 0.91                     | 1.29              |
| 4:2:297:ASN:ND2 | 4:Z:316:GLU:CD[1_556]  | 0.91                     | 1.29              |
| 4:1:294:TYR:N   | 4:Y:320:LEU:CA[1_556]  | 0.91                     | 1.29              |
| 4:2:162:ASN:C   | 4:Z:274:ILE:O[1_556]   | 0.91                     | 1.29              |
| 4:2:371:HIS:CB  | 4:Z:140:LEU:CD2[1_556] | 0.91                     | 1.29              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:208:ILE:CB  | 4:Z:198:TYR:CD1[1_556] | 0.91                     | 1.29              |
| 4:0:306:TYR:CD1 | 4:X:256:ARG:CG[1_556]  | 0.91                     | 1.29              |
| 4:1:362:TYR:CD1 | 4:Y:344:SER:O[1_556]   | 0.91                     | 1.29              |
| 4:0:153:LEU:CG  | 4:X:262:PHE:CB[1_556]  | 0.91                     | 1.29              |
| 4:0:110:LEU:CG  | 4:X:161:HIS:CB[1_556]  | 0.91                     | 1.29              |
| 4:0:148:THR:O   | 4:X:328:LYS:N[1_556]   | 0.91                     | 1.29              |
| 4:4:41:GLN:N    | 4:Z:167:GLU:CD[1_556]  | 0.92                     | 1.28              |
| 4:2:357:ILE:CG2 | 4:Z:345:ILE:CG1[1_556] | 0.92                     | 1.28              |
| 4:2:300:SER:C   | 4:Z:219:VAL:CG2[1_556] | 0.92                     | 1.28              |
| 4:0:369:ILE:N   | 4:X:346:LEU:CA[1_556]  | 0.92                     | 1.28              |
| 4:2:286:ASP:O   | 4:Z:283:MET:SD[1_556]  | 0.92                     | 1.28              |
| 4:0:371:HIS:CB  | 4:X:140:LEU:CD2[1_556] | 0.92                     | 1.28              |
| 4:1:152:VAL:N   | 4:Y:313:MET:SD[1_556]  | 0.92                     | 1.28              |
| 4:1:366:GLY:CA  | 4:Y:347:ALA:CA[1_556]  | 0.92                     | 1.28              |
| 4:2:71:ILE:O    | 4:Z:157:ASP:OD1[1_556] | 0.92                     | 1.28              |
| 4:2:177:ARG:NH2 | 4:Z:158:GLY:O[1_556]   | 0.92                     | 1.28              |
| 4:0:106:THR:CA  | 4:X:335:ARG:C[1_556]   | 0.92                     | 1.28              |
| 4:2:294:TYR:N   | 4:Z:320:LEU:N[1_556]   | 0.92                     | 1.28              |
| 4:0:79:TRP:CZ2  | 4:X:11:ASP:O[1_556]    | 0.92                     | 1.28              |
| 4:1:120:THR:OG1 | 4:Y:340:TRP:C[1_556]   | 0.92                     | 1.28              |
| 4:1:114:ALA:CB  | 4:Y:106:THR:C[1_556]   | 0.92                     | 1.28              |
| 4:0:183:ARG:O   | 4:X:187:ASP:O[1_556]   | 0.92                     | 1.28              |
| 4:1:178:LEU:O   | 4:Y:180:LEU:CG[1_556]  | 0.92                     | 1.28              |
| 4:1:338:SER:N   | 4:Y:307:PRO:C[1_556]   | 0.92                     | 1.28              |
| 4:2:116:ARG:NH1 | 4:Z:141:SER:C[1_556]   | 0.92                     | 1.28              |
| 4:2:126:THR:CB  | 4:Z:28:ARG:CB[1_556]   | 0.93                     | 1.27              |
| 4:2:183:ARG:O   | 4:Z:187:ASP:O[1_556]   | 0.93                     | 1.27              |
| 4:0:297:ASN:ND2 | 4:X:316:GLU:CD[1_556]  | 0.93                     | 1.27              |
| 4:1:281:SER:CB  | 4:Y:276:GLU:C[1_556]   | 0.93                     | 1.27              |
| 4:0:118:LYS:C   | 4:X:340:TRP:CD1[1_556] | 0.93                     | 1.27              |
| 4:1:185:LEU:CD2 | 4:Y:188:TYR:CE2[1_556] | 0.93                     | 1.27              |
| 4:0:286:ASP:O   | 4:X:283:MET:SD[1_556]  | 0.93                     | 1.27              |
| 4:0:233:SER:CA  | 4:W:367:PRO:N[1_556]   | 0.93                     | 1.27              |
| 4:0:300:SER:C   | 4:X:219:VAL:CG2[1_556] | 0.93                     | 1.27              |
| 4:2:41:GLN:N    | 4:X:167:GLU:CD[1_556]  | 0.93                     | 1.27              |
| 4:0:119:MET:C   | 4:X:340:TRP:CG[1_556]  | 0.93                     | 1.27              |
| 4:1:134:VAL:CB  | 4:Y:338:SER:CA[1_556]  | 0.93                     | 1.27              |
| 4:2:118:LYS:C   | 4:Z:340:TRP:CD1[1_556] | 0.93                     | 1.27              |
| 4:0:366:GLY:CA  | 4:X:347:ALA:CA[1_556]  | 0.93                     | 1.27              |
| 4:2:152:VAL:N   | 4:Z:313:MET:SD[1_556]  | 0.93                     | 1.27              |
| 4:1:77:THR:O    | 4:Y:33:SER:OG[1_556]   | 0.93                     | 1.27              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:119:MET:C   | 4:Z:340:TRP:CG[1_556]  | 0.93                     | 1.27              |
| 4:0:331:ALA:C   | 4:X:221:LEU:C[1_556]   | 0.93                     | 1.27              |
| 4:2:153:LEU:CG  | 4:Z:262:PHE:CB[1_556]  | 0.93                     | 1.27              |
| 4:0:294:TYR:N   | 4:X:320:LEU:N[1_556]   | 0.93                     | 1.27              |
| 4:1:281:SER:OG  | 4:Y:277:THR:CA[1_556]  | 0.93                     | 1.27              |
| 4:1:124:PHE:O   | 4:Y:24:ASP:CG[1_556]   | 0.93                     | 1.27              |
| 4:0:41:GLN:N    | 4:V:167:GLU:CD[1_556]  | 0.93                     | 1.27              |
| 4:1:292:ASP:N   | 4:Y:321:ALA:O[1_556]   | 0.93                     | 1.27              |
| 4:0:215:LYS:CG  | 4:X:196:ARG:NH2[1_556] | 0.93                     | 1.27              |
| 4:1:186:THR:CG2 | 4:Y:190:MET:O[1_556]   | 0.93                     | 1.27              |
| 4:1:286:ASP:O   | 4:Y:283:MET:SD[1_556]  | 0.93                     | 1.27              |
| 4:1:369:ILE:N   | 4:Y:346:LEU:CA[1_556]  | 0.94                     | 1.26              |
| 4:0:366:GLY:C   | 4:X:347:ALA:N[1_556]   | 0.94                     | 1.26              |
| 4:2:215:LYS:CG  | 4:Z:196:ARG:NH2[1_556] | 0.94                     | 1.26              |
| 4:1:214:GLU:N   | 4:Y:253:GLU:CG[1_556]  | 0.94                     | 1.26              |
| 4:1:105:LEU:C   | 4:Y:334:GLU:C[1_556]   | 0.94                     | 1.26              |
| 4:1:40:HIS:CE1  | 4:W:166:TYR:CG[1_556]  | 0.94                     | 1.26              |
| 4:1:300:SER:C   | 4:Y:219:VAL:CG2[1_556] | 0.94                     | 1.26              |
| 4:0:189:LEU:CB  | 4:X:195:GLU:CB[1_556]  | 0.94                     | 1.26              |
| 4:2:166:TYR:CA  | 4:Z:294:TYR:CA[1_556]  | 0.94                     | 1.26              |
| 4:2:205:GLU:O   | 4:Z:199:SER:N[1_556]   | 0.94                     | 1.26              |
| 4:2:233:SER:CA  | 4:Y:367:PRO:N[1_556]   | 0.94                     | 1.26              |
| 4:2:210:ARG:CA  | 4:Z:193:LEU:CG[1_556]  | 0.94                     | 1.26              |
| 4:0:305:MET:O   | 4:X:255:PHE:CZ[1_556]  | 0.94                     | 1.26              |
| 4:0:305:MET:O   | 4:X:255:PHE:CE1[1_556] | 0.94                     | 1.26              |
| 4:1:10:CYS:SG   | 4:Y:336:LYS:CE[1_556]  | 0.95                     | 1.25              |
| 4:2:11:ASP:CB   | 4:Z:305:MET:CE[1_556]  | 0.95                     | 1.25              |
| 4:0:72:GLU:N    | 4:X:157:ASP:CG[1_556]  | 0.95                     | 1.25              |
| 4:2:295:ALA:N   | 4:Z:319:ALA:CA[1_556]  | 0.95                     | 1.25              |
| 4:2:264:PRO:CB  | 4:Z:268:GLY:C[1_556]   | 0.95                     | 1.25              |
| 4:0:205:GLU:O   | 4:X:199:SER:N[1_556]   | 0.95                     | 1.25              |
| 4:1:294:TYR:C   | 4:Y:319:ALA:O[1_556]   | 0.95                     | 1.25              |
| 4:2:74:GLY:CA   | 4:Z:156:GLY:C[1_556]   | 0.95                     | 1.25              |
| 4:0:332:PRO:CD  | 4:X:221:LEU:CB[1_556]  | 0.95                     | 1.25              |
| 4:2:189:LEU:CB  | 4:Z:195:GLU:CB[1_556]  | 0.95                     | 1.25              |
| 4:0:152:VAL:N   | 4:X:313:MET:SD[1_556]  | 0.95                     | 1.25              |
| 4:2:366:GLY:C   | 4:Z:347:ALA:N[1_556]   | 0.95                     | 1.25              |
| 4:2:203:THR:OG1 | 4:Z:205:GLU:CG[1_556]  | 0.95                     | 1.25              |
| 4:2:296:ASN:CG  | 4:Z:318:THR:CB[1_556]  | 0.95                     | 1.25              |
| 4:0:272:ALA:N   | 4:X:270:GLU:CA[1_556]  | 0.95                     | 1.25              |
| 4:3:40:HIS:CE1  | 4:Y:166:TYR:CG[1_556]  | 0.95                     | 1.25              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:208:ILE:C   | 4:Y:198:TYR:CD2[1_556] | 0.95                     | 1.25              |
| 4:1:231:ALA:CB  | 4:X:370:VAL:CA[1_556]  | 0.95                     | 1.25              |
| 4:1:162:ASN:N   | 4:Y:274:ILE:CA[1_556]  | 0.95                     | 1.25              |
| 4:0:118:LYS:CB  | 4:X:11:ASP:N[1_556]    | 0.95                     | 1.25              |
| 4:2:331:ALA:C   | 4:Z:221:LEU:C[1_556]   | 0.95                     | 1.25              |
| 4:2:309:ILE:CD1 | 4:Z:259:GLU:CG[1_556]  | 0.95                     | 1.25              |
| 4:2:366:GLY:CA  | 4:Z:347:ALA:CA[1_556]  | 0.95                     | 1.25              |
| 4:1:266:PHE:C   | 4:X:173:HIS:N[1_556]   | 0.95                     | 1.25              |
| 4:0:74:GLY:CA   | 4:X:156:GLY:C[1_556]   | 0.95                     | 1.25              |
| 4:2:305:MET:O   | 4:Z:255:PHE:CE1[1_556] | 0.95                     | 1.25              |
| 4:2:214:GLU:N   | 4:Z:253:GLU:CG[1_556]  | 0.95                     | 1.25              |
| 4:0:166:TYR:CA  | 4:X:294:TYR:CA[1_556]  | 0.95                     | 1.25              |
| 4:2:118:LYS:CB  | 4:Z:11:ASP:N[1_556]    | 0.95                     | 1.25              |
| 4:0:213:LYS:C   | 4:X:253:GLU:OE1[1_556] | 0.95                     | 1.25              |
| 4:1:296:ASN:CG  | 4:Y:318:THR:CB[1_556]  | 0.96                     | 1.24              |
| 4:3:231:ALA:CB  | 4:Z:370:VAL:CA[1_556]  | 0.96                     | 1.24              |
| 4:1:166:TYR:CA  | 4:Y:294:TYR:CA[1_556]  | 0.96                     | 1.24              |
| 4:0:203:THR:OG1 | 4:X:205:GLU:CG[1_556]  | 0.96                     | 1.24              |
| 4:0:11:ASP:CB   | 4:X:305:MET:CE[1_556]  | 0.96                     | 1.24              |
| 4:1:117:GLU:O   | 4:Y:9:VAL:CG1[1_556]   | 0.96                     | 1.24              |
| 4:2:126:THR:OG1 | 4:Z:28:ARG:CB[1_556]   | 0.96                     | 1.24              |
| 4:1:162:ASN:CA  | 4:Y:274:ILE:C[1_556]   | 0.96                     | 1.24              |
| 4:2:305:MET:O   | 4:Z:255:PHE:CZ[1_556]  | 0.96                     | 1.24              |
| 4:0:74:GLY:N    | 4:X:156:GLY:O[1_556]   | 0.96                     | 1.24              |
| 4:1:74:GLY:CA   | 4:Y:156:GLY:O[1_556]   | 0.96                     | 1.24              |
| 4:0:296:ASN:CG  | 4:X:318:THR:CB[1_556]  | 0.96                     | 1.24              |
| 4:2:148:THR:C   | 4:Z:328:LYS:N[1_556]   | 0.96                     | 1.24              |
| 4:1:332:PRO:CD  | 4:Y:221:LEU:CB[1_556]  | 0.96                     | 1.24              |
| 4:2:113:LYS:CG  | 4:Z:136:ILE:CA[1_556]  | 0.96                     | 1.24              |
| 4:1:72:GLU:N    | 4:Y:157:ASP:CG[1_556]  | 0.96                     | 1.24              |
| 4:0:210:ARG:CA  | 4:X:193:LEU:CG[1_556]  | 0.96                     | 1.24              |
| 4:0:309:ILE:CD1 | 4:X:259:GLU:CD[1_556]  | 0.96                     | 1.24              |
| 4:1:233:SER:C   | 4:X:367:PRO:N[1_556]   | 0.96                     | 1.24              |
| 4:3:233:SER:C   | 4:Z:367:PRO:N[1_556]   | 0.96                     | 1.24              |
| 4:1:59:GLN:CG   | 4:Y:208:ILE:CB[1_556]  | 0.96                     | 1.24              |
| 4:2:168:GLY:C   | 4:Z:296:ASN:C[1_556]   | 0.96                     | 1.24              |
| 4:2:80:ASP:N    | 4:Z:31:PHE:CD1[1_556]  | 0.96                     | 1.24              |
| 4:3:40:HIS:ND1  | 4:Y:166:TYR:CD1[1_556] | 0.96                     | 1.24              |
| 4:2:213:LYS:C   | 4:Z:253:GLU:OE1[1_556] | 0.96                     | 1.24              |
| 4:0:274:ILE:CD1 | 4:X:263:GLN:C[1_556]   | 0.96                     | 1.24              |
| 4:1:81:ASP:OD2  | 4:Y:32:PRO:CG[1_556]   | 0.96                     | 1.24              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:264:PRO:CA  | 4:Y:268:GLY:CA[1_556]  | 0.96                     | 1.24              |
| 4:2:74:GLY:N    | 4:Z:156:GLY:O[1_556]   | 0.96                     | 1.24              |
| 4:3:266:PHE:C   | 4:Z:173:HIS:N[1_556]   | 0.96                     | 1.24              |
| 4:0:113:LYS:CG  | 4:X:136:ILE:CA[1_556]  | 0.97                     | 1.23              |
| 4:0:264:PRO:CB  | 4:X:268:GLY:C[1_556]   | 0.97                     | 1.23              |
| 4:2:294:TYR:N   | 4:Z:320:LEU:CA[1_556]  | 0.97                     | 1.23              |
| 4:1:309:ILE:CD1 | 4:Y:259:GLU:CG[1_556]  | 0.97                     | 1.23              |
| 4:1:153:LEU:CG  | 4:Y:262:PHE:CB[1_556]  | 0.97                     | 1.23              |
| 4:0:362:TYR:CE2 | 4:X:22:ALA:CA[1_556]   | 0.97                     | 1.23              |
| 4:2:272:ALA:N   | 4:Z:270:GLU:CA[1_556]  | 0.97                     | 1.23              |
| 4:1:148:THR:C   | 4:Y:328:LYS:N[1_556]   | 0.97                     | 1.23              |
| 4:1:62:ARG:CZ   | 4:Y:205:GLU:CA[1_556]  | 0.97                     | 1.23              |
| 4:1:141:SER:CB  | 4:Y:310:ALA:N[1_556]   | 0.97                     | 1.23              |
| 4:2:72:GLU:N    | 4:Z:157:ASP:CG[1_556]  | 0.97                     | 1.23              |
| 4:0:72:GLU:CB   | 4:X:157:ASP:OD2[1_556] | 0.97                     | 1.23              |
| 4:0:295:ALA:N   | 4:X:319:ALA:CA[1_556]  | 0.97                     | 1.23              |
| 4:0:155:SER:O   | 4:X:258:PRO:CA[1_556]  | 0.97                     | 1.23              |
| 4:1:162:ASN:OD1 | 4:Y:273:GLY:C[1_556]   | 0.97                     | 1.23              |
| 4:0:309:ILE:CD1 | 4:X:259:GLU:CG[1_556]  | 0.97                     | 1.23              |
| 4:2:279:TYR:C   | 4:Z:276:GLU:OE1[1_556] | 0.97                     | 1.23              |
| 4:2:332:PRO:CD  | 4:Z:221:LEU:CB[1_556]  | 0.97                     | 1.23              |
| 4:0:120:THR:OG1 | 4:X:340:TRP:C[1_556]   | 0.97                     | 1.23              |
| 4:0:86:TRP:CE2  | 4:X:337:TYR:CZ[1_556]  | 0.97                     | 1.23              |
| 4:0:126:THR:OG1 | 4:X:28:ARG:CB[1_556]   | 0.97                     | 1.23              |
| 4:2:72:GLU:CB   | 4:Z:157:ASP:OD2[1_556] | 0.97                     | 1.23              |
| 4:1:366:GLY:C   | 4:Y:347:ALA:N[1_556]   | 0.97                     | 1.23              |
| 4:2:362:TYR:CE2 | 4:Z:22:ALA:CA[1_556]   | 0.97                     | 1.23              |
| 4:1:73:HIS:CA   | 4:Y:157:ASP:O[1_556]   | 0.97                     | 1.23              |
| 4:0:214:GLU:N   | 4:X:253:GLU:CG[1_556]  | 0.97                     | 1.23              |
| 4:2:309:ILE:CD1 | 4:Z:259:GLU:CD[1_556]  | 0.97                     | 1.23              |
| 4:0:148:THR:OG1 | 4:X:327:ILE:O[1_556]   | 0.97                     | 1.23              |
| 4:1:177:ARG:CG  | 4:Y:178:LEU:O[1_556]   | 0.97                     | 1.23              |
| 4:1:182:GLY:C   | 4:Y:189:LEU:N[1_556]   | 0.97                     | 1.23              |
| 4:0:294:TYR:N   | 4:X:320:LEU:CA[1_556]  | 0.97                     | 1.23              |
| 4:0:168:GLY:C   | 4:X:296:ASN:C[1_556]   | 0.97                     | 1.23              |
| 4:0:64:ILE:CG1  | 4:V:291:LYS:NZ[1_556]  | 0.97                     | 1.23              |
| 4:2:64:ILE:CG1  | 4:X:291:LYS:NZ[1_556]  | 0.97                     | 1.23              |
| 4:1:33:SER:CB   | 4:Y:210:ARG:NH1[1_556] | 0.97                     | 1.23              |
| 4:1:173:HIS:NE2 | 4:Y:281:SER:O[1_556]   | 0.98                     | 1.22              |
| 4:1:40:HIS:ND1  | 4:W:166:TYR:CD1[1_556] | 0.98                     | 1.22              |
| 4:0:113:LYS:N   | 4:X:137:GLN:N[1_556]   | 0.98                     | 1.22              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:11:ASP:CG   | 4:X:305:MET:CB[1_556]  | 0.98                     | 1.22              |
| 4:2:113:LYS:N   | 4:Z:137:GLN:N[1_556]   | 0.98                     | 1.22              |
| 4:0:253:GLU:CD  | 4:W:112:PRO:C[1_556]   | 0.98                     | 1.22              |
| 4:0:59:GLN:CG   | 4:X:208:ILE:CB[1_556]  | 0.98                     | 1.22              |
| 4:1:203:THR:OG1 | 4:Y:205:GLU:CG[1_556]  | 0.98                     | 1.22              |
| 4:0:140:LEU:CD2 | 4:X:331:ALA:O[1_556]   | 0.98                     | 1.22              |
| 4:2:140:LEU:CD2 | 4:Z:331:ALA:O[1_556]   | 0.98                     | 1.22              |
| 4:1:298:VAL:CB  | 4:Y:312:ARG:C[1_556]   | 0.98                     | 1.22              |
| 4:3:191:LYS:CG  | 4:Z:110:LEU:CD1[1_556] | 0.98                     | 1.22              |
| 4:0:362:TYR:O   | 4:X:348:SER:CB[1_556]  | 0.98                     | 1.22              |
| 4:0:34:ILE:N    | 4:X:210:ARG:NH2[1_556] | 0.98                     | 1.22              |
| 4:0:299:MET:CA  | 4:X:312:ARG:CG[1_556]  | 0.98                     | 1.22              |
| 4:2:37:ARG:NH1  | 4:Z:56:ASP:CB[1_556]   | 0.98                     | 1.22              |
| 4:0:206:ARG:CA  | 4:X:199:SER:CA[1_556]  | 0.98                     | 1.22              |
| 4:0:338:SER:N   | 4:X:307:PRO:C[1_556]   | 0.98                     | 1.22              |
| 4:2:134:VAL:CG1 | 4:Z:338:SER:CA[1_556]  | 0.98                     | 1.22              |
| 4:0:177:ARG:NH1 | 4:X:159:VAL:C[1_556]   | 0.98                     | 1.22              |
| 4:2:120:THR:OG1 | 4:Z:340:TRP:C[1_556]   | 0.98                     | 1.22              |
| 4:0:279:TYR:C   | 4:X:276:GLU:OE1[1_556] | 0.98                     | 1.22              |
| 4:2:124:PHE:C   | 4:Z:24:ASP:CG[1_556]   | 0.98                     | 1.22              |
| 4:4:64:ILE:CG1  | 4:Z:291:LYS:NZ[1_556]  | 0.98                     | 1.22              |
| 4:2:86:TRP:CE2  | 4:Z:337:TYR:CZ[1_556]  | 0.98                     | 1.22              |
| 4:2:289:ILE:CG1 | 4:Z:294:TYR:OH[1_556]  | 0.98                     | 1.22              |
| 4:0:148:THR:C   | 4:X:328:LYS:N[1_556]   | 0.98                     | 1.22              |
| 4:2:148:THR:OG1 | 4:Z:327:ILE:O[1_556]   | 0.98                     | 1.22              |
| 4:1:266:PHE:O   | 4:X:173:HIS:N[1_556]   | 0.98                     | 1.22              |
| 4:0:72:GLU:CD   | 4:X:183:ARG:NE[1_556]  | 0.98                     | 1.22              |
| 4:0:80:ASP:N    | 4:X:31:PHE:CD1[1_556]  | 0.98                     | 1.22              |
| 4:1:306:TYR:CD1 | 4:Y:256:ARG:CG[1_556]  | 0.98                     | 1.22              |
| 4:2:299:MET:CA  | 4:Z:312:ARG:CG[1_556]  | 0.98                     | 1.22              |
| 4:1:261:LEU:CA  | 4:Y:266:PHE:CA[1_556]  | 0.98                     | 1.22              |
| 4:0:289:ILE:CG1 | 4:X:294:TYR:OH[1_556]  | 0.98                     | 1.22              |
| 4:2:177:ARG:NH1 | 4:Z:159:VAL:C[1_556]   | 0.98                     | 1.22              |
| 4:2:281:SER:OG  | 4:Z:277:THR:CA[1_556]  | 0.99                     | 1.21              |
| 4:1:285:CYS:SG  | 4:Y:279:TYR:C[1_556]   | 0.99                     | 1.21              |
| 4:2:274:ILE:CD1 | 4:Z:263:GLN:C[1_556]   | 0.99                     | 1.21              |
| 4:0:134:VAL:CB  | 4:X:338:SER:CA[1_556]  | 0.99                     | 1.21              |
| 4:2:253:GLU:CD  | 4:Y:112:PRO:C[1_556]   | 0.99                     | 1.21              |
| 4:1:142:LEU:CD2 | 4:Y:329:ILE:CD1[1_556] | 0.99                     | 1.21              |
| 4:0:305:MET:CA  | 4:X:255:PHE:CG[1_556]  | 0.99                     | 1.21              |
| 4:1:165:ILE:CG1 | 4:Y:297:ASN:ND2[1_556] | 0.99                     | 1.21              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:264:PRO:CA  | 4:Z:268:GLY:CA[1_556]  | 0.99                     | 1.21              |
| 4:2:362:TYR:O   | 4:Z:348:SER:CB[1_556]  | 0.99                     | 1.21              |
| 4:1:278:THR:C   | 4:Y:276:GLU:CD[1_556]  | 0.99                     | 1.21              |
| 4:1:338:SER:CA  | 4:Y:308:GLY:N[1_556]   | 0.99                     | 1.21              |
| 4:0:105:LEU:C   | 4:X:335:ARG:N[1_556]   | 0.99                     | 1.21              |
| 4:0:124:PHE:C   | 4:X:24:ASP:CG[1_556]   | 0.99                     | 1.21              |
| 4:3:233:SER:CA  | 4:Z:367:PRO:N[1_556]   | 0.99                     | 1.21              |
| 4:1:118:LYS:CD  | 4:Y:10:CYS:CA[1_556]   | 0.99                     | 1.21              |
| 4:0:166:TYR:CD1 | 4:X:294:TYR:CD2[1_556] | 0.99                     | 1.21              |
| 4:2:305:MET:CA  | 4:Z:255:PHE:CG[1_556]  | 0.99                     | 1.21              |
| 4:2:11:ASP:CG   | 4:Z:305:MET:CB[1_556]  | 0.99                     | 1.21              |
| 4:2:134:VAL:CB  | 4:Z:338:SER:CA[1_556]  | 0.99                     | 1.21              |
| 4:2:59:GLN:CG   | 4:Z:208:ILE:CB[1_556]  | 0.99                     | 1.21              |
| 4:0:32:PRO:CB   | 4:X:211:ASP:CB[1_556]  | 0.99                     | 1.21              |
| 4:2:155:SER:O   | 4:Z:258:PRO:CA[1_556]  | 0.99                     | 1.21              |
| 4:1:305:MET:O   | 4:Y:255:PHE:CZ[1_556]  | 0.99                     | 1.21              |
| 4:2:82:MET:CB   | 4:Z:30:VAL:CG1[1_556]  | 0.99                     | 1.21              |
| 4:0:37:ARG:NH1  | 4:X:56:ASP:CB[1_556]   | 0.99                     | 1.21              |
| 4:2:34:ILE:N    | 4:Z:210:ARG:NH2[1_556] | 0.99                     | 1.21              |
| 4:0:74:GLY:CA   | 4:X:156:GLY:O[1_556]   | 0.99                     | 1.21              |
| 4:0:110:LEU:CG  | 4:X:161:HIS:CA[1_556]  | 0.99                     | 1.21              |
| 4:1:191:LYS:CG  | 4:X:110:LEU:CD1[1_556] | 0.99                     | 1.21              |
| 4:1:115:ASN:CB  | 4:Y:11:ASP:OD1[1_556]  | 0.99                     | 1.21              |
| 4:2:166:TYR:CD1 | 4:Z:294:TYR:CD2[1_556] | 0.99                     | 1.21              |
| 4:1:297:ASN:ND2 | 4:Y:316:GLU:CD[1_556]  | 0.99                     | 1.21              |
| 4:1:124:PHE:C   | 4:Y:24:ASP:CG[1_556]   | 0.99                     | 1.21              |
| 4:1:211:ASP:CG  | 4:Y:249:THR:O[1_556]   | 0.99                     | 1.21              |
| 4:2:123:MET:CA  | 4:Z:26:ALA:O[1_556]    | 0.99                     | 1.21              |
| 4:1:155:SER:O   | 4:Y:258:PRO:CA[1_556]  | 0.99                     | 1.21              |
| 4:1:210:ARG:CA  | 4:Y:193:LEU:CG[1_556]  | 0.99                     | 1.21              |
| 4:0:107:GLU:C   | 4:X:300:SER:C[1_556]   | 0.99                     | 1.21              |
| 4:0:149:THR:CG2 | 4:X:327:ILE:CD1[1_556] | 0.99                     | 1.21              |
| 4:0:173:HIS:NE2 | 4:X:281:SER:O[1_556]   | 1.00                     | 1.20              |
| 4:0:294:TYR:C   | 4:X:319:ALA:O[1_556]   | 1.00                     | 1.20              |
| 4:2:338:SER:N   | 4:Z:307:PRO:C[1_556]   | 1.00                     | 1.20              |
| 4:2:294:TYR:C   | 4:Z:319:ALA:O[1_556]   | 1.00                     | 1.20              |
| 4:2:72:GLU:CD   | 4:Z:183:ARG:NE[1_556]  | 1.00                     | 1.20              |
| 4:0:81:ASP:OD2  | 4:X:32:PRO:CG[1_556]   | 1.00                     | 1.20              |
| 4:2:286:ASP:CB  | 4:Z:290:ARG:NE[1_556]  | 1.00                     | 1.20              |
| 4:1:206:ARG:CA  | 4:Y:199:SER:CA[1_556]  | 1.00                     | 1.20              |
| 4:0:82:MET:CB   | 4:X:30:VAL:CG1[1_556]  | 1.00                     | 1.20              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:124:PHE:C   | 4:X:24:ASP:CB[1_556]   | 1.00                     | 1.20              |
| 4:1:277:THR:CG2 | 4:Y:272:ALA:O[1_556]   | 1.00                     | 1.20              |
| 4:3:266:PHE:O   | 4:Z:173:HIS:N[1_556]   | 1.00                     | 1.20              |
| 4:1:34:ILE:N    | 4:Y:210:ARG:NH2[1_556] | 1.00                     | 1.20              |
| 4:0:338:SER:CA  | 4:X:308:GLY:N[1_556]   | 1.00                     | 1.20              |
| 4:1:153:LEU:CD2 | 4:Y:262:PHE:CB[1_556]  | 1.00                     | 1.20              |
| 4:2:206:ARG:CA  | 4:Z:199:SER:CA[1_556]  | 1.00                     | 1.20              |
| 4:0:124:PHE:O   | 4:X:24:ASP:CG[1_556]   | 1.00                     | 1.20              |
| 4:0:182:GLY:C   | 4:X:189:LEU:N[1_556]   | 1.00                     | 1.20              |
| 4:0:286:ASP:CB  | 4:X:290:ARG:NE[1_556]  | 1.00                     | 1.20              |
| 4:0:191:LYS:CD  | 4:W:110:LEU:CG[1_556]  | 1.00                     | 1.20              |
| 4:1:161:HIS:NE2 | 4:Y:160:THR:CB[1_556]  | 1.00                     | 1.20              |
| 4:0:134:VAL:CG1 | 4:X:338:SER:CA[1_556]  | 1.00                     | 1.20              |
| 4:2:207:GLU:OE1 | 4:Z:242:LEU:CG[1_556]  | 1.00                     | 1.20              |
| 4:0:113:LYS:CB  | 4:X:136:ILE:C[1_556]   | 1.00                     | 1.20              |
| 4:1:11:ASP:CB   | 4:Y:305:MET:CE[1_556]  | 1.00                     | 1.20              |
| 4:1:233:SER:CA  | 4:X:367:PRO:N[1_556]   | 1.00                     | 1.20              |
| 4:1:123:MET:CA  | 4:Y:26:ALA:O[1_556]    | 1.00                     | 1.20              |
| 4:0:281:SER:OG  | 4:X:277:THR:CA[1_556]  | 1.00                     | 1.20              |
| 4:0:116:ARG:CZ  | 4:X:141:SER:C[1_556]   | 1.00                     | 1.20              |
| 4:1:337:TYR:C   | 4:Y:307:PRO:CA[1_556]  | 1.00                     | 1.20              |
| 4:1:274:ILE:CD1 | 4:Y:263:GLN:C[1_556]   | 1.00                     | 1.20              |
| 4:2:182:GLY:C   | 4:Z:189:LEU:N[1_556]   | 1.00                     | 1.20              |
| 4:2:32:PRO:CB   | 4:Z:211:ASP:CB[1_556]  | 1.00                     | 1.20              |
| 4:0:123:MET:CA  | 4:X:26:ALA:O[1_556]    | 1.00                     | 1.20              |
| 4:2:124:PHE:CA  | 4:Z:24:ASP:CA[1_556]   | 1.00                     | 1.20              |
| 4:2:107:GLU:C   | 4:Z:300:SER:C[1_556]   | 1.00                     | 1.20              |
| 4:1:37:ARG:NH1  | 4:Y:56:ASP:CA[1_556]   | 1.00                     | 1.20              |
| 4:1:113:LYS:N   | 4:Y:137:GLN:N[1_556]   | 1.00                     | 1.20              |
| 4:1:279:TYR:C   | 4:Y:276:GLU:OE1[1_556] | 1.01                     | 1.19              |
| 4:2:149:THR:CG2 | 4:Z:327:ILE:CD1[1_556] | 1.01                     | 1.19              |
| 4:1:110:LEU:CG  | 4:Y:161:HIS:CA[1_556]  | 1.01                     | 1.19              |
| 4:1:189:LEU:CB  | 4:Y:195:GLU:CB[1_556]  | 1.01                     | 1.19              |
| 4:2:116:ARG:CZ  | 4:Z:141:SER:C[1_556]   | 1.01                     | 1.19              |
| 4:2:105:LEU:C   | 4:Z:335:ARG:N[1_556]   | 1.01                     | 1.19              |
| 4:0:114:ALA:CB  | 4:X:106:THR:C[1_556]   | 1.01                     | 1.19              |
| 4:1:72:GLU:CD   | 4:Y:183:ARG:NE[1_556]  | 1.01                     | 1.19              |
| 4:0:285:CYS:SG  | 4:X:279:TYR:C[1_556]   | 1.01                     | 1.19              |
| 4:1:148:THR:O   | 4:Y:328:LYS:N[1_556]   | 1.01                     | 1.19              |
| 4:2:112:PRO:CB  | 4:Z:137:GLN:NE2[1_556] | 1.01                     | 1.19              |
| 4:2:196:ARG:NE  | 4:Y:115:ASN:OD1[1_556] | 1.01                     | 1.19              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:81:ASP:OD2  | 4:Z:32:PRO:CG[1_556]   | 1.01                     | 1.19              |
| 4:0:211:ASP:CG  | 4:X:249:THR:O[1_556]   | 1.01                     | 1.19              |
| 4:2:266:PHE:C   | 4:Y:173:HIS:N[1_556]   | 1.01                     | 1.19              |
| 4:1:295:ALA:N   | 4:Y:319:ALA:CA[1_556]  | 1.01                     | 1.19              |
| 4:2:124:PHE:O   | 4:Z:24:ASP:CG[1_556]   | 1.01                     | 1.19              |
| 4:0:77:THR:OG1  | 4:X:15:GLY:N[1_556]    | 1.01                     | 1.19              |
| 4:2:77:THR:OG1  | 4:Z:15:GLY:N[1_556]    | 1.01                     | 1.19              |
| 4:0:129:VAL:CG2 | 4:X:25:ASP:CB[1_556]   | 1.01                     | 1.19              |
| 4:2:129:VAL:CG2 | 4:Z:25:ASP:CB[1_556]   | 1.01                     | 1.19              |
| 4:0:264:PRO:CA  | 4:X:268:GLY:CA[1_556]  | 1.01                     | 1.19              |
| 4:2:110:LEU:CG  | 4:Z:161:HIS:CA[1_556]  | 1.01                     | 1.19              |
| 4:0:304:THR:CB  | 4:X:223:PHE:CE2[1_556] | 1.01                     | 1.19              |
| 4:1:294:TYR:N   | 4:Y:320:LEU:N[1_556]   | 1.01                     | 1.19              |
| 4:1:122:ILE:CG1 | 4:Y:19:ALA:C[1_556]    | 1.01                     | 1.19              |
| 4:0:207:GLU:OE1 | 4:X:242:LEU:CG[1_556]  | 1.01                     | 1.19              |
| 4:2:117:GLU:O   | 4:Z:9:VAL:CG1[1_556]   | 1.01                     | 1.19              |
| 4:1:209:VAL:N   | 4:Y:198:TYR:CB[1_556]  | 1.01                     | 1.19              |
| 4:2:74:GLY:CA   | 4:Z:156:GLY:O[1_556]   | 1.01                     | 1.19              |
| 4:1:16:LEU:CD2  | 4:Y:213:LYS:C[1_556]   | 1.01                     | 1.19              |
| 4:2:304:THR:CB  | 4:Z:223:PHE:CE2[1_556] | 1.01                     | 1.19              |
| 4:1:74:GLY:N    | 4:Y:156:GLY:O[1_556]   | 1.01                     | 1.19              |
| 4:1:112:PRO:CB  | 4:Y:137:GLN:NE2[1_556] | 1.01                     | 1.19              |
| 4:1:196:ARG:NE  | 4:X:115:ASN:OD1[1_556] | 1.01                     | 1.19              |
| 4:2:285:CYS:SG  | 4:Z:279:TYR:C[1_556]   | 1.01                     | 1.19              |
| 4:1:261:LEU:CA  | 4:Y:266:PHE:N[1_556]   | 1.01                     | 1.19              |
| 4:1:80:ASP:N    | 4:Y:31:PHE:CD1[1_556]  | 1.02                     | 1.18              |
| 4:1:81:ASP:CB   | 4:Y:32:PRO:CD[1_556]   | 1.02                     | 1.18              |
| 4:2:114:ALA:CB  | 4:Z:106:THR:C[1_556]   | 1.02                     | 1.18              |
| 4:1:210:ARG:CA  | 4:Y:193:LEU:CB[1_556]  | 1.02                     | 1.18              |
| 4:2:124:PHE:C   | 4:Z:24:ASP:CB[1_556]   | 1.02                     | 1.18              |
| 4:0:124:PHE:CA  | 4:X:24:ASP:CA[1_556]   | 1.02                     | 1.18              |
| 4:2:177:ARG:CZ  | 4:Z:159:VAL:CA[1_556]  | 1.02                     | 1.18              |
| 4:2:110:LEU:CD1 | 4:Z:161:HIS:CA[1_556]  | 1.02                     | 1.18              |
| 4:2:173:HIS:NE2 | 4:Z:281:SER:O[1_556]   | 1.02                     | 1.18              |
| 4:0:266:PHE:C   | 4:W:173:HIS:N[1_556]   | 1.02                     | 1.18              |
| 4:0:32:PRO:CD   | 4:X:211:ASP:OD1[1_556] | 1.02                     | 1.18              |
| 4:1:272:ALA:N   | 4:Y:270:GLU:CA[1_556]  | 1.02                     | 1.18              |
| 4:2:211:ASP:CG  | 4:Z:249:THR:O[1_556]   | 1.02                     | 1.18              |
| 4:1:167:GLU:O   | 4:Y:295:ALA:C[1_556]   | 1.02                     | 1.18              |
| 4:1:114:ALA:C   | 4:Y:106:THR:CB[1_556]  | 1.02                     | 1.18              |
| 4:1:134:VAL:CG1 | 4:Y:338:SER:CA[1_556]  | 1.02                     | 1.18              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:186:THR:CG2 | 4:X:190:MET:O[1_556]   | 1.02                     | 1.18              |
| 4:1:147:ARG:CB  | 4:Y:314:GLN:OE1[1_556] | 1.02                     | 1.18              |
| 4:2:338:SER:CA  | 4:Z:308:GLY:N[1_556]   | 1.02                     | 1.18              |
| 4:2:115:ASN:CB  | 4:Z:11:ASP:OD1[1_556]  | 1.02                     | 1.18              |
| 4:2:209:VAL:N   | 4:Z:198:TYR:CB[1_556]  | 1.02                     | 1.18              |
| 4:0:110:LEU:CD1 | 4:X:161:HIS:CA[1_556]  | 1.02                     | 1.18              |
| 4:1:115:ASN:CA  | 4:Y:11:ASP:OD1[1_556]  | 1.02                     | 1.18              |
| 4:0:211:ASP:OD2 | 4:X:249:THR:CA[1_556]  | 1.02                     | 1.18              |
| 4:2:231:ALA:CB  | 4:Y:370:VAL:CA[1_556]  | 1.02                     | 1.18              |
| 4:2:212:ILE:C   | 4:Z:196:ARG:CG[1_556]  | 1.02                     | 1.18              |
| 4:0:78:ASN:C    | 4:X:31:PHE:O[1_556]    | 1.02                     | 1.18              |
| 4:2:191:LYS:CD  | 4:Y:110:LEU:CG[1_556]  | 1.02                     | 1.18              |
| 4:2:261:LEU:CA  | 4:Z:266:PHE:CA[1_556]  | 1.02                     | 1.18              |
| 4:2:176:MET:CG  | 4:Z:277:THR:OG1[1_556] | 1.02                     | 1.18              |
| 4:2:113:LYS:CB  | 4:Z:136:ILE:C[1_556]   | 1.02                     | 1.18              |
| 4:2:122:ILE:CG1 | 4:Z:19:ALA:C[1_556]    | 1.02                     | 1.18              |
| 4:1:307:PRO:C   | 4:Y:227:MET:CG[1_556]  | 1.02                     | 1.18              |
| 4:2:78:ASN:C    | 4:Z:31:PHE:O[1_556]    | 1.02                     | 1.18              |
| 4:0:112:PRO:CB  | 4:X:137:GLN:NE2[1_556] | 1.02                     | 1.18              |
| 4:2:126:THR:CA  | 4:Z:28:ARG:NE[1_556]   | 1.02                     | 1.18              |
| 4:1:118:LYS:C   | 4:Y:340:TRP:CD1[1_556] | 1.02                     | 1.18              |
| 4:0:209:VAL:N   | 4:X:198:TYR:CB[1_556]  | 1.03                     | 1.17              |
| 4:2:211:ASP:OD2 | 4:Z:249:THR:CA[1_556]  | 1.03                     | 1.17              |
| 4:0:231:ALA:CB  | 4:W:370:VAL:CA[1_556]  | 1.03                     | 1.17              |
| 4:1:229:THR:O   | 4:X:368:SER:CA[1_556]  | 1.03                     | 1.17              |
| 4:2:186:THR:CG2 | 4:Z:190:MET:O[1_556]   | 1.03                     | 1.17              |
| 4:2:119:MET:C   | 4:Z:340:TRP:CD2[1_556] | 1.03                     | 1.17              |
| 4:1:286:ASP:CB  | 4:Y:290:ARG:NE[1_556]  | 1.03                     | 1.17              |
| 4:1:125:GLU:CG  | 4:Y:21:PHE:CA[1_556]   | 1.03                     | 1.17              |
| 4:2:77:THR:O    | 4:Z:33:SER:OG[1_556]   | 1.03                     | 1.17              |
| 4:0:212:ILE:C   | 4:X:196:ARG:CG[1_556]  | 1.03                     | 1.17              |
| 4:2:32:PRO:CD   | 4:Z:211:ASP:OD1[1_556] | 1.03                     | 1.17              |
| 4:0:117:GLU:O   | 4:X:9:VAL:CG1[1_556]   | 1.03                     | 1.17              |
| 4:0:196:ARG:NE  | 4:W:115:ASN:OD1[1_556] | 1.03                     | 1.17              |
| 4:0:176:MET:CG  | 4:X:277:THR:OG1[1_556] | 1.03                     | 1.17              |
| 4:3:191:LYS:CD  | 4:Z:110:LEU:CG[1_556]  | 1.03                     | 1.17              |
| 4:2:298:VAL:CB  | 4:Z:312:ARG:C[1_556]   | 1.03                     | 1.17              |
| 4:0:77:THR:O    | 4:X:33:SER:OG[1_556]   | 1.03                     | 1.17              |
| 4:0:11:ASP:OD1  | 4:X:305:MET:CB[1_556]  | 1.03                     | 1.17              |
| 4:0:298:VAL:CB  | 4:X:312:ARG:C[1_556]   | 1.03                     | 1.17              |
| 4:1:166:TYR:C   | 4:Y:294:TYR:CA[1_556]  | 1.03                     | 1.17              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:261:LEU:CA  | 4:X:266:PHE:CA[1_556]  | 1.03                     | 1.17              |
| 4:0:33:SER:O    | 4:X:210:ARG:CZ[1_556]  | 1.03                     | 1.17              |
| 4:0:126:THR:CA  | 4:X:28:ARG:NE[1_556]   | 1.03                     | 1.17              |
| 4:3:196:ARG:NE  | 4:Z:115:ASN:OD1[1_556] | 1.04                     | 1.16              |
| 4:0:10:CYS:SG   | 4:X:336:LYS:CE[1_556]  | 1.04                     | 1.16              |
| 4:2:79:TRP:CD2  | 4:Z:18:LYS:N[1_556]    | 1.04                     | 1.16              |
| 4:2:153:LEU:CD2 | 4:Z:262:PHE:CB[1_556]  | 1.04                     | 1.16              |
| 4:1:116:ARG:CZ  | 4:Y:141:SER:C[1_556]   | 1.04                     | 1.16              |
| 4:1:119:MET:C   | 4:Y:340:TRP:CD2[1_556] | 1.04                     | 1.16              |
| 4:2:266:PHE:O   | 4:Y:173:HIS:N[1_556]   | 1.04                     | 1.16              |
| 4:1:298:VAL:CB  | 4:Y:312:ARG:O[1_556]   | 1.04                     | 1.16              |
| 4:0:365:ALA:N   | 4:X:349:LEU:N[1_556]   | 1.04                     | 1.16              |
| 4:0:294:TYR:CA  | 4:X:319:ALA:O[1_556]   | 1.04                     | 1.16              |
| 4:0:153:LEU:CD2 | 4:X:262:PHE:CB[1_556]  | 1.04                     | 1.16              |
| 4:0:185:LEU:CD1 | 4:X:188:TYR:CE1[1_556] | 1.04                     | 1.16              |
| 4:0:177:ARG:CZ  | 4:X:159:VAL:CA[1_556]  | 1.04                     | 1.16              |
| 4:1:86:TRP:CE2  | 4:Y:337:TYR:CZ[1_556]  | 1.04                     | 1.16              |
| 4:1:33:SER:C    | 4:Y:210:ARG:CZ[1_556]  | 1.04                     | 1.16              |
| 4:1:80:ASP:CA   | 4:Y:31:PHE:CG[1_556]   | 1.04                     | 1.16              |
| 4:0:115:ASN:CB  | 4:X:11:ASP:OD1[1_556]  | 1.04                     | 1.16              |
| 4:2:10:CYS:SG   | 4:Z:336:LYS:CE[1_556]  | 1.04                     | 1.16              |
| 4:0:79:TRP:CD2  | 4:X:18:LYS:N[1_556]    | 1.04                     | 1.16              |
| 4:0:331:ALA:CA  | 4:X:221:LEU:C[1_556]   | 1.04                     | 1.16              |
| 4:1:362:TYR:O   | 4:Y:348:SER:CB[1_556]  | 1.04                     | 1.16              |
| 4:1:140:LEU:CA  | 4:Y:331:ALA:CB[1_556]  | 1.04                     | 1.16              |
| 4:0:233:SER:C   | 4:W:367:PRO:N[1_556]   | 1.04                     | 1.16              |
| 4:1:213:LYS:C   | 4:Y:253:GLU:OE1[1_556] | 1.04                     | 1.16              |
| 4:0:191:LYS:CG  | 4:W:110:LEU:CD1[1_556] | 1.04                     | 1.16              |
| 4:0:115:ASN:CA  | 4:X:11:ASP:OD1[1_556]  | 1.04                     | 1.16              |
| 4:2:137:GLN:CB  | 4:Z:304:THR:OG1[1_556] | 1.04                     | 1.16              |
| 4:0:194:THR:O   | 4:W:75:ILE:CG1[1_556]  | 1.04                     | 1.16              |
| 4:2:119:MET:CE  | 4:Z:337:TYR:CA[1_556]  | 1.04                     | 1.16              |
| 4:1:230:ALA:CB  | 4:X:371:HIS:CB[1_556]  | 1.04                     | 1.16              |
| 4:2:76:ILE:CB   | 4:Z:18:LYS:NZ[1_556]   | 1.04                     | 1.16              |
| 4:0:167:GLU:O   | 4:X:295:ALA:C[1_556]   | 1.04                     | 1.16              |
| 4:2:33:SER:O    | 4:Z:210:ARG:CZ[1_556]  | 1.04                     | 1.16              |
| 4:1:272:ALA:CB  | 4:Y:270:GLU:C[1_556]   | 1.04                     | 1.16              |
| 4:2:233:SER:C   | 4:Y:367:PRO:N[1_556]   | 1.04                     | 1.16              |
| 4:0:119:MET:CE  | 4:X:337:TYR:CA[1_556]  | 1.04                     | 1.16              |
| 4:0:173:HIS:CD2 | 4:X:281:SER:O[1_556]   | 1.04                     | 1.16              |
| 4:1:107:GLU:C   | 4:Y:300:SER:C[1_556]   | 1.04                     | 1.16              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:194:THR:O   | 4:Y:75:ILE:CG1[1_556]  | 1.05                     | 1.15              |
| 4:1:73:HIS:N    | 4:Y:157:ASP:O[1_556]   | 1.05                     | 1.15              |
| 4:3:230:ALA:CB  | 4:Z:371:HIS:CB[1_556]  | 1.05                     | 1.15              |
| 4:3:229:THR:O   | 4:Z:368:SER:CA[1_556]  | 1.05                     | 1.15              |
| 4:1:140:LEU:CD2 | 4:Y:331:ALA:O[1_556]   | 1.05                     | 1.15              |
| 4:2:331:ALA:CA  | 4:Z:221:LEU:C[1_556]   | 1.05                     | 1.15              |
| 4:2:11:ASP:OD1  | 4:Z:305:MET:CB[1_556]  | 1.05                     | 1.15              |
| 4:0:122:ILE:CG1 | 4:X:19:ALA:C[1_556]    | 1.05                     | 1.15              |
| 4:0:266:PHE:O   | 4:W:173:HIS:N[1_556]   | 1.05                     | 1.15              |
| 4:0:62:ARG:CZ   | 4:X:205:GLU:CA[1_556]  | 1.05                     | 1.15              |
| 4:0:119:MET:C   | 4:X:340:TRP:CD2[1_556] | 1.05                     | 1.15              |
| 4:1:150:GLY:C   | 4:Y:317:ILE:CB[1_556]  | 1.05                     | 1.15              |
| 4:1:366:GLY:N   | 4:Y:347:ALA:C[1_556]   | 1.05                     | 1.15              |
| 4:0:105:LEU:N   | 4:X:334:GLU:CA[1_556]  | 1.05                     | 1.15              |
| 4:2:229:THR:O   | 4:Y:368:SER:CA[1_556]  | 1.05                     | 1.15              |
| 4:1:154:ASP:O   | 4:Y:261:LEU:CB[1_556]  | 1.05                     | 1.15              |
| 4:0:331:ALA:CB  | 4:X:222:ASP:N[1_556]   | 1.05                     | 1.15              |
| 4:2:185:LEU:CD1 | 4:Z:188:TYR:CE1[1_556] | 1.05                     | 1.15              |
| 4:2:294:TYR:CA  | 4:Z:319:ALA:O[1_556]   | 1.05                     | 1.15              |
| 4:0:305:MET:CB  | 4:X:255:PHE:CG[1_556]  | 1.05                     | 1.15              |
| 4:1:305:MET:CA  | 4:Y:255:PHE:CG[1_556]  | 1.05                     | 1.15              |
| 4:0:372:ARG:NE  | 4:X:142:LEU:O[1_556]   | 1.05                     | 1.15              |
| 4:2:177:ARG:CG  | 4:Z:178:LEU:O[1_556]   | 1.05                     | 1.15              |
| 4:1:37:ARG:NH1  | 4:Y:56:ASP:CB[1_556]   | 1.05                     | 1.15              |
| 4:2:272:ALA:CB  | 4:Z:270:GLU:C[1_556]   | 1.05                     | 1.15              |
| 4:2:118:LYS:CD  | 4:Z:10:CYS:CA[1_556]   | 1.05                     | 1.15              |
| 4:0:154:ASP:O   | 4:X:261:LEU:CB[1_556]  | 1.05                     | 1.15              |
| 4:2:277:THR:CG2 | 4:Z:272:ALA:O[1_556]   | 1.05                     | 1.15              |
| 4:1:113:LYS:CB  | 4:Y:136:ILE:C[1_556]   | 1.05                     | 1.15              |
| 4:3:192:ILE:CA  | 4:Z:110:LEU:O[1_556]   | 1.05                     | 1.15              |
| 4:1:177:ARG:CZ  | 4:Y:159:VAL:CA[1_556]  | 1.05                     | 1.15              |
| 4:1:191:LYS:CD  | 4:X:110:LEU:CG[1_556]  | 1.05                     | 1.15              |
| 4:2:73:HIS:CA   | 4:Z:157:ASP:O[1_556]   | 1.05                     | 1.15              |
| 4:1:137:GLN:CB  | 4:Y:304:THR:OG1[1_556] | 1.05                     | 1.15              |
| 4:0:118:LYS:CD  | 4:X:10:CYS:CA[1_556]   | 1.05                     | 1.15              |
| 4:1:104:LEU:CA  | 4:Y:334:GLU:CG[1_556]  | 1.05                     | 1.15              |
| 4:2:331:ALA:CB  | 4:Z:222:ASP:N[1_556]   | 1.05                     | 1.15              |
| 4:1:120:THR:OG1 | 4:Y:340:TRP:O[1_556]   | 1.05                     | 1.15              |
| 4:0:267:ILE:CA  | 4:W:173:HIS:CB[1_556]  | 1.05                     | 1.15              |
| 4:0:135:ALA:CB  | 4:X:332:PRO:CD[1_556]  | 1.05                     | 1.15              |
| 4:2:267:ILE:CA  | 4:Y:173:HIS:CB[1_556]  | 1.05                     | 1.15              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:153:LEU:CG  | 4:Y:262:PHE:CA[1_556]  | 1.05                     | 1.15              |
| 4:0:177:ARG:CG  | 4:X:178:LEU:O[1_556]   | 1.05                     | 1.15              |
| 4:2:165:ILE:CG1 | 4:Z:297:ASN:ND2[1_556] | 1.05                     | 1.15              |
| 4:1:365:ALA:N   | 4:Y:349:LEU:N[1_556]   | 1.05                     | 1.15              |
| 4:0:33:SER:C    | 4:X:210:ARG:CZ[1_556]  | 1.05                     | 1.15              |
| 4:2:167:GLU:O   | 4:Z:295:ALA:C[1_556]   | 1.05                     | 1.15              |
| 4:2:106:THR:CA  | 4:Z:335:ARG:CA[1_556]  | 1.05                     | 1.15              |
| 4:0:76:ILE:CB   | 4:X:18:LYS:NZ[1_556]   | 1.05                     | 1.15              |
| 4:2:173:HIS:CD2 | 4:Z:281:SER:O[1_556]   | 1.06                     | 1.14              |
| 4:0:123:MET:CA  | 4:X:26:ALA:C[1_556]    | 1.06                     | 1.14              |
| 4:3:64:ILE:CG1  | 4:Y:291:LYS:NZ[1_556]  | 1.06                     | 1.14              |
| 4:2:125:GLU:CG  | 4:Z:21:PHE:CB[1_556]   | 1.06                     | 1.14              |
| 4:2:115:ASN:CA  | 4:Z:11:ASP:OD1[1_556]  | 1.06                     | 1.14              |
| 4:1:183:ARG:C   | 4:Y:188:TYR:N[1_556]   | 1.06                     | 1.14              |
| 4:1:166:TYR:CD1 | 4:Y:294:TYR:CG[1_556]  | 1.06                     | 1.14              |
| 4:0:192:ILE:CA  | 4:W:110:LEU:O[1_556]   | 1.06                     | 1.14              |
| 4:1:309:ILE:CD1 | 4:Y:259:GLU:CD[1_556]  | 1.06                     | 1.14              |
| 4:1:212:ILE:CG2 | 4:Y:196:ARG:CA[1_556]  | 1.06                     | 1.14              |
| 4:1:289:ILE:CG1 | 4:Y:294:TYR:OH[1_556]  | 1.06                     | 1.14              |
| 4:2:62:ARG:CZ   | 4:Z:205:GLU:CA[1_556]  | 1.06                     | 1.14              |
| 4:2:191:LYS:CG  | 4:Y:110:LEU:CD1[1_556] | 1.06                     | 1.14              |
| 4:0:73:HIS:CA   | 4:X:157:ASP:O[1_556]   | 1.06                     | 1.14              |
| 4:2:365:ALA:N   | 4:Z:349:LEU:N[1_556]   | 1.06                     | 1.14              |
| 4:1:67:LEU:N    | 4:Y:62:ARG:NH1[1_556]  | 1.06                     | 1.14              |
| 4:2:335:ARG:O   | 4:Z:307:PRO:O[1_556]   | 1.06                     | 1.14              |
| 4:1:105:LEU:C   | 4:Y:335:ARG:N[1_556]   | 1.06                     | 1.14              |
| 4:1:76:ILE:CB   | 4:Y:18:LYS:NZ[1_556]   | 1.06                     | 1.14              |
| 4:1:80:ASP:C    | 4:Y:31:PHE:CB[1_556]   | 1.06                     | 1.14              |
| 4:1:64:ILE:CG1  | 4:W:291:LYS:NZ[1_556]  | 1.06                     | 1.14              |
| 4:0:67:LEU:CD1  | 4:X:207:GLU:CB[1_556]  | 1.06                     | 1.14              |
| 4:2:296:ASN:ND2 | 4:Z:318:THR:CB[1_556]  | 1.06                     | 1.14              |
| 4:0:185:LEU:CG  | 4:X:188:TYR:CZ[1_556]  | 1.06                     | 1.14              |
| 4:1:293:LEU:N   | 4:Y:321:ALA:N[1_556]   | 1.06                     | 1.14              |
| 4:0:165:ILE:CG1 | 4:X:297:ASN:ND2[1_556] | 1.06                     | 1.14              |
| 4:1:157:ASP:OD2 | 4:Y:186:THR:OG1[1_556] | 1.06                     | 1.14              |
| 4:2:185:LEU:CD1 | 4:Z:188:TYR:CD1[1_556] | 1.06                     | 1.14              |
| 4:1:212:ILE:C   | 4:Y:196:ARG:CG[1_556]  | 1.06                     | 1.14              |
| 4:1:372:ARG:NE  | 4:Y:142:LEU:O[1_556]   | 1.06                     | 1.14              |
| 4:2:135:ALA:CB  | 4:Z:332:PRO:CD[1_556]  | 1.06                     | 1.14              |
| 4:0:306:TYR:CD1 | 4:X:256:ARG:CD[1_556]  | 1.06                     | 1.14              |
| 4:0:307:PRO:CA  | 4:X:227:MET:CA[1_556]  | 1.06                     | 1.14              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:137:GLN:CB  | 4:X:304:THR:OG1[1_556] | 1.06                     | 1.14              |
| 4:2:105:LEU:N   | 4:Z:334:GLU:CA[1_556]  | 1.06                     | 1.14              |
| 4:2:185:LEU:CG  | 4:Z:188:TYR:CZ[1_556]  | 1.06                     | 1.14              |
| 4:2:140:LEU:CA  | 4:Z:331:ALA:CB[1_556]  | 1.06                     | 1.14              |
| 4:1:125:GLU:CG  | 4:Y:21:PHE:CB[1_556]   | 1.06                     | 1.14              |
| 4:0:272:ALA:CB  | 4:X:270:GLU:C[1_556]   | 1.07                     | 1.13              |
| 4:2:124:PHE:CA  | 4:Z:24:ASP:CB[1_556]   | 1.07                     | 1.13              |
| 4:0:178:LEU:CD2 | 4:X:264:PRO:CB[1_556]  | 1.07                     | 1.13              |
| 4:2:33:SER:CB   | 4:Z:210:ARG:NH1[1_556] | 1.07                     | 1.13              |
| 4:0:277:THR:CG2 | 4:X:272:ALA:O[1_556]   | 1.07                     | 1.13              |
| 4:0:125:GLU:CG  | 4:X:21:PHE:CB[1_556]   | 1.07                     | 1.13              |
| 4:0:33:SER:CB   | 4:X:210:ARG:NH1[1_556] | 1.07                     | 1.13              |
| 4:1:124:PHE:C   | 4:Y:24:ASP:CB[1_556]   | 1.07                     | 1.13              |
| 4:0:229:THR:O   | 4:W:368:SER:CA[1_556]  | 1.07                     | 1.13              |
| 4:0:116:ARG:NH1 | 4:X:141:SER:O[1_556]   | 1.07                     | 1.13              |
| 4:1:177:ARG:NH1 | 4:Y:159:VAL:C[1_556]   | 1.07                     | 1.13              |
| 4:0:106:THR:CA  | 4:X:335:ARG:CA[1_556]  | 1.07                     | 1.13              |
| 4:1:72:GLU:CB   | 4:Y:157:ASP:OD2[1_556] | 1.07                     | 1.13              |
| 4:1:78:ASN:C    | 4:Y:31:PHE:O[1_556]    | 1.07                     | 1.13              |
| 4:2:164:PRO:CA  | 4:Z:278:THR:CG2[1_556] | 1.07                     | 1.13              |
| 4:0:278:THR:C   | 4:X:276:GLU:CD[1_556]  | 1.07                     | 1.13              |
| 4:2:154:ASP:O   | 4:Z:261:LEU:CB[1_556]  | 1.07                     | 1.13              |
| 4:0:183:ARG:C   | 4:X:188:TYR:N[1_556]   | 1.07                     | 1.13              |
| 4:0:299:MET:CG  | 4:X:312:ARG:NE[1_556]  | 1.07                     | 1.13              |
| 4:2:305:MET:CB  | 4:Z:255:PHE:CG[1_556]  | 1.07                     | 1.13              |
| 4:1:305:MET:CB  | 4:Y:255:PHE:CG[1_556]  | 1.07                     | 1.13              |
| 4:1:192:ILE:CA  | 4:X:110:LEU:O[1_556]   | 1.07                     | 1.13              |
| 4:1:124:PHE:CA  | 4:Y:24:ASP:CB[1_556]   | 1.07                     | 1.13              |
| 4:2:372:ARG:NE  | 4:Z:142:LEU:O[1_556]   | 1.07                     | 1.13              |
| 4:0:37:ARG:NH1  | 4:X:56:ASP:CA[1_556]   | 1.07                     | 1.13              |
| 4:0:124:PHE:CA  | 4:X:24:ASP:CB[1_556]   | 1.07                     | 1.13              |
| 4:2:67:LEU:CD1  | 4:Z:207:GLU:CB[1_556]  | 1.07                     | 1.13              |
| 4:2:33:SER:C    | 4:Z:210:ARG:CZ[1_556]  | 1.07                     | 1.13              |
| 4:1:63:GLY:N    | 4:W:288:ASP:CA[1_556]  | 1.07                     | 1.13              |
| 4:2:183:ARG:C   | 4:Z:188:TYR:N[1_556]   | 1.07                     | 1.13              |
| 4:2:123:MET:CA  | 4:Z:26:ALA:C[1_556]    | 1.07                     | 1.13              |
| 4:1:123:MET:CA  | 4:Y:26:ALA:C[1_556]    | 1.07                     | 1.13              |
| 4:1:304:THR:CB  | 4:Y:223:PHE:CE2[1_556] | 1.07                     | 1.13              |
| 4:1:277:THR:OG1 | 4:Y:271:SER:O[1_556]   | 1.07                     | 1.13              |
| 4:2:37:ARG:NH1  | 4:Z:56:ASP:CA[1_556]   | 1.07                     | 1.13              |
| 4:2:122:ILE:CG1 | 4:Z:19:ALA:O[1_556]    | 1.07                     | 1.13              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:125:GLU:CG  | 4:X:21:PHE:CA[1_556]   | 1.07                     | 1.13              |
| 4:1:106:THR:CG2 | 4:Y:335:ARG:CG[1_556]  | 1.07                     | 1.13              |
| 4:0:124:PHE:CG  | 4:X:24:ASP:O[1_556]    | 1.07                     | 1.13              |
| 4:2:142:LEU:CD2 | 4:Z:329:ILE:CD1[1_556] | 1.07                     | 1.13              |
| 4:1:129:VAL:CG2 | 4:Y:25:ASP:CB[1_556]   | 1.08                     | 1.12              |
| 4:0:366:GLY:N   | 4:X:347:ALA:C[1_556]   | 1.08                     | 1.12              |
| 4:1:32:PRO:CB   | 4:Y:211:ASP:CB[1_556]  | 1.08                     | 1.12              |
| 4:0:105:LEU:O   | 4:X:335:ARG:N[1_556]   | 1.08                     | 1.12              |
| 4:2:178:LEU:CD2 | 4:Z:264:PRO:CB[1_556]  | 1.08                     | 1.12              |
| 4:2:299:MET:CG  | 4:Z:312:ARG:NE[1_556]  | 1.08                     | 1.12              |
| 4:2:116:ARG:NH1 | 4:Z:141:SER:O[1_556]   | 1.08                     | 1.12              |
| 4:0:185:LEU:CD1 | 4:X:188:TYR:CD1[1_556] | 1.08                     | 1.12              |
| 4:2:306:TYR:CD1 | 4:Z:256:ARG:CD[1_556]  | 1.08                     | 1.12              |
| 4:0:305:MET:C   | 4:X:255:PHE:CE1[1_556] | 1.08                     | 1.12              |
| 4:0:335:ARG:O   | 4:X:307:PRO:O[1_556]   | 1.08                     | 1.12              |
| 4:2:278:THR:C   | 4:Z:276:GLU:CD[1_556]  | 1.08                     | 1.12              |
| 4:1:299:MET:CA  | 4:Y:312:ARG:CG[1_556]  | 1.08                     | 1.12              |
| 4:2:192:ILE:CA  | 4:Y:110:LEU:O[1_556]   | 1.08                     | 1.12              |
| 4:2:307:PRO:CA  | 4:Z:227:MET:CA[1_556]  | 1.08                     | 1.12              |
| 4:2:307:PRO:C   | 4:Z:227:MET:CG[1_556]  | 1.08                     | 1.12              |
| 4:0:261:LEU:CB  | 4:X:266:PHE:CD1[1_556] | 1.08                     | 1.12              |
| 4:1:11:ASP:OD1  | 4:Y:305:MET:CB[1_556]  | 1.08                     | 1.12              |
| 4:2:366:GLY:N   | 4:Z:347:ALA:C[1_556]   | 1.08                     | 1.12              |
| 4:0:293:LEU:N   | 4:X:321:ALA:N[1_556]   | 1.08                     | 1.12              |
| 4:1:185:LEU:CD1 | 4:Y:188:TYR:CD1[1_556] | 1.08                     | 1.12              |
| 4:2:166:TYR:CD1 | 4:Z:294:TYR:CG[1_556]  | 1.08                     | 1.12              |
| 4:0:296:ASN:ND2 | 4:X:318:THR:CB[1_556]  | 1.08                     | 1.12              |
| 4:0:140:LEU:CA  | 4:X:331:ALA:CB[1_556]  | 1.08                     | 1.12              |
| 4:1:186:THR:OG1 | 4:Y:189:LEU:C[1_556]   | 1.08                     | 1.12              |
| 4:1:299:MET:CB  | 4:Y:312:ARG:NE[1_556]  | 1.08                     | 1.12              |
| 4:1:165:ILE:CA  | 4:Y:297:ASN:OD1[1_556] | 1.08                     | 1.12              |
| 4:2:367:PRO:CD  | 4:Z:347:ALA:CB[1_556]  | 1.08                     | 1.12              |
| 4:1:169:TYR:CD1 | 4:Y:150:GLY:O[1_556]   | 1.08                     | 1.12              |
| 4:0:80:ASP:CA   | 4:X:31:PHE:CG[1_556]   | 1.08                     | 1.12              |
| 4:1:296:ASN:OD1 | 4:Y:318:THR:OG1[1_556] | 1.08                     | 1.12              |
| 4:1:164:PRO:CA  | 4:Y:278:THR:CG2[1_556] | 1.08                     | 1.12              |
| 4:0:142:LEU:CD2 | 4:X:329:ILE:CD1[1_556] | 1.08                     | 1.12              |
| 4:1:174:ALA:CB  | 4:Y:281:SER:N[1_556]   | 1.08                     | 1.12              |
| 4:0:67:LEU:N    | 4:X:62:ARG:NH1[1_556]  | 1.08                     | 1.12              |
| 4:3:234:SER:N   | 4:Z:367:PRO:CD[1_556]  | 1.09                     | 1.11              |
| 4:0:175:ILE:C   | 4:X:277:THR:CG2[1_556] | 1.09                     | 1.11              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:166:TYR:CD1 | 4:X:294:TYR:CG[1_556]  | 1.09                     | 1.11              |
| 4:0:114:ALA:C   | 4:X:106:THR:CB[1_556]  | 1.09                     | 1.11              |
| 4:0:147:ARG:CB  | 4:X:314:GLN:OE1[1_556] | 1.09                     | 1.11              |
| 4:3:63:GLY:N    | 4:Y:288:ASP:CA[1_556]  | 1.09                     | 1.11              |
| 4:1:267:ILE:CA  | 4:X:173:HIS:CB[1_556]  | 1.09                     | 1.11              |
| 4:3:267:ILE:CA  | 4:Z:173:HIS:CB[1_556]  | 1.09                     | 1.11              |
| 4:0:129:VAL:C   | 4:X:25:ASP:OD2[1_556]  | 1.09                     | 1.11              |
| 4:2:125:GLU:CG  | 4:Z:21:PHE:CA[1_556]   | 1.09                     | 1.11              |
| 4:1:149:THR:CG2 | 4:Y:327:ILE:CD1[1_556] | 1.09                     | 1.11              |
| 4:0:253:GLU:OE1 | 4:W:112:PRO:O[1_556]   | 1.09                     | 1.11              |
| 4:1:86:TRP:NE1  | 4:Y:337:TYR:CZ[1_556]  | 1.09                     | 1.11              |
| 4:2:105:LEU:O   | 4:Z:335:ARG:N[1_556]   | 1.09                     | 1.11              |
| 4:1:82:MET:CB   | 4:Y:30:VAL:CG1[1_556]  | 1.09                     | 1.11              |
| 4:2:271:SER:C   | 4:Z:270:GLU:N[1_556]   | 1.09                     | 1.11              |
| 4:0:122:ILE:CG1 | 4:X:19:ALA:O[1_556]    | 1.09                     | 1.11              |
| 4:2:210:ARG:CA  | 4:Z:193:LEU:CB[1_556]  | 1.09                     | 1.11              |
| 4:0:16:LEU:CD2  | 4:X:213:LYS:C[1_556]   | 1.09                     | 1.11              |
| 4:0:81:ASP:CB   | 4:X:32:PRO:CD[1_556]   | 1.09                     | 1.11              |
| 4:2:293:LEU:N   | 4:Z:321:ALA:N[1_556]   | 1.09                     | 1.11              |
| 4:2:66:THR:OG1  | 4:Z:60:SER:C[1_556]    | 1.09                     | 1.11              |
| 4:2:284:LYS:O   | 4:Z:280:ASN:O[1_556]   | 1.09                     | 1.11              |
| 4:2:114:ALA:C   | 4:Z:106:THR:CB[1_556]  | 1.09                     | 1.11              |
| 4:1:234:SER:N   | 4:X:367:PRO:CD[1_556]  | 1.09                     | 1.11              |
| 4:0:164:PRO:CA  | 4:X:278:THR:CG2[1_556] | 1.09                     | 1.11              |
| 4:0:298:VAL:CB  | 4:X:312:ARG:O[1_556]   | 1.09                     | 1.11              |
| 4:1:296:ASN:ND2 | 4:Y:318:THR:CB[1_556]  | 1.09                     | 1.11              |
| 4:1:124:PHE:CA  | 4:Y:24:ASP:CA[1_556]   | 1.09                     | 1.11              |
| 4:2:16:LEU:CD2  | 4:Z:213:LYS:C[1_556]   | 1.09                     | 1.11              |
| 4:2:212:ILE:CG2 | 4:Z:196:ARG:CA[1_556]  | 1.09                     | 1.11              |
| 4:0:271:SER:C   | 4:X:270:GLU:N[1_556]   | 1.09                     | 1.11              |
| 4:0:74:GLY:C    | 4:X:156:GLY:CA[1_556]  | 1.09                     | 1.11              |
| 4:2:147:ARG:CB  | 4:Z:314:GLN:OE1[1_556] | 1.09                     | 1.11              |
| 4:1:293:LEU:CD2 | 4:Y:279:TYR:CD1[1_556] | 1.09                     | 1.11              |
| 4:1:104:LEU:C   | 4:Y:334:GLU:CA[1_556]  | 1.09                     | 1.11              |
| 4:0:210:ARG:CA  | 4:X:193:LEU:CB[1_556]  | 1.09                     | 1.11              |
| 4:2:124:PHE:CG  | 4:Z:24:ASP:O[1_556]    | 1.09                     | 1.11              |
| 4:2:261:LEU:CB  | 4:Z:266:PHE:CD1[1_556] | 1.09                     | 1.11              |
| 4:0:166:TYR:C   | 4:X:294:TYR:CA[1_556]  | 1.09                     | 1.11              |
| 4:0:337:TYR:C   | 4:X:307:PRO:CA[1_556]  | 1.09                     | 1.11              |
| 4:0:367:PRO:CD  | 4:X:347:ALA:CB[1_556]  | 1.09                     | 1.11              |
| 4:1:168:GLY:O   | 4:Y:296:ASN:C[1_556]   | 1.10                     | 1.10              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:261:LEU:CB  | 4:Z:266:PHE:CG[1_556]  | 1.10                     | 1.10              |
| 4:0:150:GLY:C   | 4:X:317:ILE:CB[1_556]  | 1.10                     | 1.10              |
| 4:2:67:LEU:N    | 4:Z:62:ARG:NH1[1_556]  | 1.10                     | 1.10              |
| 4:2:261:LEU:CA  | 4:Z:266:PHE:N[1_556]   | 1.10                     | 1.10              |
| 4:1:139:VAL:N   | 4:Y:299:MET:SD[1_556]  | 1.10                     | 1.10              |
| 4:1:178:LEU:CD2 | 4:Y:264:PRO:CB[1_556]  | 1.10                     | 1.10              |
| 4:0:307:PRO:C   | 4:X:227:MET:CG[1_556]  | 1.10                     | 1.10              |
| 4:1:209:VAL:C   | 4:Y:193:LEU:C[1_556]   | 1.10                     | 1.10              |
| 4:0:161:HIS:NE2 | 4:X:160:THR:CB[1_556]  | 1.10                     | 1.10              |
| 4:1:124:PHE:CG  | 4:Y:24:ASP:O[1_556]    | 1.10                     | 1.10              |
| 4:1:105:LEU:N   | 4:Y:334:GLU:CA[1_556]  | 1.10                     | 1.10              |
| 4:2:106:THR:C   | 4:Z:335:ARG:C[1_556]   | 1.10                     | 1.10              |
| 4:1:274:ILE:CD1 | 4:Y:264:PRO:N[1_556]   | 1.10                     | 1.10              |
| 4:2:129:VAL:C   | 4:Z:25:ASP:OD2[1_556]  | 1.10                     | 1.10              |
| 4:2:305:MET:C   | 4:Z:255:PHE:CE1[1_556] | 1.10                     | 1.10              |
| 4:2:161:HIS:NE2 | 4:Z:160:THR:CB[1_556]  | 1.10                     | 1.10              |
| 4:0:125:GLU:CA  | 4:X:24:ASP:OD2[1_556]  | 1.10                     | 1.10              |
| 4:0:73:HIS:N    | 4:X:157:ASP:O[1_556]   | 1.10                     | 1.10              |
| 4:2:337:TYR:C   | 4:Z:307:PRO:CA[1_556]  | 1.10                     | 1.10              |
| 4:1:207:GLU:OE1 | 4:Y:242:LEU:CG[1_556]  | 1.10                     | 1.10              |
| 4:1:136:ILE:O   | 4:Y:299:MET:CB[1_556]  | 1.10                     | 1.10              |
| 4:0:261:LEU:CA  | 4:X:266:PHE:N[1_556]   | 1.10                     | 1.10              |
| 4:3:253:GLU:OE1 | 4:Z:112:PRO:O[1_556]   | 1.10                     | 1.10              |
| 4:0:284:LYS:O   | 4:X:280:ASN:O[1_556]   | 1.10                     | 1.10              |
| 4:2:253:GLU:OE1 | 4:Y:112:PRO:O[1_556]   | 1.10                     | 1.10              |
| 4:1:67:LEU:CD1  | 4:Y:207:GLU:CB[1_556]  | 1.10                     | 1.10              |
| 4:2:80:ASP:CA   | 4:Z:31:PHE:CG[1_556]   | 1.10                     | 1.10              |
| 4:2:150:GLY:C   | 4:Z:317:ILE:CB[1_556]  | 1.10                     | 1.10              |
| 4:2:119:MET:N   | 4:Z:340:TRP:CD1[1_556] | 1.10                     | 1.10              |
| 4:2:74:GLY:C    | 4:Z:156:GLY:CA[1_556]  | 1.10                     | 1.10              |
| 4:2:81:ASP:CB   | 4:Z:32:PRO:CD[1_556]   | 1.10                     | 1.10              |
| 4:0:121:GLN:NE2 | 4:X:20:GLY:O[1_556]    | 1.10                     | 1.10              |
| 4:0:261:LEU:CB  | 4:X:266:PHE:CG[1_556]  | 1.10                     | 1.10              |
| 4:0:215:LYS:C   | 4:X:252:ASN:OD1[1_556] | 1.10                     | 1.10              |
| 4:0:106:THR:CB  | 4:X:335:ARG:CG[1_556]  | 1.10                     | 1.10              |
| 4:1:77:THR:OG1  | 4:Y:15:GLY:N[1_556]    | 1.11                     | 1.09              |
| 4:2:121:GLN:NE2 | 4:Z:20:GLY:O[1_556]    | 1.11                     | 1.09              |
| 4:1:227:MET:CB  | 4:X:372:ARG:O[1_556]   | 1.11                     | 1.09              |
| 4:2:175:ILE:C   | 4:Z:277:THR:CG2[1_556] | 1.11                     | 1.09              |
| 4:0:234:SER:N   | 4:W:367:PRO:CD[1_556]  | 1.11                     | 1.09              |
| 4:2:169:TYR:CA  | 4:Z:296:ASN:O[1_556]   | 1.11                     | 1.09              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:62:ARG:CG   | 4:Z:204:ALA:CB[1_556]  | 1.11                     | 1.09              |
| 4:0:183:ARG:NE  | 4:X:186:THR:CB[1_556]  | 1.11                     | 1.09              |
| 4:1:129:VAL:C   | 4:Y:25:ASP:OD2[1_556]  | 1.11                     | 1.09              |
| 4:1:75:ILE:N    | 4:Y:157:ASP:N[1_556]   | 1.11                     | 1.09              |
| 4:1:32:PRO:CD   | 4:Y:211:ASP:OD1[1_556] | 1.11                     | 1.09              |
| 4:2:165:ILE:CA  | 4:Z:297:ASN:OD1[1_556] | 1.11                     | 1.09              |
| 4:2:166:TYR:C   | 4:Z:294:TYR:CA[1_556]  | 1.11                     | 1.09              |
| 4:2:292:ASP:O   | 4:Z:318:THR:C[1_556]   | 1.11                     | 1.09              |
| 4:2:298:VAL:CB  | 4:Z:312:ARG:O[1_556]   | 1.11                     | 1.09              |
| 4:0:292:ASP:O   | 4:X:318:THR:C[1_556]   | 1.11                     | 1.09              |
| 4:0:106:THR:C   | 4:X:335:ARG:C[1_556]   | 1.11                     | 1.09              |
| 4:2:73:HIS:N    | 4:Z:157:ASP:O[1_556]   | 1.11                     | 1.09              |
| 4:1:335:ARG:O   | 4:Y:307:PRO:O[1_556]   | 1.11                     | 1.09              |
| 4:0:66:THR:OG1  | 4:X:60:SER:C[1_556]    | 1.11                     | 1.09              |
| 4:2:252:ASN:OD1 | 4:Y:113:LYS:O[1_556]   | 1.11                     | 1.09              |
| 4:0:75:ILE:N    | 4:X:157:ASP:N[1_556]   | 1.11                     | 1.09              |
| 4:1:105:LEU:O   | 4:Y:335:ARG:N[1_556]   | 1.11                     | 1.09              |
| 4:2:153:LEU:N   | 4:Z:262:PHE:CE1[1_556] | 1.11                     | 1.09              |
| 4:1:74:GLY:C    | 4:Y:156:GLY:CA[1_556]  | 1.11                     | 1.09              |
| 4:2:125:GLU:N   | 4:Z:24:ASP:OD2[1_556]  | 1.11                     | 1.09              |
| 4:2:183:ARG:NE  | 4:Z:186:THR:CB[1_556]  | 1.11                     | 1.09              |
| 4:0:212:ILE:CG2 | 4:X:196:ARG:CA[1_556]  | 1.11                     | 1.09              |
| 4:0:277:THR:OG1 | 4:X:271:SER:O[1_556]   | 1.11                     | 1.09              |
| 4:0:153:LEU:CB  | 4:X:262:PHE:CG[1_556]  | 1.11                     | 1.09              |
| 4:2:153:LEU:CB  | 4:Z:262:PHE:CG[1_556]  | 1.11                     | 1.09              |
| 4:2:215:LYS:C   | 4:Z:252:ASN:OD1[1_556] | 1.11                     | 1.09              |
| 4:2:234:SER:N   | 4:Y:367:PRO:CD[1_556]  | 1.11                     | 1.09              |
| 4:2:186:THR:OG1 | 4:Z:189:LEU:C[1_556]   | 1.11                     | 1.09              |
| 4:2:125:GLU:CB  | 4:Z:21:PHE:CB[1_556]   | 1.11                     | 1.09              |
| 4:1:209:VAL:CB  | 4:Y:194:THR:CA[1_556]  | 1.11                     | 1.09              |
| 4:3:197:GLY:C   | 4:Z:75:ILE:C[1_556]    | 1.11                     | 1.09              |
| 4:0:153:LEU:N   | 4:X:262:PHE:CE1[1_556] | 1.11                     | 1.09              |
| 4:1:331:ALA:CB  | 4:Y:222:ASP:N[1_556]   | 1.11                     | 1.09              |
| 4:1:331:ALA:CA  | 4:Y:221:LEU:C[1_556]   | 1.11                     | 1.09              |
| 4:1:125:GLU:CB  | 4:Y:21:PHE:CB[1_556]   | 1.11                     | 1.09              |
| 4:1:79:TRP:CE2  | 4:Y:11:ASP:O[1_556]    | 1.11                     | 1.09              |
| 4:0:252:ASN:ND2 | 4:W:117:GLU:CG[1_556]  | 1.11                     | 1.09              |
| 4:2:168:GLY:C   | 4:Z:296:ASN:CA[1_556]  | 1.11                     | 1.09              |
| 4:0:80:ASP:C    | 4:X:31:PHE:CB[1_556]   | 1.11                     | 1.09              |
| 4:1:306:TYR:CD1 | 4:Y:256:ARG:CD[1_556]  | 1.12                     | 1.08              |
| 4:2:125:GLU:CA  | 4:Z:24:ASP:OD2[1_556]  | 1.12                     | 1.08              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:299:MET:CB  | 4:X:312:ARG:NE[1_556]  | 1.12                     | 1.08              |
| 4:1:211:ASP:OD2 | 4:Y:249:THR:CA[1_556]  | 1.12                     | 1.08              |
| 4:1:110:LEU:CD1 | 4:Y:161:HIS:CA[1_556]  | 1.12                     | 1.08              |
| 4:1:33:SER:O    | 4:Y:210:ARG:CZ[1_556]  | 1.12                     | 1.08              |
| 4:1:253:GLU:OE1 | 4:X:112:PRO:O[1_556]   | 1.12                     | 1.08              |
| 4:1:295:ALA:N   | 4:Y:319:ALA:C[1_556]   | 1.12                     | 1.08              |
| 4:2:106:THR:CB  | 4:Z:335:ARG:CG[1_556]  | 1.12                     | 1.08              |
| 4:0:63:GLY:C    | 4:V:288:ASP:C[1_556]   | 1.12                     | 1.08              |
| 4:1:305:MET:C   | 4:Y:255:PHE:CE1[1_556] | 1.12                     | 1.08              |
| 4:0:169:TYR:CA  | 4:X:296:ASN:O[1_556]   | 1.12                     | 1.08              |
| 4:1:126:THR:CA  | 4:Y:28:ARG:NE[1_556]   | 1.12                     | 1.08              |
| 4:1:176:MET:CG  | 4:Y:277:THR:OG1[1_556] | 1.12                     | 1.08              |
| 4:2:79:TRP:CE2  | 4:Z:11:ASP:O[1_556]    | 1.12                     | 1.08              |
| 4:0:125:GLU:N   | 4:X:24:ASP:OD2[1_556]  | 1.12                     | 1.08              |
| 4:2:182:GLY:O   | 4:Z:189:LEU:CA[1_556]  | 1.12                     | 1.08              |
| 4:2:86:TRP:NE1  | 4:Z:337:TYR:CZ[1_556]  | 1.12                     | 1.08              |
| 4:2:277:THR:OG1 | 4:Z:271:SER:O[1_556]   | 1.12                     | 1.08              |
| 4:1:185:LEU:CD1 | 4:Y:188:TYR:CE1[1_556] | 1.12                     | 1.08              |
| 4:2:63:GLY:C    | 4:X:288:ASP:C[1_556]   | 1.12                     | 1.08              |
| 4:0:79:TRP:CE2  | 4:X:11:ASP:O[1_556]    | 1.12                     | 1.08              |
| 4:0:62:ARG:CG   | 4:X:204:ALA:CB[1_556]  | 1.12                     | 1.08              |
| 4:0:122:ILE:N   | 4:X:340:TRP:CZ2[1_556] | 1.12                     | 1.08              |
| 4:2:104:LEU:CA  | 4:Z:334:GLU:CG[1_556]  | 1.12                     | 1.08              |
| 4:2:120:THR:OG1 | 4:Z:340:TRP:O[1_556]   | 1.12                     | 1.08              |
| 4:1:173:HIS:CD2 | 4:Y:281:SER:O[1_556]   | 1.12                     | 1.08              |
| 4:3:231:ALA:CA  | 4:Z:370:VAL:N[1_556]   | 1.12                     | 1.08              |
| 4:0:165:ILE:CA  | 4:X:297:ASN:OD1[1_556] | 1.12                     | 1.08              |
| 4:0:119:MET:N   | 4:X:340:TRP:CD1[1_556] | 1.12                     | 1.08              |
| 4:2:122:ILE:N   | 4:Z:340:TRP:CZ2[1_556] | 1.12                     | 1.08              |
| 4:1:106:THR:CA  | 4:Y:335:ARG:CA[1_556]  | 1.12                     | 1.08              |
| 4:3:227:MET:CB  | 4:Z:372:ARG:O[1_556]   | 1.12                     | 1.08              |
| 4:0:86:TRP:NE1  | 4:X:337:TYR:CZ[1_556]  | 1.12                     | 1.08              |
| 4:1:261:LEU:N   | 4:Y:266:PHE:CA[1_556]  | 1.12                     | 1.08              |
| 4:2:170:ALA:O   | 4:Z:151:ILE:CA[1_556]  | 1.12                     | 1.08              |
| 4:1:162:ASN:CG  | 4:Y:273:GLY:O[1_556]   | 1.12                     | 1.08              |
| 4:1:147:ARG:NH1 | 4:Y:315:LYS:CD[1_556]  | 1.12                     | 1.08              |
| 4:0:338:SER:N   | 4:X:308:GLY:N[1_556]   | 1.13                     | 1.07              |
| 4:1:153:LEU:N   | 4:Y:262:PHE:CE1[1_556] | 1.13                     | 1.07              |
| 4:1:135:ALA:CB  | 4:Y:332:PRO:CD[1_556]  | 1.13                     | 1.07              |
| 4:1:291:LYS:NZ  | 4:Y:322:PRO:CA[1_556]  | 1.13                     | 1.07              |
| 4:4:63:GLY:N    | 4:Z:288:ASP:CA[1_556]  | 1.13                     | 1.07              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:63:GLY:C    | 4:Z:288:ASP:C[1_556]   | 1.13                     | 1.07              |
| 4:1:168:GLY:O   | 4:Y:297:ASN:N[1_556]   | 1.13                     | 1.07              |
| 4:0:186:THR:OG1 | 4:X:189:LEU:C[1_556]   | 1.13                     | 1.07              |
| 4:1:159:VAL:N   | 4:Y:181:ALA:O[1_556]   | 1.13                     | 1.07              |
| 4:2:331:ALA:CA  | 4:Z:221:LEU:CA[1_556]  | 1.13                     | 1.07              |
| 4:1:274:ILE:CG1 | 4:Y:263:GLN:C[1_556]   | 1.13                     | 1.07              |
| 4:0:141:SER:CA  | 4:X:310:ALA:CA[1_556]  | 1.13                     | 1.07              |
| 4:2:304:THR:CB  | 4:Z:223:PHE:CZ[1_556]  | 1.13                     | 1.07              |
| 4:0:168:GLY:C   | 4:X:296:ASN:CA[1_556]  | 1.13                     | 1.07              |
| 4:1:294:TYR:CA  | 4:Y:319:ALA:O[1_556]   | 1.13                     | 1.07              |
| 4:0:182:GLY:O   | 4:X:189:LEU:CA[1_556]  | 1.13                     | 1.07              |
| 4:1:209:VAL:CG2 | 4:Y:194:THR:CA[1_556]  | 1.13                     | 1.07              |
| 4:0:230:ALA:CB  | 4:W:371:HIS:CB[1_556]  | 1.13                     | 1.07              |
| 4:2:252:ASN:ND2 | 4:Y:117:GLU:CG[1_556]  | 1.13                     | 1.07              |
| 4:2:75:ILE:N    | 4:Z:157:ASP:N[1_556]   | 1.13                     | 1.07              |
| 4:3:267:ILE:O   | 4:Z:173:HIS:O[1_556]   | 1.13                     | 1.07              |
| 4:0:63:GLY:O    | 4:V:289:ILE:N[1_556]   | 1.13                     | 1.07              |
| 4:1:109:PRO:N   | 4:Y:154:ASP:C[1_556]   | 1.13                     | 1.07              |
| 4:1:197:GLY:C   | 4:X:75:ILE:C[1_556]    | 1.13                     | 1.07              |
| 4:2:261:LEU:N   | 4:Z:266:PHE:CA[1_556]  | 1.13                     | 1.07              |
| 4:2:230:ALA:CB  | 4:Y:371:HIS:CB[1_556]  | 1.13                     | 1.07              |
| 4:2:150:GLY:C   | 4:Z:317:ILE:CG1[1_556] | 1.13                     | 1.07              |
| 4:1:119:MET:N   | 4:Y:340:TRP:CD1[1_556] | 1.13                     | 1.07              |
| 4:3:194:THR:O   | 4:Z:75:ILE:CG1[1_556]  | 1.13                     | 1.07              |
| 4:0:304:THR:CB  | 4:X:223:PHE:CZ[1_556]  | 1.13                     | 1.07              |
| 4:0:292:ASP:O   | 4:X:318:THR:O[1_556]   | 1.13                     | 1.07              |
| 4:2:80:ASP:C    | 4:Z:31:PHE:CB[1_556]   | 1.13                     | 1.07              |
| 4:1:206:ARG:N   | 4:Y:199:SER:CA[1_556]  | 1.13                     | 1.07              |
| 4:0:252:ASN:OD1 | 4:W:113:LYS:O[1_556]   | 1.13                     | 1.07              |
| 4:2:63:GLY:O    | 4:X:289:ILE:N[1_556]   | 1.13                     | 1.07              |
| 4:0:125:GLU:CB  | 4:X:21:PHE:CB[1_556]   | 1.13                     | 1.07              |
| 4:0:296:ASN:C   | 4:X:315:LYS:O[1_556]   | 1.13                     | 1.07              |
| 4:1:338:SER:N   | 4:Y:308:GLY:N[1_556]   | 1.13                     | 1.07              |
| 4:0:104:LEU:CA  | 4:X:334:GLU:CG[1_556]  | 1.13                     | 1.07              |
| 4:1:79:TRP:CD2  | 4:Y:18:LYS:N[1_556]    | 1.13                     | 1.07              |
| 4:2:299:MET:CB  | 4:Z:312:ARG:NE[1_556]  | 1.13                     | 1.07              |
| 4:1:231:ALA:CA  | 4:X:370:VAL:N[1_556]   | 1.13                     | 1.07              |
| 4:2:157:ASP:OD2 | 4:Z:186:THR:OG1[1_556] | 1.14                     | 1.06              |
| 4:1:62:ARG:CG   | 4:Y:204:ALA:CB[1_556]  | 1.14                     | 1.06              |
| 4:3:252:ASN:O   | 4:Z:113:LYS:CD[1_556]  | 1.14                     | 1.06              |
| 4:0:139:VAL:N   | 4:X:299:MET:SD[1_556]  | 1.14                     | 1.06              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:124:PHE:CB  | 4:Z:24:ASP:N[1_556]    | 1.14                     | 1.06              |
| 4:0:120:THR:OG1 | 4:X:340:TRP:O[1_556]   | 1.14                     | 1.06              |
| 4:0:174:ALA:CB  | 4:X:281:SER:N[1_556]   | 1.14                     | 1.06              |
| 4:1:125:GLU:N   | 4:Y:24:ASP:OD2[1_556]  | 1.14                     | 1.06              |
| 4:0:168:GLY:O   | 4:X:297:ASN:N[1_556]   | 1.14                     | 1.06              |
| 4:2:292:ASP:O   | 4:Z:318:THR:O[1_556]   | 1.14                     | 1.06              |
| 4:1:252:ASN:O   | 4:X:113:LYS:CD[1_556]  | 1.14                     | 1.06              |
| 4:1:175:ILE:C   | 4:Y:277:THR:CG2[1_556] | 1.14                     | 1.06              |
| 4:0:162:ASN:CG  | 4:X:273:GLY:O[1_556]   | 1.14                     | 1.06              |
| 4:2:174:ALA:CB  | 4:Z:281:SER:N[1_556]   | 1.14                     | 1.06              |
| 4:0:106:THR:CG2 | 4:X:335:ARG:CG[1_556]  | 1.14                     | 1.06              |
| 4:4:40:HIS:C    | 4:Z:167:GLU:OE2[1_556] | 1.14                     | 1.06              |
| 4:0:267:ILE:O   | 4:W:173:HIS:O[1_556]   | 1.14                     | 1.06              |
| 4:1:307:PRO:CA  | 4:Y:227:MET:CA[1_556]  | 1.14                     | 1.06              |
| 4:1:267:ILE:O   | 4:X:173:HIS:O[1_556]   | 1.14                     | 1.06              |
| 4:1:194:THR:O   | 4:X:75:ILE:CG1[1_556]  | 1.14                     | 1.06              |
| 4:2:338:SER:N   | 4:Z:308:GLY:N[1_556]   | 1.14                     | 1.06              |
| 4:2:63:GLY:N    | 4:X:288:ASP:CA[1_556]  | 1.14                     | 1.06              |
| 4:2:114:ALA:C   | 4:Z:106:THR:CG2[1_556] | 1.14                     | 1.06              |
| 4:1:141:SER:CA  | 4:Y:310:ALA:CA[1_556]  | 1.14                     | 1.06              |
| 4:1:168:GLY:C   | 4:Y:296:ASN:CA[1_556]  | 1.14                     | 1.06              |
| 4:2:162:ASN:CG  | 4:Z:273:GLY:O[1_556]   | 1.14                     | 1.06              |
| 4:1:169:TYR:CA  | 4:Y:296:ASN:O[1_556]   | 1.14                     | 1.06              |
| 4:1:161:HIS:CE1 | 4:Y:160:THR:OG1[1_556] | 1.14                     | 1.06              |
| 4:0:153:LEU:CG  | 4:X:262:PHE:CA[1_556]  | 1.14                     | 1.06              |
| 4:1:185:LEU:CG  | 4:Y:188:TYR:CZ[1_556]  | 1.14                     | 1.06              |
| 4:0:136:ILE:O   | 4:X:299:MET:CB[1_556]  | 1.14                     | 1.06              |
| 4:1:119:MET:CE  | 4:Y:337:TYR:CA[1_556]  | 1.14                     | 1.06              |
| 4:0:150:GLY:C   | 4:X:317:ILE:CG1[1_556] | 1.14                     | 1.06              |
| 4:0:147:ARG:NH1 | 4:X:315:LYS:CD[1_556]  | 1.14                     | 1.06              |
| 4:2:296:ASN:C   | 4:Z:315:LYS:O[1_556]   | 1.14                     | 1.06              |
| 4:1:284:LYS:O   | 4:Y:280:ASN:O[1_556]   | 1.14                     | 1.06              |
| 4:2:141:SER:CA  | 4:Z:310:ALA:CA[1_556]  | 1.15                     | 1.05              |
| 4:2:209:VAL:CG2 | 4:Z:194:THR:CA[1_556]  | 1.15                     | 1.05              |
| 4:0:170:ALA:O   | 4:X:151:ILE:CA[1_556]  | 1.15                     | 1.05              |
| 4:1:215:LYS:C   | 4:Y:252:ASN:OD1[1_556] | 1.15                     | 1.05              |
| 4:1:367:PRO:CD  | 4:Y:347:ALA:CB[1_556]  | 1.15                     | 1.05              |
| 4:1:178:LEU:O   | 4:Y:180:LEU:CB[1_556]  | 1.15                     | 1.05              |
| 4:2:267:ILE:O   | 4:Y:173:HIS:O[1_556]   | 1.15                     | 1.05              |
| 4:0:168:GLY:O   | 4:X:296:ASN:C[1_556]   | 1.15                     | 1.05              |
| 4:2:233:SER:CB  | 4:Y:367:PRO:CB[1_556]  | 1.15                     | 1.05              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:63:GLY:O    | 4:Z:289:ILE:N[1_556]   | 1.15                     | 1.05              |
| 4:0:63:GLY:N    | 4:V:288:ASP:CA[1_556]  | 1.15                     | 1.05              |
| 4:0:331:ALA:CA  | 4:X:221:LEU:CA[1_556]  | 1.15                     | 1.05              |
| 4:2:307:PRO:O   | 4:Z:227:MET:CG[1_556]  | 1.15                     | 1.05              |
| 4:2:139:VAL:N   | 4:Z:299:MET:SD[1_556]  | 1.15                     | 1.05              |
| 4:1:153:LEU:CB  | 4:Y:262:PHE:CG[1_556]  | 1.15                     | 1.05              |
| 4:0:157:ASP:OD2 | 4:X:186:THR:OG1[1_556] | 1.15                     | 1.05              |
| 4:0:293:LEU:CD2 | 4:X:279:TYR:CD1[1_556] | 1.15                     | 1.05              |
| 4:0:261:LEU:N   | 4:X:266:PHE:CA[1_556]  | 1.15                     | 1.05              |
| 4:1:122:ILE:CG1 | 4:Y:19:ALA:O[1_556]    | 1.15                     | 1.05              |
| 4:1:212:ILE:CB  | 4:Y:196:ARG:CA[1_556]  | 1.15                     | 1.05              |
| 4:2:168:GLY:O   | 4:Z:296:ASN:C[1_556]   | 1.15                     | 1.05              |
| 4:0:291:LYS:NZ  | 4:X:322:PRO:CA[1_556]  | 1.15                     | 1.05              |
| 4:2:153:LEU:CG  | 4:Z:262:PHE:CA[1_556]  | 1.15                     | 1.05              |
| 4:2:106:THR:CG2 | 4:Z:335:ARG:CG[1_556]  | 1.15                     | 1.05              |
| 4:1:66:THR:OG1  | 4:Y:60:SER:C[1_556]    | 1.15                     | 1.05              |
| 4:1:152:VAL:CG2 | 4:Y:313:MET:CG[1_556]  | 1.15                     | 1.05              |
| 4:1:299:MET:CG  | 4:Y:312:ARG:NE[1_556]  | 1.15                     | 1.05              |
| 4:2:40:HIS:C    | 4:X:167:GLU:OE2[1_556] | 1.15                     | 1.05              |
| 4:0:62:ARG:NE   | 4:X:205:GLU:CA[1_556]  | 1.15                     | 1.05              |
| 4:1:177:ARG:CA  | 4:Y:178:LEU:CG[1_556]  | 1.16                     | 1.04              |
| 4:1:260:THR:O   | 4:Y:265:SER:O[1_556]   | 1.16                     | 1.04              |
| 4:0:177:ARG:C   | 4:X:178:LEU:CG[1_556]  | 1.16                     | 1.04              |
| 4:2:189:LEU:CG  | 4:Z:195:GLU:CA[1_556]  | 1.16                     | 1.04              |
| 4:1:189:LEU:CG  | 4:Y:195:GLU:CA[1_556]  | 1.16                     | 1.04              |
| 4:0:114:ALA:C   | 4:X:106:THR:CG2[1_556] | 1.16                     | 1.04              |
| 4:2:136:ILE:CA  | 4:Z:299:MET:O[1_556]   | 1.16                     | 1.04              |
| 4:0:62:ARG:O    | 4:V:288:ASP:CA[1_556]  | 1.16                     | 1.04              |
| 4:1:369:ILE:CG2 | 4:Y:346:LEU:N[1_556]   | 1.16                     | 1.04              |
| 4:0:124:PHE:CB  | 4:X:24:ASP:N[1_556]    | 1.16                     | 1.04              |
| 4:1:252:ASN:OD1 | 4:X:113:LYS:O[1_556]   | 1.16                     | 1.04              |
| 4:1:122:ILE:N   | 4:Y:340:TRP:CZ2[1_556] | 1.16                     | 1.04              |
| 4:2:177:ARG:C   | 4:Z:178:LEU:CG[1_556]  | 1.16                     | 1.04              |
| 4:0:72:GLU:O    | 4:X:157:ASP:C[1_556]   | 1.16                     | 1.04              |
| 4:1:147:ARG:CA  | 4:Y:314:GLN:NE2[1_556] | 1.16                     | 1.04              |
| 4:0:197:GLY:C   | 4:W:75:ILE:C[1_556]    | 1.16                     | 1.04              |
| 4:1:104:LEU:C   | 4:Y:334:GLU:CB[1_556]  | 1.16                     | 1.04              |
| 4:0:253:GLU:N   | 4:W:113:LYS:CB[1_556]  | 1.16                     | 1.04              |
| 4:2:168:GLY:O   | 4:Z:297:ASN:N[1_556]   | 1.16                     | 1.04              |
| 4:0:260:THR:O   | 4:X:265:SER:O[1_556]   | 1.16                     | 1.04              |
| 4:1:116:ARG:NH1 | 4:Y:141:SER:O[1_556]   | 1.16                     | 1.04              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:30:VAL:CG1  | 4:Y:215:LYS:CA[1_556]  | 1.16                     | 1.04              |
| 4:1:237:GLU:OE2 | 4:X:114:ALA:O[1_556]   | 1.16                     | 1.04              |
| 4:0:104:LEU:C   | 4:X:334:GLU:CA[1_556]  | 1.16                     | 1.04              |
| 4:0:206:ARG:N   | 4:X:199:SER:CA[1_556]  | 1.16                     | 1.04              |
| 4:0:189:LEU:CG  | 4:X:195:GLU:CA[1_556]  | 1.16                     | 1.04              |
| 4:2:62:ARG:O    | 4:X:288:ASP:CA[1_556]  | 1.16                     | 1.04              |
| 4:2:252:ASN:O   | 4:Y:113:LYS:CE[1_556]  | 1.16                     | 1.04              |
| 4:0:183:ARG:CG  | 4:X:187:ASP:N[1_556]   | 1.16                     | 1.04              |
| 4:3:252:ASN:ND2 | 4:Z:117:GLU:CG[1_556]  | 1.16                     | 1.04              |
| 4:2:136:ILE:O   | 4:Z:299:MET:CB[1_556]  | 1.16                     | 1.04              |
| 4:3:196:ARG:CA  | 4:Z:111:ASN:OD1[1_556] | 1.16                     | 1.04              |
| 4:1:261:LEU:CB  | 4:Y:266:PHE:CG[1_556]  | 1.16                     | 1.04              |
| 4:2:142:LEU:CD2 | 4:Z:329:ILE:CG1[1_556] | 1.16                     | 1.04              |
| 4:0:252:ASN:O   | 4:W:113:LYS:CE[1_556]  | 1.16                     | 1.04              |
| 4:1:183:ARG:CG  | 4:Y:187:ASP:N[1_556]   | 1.16                     | 1.04              |
| 4:1:331:ALA:CA  | 4:Y:221:LEU:CA[1_556]  | 1.16                     | 1.04              |
| 4:2:293:LEU:CD2 | 4:Z:279:TYR:CD1[1_556] | 1.16                     | 1.04              |
| 4:2:147:ARG:NH1 | 4:Z:315:LYS:CD[1_556]  | 1.16                     | 1.04              |
| 4:0:121:GLN:C   | 4:X:340:TRP:CZ2[1_556] | 1.17                     | 1.03              |
| 4:1:121:GLN:NE2 | 4:Y:20:GLY:O[1_556]    | 1.17                     | 1.03              |
| 4:0:264:PRO:CB  | 4:X:268:GLY:CA[1_556]  | 1.17                     | 1.03              |
| 4:0:209:VAL:CG2 | 4:X:194:THR:CA[1_556]  | 1.17                     | 1.03              |
| 4:0:196:ARG:CA  | 4:W:111:ASN:OD1[1_556] | 1.17                     | 1.03              |
| 4:2:264:PRO:CB  | 4:Z:268:GLY:CA[1_556]  | 1.17                     | 1.03              |
| 4:1:264:PRO:CB  | 4:Y:268:GLY:CA[1_556]  | 1.17                     | 1.03              |
| 4:3:253:GLU:N   | 4:Z:113:LYS:CB[1_556]  | 1.17                     | 1.03              |
| 4:2:260:THR:O   | 4:Z:265:SER:O[1_556]   | 1.17                     | 1.03              |
| 4:1:261:LEU:CB  | 4:Y:266:PHE:CD1[1_556] | 1.17                     | 1.03              |
| 4:2:206:ARG:N   | 4:Z:199:SER:CA[1_556]  | 1.17                     | 1.03              |
| 4:0:231:ALA:CA  | 4:W:370:VAL:N[1_556]   | 1.17                     | 1.03              |
| 4:2:119:MET:CA  | 4:Z:340:TRP:CG[1_556]  | 1.17                     | 1.03              |
| 4:0:233:SER:CB  | 4:W:367:PRO:CB[1_556]  | 1.17                     | 1.03              |
| 4:0:136:ILE:CA  | 4:X:299:MET:O[1_556]   | 1.17                     | 1.03              |
| 4:2:291:LYS:NZ  | 4:Z:322:PRO:CA[1_556]  | 1.17                     | 1.03              |
| 4:0:307:PRO:O   | 4:X:227:MET:CG[1_556]  | 1.17                     | 1.03              |
| 4:1:292:ASP:N   | 4:Y:321:ALA:C[1_556]   | 1.17                     | 1.03              |
| 4:0:274:ILE:CD1 | 4:X:264:PRO:N[1_556]   | 1.17                     | 1.03              |
| 4:0:40:HIS:C    | 4:V:167:GLU:OE2[1_556] | 1.17                     | 1.03              |
| 4:1:106:THR:CB  | 4:Y:335:ARG:CG[1_556]  | 1.17                     | 1.03              |
| 4:2:159:VAL:CG1 | 4:Z:181:ALA:CA[1_556]  | 1.17                     | 1.03              |
| 4:0:149:THR:CB  | 4:X:327:ILE:CG1[1_556] | 1.17                     | 1.03              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:170:ALA:O   | 4:Y:151:ILE:CA[1_556]  | 1.17                     | 1.03              |
| 4:4:62:ARG:O    | 4:Z:288:ASP:CA[1_556]  | 1.17                     | 1.03              |
| 4:3:252:ASN:OD1 | 4:Z:113:LYS:O[1_556]   | 1.17                     | 1.03              |
| 4:2:209:VAL:CA  | 4:Z:193:LEU:O[1_556]   | 1.17                     | 1.03              |
| 4:2:169:TYR:CD1 | 4:Z:150:GLY:O[1_556]   | 1.17                     | 1.03              |
| 4:2:227:MET:CB  | 4:Y:372:ARG:O[1_556]   | 1.17                     | 1.03              |
| 4:1:189:LEU:CD1 | 4:Y:195:GLU:CG[1_556]  | 1.17                     | 1.03              |
| 4:1:40:HIS:C    | 4:W:167:GLU:OE2[1_556] | 1.17                     | 1.03              |
| 4:2:209:VAL:C   | 4:Z:193:LEU:C[1_556]   | 1.17                     | 1.03              |
| 4:1:336:LYS:CA  | 4:Y:218:TYR:CA[1_556]  | 1.17                     | 1.03              |
| 4:2:183:ARG:CG  | 4:Z:187:ASP:N[1_556]   | 1.17                     | 1.03              |
| 4:1:114:ALA:CA  | 4:Y:106:THR:CA[1_556]  | 1.17                     | 1.03              |
| 4:0:142:LEU:CD2 | 4:X:329:ILE:CG1[1_556] | 1.17                     | 1.03              |
| 4:0:112:PRO:C   | 4:X:137:GLN:CB[1_556]  | 1.17                     | 1.03              |
| 4:2:104:LEU:C   | 4:Z:334:GLU:CA[1_556]  | 1.18                     | 1.02              |
| 4:3:198:TYR:N   | 4:Z:75:ILE:CB[1_556]   | 1.18                     | 1.02              |
| 4:0:209:VAL:CA  | 4:X:193:LEU:O[1_556]   | 1.18                     | 1.02              |
| 4:2:197:GLY:C   | 4:Y:75:ILE:C[1_556]    | 1.18                     | 1.02              |
| 4:0:300:SER:CA  | 4:X:219:VAL:CG1[1_556] | 1.18                     | 1.02              |
| 4:1:277:THR:OG1 | 4:Y:271:SER:C[1_556]   | 1.18                     | 1.02              |
| 4:2:62:ARG:NE   | 4:Z:205:GLU:CA[1_556]  | 1.18                     | 1.02              |
| 4:0:209:VAL:C   | 4:X:193:LEU:C[1_556]   | 1.18                     | 1.02              |
| 4:2:195:GLU:OE2 | 4:Y:110:LEU:N[1_556]   | 1.18                     | 1.02              |
| 4:1:62:ARG:NH2  | 4:Y:205:GLU:CA[1_556]  | 1.18                     | 1.02              |
| 4:2:72:GLU:O    | 4:Z:157:ASP:C[1_556]   | 1.18                     | 1.02              |
| 4:0:159:VAL:CG1 | 4:X:181:ALA:CA[1_556]  | 1.18                     | 1.02              |
| 4:2:197:GLY:CA  | 4:Y:75:ILE:C[1_556]    | 1.18                     | 1.02              |
| 4:2:265:SER:O   | 4:Y:173:HIS:CE1[1_556] | 1.18                     | 1.02              |
| 4:1:261:LEU:CG  | 4:Y:266:PHE:CB[1_556]  | 1.18                     | 1.02              |
| 4:1:136:ILE:C   | 4:Y:299:MET:C[1_556]   | 1.18                     | 1.02              |
| 4:2:292:ASP:N   | 4:Z:321:ALA:C[1_556]   | 1.18                     | 1.02              |
| 4:1:125:GLU:CA  | 4:Y:24:ASP:OD2[1_556]  | 1.18                     | 1.02              |
| 4:3:237:GLU:OE2 | 4:Z:114:ALA:O[1_556]   | 1.18                     | 1.02              |
| 4:2:253:GLU:N   | 4:Y:113:LYS:CB[1_556]  | 1.18                     | 1.02              |
| 4:0:177:ARG:CA  | 4:X:178:LEU:CG[1_556]  | 1.18                     | 1.02              |
| 4:0:209:VAL:CB  | 4:X:194:THR:CA[1_556]  | 1.18                     | 1.02              |
| 4:0:195:GLU:OE2 | 4:W:110:LEU:N[1_556]   | 1.18                     | 1.02              |
| 4:0:169:TYR:CD1 | 4:X:150:GLY:O[1_556]   | 1.18                     | 1.02              |
| 4:0:293:LEU:C   | 4:X:320:LEU:N[1_556]   | 1.18                     | 1.02              |
| 4:1:335:ARG:CB  | 4:Y:219:VAL:C[1_556]   | 1.18                     | 1.02              |
| 4:1:124:PHE:CB  | 4:Y:24:ASP:N[1_556]    | 1.18                     | 1.02              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:296:ASN:OD1 | 4:X:318:THR:OG1[1_556] | 1.18                     | 1.02              |
| 4:0:197:GLY:CA  | 4:W:75:ILE:C[1_556]    | 1.18                     | 1.02              |
| 4:1:252:ASN:ND2 | 4:X:117:GLU:CG[1_556]  | 1.18                     | 1.02              |
| 4:2:161:HIS:C   | 4:Z:274:ILE:CB[1_556]  | 1.18                     | 1.02              |
| 4:3:196:ARG:NH1 | 4:Z:115:ASN:CA[1_556]  | 1.18                     | 1.02              |
| 4:1:370:VAL:CG1 | 4:Y:342:GLY:C[1_556]   | 1.18                     | 1.02              |
| 4:1:150:GLY:C   | 4:Y:317:ILE:CG1[1_556] | 1.18                     | 1.02              |
| 4:1:196:ARG:CA  | 4:X:111:ASN:OD1[1_556] | 1.18                     | 1.02              |
| 4:2:209:VAL:CB  | 4:Z:194:THR:CA[1_556]  | 1.18                     | 1.02              |
| 4:0:211:ASP:OD2 | 4:X:249:THR:C[1_556]   | 1.18                     | 1.02              |
| 4:2:296:ASN:OD1 | 4:Z:318:THR:OG1[1_556] | 1.18                     | 1.02              |
| 4:1:59:GLN:NE2  | 4:Y:208:ILE:N[1_556]   | 1.18                     | 1.02              |
| 4:0:196:ARG:NH1 | 4:W:115:ASN:CA[1_556]  | 1.18                     | 1.02              |
| 4:0:161:HIS:C   | 4:X:274:ILE:CB[1_556]  | 1.18                     | 1.02              |
| 4:1:198:TYR:N   | 4:X:75:ILE:CB[1_556]   | 1.18                     | 1.02              |
| 4:0:105:LEU:CB  | 4:X:334:GLU:O[1_556]   | 1.18                     | 1.02              |
| 4:0:252:ASN:O   | 4:W:113:LYS:CD[1_556]  | 1.18                     | 1.02              |
| 4:1:296:ASN:CA  | 4:Y:315:LYS:O[1_556]   | 1.18                     | 1.02              |
| 4:2:274:ILE:CD1 | 4:Z:264:PRO:N[1_556]   | 1.18                     | 1.02              |
| 4:2:210:ARG:CB  | 4:Z:193:LEU:CD2[1_556] | 1.18                     | 1.02              |
| 4:2:231:ALA:CA  | 4:Y:370:VAL:N[1_556]   | 1.18                     | 1.02              |
| 4:0:296:ASN:CA  | 4:X:315:LYS:O[1_556]   | 1.19                     | 1.01              |
| 4:2:196:ARG:NH1 | 4:Y:115:ASN:CA[1_556]  | 1.19                     | 1.01              |
| 4:0:119:MET:CA  | 4:X:340:TRP:CG[1_556]  | 1.19                     | 1.01              |
| 4:1:106:THR:C   | 4:Y:335:ARG:C[1_556]   | 1.19                     | 1.01              |
| 4:2:196:ARG:CA  | 4:Y:111:ASN:OD1[1_556] | 1.19                     | 1.01              |
| 4:1:196:ARG:NH1 | 4:X:115:ASN:CA[1_556]  | 1.19                     | 1.01              |
| 4:1:300:SER:CA  | 4:Y:219:VAL:CG1[1_556] | 1.19                     | 1.01              |
| 4:0:227:MET:CB  | 4:W:372:ARG:O[1_556]   | 1.19                     | 1.01              |
| 4:2:121:GLN:C   | 4:Z:340:TRP:CZ2[1_556] | 1.19                     | 1.01              |
| 4:1:252:ASN:CG  | 4:X:113:LYS:O[1_556]   | 1.19                     | 1.01              |
| 4:2:112:PRO:C   | 4:Z:137:GLN:CB[1_556]  | 1.19                     | 1.01              |
| 4:1:182:GLY:O   | 4:Y:189:LEU:CA[1_556]  | 1.19                     | 1.01              |
| 4:1:114:ALA:C   | 4:Y:106:THR:CG2[1_556] | 1.19                     | 1.01              |
| 4:1:177:ARG:C   | 4:Y:178:LEU:CG[1_556]  | 1.19                     | 1.01              |
| 4:2:296:ASN:CA  | 4:Z:315:LYS:O[1_556]   | 1.19                     | 1.01              |
| 4:2:252:ASN:O   | 4:Y:113:LYS:CD[1_556]  | 1.19                     | 1.01              |
| 4:3:40:HIS:C    | 4:Y:167:GLU:OE2[1_556] | 1.19                     | 1.01              |
| 4:1:253:GLU:N   | 4:X:113:LYS:CB[1_556]  | 1.19                     | 1.01              |
| 4:0:166:TYR:CG  | 4:X:294:TYR:CB[1_556]  | 1.19                     | 1.01              |
| 4:2:166:TYR:CG  | 4:Z:294:TYR:CB[1_556]  | 1.19                     | 1.01              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:271:SER:C   | 4:Y:270:GLU:N[1_556]   | 1.19                     | 1.01              |
| 4:1:142:LEU:CD2 | 4:Y:329:ILE:CG1[1_556] | 1.19                     | 1.01              |
| 4:2:149:THR:CB  | 4:Z:327:ILE:CG1[1_556] | 1.19                     | 1.01              |
| 4:0:187:ASP:N   | 4:X:191:LYS:CA[1_556]  | 1.19                     | 1.01              |
| 4:2:293:LEU:C   | 4:Z:320:LEU:N[1_556]   | 1.19                     | 1.01              |
| 4:0:265:SER:O   | 4:W:173:HIS:CE1[1_556] | 1.19                     | 1.01              |
| 4:0:212:ILE:CD1 | 4:X:196:ARG:O[1_556]   | 1.19                     | 1.01              |
| 4:0:118:LYS:O   | 4:X:340:TRP:CD1[1_556] | 1.19                     | 1.01              |
| 4:2:141:SER:C   | 4:Z:310:ALA:CB[1_556]  | 1.19                     | 1.01              |
| 4:3:63:GLY:C    | 4:Y:288:ASP:C[1_556]   | 1.19                     | 1.01              |
| 4:1:149:THR:CB  | 4:Y:327:ILE:CG1[1_556] | 1.19                     | 1.01              |
| 4:3:227:MET:CG  | 4:Z:372:ARG:O[1_556]   | 1.19                     | 1.01              |
| 4:1:79:TRP:CB   | 4:Y:17:VAL:CB[1_556]   | 1.19                     | 1.01              |
| 4:1:233:SER:CB  | 4:X:367:PRO:CB[1_556]  | 1.20                     | 1.00              |
| 4:0:161:HIS:NE2 | 4:X:160:THR:CG2[1_556] | 1.20                     | 1.00              |
| 4:1:63:GLY:C    | 4:W:288:ASP:C[1_556]   | 1.20                     | 1.00              |
| 4:0:292:ASP:N   | 4:X:321:ALA:C[1_556]   | 1.20                     | 1.00              |
| 4:1:62:ARG:NE   | 4:Y:205:GLU:CA[1_556]  | 1.20                     | 1.00              |
| 4:0:59:GLN:NE2  | 4:X:208:ILE:N[1_556]   | 1.20                     | 1.00              |
| 4:2:212:ILE:CD1 | 4:Z:196:ARG:O[1_556]   | 1.20                     | 1.00              |
| 4:1:159:VAL:CG1 | 4:Y:181:ALA:CA[1_556]  | 1.20                     | 1.00              |
| 4:1:119:MET:CA  | 4:Y:340:TRP:CG[1_556]  | 1.20                     | 1.00              |
| 4:2:295:ALA:N   | 4:Z:319:ALA:C[1_556]   | 1.20                     | 1.00              |
| 4:2:300:SER:CA  | 4:Z:219:VAL:CG1[1_556] | 1.20                     | 1.00              |
| 4:1:307:PRO:O   | 4:Y:227:MET:CG[1_556]  | 1.20                     | 1.00              |
| 4:0:107:GLU:CA  | 4:X:301:GLY:N[1_556]   | 1.20                     | 1.00              |
| 4:1:137:GLN:NE2 | 4:Y:301:GLY:C[1_556]   | 1.20                     | 1.00              |
| 4:2:211:ASP:OD2 | 4:Z:249:THR:C[1_556]   | 1.20                     | 1.00              |
| 4:1:368:SER:CA  | 4:Y:346:LEU:CD2[1_556] | 1.20                     | 1.00              |
| 4:0:210:ARG:CB  | 4:X:193:LEU:CD2[1_556] | 1.20                     | 1.00              |
| 4:3:62:ARG:O    | 4:Y:288:ASP:CA[1_556]  | 1.20                     | 1.00              |
| 4:1:196:ARG:NE  | 4:X:115:ASN:CG[1_556]  | 1.20                     | 1.00              |
| 4:2:252:ASN:CG  | 4:Y:113:LYS:O[1_556]   | 1.20                     | 1.00              |
| 4:1:305:MET:CG  | 4:Y:255:PHE:CB[1_556]  | 1.20                     | 1.00              |
| 4:1:214:GLU:CA  | 4:Y:253:GLU:CD[1_556]  | 1.20                     | 1.00              |
| 4:1:72:GLU:O    | 4:Y:157:ASP:C[1_556]   | 1.20                     | 1.00              |
| 4:1:167:GLU:N   | 4:Y:294:TYR:O[1_556]   | 1.20                     | 1.00              |
| 4:0:164:PRO:CD  | 4:X:278:THR:CB[1_556]  | 1.20                     | 1.00              |
| 4:2:177:ARG:CA  | 4:Z:178:LEU:CG[1_556]  | 1.20                     | 1.00              |
| 4:2:164:PRO:CD  | 4:Z:278:THR:CB[1_556]  | 1.20                     | 1.00              |
| 4:0:372:ARG:CD  | 4:X:142:LEU:O[1_556]   | 1.20                     | 1.00              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:292:ASP:O   | 4:Y:318:THR:C[1_556]   | 1.20                     | 1.00              |
| 4:0:305:MET:CA  | 4:X:255:PHE:CD1[1_556] | 1.20                     | 1.00              |
| 4:0:62:ARG:CB   | 4:X:204:ALA:CA[1_556]  | 1.20                     | 1.00              |
| 4:1:214:GLU:C   | 4:Y:253:GLU:OE2[1_556] | 1.20                     | 1.00              |
| 4:1:211:ASP:OD2 | 4:Y:249:THR:C[1_556]   | 1.20                     | 1.00              |
| 4:2:237:GLU:OE2 | 4:Y:114:ALA:O[1_556]   | 1.20                     | 1.00              |
| 4:1:173:HIS:CB  | 4:Y:174:ALA:C[1_556]   | 1.20                     | 1.00              |
| 4:2:372:ARG:CA  | 4:Z:143:TYR:CB[1_556]  | 1.20                     | 1.00              |
| 4:1:209:VAL:CA  | 4:Y:193:LEU:O[1_556]   | 1.20                     | 1.00              |
| 4:2:186:THR:C   | 4:Z:191:LYS:N[1_556]   | 1.20                     | 1.00              |
| 4:1:305:MET:CA  | 4:Y:255:PHE:CD1[1_556] | 1.20                     | 1.00              |
| 4:2:272:ALA:CA  | 4:Z:270:GLU:C[1_556]   | 1.20                     | 1.00              |
| 4:0:372:ARG:CA  | 4:X:143:TYR:CB[1_556]  | 1.20                     | 1.00              |
| 4:1:227:MET:CG  | 4:X:372:ARG:O[1_556]   | 1.20                     | 1.00              |
| 4:1:77:THR:O    | 4:Y:33:SER:CB[1_556]   | 1.20                     | 1.00              |
| 4:2:153:LEU:CA  | 4:Z:262:PHE:CE1[1_556] | 1.20                     | 1.00              |
| 4:2:304:THR:C   | 4:Z:223:PHE:CE1[1_556] | 1.20                     | 1.00              |
| 4:2:309:ILE:CG1 | 4:Z:259:GLU:CD[1_556]  | 1.20                     | 1.00              |
| 4:1:161:HIS:NE2 | 4:Y:160:THR:CG2[1_556] | 1.20                     | 1.00              |
| 4:3:252:ASN:CG  | 4:Z:113:LYS:O[1_556]   | 1.20                     | 1.00              |
| 4:1:286:ASP:N   | 4:Y:283:MET:CA[1_556]  | 1.20                     | 1.00              |
| 4:2:187:ASP:N   | 4:Z:191:LYS:CA[1_556]  | 1.20                     | 1.00              |
| 4:2:368:SER:CA  | 4:Z:346:LEU:CG[1_556]  | 1.20                     | 1.00              |
| 4:0:198:TYR:N   | 4:W:75:ILE:CB[1_556]   | 1.20                     | 1.00              |
| 4:2:161:HIS:NE2 | 4:Z:160:THR:CG2[1_556] | 1.20                     | 1.00              |
| 4:2:105:LEU:CB  | 4:Z:334:GLU:O[1_556]   | 1.21                     | 0.99              |
| 4:2:372:ARG:CD  | 4:Z:142:LEU:O[1_556]   | 1.21                     | 0.99              |
| 4:0:191:LYS:CE  | 4:W:110:LEU:CG[1_556]  | 1.21                     | 0.99              |
| 4:1:292:ASP:O   | 4:Y:318:THR:O[1_556]   | 1.21                     | 0.99              |
| 4:3:41:GLN:CA   | 4:Y:167:GLU:OE2[1_556] | 1.21                     | 0.99              |
| 4:0:295:ALA:N   | 4:X:319:ALA:C[1_556]   | 1.21                     | 0.99              |
| 4:1:62:ARG:O    | 4:W:288:ASP:CA[1_556]  | 1.21                     | 0.99              |
| 4:1:183:ARG:NE  | 4:Y:186:THR:CB[1_556]  | 1.21                     | 0.99              |
| 4:2:169:TYR:N   | 4:Z:296:ASN:C[1_556]   | 1.21                     | 0.99              |
| 4:1:372:ARG:CD  | 4:Y:142:LEU:C[1_556]   | 1.21                     | 0.99              |
| 4:1:121:GLN:C   | 4:Y:340:TRP:CZ2[1_556] | 1.21                     | 0.99              |
| 4:3:196:ARG:NE  | 4:Z:115:ASN:CG[1_556]  | 1.21                     | 0.99              |
| 4:2:191:LYS:CE  | 4:Y:110:LEU:CG[1_556]  | 1.21                     | 0.99              |
| 4:0:274:ILE:CG1 | 4:X:263:GLN:C[1_556]   | 1.21                     | 0.99              |
| 4:1:337:TYR:CA  | 4:Y:307:PRO:CG[1_556]  | 1.21                     | 0.99              |
| 4:0:368:SER:CA  | 4:X:346:LEU:CG[1_556]  | 1.21                     | 0.99              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:109:PRO:CA  | 4:Z:154:ASP:CA[1_556]  | 1.21                     | 0.99              |
| 4:2:118:LYS:O   | 4:Z:340:TRP:CD1[1_556] | 1.21                     | 0.99              |
| 4:1:295:ALA:CA  | 4:Y:319:ALA:CB[1_556]  | 1.21                     | 0.99              |
| 4:1:210:ARG:O   | 4:Y:193:LEU:CD1[1_556] | 1.21                     | 0.99              |
| 4:2:82:MET:C    | 4:Z:30:VAL:CB[1_556]   | 1.21                     | 0.99              |
| 4:1:11:ASP:OD2  | 4:Y:305:MET:CB[1_556]  | 1.21                     | 0.99              |
| 4:0:153:LEU:CA  | 4:X:262:PHE:CE1[1_556] | 1.21                     | 0.99              |
| 4:1:286:ASP:C   | 4:Y:283:MET:CG[1_556]  | 1.21                     | 0.99              |
| 4:2:274:ILE:CG1 | 4:Z:263:GLN:C[1_556]   | 1.21                     | 0.99              |
| 4:0:12:ASN:ND2  | 4:X:336:LYS:CB[1_556]  | 1.21                     | 0.99              |
| 4:3:233:SER:CB  | 4:Z:367:PRO:CB[1_556]  | 1.21                     | 0.99              |
| 4:1:109:PRO:CA  | 4:Y:154:ASP:CA[1_556]  | 1.21                     | 0.99              |
| 4:0:309:ILE:CG1 | 4:X:259:GLU:CD[1_556]  | 1.21                     | 0.99              |
| 4:1:272:ALA:CA  | 4:Y:270:GLU:C[1_556]   | 1.21                     | 0.99              |
| 4:2:198:TYR:N   | 4:Y:75:ILE:CB[1_556]   | 1.21                     | 0.99              |
| 4:3:196:ARG:CD  | 4:Z:115:ASN:CB[1_556]  | 1.21                     | 0.99              |
| 4:0:167:GLU:N   | 4:X:294:TYR:O[1_556]   | 1.21                     | 0.99              |
| 4:2:274:ILE:CG1 | 4:Z:263:GLN:N[1_556]   | 1.21                     | 0.99              |
| 4:0:141:SER:C   | 4:X:310:ALA:CB[1_556]  | 1.21                     | 0.99              |
| 4:2:267:ILE:N   | 4:Y:173:HIS:CB[1_556]  | 1.22                     | 0.98              |
| 4:0:304:THR:C   | 4:X:223:PHE:CE1[1_556] | 1.22                     | 0.98              |
| 4:2:59:GLN:NE2  | 4:Z:208:ILE:N[1_556]   | 1.22                     | 0.98              |
| 4:0:60:SER:CA   | 4:X:243:PRO:CB[1_556]  | 1.22                     | 0.98              |
| 4:1:105:LEU:CB  | 4:Y:334:GLU:O[1_556]   | 1.22                     | 0.98              |
| 4:2:159:VAL:N   | 4:Z:181:ALA:O[1_556]   | 1.22                     | 0.98              |
| 4:1:82:MET:C    | 4:Y:30:VAL:CB[1_556]   | 1.22                     | 0.98              |
| 4:1:186:THR:C   | 4:Y:191:LYS:N[1_556]   | 1.22                     | 0.98              |
| 4:1:114:ALA:C   | 4:Y:106:THR:OG1[1_556] | 1.22                     | 0.98              |
| 4:2:167:GLU:N   | 4:Z:294:TYR:O[1_556]   | 1.22                     | 0.98              |
| 4:3:197:GLY:CA  | 4:Z:75:ILE:C[1_556]    | 1.22                     | 0.98              |
| 4:1:197:GLY:CA  | 4:X:75:ILE:C[1_556]    | 1.22                     | 0.98              |
| 4:2:337:TYR:CA  | 4:Z:307:PRO:CG[1_556]  | 1.22                     | 0.98              |
| 4:0:237:GLU:OE2 | 4:W:114:ALA:O[1_556]   | 1.22                     | 0.98              |
| 4:0:252:ASN:CG  | 4:W:113:LYS:O[1_556]   | 1.22                     | 0.98              |
| 4:0:82:MET:C    | 4:X:30:VAL:CB[1_556]   | 1.22                     | 0.98              |
| 4:0:272:ALA:CA  | 4:X:270:GLU:C[1_556]   | 1.22                     | 0.98              |
| 4:2:107:GLU:CA  | 4:Z:301:GLY:N[1_556]   | 1.22                     | 0.98              |
| 4:1:62:ARG:CB   | 4:Y:204:ALA:CA[1_556]  | 1.22                     | 0.98              |
| 4:1:150:GLY:CA  | 4:Y:317:ILE:CG1[1_556] | 1.22                     | 0.98              |
| 4:0:169:TYR:N   | 4:X:296:ASN:C[1_556]   | 1.22                     | 0.98              |
| 4:1:67:LEU:CA   | 4:Y:62:ARG:NH1[1_556]  | 1.22                     | 0.98              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:107:GLU:CA  | 4:Y:301:GLY:N[1_556]   | 1.22                     | 0.98              |
| 4:2:178:LEU:O   | 4:Z:180:LEU:CB[1_556]  | 1.22                     | 0.98              |
| 4:3:63:GLY:O    | 4:Y:289:ILE:N[1_556]   | 1.22                     | 0.98              |
| 4:1:41:GLN:CA   | 4:W:167:GLU:OE2[1_556] | 1.22                     | 0.98              |
| 4:1:335:ARG:CD  | 4:Y:220:ALA:N[1_556]   | 1.22                     | 0.98              |
| 4:2:79:TRP:CE3  | 4:Z:18:LYS:CA[1_556]   | 1.22                     | 0.98              |
| 4:0:30:VAL:CG1  | 4:X:215:LYS:CA[1_556]  | 1.22                     | 0.98              |
| 4:0:274:ILE:CG1 | 4:X:263:GLN:N[1_556]   | 1.22                     | 0.98              |
| 4:1:304:THR:CB  | 4:Y:223:PHE:CZ[1_556]  | 1.22                     | 0.98              |
| 4:1:169:TYR:N   | 4:Y:296:ASN:C[1_556]   | 1.22                     | 0.98              |
| 4:0:159:VAL:N   | 4:X:181:ALA:O[1_556]   | 1.22                     | 0.98              |
| 4:1:164:PRO:N   | 4:Y:278:THR:OG1[1_556] | 1.22                     | 0.98              |
| 4:2:305:MET:CA  | 4:Z:255:PHE:CD1[1_556] | 1.22                     | 0.98              |
| 4:0:368:SER:CB  | 4:X:346:LEU:CG[1_556]  | 1.22                     | 0.98              |
| 4:2:62:ARG:CB   | 4:Z:204:ALA:CA[1_556]  | 1.22                     | 0.98              |
| 4:1:265:SER:O   | 4:X:173:HIS:CE1[1_556] | 1.22                     | 0.98              |
| 4:1:267:ILE:N   | 4:X:173:HIS:CB[1_556]  | 1.22                     | 0.98              |
| 4:1:296:ASN:C   | 4:Y:315:LYS:O[1_556]   | 1.22                     | 0.98              |
| 4:0:186:THR:C   | 4:X:191:LYS:N[1_556]   | 1.22                     | 0.98              |
| 4:0:336:LYS:CA  | 4:X:218:TYR:CA[1_556]  | 1.22                     | 0.98              |
| 4:0:196:ARG:CD  | 4:W:115:ASN:CB[1_556]  | 1.22                     | 0.98              |
| 4:2:290:ARG:C   | 4:Z:320:LEU:O[1_556]   | 1.23                     | 0.97              |
| 4:2:148:THR:C   | 4:Z:327:ILE:C[1_556]   | 1.23                     | 0.97              |
| 4:1:121:GLN:CG  | 4:Y:9:VAL:N[1_556]     | 1.23                     | 0.97              |
| 4:1:295:ALA:C   | 4:Y:319:ALA:CB[1_556]  | 1.23                     | 0.97              |
| 4:0:212:ILE:CB  | 4:X:196:ARG:CA[1_556]  | 1.23                     | 0.97              |
| 4:2:189:LEU:CD1 | 4:Z:195:GLU:CG[1_556]  | 1.23                     | 0.97              |
| 4:2:136:ILE:C   | 4:Z:299:MET:C[1_556]   | 1.23                     | 0.97              |
| 4:1:74:GLY:C    | 4:Y:156:GLY:C[1_556]   | 1.23                     | 0.97              |
| 4:0:148:THR:C   | 4:X:327:ILE:C[1_556]   | 1.23                     | 0.97              |
| 4:0:163:VAL:CA  | 4:X:278:THR:OG1[1_556] | 1.23                     | 0.97              |
| 4:2:104:LEU:C   | 4:Z:334:GLU:CB[1_556]  | 1.23                     | 0.97              |
| 4:1:141:SER:C   | 4:Y:310:ALA:CB[1_556]  | 1.23                     | 0.97              |
| 4:2:332:PRO:N   | 4:Z:221:LEU:CG[1_556]  | 1.23                     | 0.97              |
| 4:1:63:GLY:O    | 4:W:289:ILE:N[1_556]   | 1.23                     | 0.97              |
| 4:2:109:PRO:N   | 4:Z:154:ASP:C[1_556]   | 1.23                     | 0.97              |
| 4:0:109:PRO:N   | 4:X:154:ASP:C[1_556]   | 1.23                     | 0.97              |
| 4:0:109:PRO:CA  | 4:X:154:ASP:CA[1_556]  | 1.23                     | 0.97              |
| 4:1:152:VAL:CA  | 4:Y:313:MET:SD[1_556]  | 1.23                     | 0.97              |
| 4:1:309:ILE:CG1 | 4:Y:259:GLU:CD[1_556]  | 1.23                     | 0.97              |
| 4:1:151:ILE:CG1 | 4:Y:275:HIS:O[1_556]   | 1.23                     | 0.97              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:210:ARG:O   | 4:Z:193:LEU:CD1[1_556] | 1.23                     | 0.97              |
| 4:1:83:GLU:N    | 4:Y:30:VAL:CA[1_556]   | 1.23                     | 0.97              |
| 4:0:296:ASN:CB  | 4:X:318:THR:OG1[1_556] | 1.23                     | 0.97              |
| 4:1:16:LEU:CA   | 4:Y:214:GLU:CG[1_556]  | 1.23                     | 0.97              |
| 4:2:12:ASN:ND2  | 4:Z:336:LYS:CB[1_556]  | 1.23                     | 0.97              |
| 4:1:232:SER:CA  | 4:X:369:ILE:CG2[1_556] | 1.23                     | 0.97              |
| 4:2:296:ASN:CB  | 4:Z:318:THR:OG1[1_556] | 1.23                     | 0.97              |
| 4:2:163:VAL:CA  | 4:Z:278:THR:OG1[1_556] | 1.23                     | 0.97              |
| 4:3:191:LYS:CE  | 4:Z:110:LEU:CG[1_556]  | 1.23                     | 0.97              |
| 4:2:137:GLN:NE2 | 4:Z:301:GLY:C[1_556]   | 1.23                     | 0.97              |
| 4:2:60:SER:CA   | 4:Z:243:PRO:CB[1_556]  | 1.23                     | 0.97              |
| 4:2:167:GLU:OE2 | 4:Z:326:LYS:CB[1_556]  | 1.23                     | 0.97              |
| 4:0:161:HIS:CE1 | 4:X:160:THR:OG1[1_556] | 1.23                     | 0.97              |
| 4:3:232:SER:CA  | 4:Z:369:ILE:CG2[1_556] | 1.23                     | 0.97              |
| 4:1:122:ILE:CB  | 4:Y:19:ALA:O[1_556]    | 1.23                     | 0.97              |
| 4:0:372:ARG:CD  | 4:X:142:LEU:C[1_556]   | 1.23                     | 0.97              |
| 4:1:196:ARG:CD  | 4:X:115:ASN:CB[1_556]  | 1.23                     | 0.97              |
| 4:2:147:ARG:CA  | 4:Z:314:GLN:NE2[1_556] | 1.23                     | 0.97              |
| 4:0:189:LEU:CD1 | 4:X:195:GLU:CG[1_556]  | 1.23                     | 0.97              |
| 4:0:178:LEU:O   | 4:X:180:LEU:CB[1_556]  | 1.23                     | 0.97              |
| 4:2:368:SER:CB  | 4:Z:346:LEU:CG[1_556]  | 1.23                     | 0.97              |
| 4:0:167:GLU:OE2 | 4:X:326:LYS:CB[1_556]  | 1.23                     | 0.97              |
| 4:3:250:ILE:C   | 4:Z:114:ALA:CB[1_556]  | 1.23                     | 0.97              |
| 4:2:212:ILE:CB  | 4:Z:196:ARG:CA[1_556]  | 1.23                     | 0.97              |
| 4:3:196:ARG:CZ  | 4:Z:115:ASN:CA[1_556]  | 1.23                     | 0.97              |
| 4:0:368:SER:CA  | 4:X:346:LEU:CD2[1_556] | 1.23                     | 0.97              |
| 4:0:162:ASN:OD1 | 4:X:273:GLY:CA[1_556]  | 1.23                     | 0.97              |
| 4:2:180:LEU:CB  | 4:Z:267:ILE:CD1[1_556] | 1.23                     | 0.97              |
| 4:0:290:ARG:C   | 4:X:320:LEU:O[1_556]   | 1.23                     | 0.97              |
| 4:2:335:ARG:CD  | 4:Z:220:ALA:N[1_556]   | 1.24                     | 0.96              |
| 4:2:164:PRO:N   | 4:Z:278:THR:OG1[1_556] | 1.24                     | 0.96              |
| 4:3:265:SER:O   | 4:Z:173:HIS:CE1[1_556] | 1.24                     | 0.96              |
| 4:1:335:ARG:NH1 | 4:Y:220:ALA:CB[1_556]  | 1.24                     | 0.96              |
| 4:0:267:ILE:N   | 4:W:173:HIS:CB[1_556]  | 1.24                     | 0.96              |
| 4:1:80:ASP:CA   | 4:Y:31:PHE:CD1[1_556]  | 1.24                     | 0.96              |
| 4:0:337:TYR:CA  | 4:X:307:PRO:CG[1_556]  | 1.24                     | 0.96              |
| 4:1:163:VAL:CA  | 4:Y:278:THR:OG1[1_556] | 1.24                     | 0.96              |
| 4:0:79:TRP:CE3  | 4:X:18:LYS:CA[1_556]   | 1.24                     | 0.96              |
| 4:2:372:ARG:CD  | 4:Z:142:LEU:C[1_556]   | 1.24                     | 0.96              |
| 4:2:30:VAL:CG1  | 4:Z:215:LYS:CA[1_556]  | 1.24                     | 0.96              |
| 4:1:191:LYS:CE  | 4:X:110:LEU:CG[1_556]  | 1.24                     | 0.96              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:293:LEU:C   | 4:Y:320:LEU:N[1_556]   | 1.24                     | 0.96              |
| 4:1:136:ILE:CA  | 4:Y:299:MET:O[1_556]   | 1.24                     | 0.96              |
| 4:3:229:THR:C   | 4:Z:368:SER:C[1_556]   | 1.24                     | 0.96              |
| 4:1:37:ARG:CA   | 4:Y:60:SER:CB[1_556]   | 1.24                     | 0.96              |
| 4:1:362:TYR:CZ  | 4:Y:22:ALA:CB[1_556]   | 1.24                     | 0.96              |
| 4:2:214:GLU:C   | 4:Z:253:GLU:OE2[1_556] | 1.24                     | 0.96              |
| 4:2:80:ASP:CA   | 4:Z:31:PHE:CD1[1_556]  | 1.24                     | 0.96              |
| 4:2:336:LYS:CA  | 4:Z:218:TYR:CA[1_556]  | 1.24                     | 0.96              |
| 4:1:12:ASN:ND2  | 4:Y:336:LYS:CB[1_556]  | 1.24                     | 0.96              |
| 4:1:168:GLY:C   | 4:Y:297:ASN:N[1_556]   | 1.24                     | 0.96              |
| 4:0:206:ARG:CB  | 4:X:199:SER:C[1_556]   | 1.24                     | 0.96              |
| 4:0:332:PRO:N   | 4:X:221:LEU:CG[1_556]  | 1.24                     | 0.96              |
| 4:0:77:THR:O    | 4:X:33:SER:CB[1_556]   | 1.24                     | 0.96              |
| 4:3:232:SER:N   | 4:Z:369:ILE:CG2[1_556] | 1.24                     | 0.96              |
| 4:3:252:ASN:O   | 4:Z:113:LYS:CE[1_556]  | 1.24                     | 0.96              |
| 4:2:161:HIS:CE1 | 4:Z:160:THR:OG1[1_556] | 1.24                     | 0.96              |
| 4:2:123:MET:CG  | 4:Z:26:ALA:CA[1_556]   | 1.24                     | 0.96              |
| 4:0:104:LEU:C   | 4:X:334:GLU:CB[1_556]  | 1.24                     | 0.96              |
| 4:1:252:ASN:O   | 4:X:113:LYS:CE[1_556]  | 1.24                     | 0.96              |
| 4:1:332:PRO:N   | 4:Y:221:LEU:CB[1_556]  | 1.24                     | 0.96              |
| 4:1:368:SER:CA  | 4:Y:346:LEU:CG[1_556]  | 1.24                     | 0.96              |
| 4:0:369:ILE:CG2 | 4:X:346:LEU:N[1_556]   | 1.24                     | 0.96              |
| 4:0:214:GLU:CA  | 4:X:253:GLU:CD[1_556]  | 1.24                     | 0.96              |
| 4:0:80:ASP:CA   | 4:X:31:PHE:CD1[1_556]  | 1.24                     | 0.96              |
| 4:1:367:PRO:N   | 4:Y:347:ALA:CB[1_556]  | 1.24                     | 0.96              |
| 4:1:60:SER:CA   | 4:Y:243:PRO:CB[1_556]  | 1.24                     | 0.96              |
| 4:1:296:ASN:O   | 4:Y:316:GLU:C[1_556]   | 1.24                     | 0.96              |
| 4:0:180:LEU:CB  | 4:X:267:ILE:CD1[1_556] | 1.24                     | 0.96              |
| 4:0:147:ARG:CA  | 4:X:314:GLN:NE2[1_556] | 1.24                     | 0.96              |
| 4:1:229:THR:C   | 4:X:368:SER:C[1_556]   | 1.24                     | 0.96              |
| 4:0:305:MET:CG  | 4:X:255:PHE:CB[1_556]  | 1.24                     | 0.96              |
| 4:0:152:VAL:CG2 | 4:X:313:MET:CG[1_556]  | 1.24                     | 0.96              |
| 4:1:250:ILE:C   | 4:X:114:ALA:CB[1_556]  | 1.24                     | 0.96              |
| 4:1:162:ASN:OD1 | 4:Y:273:GLY:CA[1_556]  | 1.24                     | 0.96              |
| 4:0:210:ARG:O   | 4:X:193:LEU:CD1[1_556] | 1.24                     | 0.96              |
| 4:0:136:ILE:C   | 4:X:299:MET:C[1_556]   | 1.24                     | 0.96              |
| 4:2:173:HIS:CB  | 4:Z:174:ALA:C[1_556]   | 1.24                     | 0.96              |
| 4:0:12:ASN:ND2  | 4:X:336:LYS:CG[1_556]  | 1.24                     | 0.96              |
| 4:1:125:GLU:CB  | 4:Y:21:PHE:CA[1_556]   | 1.24                     | 0.96              |
| 4:0:64:ILE:N    | 4:V:288:ASP:O[1_556]   | 1.24                     | 0.96              |
| 4:3:267:ILE:N   | 4:Z:173:HIS:CB[1_556]  | 1.24                     | 0.96              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:62:ARG:NH2  | 4:Z:205:GLU:CA[1_556]  | 1.25                     | 0.95              |
| 4:1:141:SER:OG  | 4:Y:309:ILE:CG2[1_556] | 1.25                     | 0.95              |
| 4:2:208:ILE:O   | 4:Z:198:TYR:CE2[1_556] | 1.25                     | 0.95              |
| 4:2:196:ARG:CD  | 4:Y:115:ASN:CB[1_556]  | 1.25                     | 0.95              |
| 4:1:118:LYS:O   | 4:Y:340:TRP:CD1[1_556] | 1.25                     | 0.95              |
| 4:1:167:GLU:CA  | 4:Y:295:ALA:N[1_556]   | 1.25                     | 0.95              |
| 4:2:152:VAL:CG2 | 4:Z:313:MET:CG[1_556]  | 1.25                     | 0.95              |
| 4:1:196:ARG:CZ  | 4:X:115:ASN:CA[1_556]  | 1.25                     | 0.95              |
| 4:2:12:ASN:ND2  | 4:Z:336:LYS:CG[1_556]  | 1.25                     | 0.95              |
| 4:0:299:MET:N   | 4:X:312:ARG:CG[1_556]  | 1.25                     | 0.95              |
| 4:2:77:THR:N    | 4:Z:16:LEU:N[1_556]    | 1.25                     | 0.95              |
| 4:1:290:ARG:C   | 4:Y:320:LEU:O[1_556]   | 1.25                     | 0.95              |
| 4:0:164:PRO:N   | 4:X:278:THR:OG1[1_556] | 1.25                     | 0.95              |
| 4:2:112:PRO:CB  | 4:Z:137:GLN:CD[1_556]  | 1.25                     | 0.95              |
| 4:2:299:MET:N   | 4:Z:312:ARG:CG[1_556]  | 1.25                     | 0.95              |
| 4:2:368:SER:CA  | 4:Z:346:LEU:CD2[1_556] | 1.25                     | 0.95              |
| 4:2:369:ILE:CG2 | 4:Z:346:LEU:N[1_556]   | 1.25                     | 0.95              |
| 4:0:365:ALA:N   | 4:X:349:LEU:CA[1_556]  | 1.25                     | 0.95              |
| 4:0:214:GLU:C   | 4:X:253:GLU:OE2[1_556] | 1.25                     | 0.95              |
| 4:1:299:MET:SD  | 4:Y:312:ARG:NH2[1_556] | 1.25                     | 0.95              |
| 4:2:120:THR:N   | 4:Z:340:TRP:CD2[1_556] | 1.25                     | 0.95              |
| 4:0:77:THR:N    | 4:X:16:LEU:N[1_556]    | 1.25                     | 0.95              |
| 4:0:120:THR:O   | 4:X:340:TRP:CZ3[1_556] | 1.25                     | 0.95              |
| 4:0:338:SER:CB  | 4:X:308:GLY:CA[1_556]  | 1.25                     | 0.95              |
| 4:1:210:ARG:CB  | 4:Y:193:LEU:CD2[1_556] | 1.25                     | 0.95              |
| 4:0:74:GLY:C    | 4:X:156:GLY:C[1_556]   | 1.25                     | 0.95              |
| 4:1:133:TYR:OH  | 4:Y:145:SER:CB[1_556]  | 1.25                     | 0.95              |
| 4:2:77:THR:O    | 4:Z:33:SER:CB[1_556]   | 1.25                     | 0.95              |
| 4:2:151:ILE:CD1 | 4:Z:275:HIS:O[1_556]   | 1.25                     | 0.95              |
| 4:2:64:ILE:N    | 4:X:288:ASP:O[1_556]   | 1.25                     | 0.95              |
| 4:2:295:ALA:CA  | 4:Z:319:ALA:CB[1_556]  | 1.25                     | 0.95              |
| 4:0:332:PRO:CG  | 4:X:221:LEU:CG[1_556]  | 1.25                     | 0.95              |
| 4:0:137:GLN:NE2 | 4:X:301:GLY:C[1_556]   | 1.25                     | 0.95              |
| 4:0:194:THR:C   | 4:W:75:ILE:CG1[1_556]  | 1.25                     | 0.95              |
| 4:1:297:ASN:CB  | 4:Y:316:GLU:OE1[1_556] | 1.25                     | 0.95              |
| 4:0:227:MET:CG  | 4:W:372:ARG:O[1_556]   | 1.25                     | 0.95              |
| 4:1:331:ALA:C   | 4:Y:221:LEU:CA[1_556]  | 1.25                     | 0.95              |
| 4:2:206:ARG:CB  | 4:Z:199:SER:C[1_556]   | 1.25                     | 0.95              |
| 4:0:208:ILE:O   | 4:X:198:TYR:CE2[1_556] | 1.25                     | 0.95              |
| 4:1:171:LEU:CG  | 4:Y:282:ILE:CG1[1_556] | 1.25                     | 0.95              |
| 4:2:214:GLU:CA  | 4:Z:253:GLU:CD[1_556]  | 1.25                     | 0.95              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:335:ARG:CD  | 4:X:220:ALA:N[1_556]   | 1.25                     | 0.95              |
| 4:1:212:ILE:CD1 | 4:Y:196:ARG:O[1_556]   | 1.25                     | 0.95              |
| 4:1:208:ILE:CA  | 4:Y:198:TYR:CG[1_556]  | 1.25                     | 0.95              |
| 4:0:112:PRO:CB  | 4:X:137:GLN:CD[1_556]  | 1.26                     | 0.94              |
| 4:1:106:THR:N   | 4:Y:335:ARG:C[1_556]   | 1.26                     | 0.94              |
| 4:0:274:ILE:CG2 | 4:X:263:GLN:CG[1_556]  | 1.26                     | 0.94              |
| 4:1:180:LEU:CB  | 4:Y:267:ILE:CD1[1_556] | 1.26                     | 0.94              |
| 4:2:162:ASN:OD1 | 4:Z:273:GLY:CA[1_556]  | 1.26                     | 0.94              |
| 4:1:186:THR:O   | 4:Y:191:LYS:CA[1_556]  | 1.26                     | 0.94              |
| 4:0:123:MET:CG  | 4:X:26:ALA:CA[1_556]   | 1.26                     | 0.94              |
| 4:2:138:ALA:CA  | 4:Z:299:MET:SD[1_556]  | 1.26                     | 0.94              |
| 4:1:142:LEU:CG  | 4:Y:329:ILE:CG1[1_556] | 1.26                     | 0.94              |
| 4:0:295:ALA:CA  | 4:X:319:ALA:CB[1_556]  | 1.26                     | 0.94              |
| 4:0:164:PRO:CG  | 4:X:279:TYR:N[1_556]   | 1.26                     | 0.94              |
| 4:0:171:LEU:CG  | 4:X:282:ILE:CG1[1_556] | 1.26                     | 0.94              |
| 4:1:212:ILE:CA  | 4:Y:196:ARG:CB[1_556]  | 1.26                     | 0.94              |
| 4:0:41:GLN:CA   | 4:V:167:GLU:OE2[1_556] | 1.26                     | 0.94              |
| 4:0:162:ASN:C   | 4:X:274:ILE:C[1_556]   | 1.26                     | 0.94              |
| 4:0:120:THR:OG1 | 4:X:341:ILE:N[1_556]   | 1.26                     | 0.94              |
| 4:1:140:LEU:CG  | 4:Y:331:ALA:CA[1_556]  | 1.26                     | 0.94              |
| 4:0:86:TRP:CE2  | 4:X:337:TYR:OH[1_556]  | 1.26                     | 0.94              |
| 4:2:147:ARG:CG  | 4:Z:314:GLN:CD[1_556]  | 1.26                     | 0.94              |
| 4:1:157:ASP:O   | 4:Y:185:LEU:CA[1_556]  | 1.26                     | 0.94              |
| 4:1:105:LEU:C   | 4:Y:334:GLU:O[1_556]   | 1.26                     | 0.94              |
| 4:0:120:THR:N   | 4:X:340:TRP:CD2[1_556] | 1.26                     | 0.94              |
| 4:2:232:SER:C   | 4:Y:366:GLY:O[1_556]   | 1.26                     | 0.94              |
| 4:0:337:TYR:C   | 4:X:307:PRO:CB[1_556]  | 1.26                     | 0.94              |
| 4:1:232:SER:N   | 4:X:369:ILE:CG2[1_556] | 1.26                     | 0.94              |
| 4:0:303:THR:CB  | 4:X:257:CYS:CA[1_556]  | 1.26                     | 0.94              |
| 4:2:184:ASP:OD1 | 4:Z:184:ASP:O[1_556]   | 1.26                     | 0.94              |
| 4:2:365:ALA:N   | 4:Z:349:LEU:CA[1_556]  | 1.26                     | 0.94              |
| 4:0:140:LEU:CG  | 4:X:331:ALA:CA[1_556]  | 1.26                     | 0.94              |
| 4:0:62:ARG:NH2  | 4:X:205:GLU:CA[1_556]  | 1.26                     | 0.94              |
| 4:2:164:PRO:CG  | 4:Z:278:THR:CA[1_556]  | 1.26                     | 0.94              |
| 4:3:192:ILE:C   | 4:Z:110:LEU:O[1_556]   | 1.26                     | 0.94              |
| 4:1:112:PRO:C   | 4:Y:137:GLN:CB[1_556]  | 1.26                     | 0.94              |
| 4:2:305:MET:CG  | 4:Z:255:PHE:CB[1_556]  | 1.26                     | 0.94              |
| 4:2:303:THR:CB  | 4:Z:257:CYS:CA[1_556]  | 1.26                     | 0.94              |
| 4:2:16:LEU:N    | 4:Z:214:GLU:CG[1_556]  | 1.26                     | 0.94              |
| 4:0:173:HIS:CB  | 4:X:174:ALA:C[1_556]   | 1.26                     | 0.94              |
| 4:1:141:SER:CA  | 4:Y:310:ALA:N[1_556]   | 1.26                     | 0.94              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:337:TYR:C   | 4:Z:307:PRO:CB[1_556]  | 1.26                     | 0.94              |
| 4:1:164:PRO:CG  | 4:Y:278:THR:CA[1_556]  | 1.26                     | 0.94              |
| 4:2:114:ALA:CA  | 4:Z:106:THR:CA[1_556]  | 1.26                     | 0.94              |
| 4:0:331:ALA:CA  | 4:X:222:ASP:N[1_556]   | 1.26                     | 0.94              |
| 4:0:79:TRP:CB   | 4:X:17:VAL:CB[1_556]   | 1.26                     | 0.94              |
| 4:2:194:THR:C   | 4:Y:75:ILE:CG1[1_556]  | 1.26                     | 0.94              |
| 4:2:140:LEU:CG  | 4:Z:331:ALA:CA[1_556]  | 1.26                     | 0.94              |
| 4:1:368:SER:C   | 4:Y:346:LEU:CG[1_556]  | 1.26                     | 0.94              |
| 4:1:157:ASP:O   | 4:Y:186:THR:N[1_556]   | 1.26                     | 0.94              |
| 4:2:168:GLY:N   | 4:Z:295:ALA:C[1_556]   | 1.26                     | 0.94              |
| 4:0:370:VAL:CG1 | 4:X:342:GLY:C[1_556]   | 1.26                     | 0.94              |
| 4:2:274:ILE:CG2 | 4:Z:263:GLN:CG[1_556]  | 1.26                     | 0.94              |
| 4:1:194:THR:CB  | 4:X:177:ARG:NH1[1_556] | 1.27                     | 0.93              |
| 4:1:206:ARG:N   | 4:Y:199:SER:CB[1_556]  | 1.27                     | 0.93              |
| 4:0:176:MET:N   | 4:X:277:THR:CG2[1_556] | 1.27                     | 0.93              |
| 4:3:195:GLU:OE2 | 4:Z:110:LEU:N[1_556]   | 1.27                     | 0.93              |
| 4:4:64:ILE:N    | 4:Z:288:ASP:O[1_556]   | 1.27                     | 0.93              |
| 4:0:150:GLY:O   | 4:X:317:ILE:CG1[1_556] | 1.27                     | 0.93              |
| 4:0:16:LEU:CB   | 4:X:214:GLU:C[1_556]   | 1.27                     | 0.93              |
| 4:2:370:VAL:CG1 | 4:Z:342:GLY:C[1_556]   | 1.27                     | 0.93              |
| 4:2:120:THR:O   | 4:Z:340:TRP:CZ3[1_556] | 1.27                     | 0.93              |
| 4:2:227:MET:CG  | 4:Y:372:ARG:O[1_556]   | 1.27                     | 0.93              |
| 4:2:152:VAL:CA  | 4:Z:313:MET:SD[1_556]  | 1.27                     | 0.93              |
| 4:2:82:MET:CG   | 4:Z:30:VAL:CG1[1_556]  | 1.27                     | 0.93              |
| 4:0:232:SER:C   | 4:W:366:GLY:O[1_556]   | 1.27                     | 0.93              |
| 4:1:332:PRO:CG  | 4:Y:221:LEU:CG[1_556]  | 1.27                     | 0.93              |
| 4:1:166:TYR:CG  | 4:Y:294:TYR:CB[1_556]  | 1.27                     | 0.93              |
| 4:2:338:SER:CB  | 4:Z:308:GLY:CA[1_556]  | 1.27                     | 0.93              |
| 4:2:164:PRO:CG  | 4:Z:279:TYR:N[1_556]   | 1.27                     | 0.93              |
| 4:2:70:PRO:CB   | 4:Z:16:LEU:CD1[1_556]  | 1.27                     | 0.93              |
| 4:2:176:MET:N   | 4:Z:277:THR:CG2[1_556] | 1.27                     | 0.93              |
| 4:1:192:ILE:C   | 4:X:110:LEU:O[1_556]   | 1.27                     | 0.93              |
| 4:0:232:SER:N   | 4:W:369:ILE:CG2[1_556] | 1.27                     | 0.93              |
| 4:2:150:GLY:O   | 4:Z:317:ILE:CG1[1_556] | 1.27                     | 0.93              |
| 4:0:209:VAL:CG1 | 4:X:194:THR:CA[1_556]  | 1.27                     | 0.93              |
| 4:1:299:MET:CG  | 4:Y:312:ARG:CZ[1_556]  | 1.27                     | 0.93              |
| 4:2:233:SER:N   | 4:Y:367:PRO:CA[1_556]  | 1.27                     | 0.93              |
| 4:2:304:THR:O   | 4:Z:223:PHE:CE1[1_556] | 1.27                     | 0.93              |
| 4:3:39:ARG:C    | 4:Y:166:TYR:CE2[1_556] | 1.27                     | 0.93              |
| 4:1:195:GLU:OE2 | 4:X:110:LEU:N[1_556]   | 1.27                     | 0.93              |
| 4:1:299:MET:N   | 4:Y:312:ARG:CG[1_556]  | 1.27                     | 0.93              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:141:SER:CB  | 4:X:309:ILE:C[1_556]   | 1.27                     | 0.93              |
| 4:1:303:THR:CB  | 4:Y:257:CYS:CA[1_556]  | 1.27                     | 0.93              |
| 4:1:161:HIS:C   | 4:Y:274:ILE:CB[1_556]  | 1.27                     | 0.93              |
| 4:1:337:TYR:C   | 4:Y:307:PRO:CB[1_556]  | 1.27                     | 0.93              |
| 4:2:105:LEU:C   | 4:Z:334:GLU:O[1_556]   | 1.27                     | 0.93              |
| 4:2:332:PRO:CG  | 4:Z:221:LEU:CG[1_556]  | 1.27                     | 0.93              |
| 4:0:59:GLN:CD   | 4:X:208:ILE:CB[1_556]  | 1.27                     | 0.93              |
| 4:1:304:THR:C   | 4:Y:223:PHE:CE1[1_556] | 1.27                     | 0.93              |
| 4:0:114:ALA:CA  | 4:X:106:THR:CA[1_556]  | 1.27                     | 0.93              |
| 4:0:168:GLY:C   | 4:X:297:ASN:N[1_556]   | 1.27                     | 0.93              |
| 4:3:194:THR:CB  | 4:Z:177:ARG:NH1[1_556] | 1.27                     | 0.93              |
| 4:0:138:ALA:CA  | 4:X:299:MET:SD[1_556]  | 1.27                     | 0.93              |
| 4:1:164:PRO:CG  | 4:Y:279:TYR:N[1_556]   | 1.27                     | 0.93              |
| 4:1:209:VAL:CG1 | 4:Y:194:THR:CA[1_556]  | 1.27                     | 0.93              |
| 4:2:277:THR:OG1 | 4:Z:271:SER:C[1_556]   | 1.27                     | 0.93              |
| 4:0:286:ASP:C   | 4:X:283:MET:CG[1_556]  | 1.27                     | 0.93              |
| 4:2:286:ASP:C   | 4:Z:283:MET:CG[1_556]  | 1.27                     | 0.93              |
| 4:2:184:ASP:N   | 4:Z:187:ASP:C[1_556]   | 1.27                     | 0.93              |
| 4:2:74:GLY:C    | 4:Z:156:GLY:C[1_556]   | 1.27                     | 0.93              |
| 4:1:184:ASP:N   | 4:Y:187:ASP:C[1_556]   | 1.27                     | 0.93              |
| 4:1:120:THR:N   | 4:Y:340:TRP:CD2[1_556] | 1.27                     | 0.93              |
| 4:2:16:LEU:CB   | 4:Z:214:GLU:C[1_556]   | 1.27                     | 0.93              |
| 4:0:261:LEU:CG  | 4:X:266:PHE:CB[1_556]  | 1.27                     | 0.93              |
| 4:2:86:TRP:CE2  | 4:Z:337:TYR:OH[1_556]  | 1.27                     | 0.93              |
| 4:1:141:SER:CB  | 4:Y:309:ILE:C[1_556]   | 1.27                     | 0.93              |
| 4:2:179:ASP:N   | 4:Z:180:LEU:CB[1_556]  | 1.27                     | 0.93              |
| 4:0:141:SER:CA  | 4:X:310:ALA:N[1_556]   | 1.27                     | 0.93              |
| 4:1:366:GLY:O   | 4:Y:346:LEU:C[1_556]   | 1.27                     | 0.93              |
| 4:1:187:ASP:N   | 4:Y:191:LYS:CA[1_556]  | 1.27                     | 0.93              |
| 4:1:372:ARG:CD  | 4:Y:142:LEU:O[1_556]   | 1.27                     | 0.93              |
| 4:0:298:VAL:CG1 | 4:X:312:ARG:N[1_556]   | 1.27                     | 0.93              |
| 4:0:151:ILE:CD1 | 4:X:275:HIS:O[1_556]   | 1.28                     | 0.92              |
| 4:2:161:HIS:O   | 4:Z:274:ILE:CB[1_556]  | 1.28                     | 0.92              |
| 4:2:298:VAL:CG1 | 4:Z:312:ARG:N[1_556]   | 1.28                     | 0.92              |
| 4:2:186:THR:O   | 4:Z:191:LYS:CA[1_556]  | 1.28                     | 0.92              |
| 4:1:37:ARG:CG   | 4:Y:60:SER:OG[1_556]   | 1.28                     | 0.92              |
| 4:1:164:PRO:CG  | 4:Y:278:THR:C[1_556]   | 1.28                     | 0.92              |
| 4:2:158:GLY:O   | 4:Z:181:ALA:O[1_556]   | 1.28                     | 0.92              |
| 4:2:41:GLN:CA   | 4:X:167:GLU:OE2[1_556] | 1.28                     | 0.92              |
| 4:2:362:TYR:CZ  | 4:Z:22:ALA:CB[1_556]   | 1.28                     | 0.92              |
| 4:1:120:THR:N   | 4:Y:340:TRP:CG[1_556]  | 1.28                     | 0.92              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:277:THR:OG1 | 4:X:271:SER:C[1_556]   | 1.28                     | 0.92              |
| 4:2:367:PRO:N   | 4:Z:347:ALA:CB[1_556]  | 1.28                     | 0.92              |
| 4:1:82:MET:CG   | 4:Y:30:VAL:CG1[1_556]  | 1.28                     | 0.92              |
| 4:2:265:SER:C   | 4:Y:173:HIS:ND1[1_556] | 1.28                     | 0.92              |
| 4:0:184:ASP:OD1 | 4:X:184:ASP:O[1_556]   | 1.28                     | 0.92              |
| 4:1:151:ILE:CD1 | 4:Y:275:HIS:O[1_556]   | 1.28                     | 0.92              |
| 4:2:59:GLN:CD   | 4:Z:208:ILE:CB[1_556]  | 1.28                     | 0.92              |
| 4:0:183:ARG:CG  | 4:X:186:THR:C[1_556]   | 1.28                     | 0.92              |
| 4:2:79:TRP:CB   | 4:Z:17:VAL:CB[1_556]   | 1.28                     | 0.92              |
| 4:2:171:LEU:CG  | 4:Z:282:ILE:CG1[1_556] | 1.28                     | 0.92              |
| 4:2:261:LEU:CG  | 4:Z:266:PHE:CB[1_556]  | 1.28                     | 0.92              |
| 4:0:272:ALA:O   | 4:X:269:MET:O[1_556]   | 1.28                     | 0.92              |
| 4:2:120:THR:OG1 | 4:Z:341:ILE:N[1_556]   | 1.28                     | 0.92              |
| 4:2:151:ILE:CD1 | 4:Z:275:HIS:C[1_556]   | 1.28                     | 0.92              |
| 4:1:151:ILE:CD1 | 4:Y:275:HIS:C[1_556]   | 1.28                     | 0.92              |
| 4:0:40:HIS:NE2  | 4:V:166:TYR:CB[1_556]  | 1.28                     | 0.92              |
| 4:2:335:ARG:CB  | 4:Z:219:VAL:C[1_556]   | 1.28                     | 0.92              |
| 4:2:162:ASN:C   | 4:Z:274:ILE:C[1_556]   | 1.28                     | 0.92              |
| 4:2:332:PRO:N   | 4:Z:221:LEU:CB[1_556]  | 1.28                     | 0.92              |
| 4:2:141:SER:OG  | 4:Z:309:ILE:CG2[1_556] | 1.28                     | 0.92              |
| 4:1:176:MET:N   | 4:Y:277:THR:CG2[1_556] | 1.28                     | 0.92              |
| 4:2:150:GLY:CA  | 4:Z:317:ILE:CG1[1_556] | 1.28                     | 0.92              |
| 4:0:114:ALA:C   | 4:X:106:THR:OG1[1_556] | 1.28                     | 0.92              |
| 4:0:335:ARG:CB  | 4:X:219:VAL:C[1_556]   | 1.28                     | 0.92              |
| 4:0:152:VAL:CA  | 4:X:313:MET:SD[1_556]  | 1.28                     | 0.92              |
| 4:2:164:PRO:CG  | 4:Z:278:THR:C[1_556]   | 1.28                     | 0.92              |
| 4:0:179:ASP:N   | 4:X:180:LEU:CB[1_556]  | 1.28                     | 0.92              |
| 4:0:168:GLY:N   | 4:X:295:ALA:C[1_556]   | 1.28                     | 0.92              |
| 4:1:70:PRO:CB   | 4:Y:16:LEU:CD1[1_556]  | 1.28                     | 0.92              |
| 4:1:331:ALA:CA  | 4:Y:222:ASP:N[1_556]   | 1.28                     | 0.92              |
| 4:0:208:ILE:CA  | 4:X:198:TYR:CG[1_556]  | 1.28                     | 0.92              |
| 4:0:147:ARG:CG  | 4:X:314:GLN:CD[1_556]  | 1.28                     | 0.92              |
| 4:0:153:LEU:C   | 4:X:262:PHE:CE1[1_556] | 1.28                     | 0.92              |
| 4:2:168:GLY:C   | 4:Z:297:ASN:N[1_556]   | 1.28                     | 0.92              |
| 4:0:164:PRO:CG  | 4:X:278:THR:CA[1_556]  | 1.28                     | 0.92              |
| 4:0:299:MET:CG  | 4:X:312:ARG:CZ[1_556]  | 1.28                     | 0.92              |
| 4:0:332:PRO:N   | 4:X:221:LEU:CB[1_556]  | 1.28                     | 0.92              |
| 4:0:366:GLY:O   | 4:X:346:LEU:C[1_556]   | 1.28                     | 0.92              |
| 4:2:122:ILE:CB  | 4:Z:19:ALA:O[1_556]    | 1.28                     | 0.92              |
| 4:0:133:TYR:O   | 4:X:334:GLU:OE1[1_556] | 1.28                     | 0.92              |
| 4:1:148:THR:C   | 4:Y:327:ILE:C[1_556]   | 1.28                     | 0.92              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:184:ASP:N   | 4:X:187:ASP:C[1_556]   | 1.28                     | 0.92              |
| 4:1:127:PHE:CE2 | 4:Y:27:PRO:O[1_556]    | 1.28                     | 0.92              |
| 4:0:261:LEU:CD1 | 4:X:266:PHE:CE2[1_556] | 1.28                     | 0.92              |
| 4:2:196:ARG:NE  | 4:Y:115:ASN:CG[1_556]  | 1.28                     | 0.92              |
| 4:2:183:ARG:CG  | 4:Z:186:THR:C[1_556]   | 1.28                     | 0.92              |
| 4:0:335:ARG:CG  | 4:X:220:ALA:CA[1_556]  | 1.28                     | 0.92              |
| 4:0:82:MET:CG   | 4:X:30:VAL:CG1[1_556]  | 1.28                     | 0.92              |
| 4:0:186:THR:O   | 4:X:191:LYS:CA[1_556]  | 1.28                     | 0.92              |
| 4:0:70:PRO:CB   | 4:X:16:LEU:CD1[1_556]  | 1.28                     | 0.92              |
| 4:2:167:GLU:O   | 4:Z:295:ALA:O[1_556]   | 1.28                     | 0.92              |
| 4:1:372:ARG:CA  | 4:Y:143:TYR:CB[1_556]  | 1.28                     | 0.92              |
| 4:0:157:ASP:O   | 4:X:185:LEU:CA[1_556]  | 1.28                     | 0.92              |
| 4:1:39:ARG:C    | 4:W:166:TYR:CE2[1_556] | 1.28                     | 0.92              |
| 4:2:332:PRO:CG  | 4:Z:221:LEU:CD2[1_556] | 1.28                     | 0.92              |
| 4:0:16:LEU:N    | 4:X:214:GLU:CG[1_556]  | 1.28                     | 0.92              |
| 4:1:120:THR:O   | 4:Y:340:TRP:CH2[1_556] | 1.28                     | 0.92              |
| 4:1:304:THR:O   | 4:Y:223:PHE:CE1[1_556] | 1.28                     | 0.92              |
| 4:1:365:ALA:N   | 4:Y:349:LEU:CA[1_556]  | 1.29                     | 0.91              |
| 4:2:331:ALA:CA  | 4:Z:222:ASP:N[1_556]   | 1.29                     | 0.91              |
| 4:2:366:GLY:O   | 4:Z:346:LEU:C[1_556]   | 1.29                     | 0.91              |
| 4:0:167:GLU:OE2 | 4:X:326:LYS:CA[1_556]  | 1.29                     | 0.91              |
| 4:0:233:SER:N   | 4:W:367:PRO:CA[1_556]  | 1.29                     | 0.91              |
| 4:4:41:GLN:CA   | 4:Z:167:GLU:OE2[1_556] | 1.29                     | 0.91              |
| 4:2:40:HIS:NE2  | 4:X:166:TYR:CB[1_556]  | 1.29                     | 0.91              |
| 4:0:32:PRO:N    | 4:X:211:ASP:CG[1_556]  | 1.29                     | 0.91              |
| 4:2:153:LEU:C   | 4:Z:262:PHE:CE1[1_556] | 1.29                     | 0.91              |
| 4:0:161:HIS:O   | 4:X:274:ILE:CB[1_556]  | 1.29                     | 0.91              |
| 4:2:142:LEU:CG  | 4:Z:329:ILE:CG1[1_556] | 1.29                     | 0.91              |
| 4:0:196:ARG:NE  | 4:W:115:ASN:CG[1_556]  | 1.29                     | 0.91              |
| 4:0:167:GLU:O   | 4:X:295:ALA:O[1_556]   | 1.29                     | 0.91              |
| 4:2:141:SER:CA  | 4:Z:310:ALA:CB[1_556]  | 1.29                     | 0.91              |
| 4:1:233:SER:N   | 4:X:367:PRO:CA[1_556]  | 1.29                     | 0.91              |
| 4:2:232:SER:N   | 4:Y:369:ILE:CG2[1_556] | 1.29                     | 0.91              |
| 4:0:158:GLY:O   | 4:X:181:ALA:O[1_556]   | 1.29                     | 0.91              |
| 4:1:171:LEU:N   | 4:Y:151:ILE:CD1[1_556] | 1.29                     | 0.91              |
| 4:2:157:ASP:O   | 4:Z:186:THR:N[1_556]   | 1.29                     | 0.91              |
| 4:0:304:THR:O   | 4:X:223:PHE:CE1[1_556] | 1.29                     | 0.91              |
| 4:2:133:TYR:O   | 4:Z:334:GLU:OE1[1_556] | 1.29                     | 0.91              |
| 4:1:73:HIS:CE1  | 4:Y:184:ASP:OD1[1_556] | 1.29                     | 0.91              |
| 4:0:105:LEU:C   | 4:X:334:GLU:O[1_556]   | 1.29                     | 0.91              |
| 4:2:286:ASP:N   | 4:Z:283:MET:CA[1_556]  | 1.29                     | 0.91              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:16:LEU:N    | 4:Y:214:GLU:CG[1_556]  | 1.29                     | 0.91              |
| 4:0:332:PRO:CG  | 4:X:221:LEU:CD2[1_556] | 1.29                     | 0.91              |
| 4:2:141:SER:CB  | 4:Z:309:ILE:C[1_556]   | 1.29                     | 0.91              |
| 4:2:121:GLN:CG  | 4:Z:9:VAL:N[1_556]     | 1.29                     | 0.91              |
| 4:1:147:ARG:CG  | 4:Y:314:GLN:CD[1_556]  | 1.29                     | 0.91              |
| 4:2:335:ARG:NH1 | 4:Z:220:ALA:CB[1_556]  | 1.29                     | 0.91              |
| 4:2:272:ALA:O   | 4:Z:269:MET:O[1_556]   | 1.29                     | 0.91              |
| 4:2:114:ALA:C   | 4:Z:106:THR:OG1[1_556] | 1.29                     | 0.91              |
| 4:0:164:PRO:CG  | 4:X:278:THR:C[1_556]   | 1.29                     | 0.91              |
| 4:1:298:VAL:CG1 | 4:Y:312:ARG:C[1_556]   | 1.29                     | 0.91              |
| 4:2:157:ASP:O   | 4:Z:185:LEU:CA[1_556]  | 1.29                     | 0.91              |
| 4:2:209:VAL:CG1 | 4:Z:194:THR:CA[1_556]  | 1.29                     | 0.91              |
| 4:0:362:TYR:CZ  | 4:X:22:ALA:CB[1_556]   | 1.29                     | 0.91              |
| 4:1:332:PRO:CG  | 4:Y:221:LEU:CD2[1_556] | 1.29                     | 0.91              |
| 4:1:266:PHE:N   | 4:X:173:HIS:ND1[1_556] | 1.29                     | 0.91              |
| 4:1:162:ASN:CB  | 4:Y:273:GLY:O[1_556]   | 1.29                     | 0.91              |
| 4:0:150:GLY:CA  | 4:X:317:ILE:CG1[1_556] | 1.29                     | 0.91              |
| 4:1:136:ILE:CA  | 4:Y:300:SER:N[1_556]   | 1.29                     | 0.91              |
| 4:1:272:ALA:O   | 4:Y:269:MET:O[1_556]   | 1.29                     | 0.91              |
| 4:1:72:GLU:OE2  | 4:Y:183:ARG:CD[1_556]  | 1.29                     | 0.91              |
| 4:0:265:SER:C   | 4:W:173:HIS:ND1[1_556] | 1.29                     | 0.91              |
| 4:2:261:LEU:CD1 | 4:Z:266:PHE:CE2[1_556] | 1.29                     | 0.91              |
| 4:1:161:HIS:O   | 4:Y:274:ILE:CB[1_556]  | 1.29                     | 0.91              |
| 4:0:121:GLN:CG  | 4:X:9:VAL:N[1_556]     | 1.29                     | 0.91              |
| 4:0:151:ILE:CD1 | 4:X:275:HIS:C[1_556]   | 1.29                     | 0.91              |
| 4:2:141:SER:CA  | 4:Z:310:ALA:N[1_556]   | 1.29                     | 0.91              |
| 4:1:134:VAL:C   | 4:Y:338:SER:OG[1_556]  | 1.29                     | 0.91              |
| 4:0:367:PRO:N   | 4:X:347:ALA:CB[1_556]  | 1.29                     | 0.91              |
| 4:2:138:ALA:N   | 4:Z:299:MET:CG[1_556]  | 1.30                     | 0.90              |
| 4:0:72:GLU:OE1  | 4:X:183:ARG:CZ[1_556]  | 1.30                     | 0.90              |
| 4:1:162:ASN:C   | 4:Y:274:ILE:C[1_556]   | 1.30                     | 0.90              |
| 4:2:32:PRO:N    | 4:Z:211:ASP:CG[1_556]  | 1.30                     | 0.90              |
| 4:0:141:SER:CA  | 4:X:310:ALA:CB[1_556]  | 1.30                     | 0.90              |
| 4:0:331:ALA:C   | 4:X:221:LEU:O[1_556]   | 1.30                     | 0.90              |
| 4:0:113:LYS:CG  | 4:X:136:ILE:C[1_556]   | 1.30                     | 0.90              |
| 4:1:138:ALA:CA  | 4:Y:299:MET:SD[1_556]  | 1.30                     | 0.90              |
| 4:0:141:SER:OG  | 4:X:309:ILE:CG2[1_556] | 1.30                     | 0.90              |
| 4:2:112:PRO:CD  | 4:Z:137:GLN:OE1[1_556] | 1.30                     | 0.90              |
| 4:0:174:ALA:C   | 4:X:277:THR:O[1_556]   | 1.30                     | 0.90              |
| 4:1:120:THR:O   | 4:Y:340:TRP:CZ3[1_556] | 1.30                     | 0.90              |
| 4:0:157:ASP:O   | 4:X:186:THR:N[1_556]   | 1.30                     | 0.90              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:83:GLU:N    | 4:X:30:VAL:CA[1_556]   | 1.30                     | 0.90              |
| 4:2:83:GLU:N    | 4:Z:30:VAL:CA[1_556]   | 1.30                     | 0.90              |
| 4:2:72:GLU:OE1  | 4:Z:183:ARG:CZ[1_556]  | 1.30                     | 0.90              |
| 4:2:153:LEU:CG  | 4:Z:262:PHE:CG[1_556]  | 1.30                     | 0.90              |
| 4:1:168:GLY:N   | 4:Y:295:ALA:C[1_556]   | 1.30                     | 0.90              |
| 4:2:372:ARG:NH2 | 4:Z:144:ALA:C[1_556]   | 1.30                     | 0.90              |
| 4:3:194:THR:C   | 4:Z:75:ILE:CG1[1_556]  | 1.30                     | 0.90              |
| 4:0:122:ILE:CB  | 4:X:19:ALA:O[1_556]    | 1.30                     | 0.90              |
| 4:2:335:ARG:CG  | 4:Z:220:ALA:CA[1_556]  | 1.30                     | 0.90              |
| 4:0:196:ARG:CZ  | 4:W:115:ASN:CA[1_556]  | 1.30                     | 0.90              |
| 4:2:11:ASP:OD2  | 4:Z:305:MET:CB[1_556]  | 1.30                     | 0.90              |
| 4:2:177:ARG:NH2 | 4:Z:158:GLY:C[1_556]   | 1.30                     | 0.90              |
| 4:0:286:ASP:N   | 4:X:283:MET:CA[1_556]  | 1.30                     | 0.90              |
| 4:0:295:ALA:C   | 4:X:319:ALA:CB[1_556]  | 1.30                     | 0.90              |
| 4:0:125:GLU:CB  | 4:X:21:PHE:CA[1_556]   | 1.30                     | 0.90              |
| 4:2:299:MET:CG  | 4:Z:312:ARG:CZ[1_556]  | 1.30                     | 0.90              |
| 4:0:212:ILE:CA  | 4:X:196:ARG:CD[1_556]  | 1.30                     | 0.90              |
| 4:2:113:LYS:CG  | 4:Z:136:ILE:C[1_556]   | 1.30                     | 0.90              |
| 4:1:138:ALA:N   | 4:Y:299:MET:CG[1_556]  | 1.30                     | 0.90              |
| 4:1:164:PRO:CD  | 4:Y:278:THR:CB[1_556]  | 1.30                     | 0.90              |
| 4:2:212:ILE:CA  | 4:Z:196:ARG:CD[1_556]  | 1.30                     | 0.90              |
| 4:1:338:SER:OG  | 4:Y:308:GLY:C[1_556]   | 1.30                     | 0.90              |
| 4:0:73:HIS:CE1  | 4:X:184:ASP:OD1[1_556] | 1.30                     | 0.90              |
| 4:0:123:MET:CB  | 4:X:26:ALA:CA[1_556]   | 1.30                     | 0.90              |
| 4:1:274:ILE:CG1 | 4:Y:263:GLN:N[1_556]   | 1.30                     | 0.90              |
| 4:1:364:GLU:N   | 4:Y:348:SER:O[1_556]   | 1.30                     | 0.90              |
| 4:1:357:ILE:CG1 | 4:Y:345:ILE:CD1[1_556] | 1.30                     | 0.90              |
| 4:2:210:ARG:NH1 | 4:Z:212:ILE:CG2[1_556] | 1.30                     | 0.90              |
| 4:1:107:GLU:O   | 4:Y:300:SER:O[1_556]   | 1.30                     | 0.90              |
| 4:1:153:LEU:CA  | 4:Y:262:PHE:CE1[1_556] | 1.30                     | 0.90              |
| 4:0:109:PRO:C   | 4:X:154:ASP:N[1_556]   | 1.30                     | 0.90              |
| 4:1:126:THR:O   | 4:Y:28:ARG:CD[1_556]   | 1.30                     | 0.90              |
| 4:2:208:ILE:CA  | 4:Z:198:TYR:CG[1_556]  | 1.30                     | 0.90              |
| 4:1:32:PRO:N    | 4:Y:211:ASP:CG[1_556]  | 1.30                     | 0.90              |
| 4:1:210:ARG:NH1 | 4:Y:212:ILE:CG2[1_556] | 1.30                     | 0.90              |
| 4:4:40:HIS:NE2  | 4:Z:166:TYR:CB[1_556]  | 1.30                     | 0.90              |
| 4:0:79:TRP:CG   | 4:X:17:VAL:CA[1_556]   | 1.30                     | 0.90              |
| 4:2:125:GLU:CB  | 4:Z:21:PHE:CA[1_556]   | 1.30                     | 0.90              |
| 4:0:299:MET:SD  | 4:X:312:ARG:NH2[1_556] | 1.30                     | 0.90              |
| 4:2:229:THR:O   | 4:Y:368:SER:CB[1_556]  | 1.30                     | 0.90              |
| 4:0:155:SER:CB  | 4:X:258:PRO:O[1_556]   | 1.30                     | 0.90              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:107:GLU:CG  | 4:X:300:SER:CB[1_556]  | 1.30                     | 0.90              |
| 4:3:233:SER:N   | 4:Z:367:PRO:CA[1_556]  | 1.30                     | 0.90              |
| 4:1:332:PRO:N   | 4:Y:221:LEU:CG[1_556]  | 1.30                     | 0.90              |
| 4:1:209:VAL:O   | 4:Y:193:LEU:O[1_556]   | 1.31                     | 0.89              |
| 4:0:83:GLU:OE1  | 4:X:29:ALA:CA[1_556]   | 1.31                     | 0.89              |
| 4:1:123:MET:CG  | 4:Y:26:ALA:CA[1_556]   | 1.31                     | 0.89              |
| 4:0:291:LYS:NZ  | 4:X:322:PRO:C[1_556]   | 1.31                     | 0.89              |
| 4:0:153:LEU:CG  | 4:X:262:PHE:CG[1_556]  | 1.31                     | 0.89              |
| 4:0:11:ASP:OD2  | 4:X:305:MET:CB[1_556]  | 1.31                     | 0.89              |
| 4:2:16:LEU:CG   | 4:Z:215:LYS:N[1_556]   | 1.31                     | 0.89              |
| 4:1:167:GLU:OE2 | 4:Y:326:LYS:CB[1_556]  | 1.31                     | 0.89              |
| 4:1:113:LYS:CB  | 4:Y:136:ILE:CA[1_556]  | 1.31                     | 0.89              |
| 4:2:211:ASP:CG  | 4:Z:249:THR:C[1_556]   | 1.31                     | 0.89              |
| 4:2:299:MET:SD  | 4:Z:312:ARG:NH2[1_556] | 1.31                     | 0.89              |
| 4:0:39:ARG:C    | 4:V:166:TYR:CE2[1_556] | 1.31                     | 0.89              |
| 4:0:214:GLU:CA  | 4:X:253:GLU:OE2[1_556] | 1.31                     | 0.89              |
| 4:2:123:MET:CB  | 4:Z:26:ALA:CA[1_556]   | 1.31                     | 0.89              |
| 4:0:335:ARG:NH1 | 4:X:220:ALA:CB[1_556]  | 1.31                     | 0.89              |
| 4:0:370:VAL:CG1 | 4:X:342:GLY:CA[1_556]  | 1.31                     | 0.89              |
| 4:1:232:SER:C   | 4:X:366:GLY:O[1_556]   | 1.31                     | 0.89              |
| 4:1:79:TRP:CE3  | 4:Y:18:LYS:CA[1_556]   | 1.31                     | 0.89              |
| 4:1:161:HIS:NE2 | 4:Y:160:THR:OG1[1_556] | 1.31                     | 0.89              |
| 4:0:369:ILE:CG2 | 4:X:345:ILE:CA[1_556]  | 1.31                     | 0.89              |
| 4:0:229:THR:C   | 4:W:368:SER:C[1_556]   | 1.31                     | 0.89              |
| 4:2:167:GLU:OE2 | 4:Z:326:LYS:CA[1_556]  | 1.31                     | 0.89              |
| 4:2:174:ALA:C   | 4:Z:277:THR:O[1_556]   | 1.31                     | 0.89              |
| 4:1:86:TRP:CD1  | 4:Y:337:TYR:OH[1_556]  | 1.31                     | 0.89              |
| 4:2:16:LEU:CA   | 4:Z:214:GLU:CG[1_556]  | 1.31                     | 0.89              |
| 4:0:142:LEU:CG  | 4:X:329:ILE:CG1[1_556] | 1.31                     | 0.89              |
| 4:2:167:GLU:CB  | 4:Z:295:ALA:CB[1_556]  | 1.31                     | 0.89              |
| 4:1:135:ALA:C   | 4:Y:299:MET:O[1_556]   | 1.31                     | 0.89              |
| 4:1:131:ALA:N   | 4:Y:25:ASP:OD1[1_556]  | 1.31                     | 0.89              |
| 4:2:120:THR:O   | 4:Z:340:TRP:CH2[1_556] | 1.31                     | 0.89              |
| 4:2:151:ILE:CG1 | 4:Z:275:HIS:O[1_556]   | 1.31                     | 0.89              |
| 4:0:72:GLU:OE2  | 4:X:183:ARG:CD[1_556]  | 1.31                     | 0.89              |
| 4:0:211:ASP:CG  | 4:X:249:THR:C[1_556]   | 1.31                     | 0.89              |
| 4:0:141:SER:C   | 4:X:310:ALA:C[1_556]   | 1.31                     | 0.89              |
| 4:2:206:ARG:CD  | 4:Z:200:PHE:CB[1_556]  | 1.31                     | 0.89              |
| 4:0:120:THR:O   | 4:X:340:TRP:CH2[1_556] | 1.31                     | 0.89              |
| 4:0:138:ALA:N   | 4:X:299:MET:CG[1_556]  | 1.31                     | 0.89              |
| 4:2:73:HIS:CE1  | 4:Z:184:ASP:OD1[1_556] | 1.31                     | 0.89              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:338:SER:CB  | 4:Y:308:GLY:CA[1_556]  | 1.31                     | 0.89              |
| 4:2:280:ASN:N   | 4:Z:276:GLU:OE1[1_556] | 1.31                     | 0.89              |
| 4:2:155:SER:CB  | 4:Z:258:PRO:O[1_556]   | 1.31                     | 0.89              |
| 4:2:369:ILE:CG2 | 4:Z:345:ILE:CA[1_556]  | 1.31                     | 0.89              |
| 4:1:32:PRO:CD   | 4:Y:211:ASP:OD2[1_556] | 1.31                     | 0.89              |
| 4:1:177:ARG:CA  | 4:Y:178:LEU:CB[1_556]  | 1.31                     | 0.89              |
| 4:3:232:SER:C   | 4:Z:366:GLY:O[1_556]   | 1.31                     | 0.89              |
| 4:2:331:ALA:C   | 4:Z:221:LEU:O[1_556]   | 1.31                     | 0.89              |
| 4:2:295:ALA:C   | 4:Z:319:ALA:CB[1_556]  | 1.31                     | 0.89              |
| 4:0:177:ARG:NH2 | 4:X:158:GLY:C[1_556]   | 1.31                     | 0.89              |
| 4:2:109:PRO:C   | 4:Z:154:ASP:N[1_556]   | 1.31                     | 0.89              |
| 4:1:186:THR:CB  | 4:Y:190:MET:C[1_556]   | 1.31                     | 0.89              |
| 4:1:141:SER:O   | 4:Y:310:ALA:C[1_556]   | 1.31                     | 0.89              |
| 4:0:151:ILE:CG1 | 4:X:275:HIS:O[1_556]   | 1.31                     | 0.89              |
| 4:0:372:ARG:NH2 | 4:X:144:ALA:C[1_556]   | 1.31                     | 0.89              |
| 4:1:331:ALA:O   | 4:Y:221:LEU:C[1_556]   | 1.31                     | 0.89              |
| 4:0:250:ILE:C   | 4:W:114:ALA:CB[1_556]  | 1.31                     | 0.89              |
| 4:1:86:TRP:CE2  | 4:Y:337:TYR:OH[1_556]  | 1.31                     | 0.89              |
| 4:1:194:THR:C   | 4:X:75:ILE:CG1[1_556]  | 1.31                     | 0.89              |
| 4:0:211:ASP:O   | 4:X:196:ARG:NE[1_556]  | 1.31                     | 0.89              |
| 4:1:77:THR:N    | 4:Y:16:LEU:N[1_556]    | 1.31                     | 0.89              |
| 4:3:266:PHE:N   | 4:Z:173:HIS:ND1[1_556] | 1.31                     | 0.89              |
| 4:1:261:LEU:C   | 4:Y:266:PHE:N[1_556]   | 1.31                     | 0.89              |
| 4:0:280:ASN:N   | 4:X:276:GLU:OE1[1_556] | 1.31                     | 0.89              |
| 4:2:291:LYS:NZ  | 4:Z:322:PRO:C[1_556]   | 1.32                     | 0.88              |
| 4:2:196:ARG:CZ  | 4:Y:115:ASN:CA[1_556]  | 1.32                     | 0.88              |
| 4:0:149:THR:N   | 4:X:327:ILE:CG2[1_556] | 1.32                     | 0.88              |
| 4:2:214:GLU:CA  | 4:Z:253:GLU:OE2[1_556] | 1.32                     | 0.88              |
| 4:0:67:LEU:CA   | 4:X:62:ARG:NH1[1_556]  | 1.32                     | 0.88              |
| 4:1:368:SER:CB  | 4:Y:346:LEU:CG[1_556]  | 1.32                     | 0.88              |
| 4:0:16:LEU:CG   | 4:X:215:LYS:N[1_556]   | 1.32                     | 0.88              |
| 4:1:170:ALA:C   | 4:Y:151:ILE:CB[1_556]  | 1.32                     | 0.88              |
| 4:3:40:HIS:CG   | 4:Y:166:TYR:CG[1_556]  | 1.32                     | 0.88              |
| 4:2:32:PRO:CD   | 4:Z:211:ASP:OD2[1_556] | 1.32                     | 0.88              |
| 4:1:153:LEU:CD1 | 4:Y:262:PHE:C[1_556]   | 1.32                     | 0.88              |
| 4:1:164:PRO:CB  | 4:Y:279:TYR:N[1_556]   | 1.32                     | 0.88              |
| 4:2:32:PRO:N    | 4:Z:211:ASP:OD2[1_556] | 1.32                     | 0.88              |
| 4:1:370:VAL:CG1 | 4:Y:342:GLY:CA[1_556]  | 1.32                     | 0.88              |
| 4:2:229:THR:C   | 4:Y:368:SER:C[1_556]   | 1.32                     | 0.88              |
| 4:0:132:MET:SD  | 4:X:341:ILE:CG2[1_556] | 1.32                     | 0.88              |
| 4:0:112:PRO:CD  | 4:X:137:GLN:OE1[1_556] | 1.32                     | 0.88              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:116:ARG:C   | 4:X:339:VAL:O[1_556]   | 1.32                     | 0.88              |
| 4:0:16:LEU:CA   | 4:X:214:GLU:CG[1_556]  | 1.32                     | 0.88              |
| 4:0:229:THR:O   | 4:W:368:SER:CB[1_556]  | 1.32                     | 0.88              |
| 4:1:113:LYS:CG  | 4:Y:136:ILE:CB[1_556]  | 1.32                     | 0.88              |
| 4:2:107:GLU:CG  | 4:Z:300:SER:CB[1_556]  | 1.32                     | 0.88              |
| 4:0:206:ARG:CD  | 4:X:200:PHE:CB[1_556]  | 1.32                     | 0.88              |
| 4:1:196:ARG:CD  | 4:X:115:ASN:ND2[1_556] | 1.32                     | 0.88              |
| 4:2:67:LEU:CA   | 4:Z:62:ARG:NH1[1_556]  | 1.32                     | 0.88              |
| 4:1:108:ALA:O   | 4:Y:154:ASP:OD1[1_556] | 1.32                     | 0.88              |
| 4:1:120:THR:OG1 | 4:Y:341:ILE:N[1_556]   | 1.32                     | 0.88              |
| 4:2:282:ILE:CD1 | 4:Z:320:LEU:CD1[1_556] | 1.32                     | 0.88              |
| 4:0:162:ASN:CB  | 4:X:273:GLY:O[1_556]   | 1.32                     | 0.88              |
| 4:0:120:THR:N   | 4:X:340:TRP:CG[1_556]  | 1.32                     | 0.88              |
| 4:1:292:ASP:CB  | 4:Y:321:ALA:CB[1_556]  | 1.32                     | 0.88              |
| 4:0:277:THR:CG2 | 4:X:273:GLY:N[1_556]   | 1.32                     | 0.88              |
| 4:1:335:ARG:CG  | 4:Y:220:ALA:CA[1_556]  | 1.32                     | 0.88              |
| 4:1:167:GLU:OE2 | 4:Y:326:LYS:CA[1_556]  | 1.32                     | 0.88              |
| 4:1:213:LYS:CB  | 4:Y:192:ILE:O[1_556]   | 1.32                     | 0.88              |
| 4:2:39:ARG:C    | 4:X:166:TYR:CE2[1_556] | 1.32                     | 0.88              |
| 4:0:37:ARG:CG   | 4:X:60:SER:OG[1_556]   | 1.32                     | 0.88              |
| 4:1:167:GLU:N   | 4:Y:295:ALA:N[1_556]   | 1.32                     | 0.88              |
| 4:0:206:ARG:N   | 4:X:199:SER:CB[1_556]  | 1.32                     | 0.88              |
| 4:1:302:GLY:N   | 4:Y:258:PRO:CG[1_556]  | 1.32                     | 0.88              |
| 4:2:116:ARG:C   | 4:Z:339:VAL:O[1_556]   | 1.32                     | 0.88              |
| 4:0:210:ARG:NH1 | 4:X:212:ILE:CG2[1_556] | 1.32                     | 0.88              |
| 4:2:277:THR:CG2 | 4:Z:273:GLY:N[1_556]   | 1.32                     | 0.88              |
| 4:1:79:TRP:CG   | 4:Y:17:VAL:CA[1_556]   | 1.32                     | 0.88              |
| 4:2:72:GLU:OE2  | 4:Z:183:ARG:CD[1_556]  | 1.32                     | 0.88              |
| 4:2:62:ARG:NE   | 4:Z:204:ALA:C[1_556]   | 1.32                     | 0.88              |
| 4:1:113:LYS:CA  | 4:Y:137:GLN:N[1_556]   | 1.32                     | 0.88              |
| 4:2:79:TRP:CG   | 4:Z:17:VAL:CA[1_556]   | 1.32                     | 0.88              |
| 4:1:265:SER:C   | 4:X:173:HIS:ND1[1_556] | 1.33                     | 0.87              |
| 4:0:167:GLU:CB  | 4:X:295:ALA:CB[1_556]  | 1.33                     | 0.87              |
| 4:2:83:GLU:OE1  | 4:Z:29:ALA:CA[1_556]   | 1.33                     | 0.87              |
| 4:0:232:SER:CA  | 4:W:369:ILE:CG2[1_556] | 1.33                     | 0.87              |
| 4:3:64:ILE:N    | 4:Y:288:ASP:O[1_556]   | 1.33                     | 0.87              |
| 4:2:297:ASN:CA  | 4:Z:316:GLU:CA[1_556]  | 1.33                     | 0.87              |
| 4:2:331:ALA:C   | 4:Z:221:LEU:CA[1_556]  | 1.33                     | 0.87              |
| 4:2:170:ALA:C   | 4:Z:151:ILE:CB[1_556]  | 1.33                     | 0.87              |
| 4:2:250:ILE:C   | 4:Y:114:ALA:CB[1_556]  | 1.33                     | 0.87              |
| 4:4:40:HIS:CE1  | 4:Z:166:TYR:CB[1_556]  | 1.33                     | 0.87              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:370:VAL:CG1 | 4:Z:342:GLY:CA[1_556]  | 1.33                     | 0.87              |
| 4:1:331:ALA:C   | 4:Y:221:LEU:O[1_556]   | 1.33                     | 0.87              |
| 4:0:32:PRO:N    | 4:X:211:ASP:OD2[1_556] | 1.33                     | 0.87              |
| 4:2:140:LEU:CG  | 4:Z:331:ALA:C[1_556]   | 1.33                     | 0.87              |
| 4:1:303:THR:CB  | 4:Y:257:CYS:O[1_556]   | 1.33                     | 0.87              |
| 4:2:120:THR:N   | 4:Z:340:TRP:CG[1_556]  | 1.33                     | 0.87              |
| 4:1:167:GLU:O   | 4:Y:295:ALA:O[1_556]   | 1.33                     | 0.87              |
| 4:0:64:ILE:N    | 4:V:288:ASP:C[1_556]   | 1.33                     | 0.87              |
| 4:1:296:ASN:CB  | 4:Y:318:THR:OG1[1_556] | 1.33                     | 0.87              |
| 4:1:206:ARG:CB  | 4:Y:199:SER:C[1_556]   | 1.33                     | 0.87              |
| 4:0:297:ASN:ND2 | 4:X:316:GLU:OE1[1_556] | 1.33                     | 0.87              |
| 4:0:296:ASN:O   | 4:X:316:GLU:C[1_556]   | 1.33                     | 0.87              |
| 4:2:368:SER:C   | 4:Z:346:LEU:CG[1_556]  | 1.33                     | 0.87              |
| 4:1:72:GLU:OE1  | 4:Y:183:ARG:CZ[1_556]  | 1.33                     | 0.87              |
| 4:1:149:THR:N   | 4:Y:327:ILE:CG2[1_556] | 1.33                     | 0.87              |
| 4:1:274:ILE:CG2 | 4:Y:263:GLN:CB[1_556]  | 1.33                     | 0.87              |
| 4:2:40:HIS:CE1  | 4:X:166:TYR:CB[1_556]  | 1.33                     | 0.87              |
| 4:1:32:PRO:N    | 4:Y:211:ASP:OD2[1_556] | 1.33                     | 0.87              |
| 4:0:365:ALA:O   | 4:X:346:LEU:O[1_556]   | 1.33                     | 0.87              |
| 4:2:37:ARG:CG   | 4:Z:60:SER:OG[1_556]   | 1.33                     | 0.87              |
| 4:0:142:LEU:CD1 | 4:X:314:GLN:CA[1_556]  | 1.33                     | 0.87              |
| 4:2:211:ASP:O   | 4:Z:196:ARG:NE[1_556]  | 1.33                     | 0.87              |
| 4:1:303:THR:N   | 4:Y:258:PRO:N[1_556]   | 1.33                     | 0.87              |
| 4:2:132:MET:SD  | 4:Z:341:ILE:CG2[1_556] | 1.33                     | 0.87              |
| 4:1:130:PRO:N   | 4:Y:25:ASP:OD2[1_556]  | 1.33                     | 0.87              |
| 4:2:232:SER:CA  | 4:Y:369:ILE:CG2[1_556] | 1.33                     | 0.87              |
| 4:4:39:ARG:C    | 4:Z:166:TYR:CE2[1_556] | 1.33                     | 0.87              |
| 4:0:16:LEU:C    | 4:X:214:GLU:CB[1_556]  | 1.33                     | 0.87              |
| 4:3:196:ARG:CD  | 4:Z:115:ASN:ND2[1_556] | 1.33                     | 0.87              |
| 4:1:332:PRO:CA  | 4:Y:221:LEU:CG[1_556]  | 1.33                     | 0.87              |
| 4:1:116:ARG:CA  | 4:Y:339:VAL:CG1[1_556] | 1.33                     | 0.87              |
| 4:2:297:ASN:ND2 | 4:Z:316:GLU:OE1[1_556] | 1.33                     | 0.87              |
| 4:2:149:THR:N   | 4:Z:327:ILE:CG2[1_556] | 1.33                     | 0.87              |
| 4:1:40:HIS:CE1  | 4:W:166:TYR:CB[1_556]  | 1.33                     | 0.87              |
| 4:0:81:ASP:N    | 4:X:31:PHE:CA[1_556]   | 1.33                     | 0.87              |
| 4:1:141:SER:C   | 4:Y:310:ALA:C[1_556]   | 1.33                     | 0.87              |
| 4:0:148:THR:CB  | 4:X:327:ILE:O[1_556]   | 1.33                     | 0.87              |
| 4:1:372:ARG:NH2 | 4:Y:144:ALA:C[1_556]   | 1.33                     | 0.87              |
| 4:2:141:SER:C   | 4:Z:310:ALA:C[1_556]   | 1.33                     | 0.87              |
| 4:1:150:GLY:N   | 4:Y:317:ILE:CG1[1_556] | 1.33                     | 0.87              |
| 4:0:192:ILE:C   | 4:W:110:LEU:O[1_556]   | 1.33                     | 0.87              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:40:HIS:NE2  | 4:Y:166:TYR:CB[1_556]  | 1.33                     | 0.87              |
| 4:1:62:ARG:CD   | 4:Y:204:ALA:CA[1_556]  | 1.34                     | 0.86              |
| 4:1:149:THR:CB  | 4:Y:327:ILE:CD1[1_556] | 1.34                     | 0.86              |
| 4:3:196:ARG:NH2 | 4:Z:114:ALA:C[1_556]   | 1.34                     | 0.86              |
| 4:1:274:ILE:CG2 | 4:Y:263:GLN:CG[1_556]  | 1.34                     | 0.86              |
| 4:1:212:ILE:CB  | 4:Y:196:ARG:CB[1_556]  | 1.34                     | 0.86              |
| 4:1:40:HIS:CG   | 4:W:166:TYR:CG[1_556]  | 1.34                     | 0.86              |
| 4:1:170:ALA:C   | 4:Y:151:ILE:CG1[1_556] | 1.34                     | 0.86              |
| 4:2:37:ARG:CA   | 4:Z:60:SER:CB[1_556]   | 1.34                     | 0.86              |
| 4:0:282:ILE:CD1 | 4:X:320:LEU:CD1[1_556] | 1.34                     | 0.86              |
| 4:3:40:HIS:CE1  | 4:Y:166:TYR:CB[1_556]  | 1.34                     | 0.86              |
| 4:1:297:ASN:CA  | 4:Y:316:GLU:CA[1_556]  | 1.34                     | 0.86              |
| 4:1:64:ILE:N    | 4:W:288:ASP:O[1_556]   | 1.34                     | 0.86              |
| 4:0:32:PRO:CD   | 4:X:211:ASP:OD2[1_556] | 1.34                     | 0.86              |
| 4:0:135:ALA:C   | 4:X:299:MET:O[1_556]   | 1.34                     | 0.86              |
| 4:0:40:HIS:CE1  | 4:V:166:TYR:CB[1_556]  | 1.34                     | 0.86              |
| 4:1:153:LEU:C   | 4:Y:262:PHE:CE1[1_556] | 1.34                     | 0.86              |
| 4:0:37:ARG:CA   | 4:X:60:SER:CB[1_556]   | 1.34                     | 0.86              |
| 4:2:167:GLU:N   | 4:Z:295:ALA:N[1_556]   | 1.34                     | 0.86              |
| 4:1:207:GLU:O   | 4:Y:200:PHE:CZ[1_556]  | 1.34                     | 0.86              |
| 4:2:212:ILE:CB  | 4:Z:196:ARG:CB[1_556]  | 1.34                     | 0.86              |
| 4:0:104:LEU:CD2 | 4:X:333:PRO:N[1_556]   | 1.34                     | 0.86              |
| 4:2:296:ASN:O   | 4:Z:316:GLU:C[1_556]   | 1.34                     | 0.86              |
| 4:0:170:ALA:C   | 4:X:151:ILE:CB[1_556]  | 1.34                     | 0.86              |
| 4:1:165:ILE:CB  | 4:Y:297:ASN:OD1[1_556] | 1.34                     | 0.86              |
| 4:2:111:ASN:N   | 4:Z:154:ASP:OD2[1_556] | 1.34                     | 0.86              |
| 4:0:331:ALA:C   | 4:X:221:LEU:CA[1_556]  | 1.34                     | 0.86              |
| 4:0:161:HIS:NE2 | 4:X:160:THR:OG1[1_556] | 1.34                     | 0.86              |
| 4:1:177:ARG:NH2 | 4:Y:158:GLY:C[1_556]   | 1.34                     | 0.86              |
| 4:2:206:ARG:N   | 4:Z:199:SER:CB[1_556]  | 1.34                     | 0.86              |
| 4:3:64:ILE:N    | 4:Y:288:ASP:C[1_556]   | 1.34                     | 0.86              |
| 4:1:109:PRO:N   | 4:Y:154:ASP:CA[1_556]  | 1.34                     | 0.86              |
| 4:2:162:ASN:CB  | 4:Z:273:GLY:O[1_556]   | 1.34                     | 0.86              |
| 4:2:274:ILE:CG2 | 4:Z:263:GLN:CB[1_556]  | 1.34                     | 0.86              |
| 4:1:113:LYS:CG  | 4:Y:136:ILE:C[1_556]   | 1.34                     | 0.86              |
| 4:1:184:ASP:OD1 | 4:Y:184:ASP:O[1_556]   | 1.34                     | 0.86              |
| 4:2:161:HIS:NE2 | 4:Z:160:THR:OG1[1_556] | 1.34                     | 0.86              |
| 4:1:298:VAL:CG1 | 4:Y:312:ARG:N[1_556]   | 1.34                     | 0.86              |
| 4:3:265:SER:C   | 4:Z:173:HIS:ND1[1_556] | 1.34                     | 0.86              |
| 4:1:336:LYS:CB  | 4:Y:218:TYR:CA[1_556]  | 1.34                     | 0.86              |
| 4:1:79:TRP:CG   | 4:Y:17:VAL:CB[1_556]   | 1.34                     | 0.86              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:209:VAL:O   | 4:Z:193:LEU:O[1_556]   | 1.34                     | 0.86              |
| 4:1:208:ILE:O   | 4:Y:198:TYR:CE2[1_556] | 1.34                     | 0.86              |
| 4:2:213:LYS:O   | 4:Z:253:GLU:OE1[1_556] | 1.34                     | 0.86              |
| 4:1:132:MET:SD  | 4:Y:341:ILE:CG2[1_556] | 1.34                     | 0.86              |
| 4:2:266:PHE:N   | 4:Y:173:HIS:ND1[1_556] | 1.34                     | 0.86              |
| 4:2:127:PHE:CE2 | 4:Z:27:PRO:O[1_556]    | 1.34                     | 0.86              |
| 4:0:368:SER:C   | 4:X:346:LEU:CG[1_556]  | 1.34                     | 0.86              |
| 4:1:112:PRO:CD  | 4:Y:137:GLN:OE1[1_556] | 1.34                     | 0.86              |
| 4:0:142:LEU:CD1 | 4:X:314:GLN:N[1_556]   | 1.34                     | 0.86              |
| 4:2:162:ASN:CG  | 4:Z:274:ILE:N[1_556]   | 1.34                     | 0.86              |
| 4:0:274:ILE:CG2 | 4:X:263:GLN:CB[1_556]  | 1.34                     | 0.86              |
| 4:0:106:THR:N   | 4:X:335:ARG:C[1_556]   | 1.34                     | 0.86              |
| 4:1:107:GLU:O   | 4:Y:301:GLY:N[1_556]   | 1.34                     | 0.86              |
| 4:2:261:LEU:C   | 4:Z:266:PHE:N[1_556]   | 1.34                     | 0.86              |
| 4:0:155:SER:O   | 4:X:258:PRO:CB[1_556]  | 1.34                     | 0.86              |
| 4:0:113:LYS:CA  | 4:X:137:GLN:N[1_556]   | 1.34                     | 0.86              |
| 4:1:112:PRO:CB  | 4:Y:137:GLN:CD[1_556]  | 1.34                     | 0.86              |
| 4:1:16:LEU:C    | 4:Y:214:GLU:CB[1_556]  | 1.34                     | 0.86              |
| 4:2:335:ARG:CZ  | 4:Z:220:ALA:CB[1_556]  | 1.34                     | 0.86              |
| 4:2:167:GLU:CA  | 4:Z:295:ALA:N[1_556]   | 1.34                     | 0.86              |
| 4:0:40:HIS:CG   | 4:V:166:TYR:CG[1_556]  | 1.34                     | 0.86              |
| 4:0:127:PHE:CE2 | 4:X:27:PRO:O[1_556]    | 1.34                     | 0.86              |
| 4:1:115:ASN:N   | 4:Y:106:THR:OG1[1_556] | 1.34                     | 0.86              |
| 4:1:371:HIS:O   | 4:Y:139:VAL:O[1_556]   | 1.34                     | 0.86              |
| 4:0:62:ARG:NE   | 4:X:204:ALA:C[1_556]   | 1.34                     | 0.86              |
| 4:2:297:ASN:CB  | 4:Z:316:GLU:OE1[1_556] | 1.34                     | 0.86              |
| 4:2:155:SER:O   | 4:Z:258:PRO:CB[1_556]  | 1.35                     | 0.85              |
| 4:0:133:TYR:OH  | 4:X:145:SER:CB[1_556]  | 1.35                     | 0.85              |
| 4:0:147:ARG:O   | 4:X:314:GLN:NE2[1_556] | 1.35                     | 0.85              |
| 4:1:12:ASN:ND2  | 4:Y:336:LYS:CG[1_556]  | 1.35                     | 0.85              |
| 4:0:167:GLU:CA  | 4:X:295:ALA:N[1_556]   | 1.35                     | 0.85              |
| 4:1:211:ASP:O   | 4:Y:196:ARG:NE[1_556]  | 1.35                     | 0.85              |
| 4:1:106:THR:N   | 4:Y:336:LYS:N[1_556]   | 1.35                     | 0.85              |
| 4:2:142:LEU:CD1 | 4:Z:314:GLN:CA[1_556]  | 1.35                     | 0.85              |
| 4:0:140:LEU:CG  | 4:X:331:ALA:C[1_556]   | 1.35                     | 0.85              |
| 4:2:192:ILE:C   | 4:Y:110:LEU:O[1_556]   | 1.35                     | 0.85              |
| 4:2:81:ASP:N    | 4:Z:31:PHE:CA[1_556]   | 1.35                     | 0.85              |
| 4:1:215:LYS:N   | 4:Y:253:GLU:OE2[1_556] | 1.35                     | 0.85              |
| 4:0:213:LYS:O   | 4:X:253:GLU:OE1[1_556] | 1.35                     | 0.85              |
| 4:0:297:ASN:CA  | 4:X:316:GLU:CA[1_556]  | 1.35                     | 0.85              |
| 4:1:196:ARG:NH2 | 4:X:114:ALA:C[1_556]   | 1.35                     | 0.85              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:106:THR:N   | 4:Z:335:ARG:C[1_556]   | 1.35                     | 0.85              |
| 4:2:16:LEU:C    | 4:Z:214:GLU:CB[1_556]  | 1.35                     | 0.85              |
| 4:2:365:ALA:O   | 4:Z:346:LEU:O[1_556]   | 1.35                     | 0.85              |
| 4:1:148:THR:CB  | 4:Y:327:ILE:O[1_556]   | 1.35                     | 0.85              |
| 4:1:40:HIS:NE2  | 4:W:166:TYR:CB[1_556]  | 1.35                     | 0.85              |
| 4:1:158:GLY:O   | 4:Y:181:ALA:O[1_556]   | 1.35                     | 0.85              |
| 4:1:171:LEU:N   | 4:Y:151:ILE:CG1[1_556] | 1.35                     | 0.85              |
| 4:2:187:ASP:N   | 4:Z:191:LYS:N[1_556]   | 1.35                     | 0.85              |
| 4:2:62:ARG:CD   | 4:Z:204:ALA:CA[1_556]  | 1.35                     | 0.85              |
| 4:2:161:HIS:C   | 4:Z:274:ILE:CG1[1_556] | 1.35                     | 0.85              |
| 4:2:133:TYR:OH  | 4:Z:145:SER:CB[1_556]  | 1.35                     | 0.85              |
| 4:2:64:ILE:N    | 4:X:288:ASP:C[1_556]   | 1.35                     | 0.85              |
| 4:0:297:ASN:CB  | 4:X:316:GLU:OE1[1_556] | 1.35                     | 0.85              |
| 4:0:212:ILE:CB  | 4:X:196:ARG:CB[1_556]  | 1.35                     | 0.85              |
| 4:0:282:ILE:CG1 | 4:X:320:LEU:CD1[1_556] | 1.35                     | 0.85              |
| 4:2:108:ALA:O   | 4:Z:154:ASP:OD1[1_556] | 1.35                     | 0.85              |
| 4:0:209:VAL:O   | 4:X:193:LEU:O[1_556]   | 1.35                     | 0.85              |
| 4:1:67:LEU:O    | 4:Y:59:GLN:OE1[1_556]  | 1.35                     | 0.85              |
| 4:0:111:ASN:N   | 4:X:154:ASP:OD2[1_556] | 1.35                     | 0.85              |
| 4:1:126:THR:C   | 4:Y:28:ARG:CD[1_556]   | 1.35                     | 0.85              |
| 4:2:104:LEU:CD2 | 4:Z:333:PRO:N[1_556]   | 1.35                     | 0.85              |
| 4:1:206:ARG:NH2 | 4:Y:190:MET:CE[1_556]  | 1.35                     | 0.85              |
| 4:1:285:CYS:C   | 4:Y:283:MET:CA[1_556]  | 1.35                     | 0.85              |
| 4:2:215:LYS:CE  | 4:Z:249:THR:OG1[1_556] | 1.35                     | 0.85              |
| 4:0:153:LEU:CD1 | 4:X:262:PHE:C[1_556]   | 1.35                     | 0.85              |
| 4:2:142:LEU:CD1 | 4:Z:314:GLN:N[1_556]   | 1.35                     | 0.85              |
| 4:1:180:LEU:CG  | 4:Y:267:ILE:CB[1_556]  | 1.35                     | 0.85              |
| 4:2:212:ILE:CA  | 4:Z:196:ARG:CB[1_556]  | 1.35                     | 0.85              |
| 4:2:148:THR:CB  | 4:Z:327:ILE:O[1_556]   | 1.35                     | 0.85              |
| 4:0:196:ARG:NH2 | 4:W:114:ALA:C[1_556]   | 1.35                     | 0.85              |
| 4:2:357:ILE:CG1 | 4:Z:345:ILE:CD1[1_556] | 1.35                     | 0.85              |
| 4:1:214:GLU:CA  | 4:Y:253:GLU:OE2[1_556] | 1.35                     | 0.85              |
| 4:2:107:GLU:O   | 4:Z:301:GLY:N[1_556]   | 1.35                     | 0.85              |
| 4:1:182:GLY:O   | 4:Y:188:TYR:C[1_556]   | 1.36                     | 0.84              |
| 4:2:282:ILE:CG1 | 4:Z:320:LEU:CD1[1_556] | 1.36                     | 0.84              |
| 4:0:150:GLY:O   | 4:X:317:ILE:CB[1_556]  | 1.36                     | 0.84              |
| 4:0:167:GLU:N   | 4:X:295:ALA:N[1_556]   | 1.36                     | 0.84              |
| 4:2:196:ARG:CD  | 4:Y:115:ASN:ND2[1_556] | 1.36                     | 0.84              |
| 4:1:291:LYS:NZ  | 4:Y:322:PRO:CB[1_556]  | 1.36                     | 0.84              |
| 4:2:135:ALA:C   | 4:Z:299:MET:O[1_556]   | 1.36                     | 0.84              |
| 4:0:212:ILE:CA  | 4:X:196:ARG:CB[1_556]  | 1.36                     | 0.84              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:149:THR:CB  | 4:X:327:ILE:CD1[1_556] | 1.36                     | 0.84              |
| 4:2:194:THR:CB  | 4:Y:177:ARG:NH1[1_556] | 1.36                     | 0.84              |
| 4:1:338:SER:N   | 4:Y:307:PRO:CA[1_556]  | 1.36                     | 0.84              |
| 4:1:151:ILE:CG1 | 4:Y:275:HIS:C[1_556]   | 1.36                     | 0.84              |
| 4:2:332:PRO:CA  | 4:Z:221:LEU:CG[1_556]  | 1.36                     | 0.84              |
| 4:1:83:GLU:OE1  | 4:Y:29:ALA:CA[1_556]   | 1.36                     | 0.84              |
| 4:2:299:MET:CB  | 4:Z:312:ARG:CD[1_556]  | 1.36                     | 0.84              |
| 4:1:164:PRO:CA  | 4:Y:278:THR:CB[1_556]  | 1.36                     | 0.84              |
| 4:1:71:ILE:C    | 4:Y:157:ASP:OD1[1_556] | 1.36                     | 0.84              |
| 4:1:299:MET:CB  | 4:Y:312:ARG:CD[1_556]  | 1.36                     | 0.84              |
| 4:0:299:MET:CB  | 4:X:312:ARG:CD[1_556]  | 1.36                     | 0.84              |
| 4:2:372:ARG:CB  | 4:Z:143:TYR:CB[1_556]  | 1.36                     | 0.84              |
| 4:0:371:HIS:O   | 4:X:139:VAL:O[1_556]   | 1.36                     | 0.84              |
| 4:1:116:ARG:NE  | 4:Y:141:SER:N[1_556]   | 1.36                     | 0.84              |
| 4:0:194:THR:CB  | 4:W:177:ARG:NH1[1_556] | 1.36                     | 0.84              |
| 4:0:357:ILE:CG1 | 4:X:345:ILE:CD1[1_556] | 1.36                     | 0.84              |
| 4:0:266:PHE:N   | 4:W:173:HIS:ND1[1_556] | 1.36                     | 0.84              |
| 4:1:64:ILE:N    | 4:W:288:ASP:C[1_556]   | 1.36                     | 0.84              |
| 4:1:123:MET:CB  | 4:Y:26:ALA:CA[1_556]   | 1.36                     | 0.84              |
| 4:1:32:PRO:CG   | 4:Y:211:ASP:CB[1_556]  | 1.36                     | 0.84              |
| 4:0:154:ASP:OD2 | 4:X:309:ILE:CD1[1_556] | 1.36                     | 0.84              |
| 4:2:281:SER:CB  | 4:Z:277:THR:N[1_556]   | 1.36                     | 0.84              |
| 4:2:229:THR:C   | 4:Y:368:SER:CA[1_556]  | 1.36                     | 0.84              |
| 4:1:16:LEU:CB   | 4:Y:214:GLU:CB[1_556]  | 1.36                     | 0.84              |
| 4:1:150:GLY:O   | 4:Y:317:ILE:CG1[1_556] | 1.36                     | 0.84              |
| 4:1:62:ARG:NE   | 4:Y:204:ALA:C[1_556]   | 1.36                     | 0.84              |
| 4:0:332:PRO:CA  | 4:X:221:LEU:CG[1_556]  | 1.36                     | 0.84              |
| 4:2:106:THR:O   | 4:Z:335:ARG:O[1_556]   | 1.36                     | 0.84              |
| 4:0:261:LEU:C   | 4:X:266:PHE:N[1_556]   | 1.36                     | 0.84              |
| 4:1:282:ILE:CD1 | 4:Y:320:LEU:CD1[1_556] | 1.36                     | 0.84              |
| 4:0:32:PRO:CG   | 4:X:211:ASP:CB[1_556]  | 1.36                     | 0.84              |
| 4:1:72:GLU:OE2  | 4:Y:183:ARG:NE[1_556]  | 1.36                     | 0.84              |
| 4:1:141:SER:CA  | 4:Y:310:ALA:CB[1_556]  | 1.36                     | 0.84              |
| 4:0:187:ASP:N   | 4:X:191:LYS:N[1_556]   | 1.36                     | 0.84              |
| 4:0:298:VAL:CG1 | 4:X:312:ARG:C[1_556]   | 1.36                     | 0.84              |
| 4:1:16:LEU:CB   | 4:Y:214:GLU:C[1_556]   | 1.36                     | 0.84              |
| 4:0:162:ASN:CG  | 4:X:274:ILE:N[1_556]   | 1.36                     | 0.84              |
| 4:1:162:ASN:CG  | 4:Y:274:ILE:N[1_556]   | 1.36                     | 0.84              |
| 4:0:106:THR:O   | 4:X:335:ARG:O[1_556]   | 1.36                     | 0.84              |
| 4:1:362:TYR:CD2 | 4:Y:22:ALA:C[1_556]    | 1.36                     | 0.84              |
| 4:0:111:ASN:CA  | 4:X:154:ASP:OD2[1_556] | 1.36                     | 0.84              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:209:VAL:CG2 | 4:X:194:THR:O[1_556]   | 1.36                     | 0.84              |
| 4:1:291:LYS:CE  | 4:Y:322:PRO:CB[1_556]  | 1.36                     | 0.84              |
| 4:1:81:ASP:N    | 4:Y:31:PHE:CA[1_556]   | 1.36                     | 0.84              |
| 4:0:180:LEU:CG  | 4:X:267:ILE:CB[1_556]  | 1.36                     | 0.84              |
| 4:2:113:LYS:CA  | 4:Z:137:GLN:N[1_556]   | 1.36                     | 0.84              |
| 4:0:335:ARG:CZ  | 4:X:220:ALA:CB[1_556]  | 1.36                     | 0.84              |
| 4:1:177:ARG:N   | 4:Y:178:LEU:CG[1_556]  | 1.36                     | 0.84              |
| 4:0:62:ARG:CD   | 4:X:204:ALA:CA[1_556]  | 1.36                     | 0.84              |
| 4:2:147:ARG:O   | 4:Z:314:GLN:NE2[1_556] | 1.36                     | 0.84              |
| 4:3:267:ILE:C   | 4:Z:173:HIS:C[1_556]   | 1.36                     | 0.84              |
| 4:0:261:LEU:CG  | 4:X:266:PHE:CD2[1_556] | 1.36                     | 0.84              |
| 4:1:83:GLU:CB   | 4:Y:30:VAL:N[1_556]    | 1.36                     | 0.84              |
| 4:2:365:ALA:CA  | 4:Z:349:LEU:CA[1_556]  | 1.36                     | 0.84              |
| 4:2:303:THR:OG1 | 4:Z:257:CYS:CB[1_556]  | 1.37                     | 0.83              |
| 4:0:134:VAL:C   | 4:X:338:SER:OG[1_556]  | 1.37                     | 0.83              |
| 4:0:229:THR:C   | 4:W:368:SER:CA[1_556]  | 1.37                     | 0.83              |
| 4:2:261:LEU:CG  | 4:Z:266:PHE:CD2[1_556] | 1.37                     | 0.83              |
| 4:0:364:GLU:N   | 4:X:348:SER:O[1_556]   | 1.37                     | 0.83              |
| 4:2:177:ARG:CA  | 4:Z:178:LEU:CB[1_556]  | 1.37                     | 0.83              |
| 4:1:142:LEU:CD1 | 4:Y:314:GLN:N[1_556]   | 1.37                     | 0.83              |
| 4:1:59:GLN:CD   | 4:Y:208:ILE:CB[1_556]  | 1.37                     | 0.83              |
| 4:0:71:ILE:C    | 4:X:157:ASP:OD1[1_556] | 1.37                     | 0.83              |
| 4:0:108:ALA:O   | 4:X:154:ASP:OD1[1_556] | 1.37                     | 0.83              |
| 4:2:40:HIS:CG   | 4:X:166:TYR:CG[1_556]  | 1.37                     | 0.83              |
| 4:2:154:ASP:OD2 | 4:Z:309:ILE:CD1[1_556] | 1.37                     | 0.83              |
| 4:2:111:ASN:CA  | 4:Z:154:ASP:OD2[1_556] | 1.37                     | 0.83              |
| 4:0:196:ARG:CD  | 4:W:115:ASN:ND2[1_556] | 1.37                     | 0.83              |
| 4:0:365:ALA:CA  | 4:X:349:LEU:CA[1_556]  | 1.37                     | 0.83              |
| 4:1:261:LEU:CD1 | 4:Y:266:PHE:CE2[1_556] | 1.37                     | 0.83              |
| 4:1:206:ARG:CG  | 4:Y:200:PHE:C[1_556]   | 1.37                     | 0.83              |
| 4:0:177:ARG:CA  | 4:X:178:LEU:CB[1_556]  | 1.37                     | 0.83              |
| 4:1:212:ILE:CB  | 4:Y:196:ARG:C[1_556]   | 1.37                     | 0.83              |
| 4:2:196:ARG:NH2 | 4:Y:114:ALA:C[1_556]   | 1.37                     | 0.83              |
| 4:2:72:GLU:OE2  | 4:Z:183:ARG:NE[1_556]  | 1.37                     | 0.83              |
| 4:1:183:ARG:CG  | 4:Y:186:THR:C[1_556]   | 1.37                     | 0.83              |
| 4:0:113:LYS:CB  | 4:X:136:ILE:CA[1_556]  | 1.37                     | 0.83              |
| 4:4:64:ILE:N    | 4:Z:288:ASP:C[1_556]   | 1.37                     | 0.83              |
| 4:1:215:LYS:CE  | 4:Y:249:THR:OG1[1_556] | 1.37                     | 0.83              |
| 4:2:73:HIS:CB   | 4:Z:157:ASP:O[1_556]   | 1.37                     | 0.83              |
| 4:1:179:ASP:N   | 4:Y:180:LEU:CB[1_556]  | 1.37                     | 0.83              |
| 4:1:177:ARG:CD  | 4:Y:178:LEU:O[1_556]   | 1.37                     | 0.83              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:109:PRO:N   | 4:Z:154:ASP:CA[1_556]  | 1.37                     | 0.83              |
| 4:2:134:VAL:C   | 4:Z:338:SER:OG[1_556]  | 1.37                     | 0.83              |
| 4:0:301:GLY:N   | 4:X:219:VAL:CB[1_556]  | 1.37                     | 0.83              |
| 4:2:180:LEU:CG  | 4:Z:267:ILE:CB[1_556]  | 1.37                     | 0.83              |
| 4:2:67:LEU:O    | 4:Z:59:GLN:OE1[1_556]  | 1.37                     | 0.83              |
| 4:0:303:THR:OG1 | 4:X:257:CYS:CB[1_556]  | 1.37                     | 0.83              |
| 4:0:267:ILE:C   | 4:W:173:HIS:C[1_556]   | 1.37                     | 0.83              |
| 4:0:161:HIS:C   | 4:X:274:ILE:CG1[1_556] | 1.37                     | 0.83              |
| 4:1:133:TYR:O   | 4:Y:334:GLU:OE1[1_556] | 1.37                     | 0.83              |
| 4:0:107:GLU:O   | 4:X:301:GLY:N[1_556]   | 1.37                     | 0.83              |
| 4:0:335:ARG:CD  | 4:X:220:ALA:C[1_556]   | 1.37                     | 0.83              |
| 4:1:118:LYS:CG  | 4:Y:11:ASP:N[1_556]    | 1.37                     | 0.83              |
| 4:0:272:ALA:N   | 4:X:270:GLU:N[1_556]   | 1.37                     | 0.83              |
| 4:1:167:GLU:CB  | 4:Y:295:ALA:CB[1_556]  | 1.37                     | 0.83              |
| 4:2:153:LEU:CD1 | 4:Z:262:PHE:C[1_556]   | 1.37                     | 0.83              |
| 4:2:272:ALA:N   | 4:Z:270:GLU:N[1_556]   | 1.37                     | 0.83              |
| 4:0:171:LEU:N   | 4:X:151:ILE:CD1[1_556] | 1.37                     | 0.83              |
| 4:3:270:GLU:CD  | 4:Z:286:ASP:CB[1_556]  | 1.37                     | 0.83              |
| 4:1:116:ARG:CD  | 4:Y:141:SER:N[1_556]   | 1.37                     | 0.83              |
| 4:1:229:THR:O   | 4:X:368:SER:CB[1_556]  | 1.37                     | 0.83              |
| 4:0:304:THR:N   | 4:X:255:PHE:O[1_556]   | 1.37                     | 0.83              |
| 4:1:209:VAL:CG2 | 4:Y:194:THR:O[1_556]   | 1.37                     | 0.83              |
| 4:1:164:PRO:CB  | 4:Y:278:THR:C[1_556]   | 1.37                     | 0.83              |
| 4:2:371:HIS:O   | 4:Z:139:VAL:O[1_556]   | 1.37                     | 0.83              |
| 4:1:267:ILE:C   | 4:X:173:HIS:C[1_556]   | 1.37                     | 0.83              |
| 4:1:211:ASP:CG  | 4:Y:249:THR:C[1_556]   | 1.37                     | 0.83              |
| 4:0:116:ARG:CD  | 4:X:141:SER:N[1_556]   | 1.37                     | 0.83              |
| 4:0:136:ILE:CA  | 4:X:300:SER:N[1_556]   | 1.37                     | 0.83              |
| 4:0:131:ALA:N   | 4:X:25:ASP:OD1[1_556]  | 1.37                     | 0.83              |
| 4:2:285:CYS:C   | 4:Z:283:MET:CA[1_556]  | 1.37                     | 0.83              |
| 4:1:164:PRO:CD  | 4:Y:278:THR:N[1_556]   | 1.37                     | 0.83              |
| 4:0:67:LEU:O    | 4:X:59:GLN:OE1[1_556]  | 1.38                     | 0.82              |
| 4:2:107:GLU:N   | 4:Z:335:ARG:O[1_556]   | 1.38                     | 0.82              |
| 4:3:230:ALA:N   | 4:Z:368:SER:O[1_556]   | 1.38                     | 0.82              |
| 4:2:335:ARG:CD  | 4:Z:220:ALA:C[1_556]   | 1.38                     | 0.82              |
| 4:1:364:GLU:O   | 4:Y:349:LEU:O[1_556]   | 1.38                     | 0.82              |
| 4:1:206:ARG:CA  | 4:Y:200:PHE:N[1_556]   | 1.38                     | 0.82              |
| 4:1:213:LYS:O   | 4:Y:253:GLU:OE1[1_556] | 1.38                     | 0.82              |
| 4:2:149:THR:CB  | 4:Z:327:ILE:CD1[1_556] | 1.38                     | 0.82              |
| 4:0:107:GLU:O   | 4:X:300:SER:O[1_556]   | 1.38                     | 0.82              |
| 4:1:372:ARG:CB  | 4:Y:143:TYR:CB[1_556]  | 1.38                     | 0.82              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:296:ASN:O   | 4:Y:317:ILE:N[1_556]   | 1.38                     | 0.82              |
| 4:1:170:ALA:O   | 4:Y:151:ILE:CG1[1_556] | 1.38                     | 0.82              |
| 4:2:150:GLY:O   | 4:Z:317:ILE:CB[1_556]  | 1.38                     | 0.82              |
| 4:2:298:VAL:CG1 | 4:Z:312:ARG:C[1_556]   | 1.38                     | 0.82              |
| 4:0:177:ARG:N   | 4:X:178:LEU:CG[1_556]  | 1.38                     | 0.82              |
| 4:1:369:ILE:CG2 | 4:Y:345:ILE:CA[1_556]  | 1.38                     | 0.82              |
| 4:0:362:TYR:C   | 4:X:348:SER:OG[1_556]  | 1.38                     | 0.82              |
| 4:2:364:GLU:N   | 4:Z:348:SER:O[1_556]   | 1.38                     | 0.82              |
| 4:2:171:LEU:N   | 4:Z:151:ILE:CD1[1_556] | 1.38                     | 0.82              |
| 4:2:206:ARG:NE  | 4:Z:200:PHE:CB[1_556]  | 1.38                     | 0.82              |
| 4:2:267:ILE:C   | 4:Y:173:HIS:C[1_556]   | 1.38                     | 0.82              |
| 4:3:197:GLY:O   | 4:Z:75:ILE:C[1_556]    | 1.38                     | 0.82              |
| 4:2:32:PRO:CG   | 4:Z:211:ASP:CB[1_556]  | 1.38                     | 0.82              |
| 4:1:129:VAL:CG2 | 4:Y:25:ASP:CA[1_556]   | 1.38                     | 0.82              |
| 4:2:136:ILE:CA  | 4:Z:300:SER:N[1_556]   | 1.38                     | 0.82              |
| 4:0:215:LYS:CE  | 4:X:249:THR:OG1[1_556] | 1.38                     | 0.82              |
| 4:1:304:THR:OG1 | 4:Y:223:PHE:CE2[1_556] | 1.38                     | 0.82              |
| 4:0:281:SER:CB  | 4:X:277:THR:N[1_556]   | 1.38                     | 0.82              |
| 4:0:86:TRP:CD1  | 4:X:337:TYR:OH[1_556]  | 1.38                     | 0.82              |
| 4:2:306:TYR:CE1 | 4:Z:256:ARG:CB[1_556]  | 1.38                     | 0.82              |
| 4:1:122:ILE:CG1 | 4:Y:19:ALA:CA[1_556]   | 1.38                     | 0.82              |
| 4:1:267:ILE:C   | 4:X:173:HIS:O[1_556]   | 1.38                     | 0.82              |
| 4:1:150:GLY:O   | 4:Y:317:ILE:CB[1_556]  | 1.38                     | 0.82              |
| 4:2:113:LYS:CB  | 4:Z:136:ILE:CA[1_556]  | 1.38                     | 0.82              |
| 4:0:288:ASP:OD2 | 4:Z:205:GLU:CD[1_556]  | 1.38                     | 0.82              |
| 4:0:141:SER:O   | 4:X:310:ALA:C[1_556]   | 1.38                     | 0.82              |
| 4:0:72:GLU:OE2  | 4:X:183:ARG:NE[1_556]  | 1.38                     | 0.82              |
| 4:0:372:ARG:CB  | 4:X:143:TYR:CB[1_556]  | 1.38                     | 0.82              |
| 4:2:209:VAL:CG2 | 4:Z:194:THR:O[1_556]   | 1.38                     | 0.82              |
| 4:0:206:ARG:NE  | 4:X:200:PHE:CB[1_556]  | 1.38                     | 0.82              |
| 4:2:301:GLY:N   | 4:Z:219:VAL:CB[1_556]  | 1.38                     | 0.82              |
| 4:0:213:LYS:CB  | 4:X:192:ILE:O[1_556]   | 1.38                     | 0.82              |
| 4:0:166:TYR:CG  | 4:X:294:TYR:CG[1_556]  | 1.38                     | 0.82              |
| 4:1:186:THR:CA  | 4:Y:191:LYS:C[1_556]   | 1.38                     | 0.82              |
| 4:0:109:PRO:N   | 4:X:154:ASP:CA[1_556]  | 1.38                     | 0.82              |
| 4:4:40:HIS:CG   | 4:Z:166:TYR:CG[1_556]  | 1.38                     | 0.82              |
| 4:0:186:THR:CA  | 4:X:191:LYS:C[1_556]   | 1.38                     | 0.82              |
| 4:3:229:THR:O   | 4:Z:368:SER:CB[1_556]  | 1.38                     | 0.82              |
| 4:1:229:THR:C   | 4:X:368:SER:CA[1_556]  | 1.38                     | 0.82              |
| 4:1:270:GLU:CD  | 4:X:286:ASP:CB[1_556]  | 1.38                     | 0.82              |
| 4:1:180:LEU:CD1 | 4:Y:267:ILE:CB[1_556]  | 1.38                     | 0.82              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:297:ASN:ND2 | 4:Y:316:GLU:OE1[1_556] | 1.38                     | 0.82              |
| 4:0:113:LYS:CG  | 4:X:136:ILE:CB[1_556]  | 1.38                     | 0.82              |
| 4:2:294:TYR:C   | 4:Z:319:ALA:C[1_556]   | 1.38                     | 0.82              |
| 4:0:73:HIS:CB   | 4:X:157:ASP:O[1_556]   | 1.38                     | 0.82              |
| 4:2:304:THR:N   | 4:Z:255:PHE:O[1_556]   | 1.38                     | 0.82              |
| 4:1:197:GLY:O   | 4:X:75:ILE:C[1_556]    | 1.38                     | 0.82              |
| 4:1:175:ILE:CA  | 4:Y:162:ASN:OD1[1_556] | 1.38                     | 0.82              |
| 4:1:107:GLU:CG  | 4:Y:300:SER:CB[1_556]  | 1.38                     | 0.82              |
| 4:2:107:GLU:O   | 4:Z:300:SER:O[1_556]   | 1.39                     | 0.81              |
| 4:0:68:LYS:CG   | 4:X:59:GLN:CD[1_556]   | 1.39                     | 0.81              |
| 4:2:131:ALA:N   | 4:Z:25:ASP:OD1[1_556]  | 1.39                     | 0.81              |
| 4:0:173:HIS:N   | 4:X:281:SER:OG[1_556]  | 1.39                     | 0.81              |
| 4:1:230:ALA:N   | 4:X:368:SER:O[1_556]   | 1.39                     | 0.81              |
| 4:3:229:THR:C   | 4:Z:368:SER:CA[1_556]  | 1.39                     | 0.81              |
| 4:2:116:ARG:CD  | 4:Z:141:SER:N[1_556]   | 1.39                     | 0.81              |
| 4:2:298:VAL:N   | 4:Z:312:ARG:O[1_556]   | 1.39                     | 0.81              |
| 4:1:372:ARG:CZ  | 4:Y:142:LEU:O[1_556]   | 1.39                     | 0.81              |
| 4:1:174:ALA:C   | 4:Y:277:THR:O[1_556]   | 1.39                     | 0.81              |
| 4:2:186:THR:N   | 4:Z:188:TYR:O[1_556]   | 1.39                     | 0.81              |
| 4:1:147:ARG:O   | 4:Y:314:GLN:NE2[1_556] | 1.39                     | 0.81              |
| 4:2:86:TRP:CD1  | 4:Z:337:TYR:OH[1_556]  | 1.39                     | 0.81              |
| 4:0:83:GLU:N    | 4:X:30:VAL:CB[1_556]   | 1.39                     | 0.81              |
| 4:0:177:ARG:CD  | 4:X:178:LEU:O[1_556]   | 1.39                     | 0.81              |
| 4:0:306:TYR:CE1 | 4:X:256:ARG:CB[1_556]  | 1.39                     | 0.81              |
| 4:1:335:ARG:CZ  | 4:Y:220:ALA:CB[1_556]  | 1.39                     | 0.81              |
| 4:2:71:ILE:C    | 4:Z:157:ASP:OD1[1_556] | 1.39                     | 0.81              |
| 4:0:62:ARG:CD   | 4:X:205:GLU:N[1_556]   | 1.39                     | 0.81              |
| 4:2:174:ALA:O   | 4:Z:277:THR:O[1_556]   | 1.39                     | 0.81              |
| 4:2:177:ARG:N   | 4:Z:178:LEU:CG[1_556]  | 1.39                     | 0.81              |
| 4:2:338:SER:N   | 4:Z:307:PRO:CA[1_556]  | 1.39                     | 0.81              |
| 4:0:79:TRP:CG   | 4:X:17:VAL:CB[1_556]   | 1.39                     | 0.81              |
| 4:2:186:THR:CB  | 4:Z:190:MET:C[1_556]   | 1.39                     | 0.81              |
| 4:2:365:ALA:N   | 4:Z:348:SER:C[1_556]   | 1.39                     | 0.81              |
| 4:2:213:LYS:CB  | 4:Z:192:ILE:O[1_556]   | 1.39                     | 0.81              |
| 4:0:365:ALA:N   | 4:X:348:SER:C[1_556]   | 1.39                     | 0.81              |
| 4:0:164:PRO:CB  | 4:X:279:TYR:N[1_556]   | 1.39                     | 0.81              |
| 4:0:151:ILE:O   | 4:X:316:GLU:CB[1_556]  | 1.39                     | 0.81              |
| 4:2:79:TRP:CG   | 4:Z:17:VAL:CB[1_556]   | 1.39                     | 0.81              |
| 4:2:149:THR:OG1 | 4:Z:327:ILE:CA[1_556]  | 1.39                     | 0.81              |
| 4:0:161:HIS:CB  | 4:X:274:ILE:CG1[1_556] | 1.39                     | 0.81              |
| 4:1:106:THR:O   | 4:Y:335:ARG:O[1_556]   | 1.39                     | 0.81              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:166:TYR:CG  | 4:Y:294:TYR:CG[1_556]  | 1.39                     | 0.81              |
| 4:1:212:ILE:CA  | 4:Y:196:ARG:CD[1_556]  | 1.39                     | 0.81              |
| 4:1:291:LYS:NZ  | 4:Y:322:PRO:C[1_556]   | 1.39                     | 0.81              |
| 4:2:267:ILE:C   | 4:Y:173:HIS:O[1_556]   | 1.39                     | 0.81              |
| 4:1:140:LEU:CG  | 4:Y:331:ALA:C[1_556]   | 1.39                     | 0.81              |
| 4:1:161:HIS:C   | 4:Y:274:ILE:CG1[1_556] | 1.39                     | 0.81              |
| 4:0:126:THR:O   | 4:X:28:ARG:CD[1_556]   | 1.39                     | 0.81              |
| 4:2:141:SER:O   | 4:Z:310:ALA:C[1_556]   | 1.39                     | 0.81              |
| 4:0:187:ASP:N   | 4:X:191:LYS:CB[1_556]  | 1.39                     | 0.81              |
| 4:1:294:TYR:C   | 4:Y:319:ALA:C[1_556]   | 1.39                     | 0.81              |
| 4:1:165:ILE:CG2 | 4:Y:297:ASN:CB[1_556]  | 1.39                     | 0.81              |
| 4:1:79:TRP:CG   | 4:Y:17:VAL:CG1[1_556]  | 1.39                     | 0.81              |
| 4:3:267:ILE:C   | 4:Z:173:HIS:O[1_556]   | 1.39                     | 0.81              |
| 4:0:186:THR:CB  | 4:X:190:MET:C[1_556]   | 1.39                     | 0.81              |
| 4:0:107:GLU:N   | 4:X:335:ARG:O[1_556]   | 1.39                     | 0.81              |
| 4:0:338:SER:OG  | 4:X:308:GLY:C[1_556]   | 1.39                     | 0.81              |
| 4:0:171:LEU:C   | 4:X:151:ILE:CD1[1_556] | 1.39                     | 0.81              |
| 4:0:149:THR:OG1 | 4:X:327:ILE:CA[1_556]  | 1.39                     | 0.81              |
| 4:2:175:ILE:CA  | 4:Z:162:ASN:OD1[1_556] | 1.39                     | 0.81              |
| 4:1:295:ALA:CA  | 4:Y:319:ALA:CA[1_556]  | 1.39                     | 0.81              |
| 4:0:285:CYS:C   | 4:X:283:MET:CA[1_556]  | 1.39                     | 0.81              |
| 4:1:187:ASP:N   | 4:Y:191:LYS:CB[1_556]  | 1.39                     | 0.81              |
| 4:4:63:GLY:CA   | 4:Z:288:ASP:C[1_556]   | 1.39                     | 0.81              |
| 4:2:113:LYS:CG  | 4:Z:136:ILE:CB[1_556]  | 1.40                     | 0.80              |
| 4:2:280:ASN:O   | 4:Z:280:ASN:OD1[1_556] | 1.40                     | 0.80              |
| 4:0:271:SER:OG  | 4:X:269:MET:CA[1_556]  | 1.40                     | 0.80              |
| 4:1:281:SER:CB  | 4:Y:277:THR:N[1_556]   | 1.40                     | 0.80              |
| 4:1:62:ARG:CD   | 4:Y:205:GLU:N[1_556]   | 1.40                     | 0.80              |
| 4:0:255:PHE:N   | 4:W:113:LYS:NZ[1_556]  | 1.40                     | 0.80              |
| 4:2:162:ASN:OD1 | 4:Z:274:ILE:N[1_556]   | 1.40                     | 0.80              |
| 4:1:211:ASP:OD1 | 4:Y:249:THR:O[1_556]   | 1.40                     | 0.80              |
| 4:0:186:THR:N   | 4:X:188:TYR:O[1_556]   | 1.40                     | 0.80              |
| 4:2:178:LEU:CB  | 4:Z:180:LEU:CD2[1_556] | 1.40                     | 0.80              |
| 4:0:68:LYS:CD   | 4:X:59:GLN:CB[1_556]   | 1.40                     | 0.80              |
| 4:1:161:HIS:CB  | 4:Y:274:ILE:CD1[1_556] | 1.40                     | 0.80              |
| 4:0:174:ALA:O   | 4:X:277:THR:O[1_556]   | 1.40                     | 0.80              |
| 4:1:307:PRO:CA  | 4:Y:227:MET:CB[1_556]  | 1.40                     | 0.80              |
| 4:2:338:SER:OG  | 4:Z:308:GLY:C[1_556]   | 1.40                     | 0.80              |
| 4:0:214:GLU:OE1 | 4:X:250:ILE:CB[1_556]  | 1.40                     | 0.80              |
| 4:2:362:TYR:C   | 4:Z:348:SER:OG[1_556]  | 1.40                     | 0.80              |
| 4:0:116:ARG:CA  | 4:X:339:VAL:CG1[1_556] | 1.40                     | 0.80              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:251:GLY:N   | 4:Z:114:ALA:CA[1_556]  | 1.40                     | 0.80              |
| 4:0:306:TYR:CZ  | 4:X:256:ARG:CB[1_556]  | 1.40                     | 0.80              |
| 4:0:300:SER:C   | 4:X:219:VAL:CB[1_556]  | 1.40                     | 0.80              |
| 4:1:109:PRO:C   | 4:Y:154:ASP:N[1_556]   | 1.40                     | 0.80              |
| 4:1:153:LEU:CG  | 4:Y:262:PHE:CG[1_556]  | 1.40                     | 0.80              |
| 4:2:303:THR:CB  | 4:Z:257:CYS:O[1_556]   | 1.40                     | 0.80              |
| 4:2:171:LEU:C   | 4:Z:151:ILE:CD1[1_556] | 1.40                     | 0.80              |
| 4:1:357:ILE:CB  | 4:Y:345:ILE:CD1[1_556] | 1.40                     | 0.80              |
| 4:2:171:LEU:N   | 4:Z:151:ILE:CG1[1_556] | 1.40                     | 0.80              |
| 4:1:362:TYR:C   | 4:Y:348:SER:OG[1_556]  | 1.40                     | 0.80              |
| 4:1:111:ASN:CB  | 4:Y:154:ASP:OD2[1_556] | 1.40                     | 0.80              |
| 4:1:116:ARG:C   | 4:Y:339:VAL:O[1_556]   | 1.40                     | 0.80              |
| 4:2:300:SER:C   | 4:Z:219:VAL:CB[1_556]  | 1.40                     | 0.80              |
| 4:2:166:TYR:CG  | 4:Z:294:TYR:CG[1_556]  | 1.40                     | 0.80              |
| 4:2:306:TYR:CZ  | 4:Z:256:ARG:CB[1_556]  | 1.40                     | 0.80              |
| 4:0:338:SER:N   | 4:X:307:PRO:CA[1_556]  | 1.40                     | 0.80              |
| 4:2:126:THR:O   | 4:Z:28:ARG:CD[1_556]   | 1.40                     | 0.80              |
| 4:1:16:LEU:CG   | 4:Y:215:LYS:N[1_556]   | 1.40                     | 0.80              |
| 4:1:155:SER:CB  | 4:Y:258:PRO:O[1_556]   | 1.40                     | 0.80              |
| 4:1:206:ARG:CD  | 4:Y:200:PHE:CB[1_556]  | 1.40                     | 0.80              |
| 4:0:230:ALA:O   | 4:W:367:PRO:C[1_556]   | 1.40                     | 0.80              |
| 4:0:294:TYR:C   | 4:X:319:ALA:C[1_556]   | 1.40                     | 0.80              |
| 4:2:83:GLU:N    | 4:Z:30:VAL:CB[1_556]   | 1.40                     | 0.80              |
| 4:2:39:ARG:N    | 4:X:166:TYR:OH[1_556]  | 1.40                     | 0.80              |
| 4:1:332:PRO:CB  | 4:Y:221:LEU:CG[1_556]  | 1.40                     | 0.80              |
| 4:2:286:ASP:O   | 4:Z:283:MET:CE[1_556]  | 1.40                     | 0.80              |
| 4:0:336:LYS:CB  | 4:X:218:TYR:CA[1_556]  | 1.40                     | 0.80              |
| 4:2:164:PRO:CB  | 4:Z:279:TYR:N[1_556]   | 1.40                     | 0.80              |
| 4:4:39:ARG:N    | 4:Z:166:TYR:OH[1_556]  | 1.40                     | 0.80              |
| 4:1:104:LEU:O   | 4:Y:334:GLU:CA[1_556]  | 1.40                     | 0.80              |
| 4:2:68:LYS:CD   | 4:Z:59:GLN:CB[1_556]   | 1.40                     | 0.80              |
| 4:1:183:ARG:O   | 4:Y:187:ASP:C[1_556]   | 1.40                     | 0.80              |
| 4:1:365:ALA:O   | 4:Y:346:LEU:O[1_556]   | 1.40                     | 0.80              |
| 4:2:186:THR:CA  | 4:Z:191:LYS:C[1_556]   | 1.40                     | 0.80              |
| 4:1:365:ALA:N   | 4:Y:348:SER:C[1_556]   | 1.40                     | 0.80              |
| 4:0:298:VAL:N   | 4:X:312:ARG:O[1_556]   | 1.40                     | 0.80              |
| 4:2:173:HIS:N   | 4:Z:281:SER:OG[1_556]  | 1.40                     | 0.80              |
| 4:2:206:ARG:NH2 | 4:Z:190:MET:CE[1_556]  | 1.40                     | 0.80              |
| 4:2:292:ASP:CB  | 4:Z:321:ALA:CB[1_556]  | 1.40                     | 0.80              |
| 4:0:39:ARG:N    | 4:V:166:TYR:OH[1_556]  | 1.40                     | 0.80              |
| 4:0:111:ASN:CB  | 4:X:154:ASP:OD2[1_556] | 1.40                     | 0.80              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:118:LYS:CG  | 4:X:11:ASP:N[1_556]    | 1.40                     | 0.80              |
| 4:1:335:ARG:CD  | 4:Y:220:ALA:C[1_556]   | 1.40                     | 0.80              |
| 4:1:168:GLY:N   | 4:Y:296:ASN:N[1_556]   | 1.40                     | 0.80              |
| 4:0:32:PRO:CG   | 4:X:211:ASP:CG[1_556]  | 1.41                     | 0.79              |
| 4:2:331:ALA:O   | 4:Z:221:LEU:C[1_556]   | 1.41                     | 0.79              |
| 4:0:164:PRO:O   | 4:X:278:THR:CG2[1_556] | 1.41                     | 0.79              |
| 4:0:267:ILE:C   | 4:W:173:HIS:O[1_556]   | 1.41                     | 0.79              |
| 4:2:161:HIS:CB  | 4:Z:274:ILE:CG1[1_556] | 1.41                     | 0.79              |
| 4:2:215:LYS:N   | 4:Z:253:GLU:OE2[1_556] | 1.41                     | 0.79              |
| 4:2:303:THR:N   | 4:Z:258:PRO:N[1_556]   | 1.41                     | 0.79              |
| 4:2:16:LEU:CB   | 4:Z:214:GLU:CB[1_556]  | 1.41                     | 0.79              |
| 4:0:303:THR:CB  | 4:X:257:CYS:O[1_556]   | 1.41                     | 0.79              |
| 4:0:331:ALA:O   | 4:X:221:LEU:C[1_556]   | 1.41                     | 0.79              |
| 4:2:169:TYR:N   | 4:Z:296:ASN:CA[1_556]  | 1.41                     | 0.79              |
| 4:0:286:ASP:O   | 4:X:283:MET:CE[1_556]  | 1.41                     | 0.79              |
| 4:0:178:LEU:CB  | 4:X:180:LEU:CD2[1_556] | 1.41                     | 0.79              |
| 4:1:37:ARG:CB   | 4:Y:60:SER:OG[1_556]   | 1.41                     | 0.79              |
| 4:0:15:GLY:O    | 4:X:210:ARG:O[1_556]   | 1.41                     | 0.79              |
| 4:2:255:PHE:N   | 4:Y:113:LYS:NZ[1_556]  | 1.41                     | 0.79              |
| 4:0:83:GLU:CB   | 4:X:30:VAL:N[1_556]    | 1.41                     | 0.79              |
| 4:2:68:LYS:CG   | 4:Z:59:GLN:CD[1_556]   | 1.41                     | 0.79              |
| 4:3:39:ARG:N    | 4:Y:166:TYR:OH[1_556]  | 1.41                     | 0.79              |
| 4:0:299:MET:CA  | 4:X:312:ARG:CD[1_556]  | 1.41                     | 0.79              |
| 4:0:303:THR:N   | 4:X:258:PRO:N[1_556]   | 1.41                     | 0.79              |
| 4:2:177:ARG:CD  | 4:Z:178:LEU:O[1_556]   | 1.41                     | 0.79              |
| 4:1:251:GLY:N   | 4:X:114:ALA:CA[1_556]  | 1.41                     | 0.79              |
| 4:2:32:PRO:CG   | 4:Z:211:ASP:CG[1_556]  | 1.41                     | 0.79              |
| 4:0:145:SER:N   | 4:X:311:ASP:OD1[1_556] | 1.41                     | 0.79              |
| 4:0:307:PRO:CB  | 4:X:227:MET:C[1_556]   | 1.41                     | 0.79              |
| 4:1:186:THR:N   | 4:Y:188:TYR:O[1_556]   | 1.41                     | 0.79              |
| 4:0:130:PRO:N   | 4:X:25:ASP:OD2[1_556]  | 1.41                     | 0.79              |
| 4:2:166:TYR:CB  | 4:Z:294:TYR:CA[1_556]  | 1.41                     | 0.79              |
| 4:1:39:ARG:N    | 4:W:166:TYR:OH[1_556]  | 1.41                     | 0.79              |
| 4:3:253:GLU:CD  | 4:Z:113:LYS:N[1_556]   | 1.41                     | 0.79              |
| 4:2:336:LYS:CB  | 4:Z:218:TYR:CA[1_556]  | 1.41                     | 0.79              |
| 4:1:148:THR:CG2 | 4:Y:328:LYS:CB[1_556]  | 1.41                     | 0.79              |
| 4:1:167:GLU:OE2 | 4:Y:326:LYS:C[1_556]   | 1.41                     | 0.79              |
| 4:2:299:MET:N   | 4:Z:312:ARG:CB[1_556]  | 1.41                     | 0.79              |
| 4:2:116:ARG:NE  | 4:Z:141:SER:N[1_556]   | 1.41                     | 0.79              |
| 4:1:277:THR:CG2 | 4:Y:273:GLY:N[1_556]   | 1.41                     | 0.79              |
| 4:1:272:ALA:N   | 4:Y:270:GLU:N[1_556]   | 1.41                     | 0.79              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:151:ILE:O   | 4:Z:316:GLU:CB[1_556]  | 1.41                     | 0.79              |
| 4:1:82:MET:N    | 4:Y:31:PHE:N[1_556]    | 1.41                     | 0.79              |
| 4:2:62:ARG:CD   | 4:Z:205:GLU:N[1_556]   | 1.41                     | 0.79              |
| 4:0:304:THR:OG1 | 4:X:223:PHE:CE2[1_556] | 1.41                     | 0.79              |
| 4:2:271:SER:OG  | 4:Z:269:MET:CA[1_556]  | 1.41                     | 0.79              |
| 4:2:338:SER:CB  | 4:Z:308:GLY:N[1_556]   | 1.41                     | 0.79              |
| 4:0:162:ASN:OD1 | 4:X:274:ILE:N[1_556]   | 1.41                     | 0.79              |
| 4:0:280:ASN:O   | 4:X:280:ASN:OD1[1_556] | 1.41                     | 0.79              |
| 4:2:362:TYR:CD2 | 4:Z:22:ALA:C[1_556]    | 1.41                     | 0.79              |
| 4:0:115:ASN:CA  | 4:X:11:ASP:CG[1_556]   | 1.41                     | 0.79              |
| 4:2:214:GLU:OE1 | 4:Z:250:ILE:CB[1_556]  | 1.41                     | 0.79              |
| 4:2:211:ASP:OD2 | 4:Z:249:THR:N[1_556]   | 1.41                     | 0.79              |
| 4:2:115:ASN:CA  | 4:Z:11:ASP:CG[1_556]   | 1.41                     | 0.79              |
| 4:2:63:GLY:CA   | 4:X:288:ASP:C[1_556]   | 1.41                     | 0.79              |
| 4:0:150:GLY:N   | 4:X:317:ILE:CG1[1_556] | 1.41                     | 0.79              |
| 4:1:280:ASN:N   | 4:Y:276:GLU:OE1[1_556] | 1.41                     | 0.79              |
| 4:0:292:ASP:CB  | 4:X:321:ALA:CB[1_556]  | 1.41                     | 0.79              |
| 4:1:12:ASN:O    | 4:Y:302:GLY:CA[1_556]  | 1.41                     | 0.79              |
| 4:2:187:ASP:N   | 4:Z:191:LYS:CB[1_556]  | 1.41                     | 0.79              |
| 4:1:281:SER:O   | 4:Y:280:ASN:CG[1_556]  | 1.41                     | 0.79              |
| 4:4:40:HIS:CD2  | 4:Z:166:TYR:C[1_556]   | 1.41                     | 0.79              |
| 4:0:78:ASN:CB   | 4:X:32:PRO:CA[1_556]   | 1.41                     | 0.79              |
| 4:1:40:HIS:CD2  | 4:W:166:TYR:C[1_556]   | 1.41                     | 0.79              |
| 4:2:150:GLY:N   | 4:Z:317:ILE:CG1[1_556] | 1.41                     | 0.79              |
| 4:1:159:VAL:CG1 | 4:Y:181:ALA:N[1_556]   | 1.41                     | 0.79              |
| 4:0:338:SER:CB  | 4:X:308:GLY:N[1_556]   | 1.41                     | 0.79              |
| 4:0:126:THR:C   | 4:X:28:ARG:CD[1_556]   | 1.41                     | 0.79              |
| 4:1:306:TYR:CE1 | 4:Y:256:ARG:CB[1_556]  | 1.41                     | 0.79              |
| 4:2:126:THR:C   | 4:Z:28:ARG:CD[1_556]   | 1.41                     | 0.79              |
| 4:2:116:ARG:CA  | 4:Z:339:VAL:CG1[1_556] | 1.41                     | 0.79              |
| 4:2:178:LEU:C   | 4:Z:180:LEU:CG[1_556]  | 1.41                     | 0.79              |
| 4:1:10:CYS:SG   | 4:Y:336:LYS:NZ[1_556]  | 1.41                     | 0.79              |
| 4:0:175:ILE:CA  | 4:X:162:ASN:OD1[1_556] | 1.41                     | 0.79              |
| 4:1:172:PRO:CB  | 4:Y:164:PRO:CD[1_556]  | 1.42                     | 0.78              |
| 4:0:106:THR:N   | 4:X:336:LYS:N[1_556]   | 1.42                     | 0.78              |
| 4:1:73:HIS:CB   | 4:Y:157:ASP:O[1_556]   | 1.42                     | 0.78              |
| 4:2:111:ASN:CB  | 4:Z:154:ASP:OD2[1_556] | 1.42                     | 0.78              |
| 4:0:211:ASP:OD2 | 4:X:249:THR:N[1_556]   | 1.42                     | 0.78              |
| 4:1:72:GLU:N    | 4:Y:157:ASP:OD2[1_556] | 1.42                     | 0.78              |
| 4:2:130:PRO:N   | 4:Z:25:ASP:OD2[1_556]  | 1.42                     | 0.78              |
| 4:1:253:GLU:CD  | 4:X:113:LYS:N[1_556]   | 1.42                     | 0.78              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:118:LYS:CG  | 4:Z:11:ASP:N[1_556]    | 1.42                     | 0.78              |
| 4:2:16:LEU:CG   | 4:Z:214:GLU:C[1_556]   | 1.42                     | 0.78              |
| 4:1:68:LYS:CG   | 4:Y:59:GLN:NE2[1_556]  | 1.42                     | 0.78              |
| 4:0:116:ARG:NE  | 4:X:141:SER:N[1_556]   | 1.42                     | 0.78              |
| 4:2:230:ALA:O   | 4:Y:367:PRO:C[1_556]   | 1.42                     | 0.78              |
| 4:0:171:LEU:N   | 4:X:151:ILE:CG1[1_556] | 1.42                     | 0.78              |
| 4:0:178:LEU:C   | 4:X:180:LEU:CG[1_556]  | 1.42                     | 0.78              |
| 4:2:145:SER:N   | 4:Z:311:ASP:OD1[1_556] | 1.42                     | 0.78              |
| 4:1:119:MET:O   | 4:Y:340:TRP:CD2[1_556] | 1.42                     | 0.78              |
| 4:3:255:PHE:N   | 4:Z:113:LYS:NZ[1_556]  | 1.42                     | 0.78              |
| 4:1:267:ILE:N   | 4:X:173:HIS:CG[1_556]  | 1.42                     | 0.78              |
| 4:0:302:GLY:N   | 4:X:258:PRO:CG[1_556]  | 1.42                     | 0.78              |
| 4:1:111:ASN:N   | 4:Y:154:ASP:OD2[1_556] | 1.42                     | 0.78              |
| 4:1:63:GLY:CA   | 4:W:289:ILE:N[1_556]   | 1.42                     | 0.78              |
| 4:0:302:GLY:O   | 4:X:255:PHE:CA[1_556]  | 1.42                     | 0.78              |
| 4:2:302:GLY:N   | 4:Z:258:PRO:CG[1_556]  | 1.42                     | 0.78              |
| 4:1:303:THR:OG1 | 4:Y:257:CYS:CB[1_556]  | 1.42                     | 0.78              |
| 4:0:369:ILE:C   | 4:X:143:TYR:CE2[1_556] | 1.42                     | 0.78              |
| 4:2:229:THR:C   | 4:Y:368:SER:CB[1_556]  | 1.42                     | 0.78              |
| 4:1:336:LYS:NZ  | 4:Y:254:ARG:CZ[1_556]  | 1.42                     | 0.78              |
| 4:0:362:TYR:CD2 | 4:X:22:ALA:C[1_556]    | 1.42                     | 0.78              |
| 4:2:206:ARG:CA  | 4:Z:200:PHE:N[1_556]   | 1.42                     | 0.78              |
| 4:1:30:VAL:O    | 4:Y:215:LYS:CD[1_556]  | 1.42                     | 0.78              |
| 4:0:149:THR:CA  | 4:X:327:ILE:CB[1_556]  | 1.42                     | 0.78              |
| 4:0:206:ARG:NH2 | 4:X:190:MET:CE[1_556]  | 1.42                     | 0.78              |
| 4:2:164:PRO:CA  | 4:Z:278:THR:CB[1_556]  | 1.42                     | 0.78              |
| 4:0:169:TYR:N   | 4:X:296:ASN:CA[1_556]  | 1.42                     | 0.78              |
| 4:2:149:THR:O   | 4:Z:327:ILE:CG2[1_556] | 1.42                     | 0.78              |
| 4:0:364:GLU:O   | 4:X:349:LEU:O[1_556]   | 1.42                     | 0.78              |
| 4:2:106:THR:N   | 4:Z:336:LYS:N[1_556]   | 1.42                     | 0.78              |
| 4:0:215:LYS:N   | 4:X:253:GLU:OE2[1_556] | 1.42                     | 0.78              |
| 4:1:107:GLU:N   | 4:Y:335:ARG:O[1_556]   | 1.42                     | 0.78              |
| 4:1:83:GLU:N    | 4:Y:30:VAL:CB[1_556]   | 1.42                     | 0.78              |
| 4:1:68:LYS:CG   | 4:Y:59:GLN:CD[1_556]   | 1.42                     | 0.78              |
| 4:2:154:ASP:CG  | 4:Z:309:ILE:CD1[1_556] | 1.42                     | 0.78              |
| 4:2:40:HIS:CD2  | 4:X:166:TYR:C[1_556]   | 1.42                     | 0.78              |
| 4:0:307:PRO:CA  | 4:X:227:MET:CB[1_556]  | 1.42                     | 0.78              |
| 4:1:142:LEU:CD1 | 4:Y:314:GLN:CA[1_556]  | 1.42                     | 0.78              |
| 4:3:40:HIS:CD2  | 4:Y:166:TYR:C[1_556]   | 1.42                     | 0.78              |
| 4:2:107:GLU:CD  | 4:Z:141:SER:OG[1_556]  | 1.42                     | 0.78              |
| 4:2:366:GLY:CA  | 4:Z:347:ALA:O[1_556]   | 1.42                     | 0.78              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:77:THR:OG1  | 4:Y:14:SER:O[1_556]    | 1.42                     | 0.78              |
| 4:2:372:ARG:CB  | 4:Z:143:TYR:CA[1_556]  | 1.42                     | 0.78              |
| 4:2:78:ASN:CB   | 4:Z:32:PRO:CA[1_556]   | 1.42                     | 0.78              |
| 4:1:299:MET:CA  | 4:Y:312:ARG:CD[1_556]  | 1.42                     | 0.78              |
| 4:2:207:GLU:O   | 4:Z:200:PHE:CZ[1_556]  | 1.42                     | 0.78              |
| 4:2:83:GLU:CB   | 4:Z:30:VAL:N[1_556]    | 1.42                     | 0.78              |
| 4:0:166:TYR:CB  | 4:X:294:TYR:CA[1_556]  | 1.42                     | 0.78              |
| 4:1:304:THR:N   | 4:Y:255:PHE:O[1_556]   | 1.42                     | 0.78              |
| 4:2:119:MET:O   | 4:Z:340:TRP:CE3[1_556] | 1.42                     | 0.78              |
| 4:2:164:PRO:O   | 4:Z:278:THR:CG2[1_556] | 1.42                     | 0.78              |
| 4:0:16:LEU:CB   | 4:X:214:GLU:CB[1_556]  | 1.42                     | 0.78              |
| 4:0:281:SER:OG  | 4:X:276:GLU:C[1_556]   | 1.42                     | 0.78              |
| 4:1:104:LEU:CD2 | 4:Y:333:PRO:N[1_556]   | 1.42                     | 0.78              |
| 4:0:332:PRO:CD  | 4:X:221:LEU:CG[1_556]  | 1.43                     | 0.77              |
| 4:2:307:PRO:CB  | 4:Z:227:MET:C[1_556]   | 1.43                     | 0.77              |
| 4:0:229:THR:C   | 4:W:368:SER:CB[1_556]  | 1.43                     | 0.77              |
| 4:0:208:ILE:CA  | 4:X:198:TYR:CD1[1_556] | 1.43                     | 0.77              |
| 4:1:177:ARG:CB  | 4:Y:178:LEU:O[1_556]   | 1.43                     | 0.77              |
| 4:0:170:ALA:O   | 4:X:151:ILE:CG1[1_556] | 1.43                     | 0.77              |
| 4:2:153:LEU:C   | 4:Z:262:PHE:CZ[1_556]  | 1.43                     | 0.77              |
| 4:0:153:LEU:C   | 4:X:262:PHE:CZ[1_556]  | 1.43                     | 0.77              |
| 4:2:256:ARG:NH2 | 4:Y:111:ASN:O[1_556]   | 1.43                     | 0.77              |
| 4:3:267:ILE:N   | 4:Z:173:HIS:CG[1_556]  | 1.43                     | 0.77              |
| 4:1:211:ASP:OD2 | 4:Y:249:THR:N[1_556]   | 1.43                     | 0.77              |
| 4:0:164:PRO:CA  | 4:X:278:THR:CB[1_556]  | 1.43                     | 0.77              |
| 4:0:16:LEU:CG   | 4:X:214:GLU:C[1_556]   | 1.43                     | 0.77              |
| 4:0:110:LEU:CD2 | 4:X:162:ASN:N[1_556]   | 1.43                     | 0.77              |
| 4:2:304:THR:OG1 | 4:Z:223:PHE:CE2[1_556] | 1.43                     | 0.77              |
| 4:0:256:ARG:NH2 | 4:W:111:ASN:O[1_556]   | 1.43                     | 0.77              |
| 4:1:206:ARG:NE  | 4:Y:200:PHE:CB[1_556]  | 1.43                     | 0.77              |
| 4:1:306:TYR:C   | 4:Y:227:MET:SD[1_556]  | 1.43                     | 0.77              |
| 4:1:164:PRO:O   | 4:Y:278:THR:CG2[1_556] | 1.43                     | 0.77              |
| 4:3:197:GLY:C   | 4:Z:75:ILE:CA[1_556]   | 1.43                     | 0.77              |
| 4:2:149:THR:CA  | 4:Z:327:ILE:CB[1_556]  | 1.43                     | 0.77              |
| 4:2:299:MET:CA  | 4:Z:312:ARG:CD[1_556]  | 1.43                     | 0.77              |
| 4:0:212:ILE:CB  | 4:X:196:ARG:C[1_556]   | 1.43                     | 0.77              |
| 4:1:15:GLY:O    | 4:Y:210:ARG:O[1_556]   | 1.43                     | 0.77              |
| 4:0:39:ARG:O    | 4:V:166:TYR:CE2[1_556] | 1.43                     | 0.77              |
| 4:1:307:PRO:N   | 4:Y:227:MET:SD[1_556]  | 1.43                     | 0.77              |
| 4:1:298:VAL:CG1 | 4:Y:312:ARG:CA[1_556]  | 1.43                     | 0.77              |
| 4:0:372:ARG:CB  | 4:X:143:TYR:CA[1_556]  | 1.43                     | 0.77              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:197:GLY:C   | 4:X:75:ILE:CA[1_556]   | 1.43                     | 0.77              |
| 4:0:106:THR:N   | 4:X:335:ARG:CA[1_556]  | 1.43                     | 0.77              |
| 4:2:15:GLY:O    | 4:Z:210:ARG:O[1_556]   | 1.43                     | 0.77              |
| 4:0:372:ARG:CB  | 4:X:143:TYR:N[1_556]   | 1.43                     | 0.77              |
| 4:1:369:ILE:C   | 4:Y:143:TYR:CE2[1_556] | 1.43                     | 0.77              |
| 4:2:165:ILE:CB  | 4:Z:297:ASN:OD1[1_556] | 1.43                     | 0.77              |
| 4:2:332:PRO:CD  | 4:Z:221:LEU:CG[1_556]  | 1.43                     | 0.77              |
| 4:2:115:ASN:N   | 4:Z:106:THR:OG1[1_556] | 1.43                     | 0.77              |
| 4:0:170:ALA:C   | 4:X:151:ILE:CG1[1_556] | 1.43                     | 0.77              |
| 4:0:299:MET:N   | 4:X:312:ARG:CB[1_556]  | 1.43                     | 0.77              |
| 4:4:63:GLY:CA   | 4:Z:289:ILE:N[1_556]   | 1.43                     | 0.77              |
| 4:0:298:VAL:CG1 | 4:X:312:ARG:CA[1_556]  | 1.43                     | 0.77              |
| 4:1:255:PHE:N   | 4:X:113:LYS:NZ[1_556]  | 1.43                     | 0.77              |
| 4:0:207:GLU:O   | 4:X:200:PHE:CZ[1_556]  | 1.43                     | 0.77              |
| 4:0:40:HIS:CD2  | 4:V:166:TYR:C[1_556]   | 1.43                     | 0.77              |
| 4:2:170:ALA:C   | 4:Z:151:ILE:CG1[1_556] | 1.43                     | 0.77              |
| 4:2:296:ASN:C   | 4:Z:315:LYS:C[1_556]   | 1.43                     | 0.77              |
| 4:2:369:ILE:C   | 4:Z:143:TYR:CE2[1_556] | 1.43                     | 0.77              |
| 4:0:79:TRP:CD2  | 4:X:17:VAL:C[1_556]    | 1.43                     | 0.77              |
| 4:0:141:SER:O   | 4:X:311:ASP:N[1_556]   | 1.43                     | 0.77              |
| 4:2:149:THR:C   | 4:Z:327:ILE:CG2[1_556] | 1.43                     | 0.77              |
| 4:2:165:ILE:CG2 | 4:Z:297:ASN:CB[1_556]  | 1.43                     | 0.77              |
| 4:2:302:GLY:O   | 4:Z:255:PHE:CA[1_556]  | 1.43                     | 0.77              |
| 4:1:278:THR:O   | 4:Y:276:GLU:CB[1_556]  | 1.43                     | 0.77              |
| 4:0:63:GLY:CA   | 4:V:288:ASP:C[1_556]   | 1.43                     | 0.77              |
| 4:0:154:ASP:CG  | 4:X:309:ILE:CD1[1_556] | 1.43                     | 0.77              |
| 4:2:297:ASN:CG  | 4:Z:316:GLU:CD[1_556]  | 1.43                     | 0.77              |
| 4:0:339:VAL:CG1 | 4:X:335:ARG:NH2[1_556] | 1.43                     | 0.77              |
| 4:0:165:ILE:CB  | 4:X:297:ASN:OD1[1_556] | 1.43                     | 0.77              |
| 4:0:68:LYS:CG   | 4:X:59:GLN:CG[1_556]   | 1.43                     | 0.77              |
| 4:2:212:ILE:CB  | 4:Z:196:ARG:C[1_556]   | 1.43                     | 0.77              |
| 4:2:211:ASP:OD1 | 4:Z:249:THR:O[1_556]   | 1.44                     | 0.76              |
| 4:0:372:ARG:CZ  | 4:X:142:LEU:O[1_556]   | 1.44                     | 0.76              |
| 4:0:129:VAL:CG2 | 4:X:25:ASP:CA[1_556]   | 1.44                     | 0.76              |
| 4:0:206:ARG:CA  | 4:X:200:PHE:N[1_556]   | 1.44                     | 0.76              |
| 4:0:291:LYS:NZ  | 4:X:322:PRO:CB[1_556]  | 1.44                     | 0.76              |
| 4:1:277:THR:CA  | 4:Y:272:ALA:CA[1_556]  | 1.44                     | 0.76              |
| 4:2:129:VAL:CG2 | 4:Z:25:ASP:CA[1_556]   | 1.44                     | 0.76              |
| 4:1:206:ARG:CZ  | 4:Y:190:MET:CE[1_556]  | 1.44                     | 0.76              |
| 4:0:206:ARG:CG  | 4:X:200:PHE:N[1_556]   | 1.44                     | 0.76              |
| 4:1:265:SER:CA  | 4:X:173:HIS:CE1[1_556] | 1.44                     | 0.76              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:299:MET:N   | 4:Y:312:ARG:CD[1_556]  | 1.44                     | 0.76              |
| 4:0:172:PRO:CB  | 4:X:164:PRO:CD[1_556]  | 1.44                     | 0.76              |
| 4:0:336:LYS:NZ  | 4:X:254:ARG:CZ[1_556]  | 1.44                     | 0.76              |
| 4:2:79:TRP:CD2  | 4:Z:17:VAL:C[1_556]    | 1.44                     | 0.76              |
| 4:0:164:PRO:CD  | 4:X:278:THR:N[1_556]   | 1.44                     | 0.76              |
| 4:2:301:GLY:O   | 4:Z:218:TYR:O[1_556]   | 1.44                     | 0.76              |
| 4:2:106:THR:N   | 4:Z:335:ARG:CA[1_556]  | 1.44                     | 0.76              |
| 4:2:339:VAL:CG1 | 4:Z:335:ARG:NH2[1_556] | 1.44                     | 0.76              |
| 4:1:151:ILE:O   | 4:Y:316:GLU:CB[1_556]  | 1.44                     | 0.76              |
| 4:3:63:GLY:CA   | 4:Y:289:ILE:N[1_556]   | 1.44                     | 0.76              |
| 4:2:172:PRO:CB  | 4:Z:164:PRO:CD[1_556]  | 1.44                     | 0.76              |
| 4:0:214:GLU:CD  | 4:X:250:ILE:CG2[1_556] | 1.44                     | 0.76              |
| 4:3:265:SER:CA  | 4:Z:173:HIS:CE1[1_556] | 1.44                     | 0.76              |
| 4:2:364:GLU:O   | 4:Z:349:LEU:O[1_556]   | 1.44                     | 0.76              |
| 4:0:296:ASN:C   | 4:X:315:LYS:C[1_556]   | 1.44                     | 0.76              |
| 4:1:366:GLY:CA  | 4:Y:347:ALA:O[1_556]   | 1.44                     | 0.76              |
| 4:1:196:ARG:N   | 4:X:75:ILE:CD1[1_556]  | 1.44                     | 0.76              |
| 4:0:115:ASN:N   | 4:X:106:THR:OG1[1_556] | 1.44                     | 0.76              |
| 4:0:253:GLU:CD  | 4:W:113:LYS:N[1_556]   | 1.44                     | 0.76              |
| 4:2:291:LYS:CE  | 4:Z:322:PRO:CB[1_556]  | 1.44                     | 0.76              |
| 4:1:106:THR:N   | 4:Y:335:ARG:CA[1_556]  | 1.44                     | 0.76              |
| 4:0:107:GLU:CD  | 4:X:141:SER:OG[1_556]  | 1.44                     | 0.76              |
| 4:1:150:GLY:O   | 4:Y:317:ILE:CG2[1_556] | 1.44                     | 0.76              |
| 4:1:149:THR:O   | 4:Y:327:ILE:CG2[1_556] | 1.44                     | 0.76              |
| 4:1:305:MET:O   | 4:Y:255:PHE:CD1[1_556] | 1.44                     | 0.76              |
| 4:0:336:LYS:CB  | 4:X:218:TYR:CB[1_556]  | 1.44                     | 0.76              |
| 4:0:119:MET:O   | 4:X:340:TRP:CE3[1_556] | 1.44                     | 0.76              |
| 4:2:68:LYS:CG   | 4:Z:59:GLN:CG[1_556]   | 1.44                     | 0.76              |
| 4:1:267:ILE:N   | 4:X:173:HIS:CA[1_556]  | 1.44                     | 0.76              |
| 4:0:306:TYR:C   | 4:X:227:MET:SD[1_556]  | 1.44                     | 0.76              |
| 4:1:78:ASN:CG   | 4:Y:32:PRO:C[1_556]    | 1.44                     | 0.76              |
| 4:2:104:LEU:CG  | 4:Z:334:GLU:OE2[1_556] | 1.44                     | 0.76              |
| 4:1:145:SER:N   | 4:Y:311:ASP:OD1[1_556] | 1.44                     | 0.76              |
| 4:1:155:SER:O   | 4:Y:258:PRO:CB[1_556]  | 1.44                     | 0.76              |
| 4:0:166:TYR:CZ  | 4:X:325:MET:SD[1_556]  | 1.44                     | 0.76              |
| 4:1:142:LEU:CB  | 4:Y:329:ILE:CG1[1_556] | 1.44                     | 0.76              |
| 4:1:302:GLY:C   | 4:Y:258:PRO:CD[1_556]  | 1.44                     | 0.76              |
| 4:1:126:THR:O   | 4:Y:28:ARG:NE[1_556]   | 1.44                     | 0.76              |
| 4:2:253:GLU:OE1 | 4:Y:113:LYS:N[1_556]   | 1.44                     | 0.76              |
| 4:0:253:GLU:OE1 | 4:W:113:LYS:N[1_556]   | 1.44                     | 0.76              |
| 4:2:291:LYS:NZ  | 4:Z:322:PRO:CB[1_556]  | 1.44                     | 0.76              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:301:GLY:N   | 4:Y:219:VAL:CB[1_556]  | 1.44                     | 0.76              |
| 4:0:332:PRO:CB  | 4:X:221:LEU:CG[1_556]  | 1.44                     | 0.76              |
| 4:2:281:SER:OG  | 4:Z:276:GLU:C[1_556]   | 1.44                     | 0.76              |
| 4:2:74:GLY:N    | 4:Z:156:GLY:C[1_556]   | 1.44                     | 0.76              |
| 4:1:63:GLY:CA   | 4:W:288:ASP:C[1_556]   | 1.44                     | 0.76              |
| 4:2:233:SER:OG  | 4:Y:367:PRO:CB[1_556]  | 1.44                     | 0.76              |
| 4:2:208:ILE:CA  | 4:Z:198:TYR:CD1[1_556] | 1.44                     | 0.76              |
| 4:0:233:SER:OG  | 4:W:367:PRO:CB[1_556]  | 1.44                     | 0.76              |
| 4:1:187:ASP:N   | 4:Y:191:LYS:N[1_556]   | 1.44                     | 0.76              |
| 4:0:161:HIS:CB  | 4:X:274:ILE:CD1[1_556] | 1.44                     | 0.76              |
| 4:1:74:GLY:O    | 4:Y:156:GLY:CA[1_556]  | 1.44                     | 0.76              |
| 4:1:72:GLU:O    | 4:Y:158:GLY:N[1_556]   | 1.44                     | 0.76              |
| 4:2:372:ARG:CB  | 4:Z:143:TYR:N[1_556]   | 1.44                     | 0.76              |
| 4:2:307:PRO:CA  | 4:Z:227:MET:CB[1_556]  | 1.44                     | 0.76              |
| 4:1:172:PRO:CG  | 4:Y:164:PRO:CG[1_556]  | 1.44                     | 0.76              |
| 4:0:149:THR:O   | 4:X:327:ILE:CG2[1_556] | 1.44                     | 0.76              |
| 4:2:68:LYS:CB   | 4:Z:59:GLN:CG[1_556]   | 1.44                     | 0.76              |
| 4:2:372:ARG:CZ  | 4:Z:142:LEU:O[1_556]   | 1.44                     | 0.76              |
| 4:2:362:TYR:OH  | 4:Z:22:ALA:CA[1_556]   | 1.44                     | 0.76              |
| 4:1:272:ALA:O   | 4:Y:269:MET:C[1_556]   | 1.44                     | 0.76              |
| 4:2:170:ALA:O   | 4:Z:151:ILE:CG1[1_556] | 1.44                     | 0.76              |
| 4:2:206:ARG:CZ  | 4:Z:190:MET:CE[1_556]  | 1.44                     | 0.76              |
| 4:2:296:ASN:O   | 4:Z:317:ILE:N[1_556]   | 1.44                     | 0.76              |
| 4:1:252:ASN:C   | 4:X:113:LYS:CG[1_556]  | 1.44                     | 0.76              |
| 4:0:68:LYS:CB   | 4:X:59:GLN:CG[1_556]   | 1.44                     | 0.76              |
| 4:0:301:GLY:O   | 4:X:218:TYR:O[1_556]   | 1.44                     | 0.76              |
| 4:1:161:HIS:CB  | 4:Y:274:ILE:CG1[1_556] | 1.45                     | 0.75              |
| 4:2:79:TRP:CZ3  | 4:Z:18:LYS:CB[1_556]   | 1.45                     | 0.75              |
| 4:1:298:VAL:N   | 4:Y:312:ARG:O[1_556]   | 1.45                     | 0.75              |
| 4:0:366:GLY:CA  | 4:X:347:ALA:O[1_556]   | 1.45                     | 0.75              |
| 4:2:110:LEU:CD2 | 4:Z:162:ASN:N[1_556]   | 1.45                     | 0.75              |
| 4:0:172:PRO:CG  | 4:X:164:PRO:CG[1_556]  | 1.45                     | 0.75              |
| 4:1:299:MET:N   | 4:Y:312:ARG:CB[1_556]  | 1.45                     | 0.75              |
| 4:2:121:GLN:CD  | 4:Z:20:GLY:O[1_556]    | 1.45                     | 0.75              |
| 4:1:16:LEU:CD2  | 4:Y:214:GLU:N[1_556]   | 1.45                     | 0.75              |
| 4:2:39:ARG:O    | 4:X:166:TYR:CE2[1_556] | 1.45                     | 0.75              |
| 4:2:183:ARG:O   | 4:Z:187:ASP:C[1_556]   | 1.45                     | 0.75              |
| 4:0:270:GLU:CD  | 4:W:286:ASP:CB[1_556]  | 1.45                     | 0.75              |
| 4:2:295:ALA:CA  | 4:Z:319:ALA:CA[1_556]  | 1.45                     | 0.75              |
| 4:0:182:GLY:O   | 4:X:188:TYR:C[1_556]   | 1.45                     | 0.75              |
| 4:1:229:THR:O   | 4:X:368:SER:C[1_556]   | 1.45                     | 0.75              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:211:ASP:OD1 | 4:X:249:THR:O[1_556]   | 1.45                     | 0.75              |
| 4:0:149:THR:C   | 4:X:327:ILE:CG2[1_556] | 1.45                     | 0.75              |
| 4:0:165:ILE:CG2 | 4:X:297:ASN:CB[1_556]  | 1.45                     | 0.75              |
| 4:1:291:LYS:CE  | 4:Y:322:PRO:CA[1_556]  | 1.45                     | 0.75              |
| 4:0:77:THR:CB   | 4:X:15:GLY:N[1_556]    | 1.45                     | 0.75              |
| 4:1:282:ILE:CG1 | 4:Y:320:LEU:CD1[1_556] | 1.45                     | 0.75              |
| 4:0:167:GLU:OE2 | 4:X:326:LYS:C[1_556]   | 1.45                     | 0.75              |
| 4:2:298:VAL:CG1 | 4:Z:312:ARG:CA[1_556]  | 1.45                     | 0.75              |
| 4:2:297:ASN:N   | 4:Z:315:LYS:O[1_556]   | 1.45                     | 0.75              |
| 4:0:151:ILE:CG1 | 4:X:275:HIS:C[1_556]   | 1.45                     | 0.75              |
| 4:2:253:GLU:CD  | 4:Y:113:LYS:N[1_556]   | 1.45                     | 0.75              |
| 4:1:111:ASN:CA  | 4:Y:154:ASP:OD2[1_556] | 1.45                     | 0.75              |
| 4:0:62:ARG:CG   | 4:X:204:ALA:C[1_556]   | 1.45                     | 0.75              |
| 4:0:297:ASN:CG  | 4:X:316:GLU:CD[1_556]  | 1.45                     | 0.75              |
| 4:1:141:SER:O   | 4:Y:311:ASP:N[1_556]   | 1.45                     | 0.75              |
| 4:2:151:ILE:CG1 | 4:Z:275:HIS:C[1_556]   | 1.45                     | 0.75              |
| 4:2:367:PRO:C   | 4:Z:343:GLY:O[1_556]   | 1.45                     | 0.75              |
| 4:0:105:LEU:CA  | 4:X:334:GLU:CA[1_556]  | 1.45                     | 0.75              |
| 4:2:214:GLU:CD  | 4:Z:250:ILE:CG2[1_556] | 1.45                     | 0.75              |
| 4:1:125:GLU:CB  | 4:Y:21:PHE:N[1_556]    | 1.45                     | 0.75              |
| 4:1:154:ASP:OD2 | 4:Y:309:ILE:CD1[1_556] | 1.45                     | 0.75              |
| 4:0:78:ASN:CG   | 4:X:32:PRO:C[1_556]    | 1.45                     | 0.75              |
| 4:2:164:PRO:CD  | 4:Z:278:THR:N[1_556]   | 1.45                     | 0.75              |
| 4:2:63:GLY:CA   | 4:X:289:ILE:N[1_556]   | 1.45                     | 0.75              |
| 4:0:12:ASN:OD1  | 4:X:336:LYS:CD[1_556]  | 1.45                     | 0.75              |
| 4:1:173:HIS:N   | 4:Y:281:SER:OG[1_556]  | 1.45                     | 0.75              |
| 4:2:105:LEU:CA  | 4:Z:334:GLU:CA[1_556]  | 1.45                     | 0.75              |
| 4:0:186:THR:C   | 4:X:191:LYS:C[1_556]   | 1.45                     | 0.75              |
| 4:0:362:TYR:OH  | 4:X:22:ALA:CA[1_556]   | 1.45                     | 0.75              |
| 4:1:338:SER:CB  | 4:Y:308:GLY:N[1_556]   | 1.45                     | 0.75              |
| 4:1:165:ILE:CB  | 4:Y:297:ASN:CG[1_556]  | 1.45                     | 0.75              |
| 4:3:196:ARG:N   | 4:Z:75:ILE:CD1[1_556]  | 1.45                     | 0.75              |
| 4:3:267:ILE:N   | 4:Z:173:HIS:CA[1_556]  | 1.45                     | 0.75              |
| 4:3:252:ASN:C   | 4:Z:113:LYS:CG[1_556]  | 1.45                     | 0.75              |
| 4:1:178:LEU:CB  | 4:Y:180:LEU:CD2[1_556] | 1.45                     | 0.75              |
| 4:0:230:ALA:N   | 4:W:368:SER:O[1_556]   | 1.45                     | 0.75              |
| 4:0:162:ASN:O   | 4:X:274:ILE:O[1_556]   | 1.45                     | 0.75              |
| 4:2:206:ARG:CG  | 4:Z:200:PHE:C[1_556]   | 1.45                     | 0.75              |
| 4:1:154:ASP:O   | 4:Y:261:LEU:CG[1_556]  | 1.45                     | 0.75              |
| 4:0:291:LYS:CE  | 4:X:322:PRO:CB[1_556]  | 1.45                     | 0.75              |
| 4:2:265:SER:CA  | 4:Y:173:HIS:CE1[1_556] | 1.45                     | 0.75              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:68:LYS:CB   | 4:Y:59:GLN:CG[1_556]   | 1.45                     | 0.75              |
| 4:1:119:MET:O   | 4:Y:340:TRP:CE3[1_556] | 1.45                     | 0.75              |
| 4:1:136:ILE:C   | 4:Y:299:MET:CA[1_556]  | 1.45                     | 0.75              |
| 4:2:79:TRP:CG   | 4:Z:17:VAL:CG1[1_556]  | 1.45                     | 0.75              |
| 4:2:182:GLY:O   | 4:Z:188:TYR:C[1_556]   | 1.46                     | 0.74              |
| 4:0:72:GLU:C    | 4:X:157:ASP:C[1_556]   | 1.46                     | 0.74              |
| 4:0:297:ASN:N   | 4:X:315:LYS:O[1_556]   | 1.46                     | 0.74              |
| 4:0:296:ASN:O   | 4:X:317:ILE:N[1_556]   | 1.46                     | 0.74              |
| 4:0:79:TRP:CZ3  | 4:X:18:LYS:CB[1_556]   | 1.46                     | 0.74              |
| 4:2:281:SER:CB  | 4:Z:276:GLU:O[1_556]   | 1.46                     | 0.74              |
| 4:3:229:THR:O   | 4:Z:368:SER:C[1_556]   | 1.46                     | 0.74              |
| 4:0:74:GLY:N    | 4:X:156:GLY:C[1_556]   | 1.46                     | 0.74              |
| 4:2:141:SER:O   | 4:Z:311:ASP:N[1_556]   | 1.46                     | 0.74              |
| 4:2:336:LYS:NZ  | 4:Z:254:ARG:CZ[1_556]  | 1.46                     | 0.74              |
| 4:0:265:SER:CA  | 4:W:173:HIS:CE1[1_556] | 1.46                     | 0.74              |
| 4:2:277:THR:CB  | 4:Z:272:ALA:C[1_556]   | 1.46                     | 0.74              |
| 4:0:68:LYS:CG   | 4:X:59:GLN:NE2[1_556]  | 1.46                     | 0.74              |
| 4:0:231:ALA:CB  | 4:W:369:ILE:C[1_556]   | 1.46                     | 0.74              |
| 4:1:74:GLY:N    | 4:Y:156:GLY:C[1_556]   | 1.46                     | 0.74              |
| 4:0:206:ARG:CG  | 4:X:200:PHE:C[1_556]   | 1.46                     | 0.74              |
| 4:2:12:ASN:OD1  | 4:Z:336:LYS:CD[1_556]  | 1.46                     | 0.74              |
| 4:1:261:LEU:CG  | 4:Y:266:PHE:CD2[1_556] | 1.46                     | 0.74              |
| 4:0:183:ARG:O   | 4:X:187:ASP:C[1_556]   | 1.46                     | 0.74              |
| 4:3:267:ILE:N   | 4:Z:173:HIS:N[1_556]   | 1.46                     | 0.74              |
| 4:1:78:ASN:CB   | 4:Y:33:SER:N[1_556]    | 1.46                     | 0.74              |
| 4:2:166:TYR:CZ  | 4:Z:325:MET:SD[1_556]  | 1.46                     | 0.74              |
| 4:0:215:LYS:CE  | 4:X:237:GLU:OE1[1_556] | 1.46                     | 0.74              |
| 4:0:125:GLU:CG  | 4:X:21:PHE:C[1_556]    | 1.46                     | 0.74              |
| 4:2:306:TYR:C   | 4:Z:227:MET:SD[1_556]  | 1.46                     | 0.74              |
| 4:2:206:ARG:CG  | 4:Z:200:PHE:N[1_556]   | 1.46                     | 0.74              |
| 4:3:230:ALA:O   | 4:Z:367:PRO:C[1_556]   | 1.46                     | 0.74              |
| 4:1:208:ILE:CA  | 4:Y:198:TYR:CD1[1_556] | 1.46                     | 0.74              |
| 4:2:233:SER:CB  | 4:Y:367:PRO:CA[1_556]  | 1.46                     | 0.74              |
| 4:2:336:LYS:CB  | 4:Z:218:TYR:CB[1_556]  | 1.46                     | 0.74              |
| 4:0:233:SER:CB  | 4:W:367:PRO:CA[1_556]  | 1.46                     | 0.74              |
| 4:2:297:ASN:OD1 | 4:Z:316:GLU:OE1[1_556] | 1.46                     | 0.74              |
| 4:1:297:ASN:CG  | 4:Y:316:GLU:CD[1_556]  | 1.46                     | 0.74              |
| 4:1:107:GLU:CD  | 4:Y:141:SER:OG[1_556]  | 1.46                     | 0.74              |
| 4:2:169:TYR:CD1 | 4:Z:150:GLY:CA[1_556]  | 1.46                     | 0.74              |
| 4:2:267:ILE:N   | 4:Y:173:HIS:CA[1_556]  | 1.46                     | 0.74              |
| 4:2:270:GLU:CD  | 4:Y:286:ASP:CB[1_556]  | 1.46                     | 0.74              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:115:ASN:CA  | 4:Y:11:ASP:CG[1_556]   | 1.46                     | 0.74              |
| 4:0:149:THR:N   | 4:X:327:ILE:CB[1_556]  | 1.46                     | 0.74              |
| 4:1:104:LEU:CG  | 4:Y:334:GLU:OE2[1_556] | 1.46                     | 0.74              |
| 4:0:281:SER:CB  | 4:X:276:GLU:O[1_556]   | 1.46                     | 0.74              |
| 4:1:134:VAL:CG2 | 4:Y:338:SER:CA[1_556]  | 1.46                     | 0.74              |
| 4:2:332:PRO:CB  | 4:Z:221:LEU:CG[1_556]  | 1.46                     | 0.74              |
| 4:0:367:PRO:C   | 4:X:343:GLY:O[1_556]   | 1.46                     | 0.74              |
| 4:1:280:ASN:O   | 4:Y:280:ASN:OD1[1_556] | 1.46                     | 0.74              |
| 4:1:70:PRO:O    | 4:Y:15:GLY:C[1_556]    | 1.46                     | 0.74              |
| 4:2:161:HIS:CB  | 4:Z:274:ILE:CD1[1_556] | 1.46                     | 0.74              |
| 4:2:164:PRO:CB  | 4:Z:278:THR:C[1_556]   | 1.46                     | 0.74              |
| 4:1:233:SER:CB  | 4:X:367:PRO:CA[1_556]  | 1.46                     | 0.74              |
| 4:1:364:GLU:CA  | 4:Y:348:SER:O[1_556]   | 1.46                     | 0.74              |
| 4:2:77:THR:CB   | 4:Z:15:GLY:N[1_556]    | 1.46                     | 0.74              |
| 4:3:63:GLY:CA   | 4:Y:288:ASP:C[1_556]   | 1.46                     | 0.74              |
| 4:1:149:THR:OG1 | 4:Y:327:ILE:CA[1_556]  | 1.46                     | 0.74              |
| 4:1:72:GLU:C    | 4:Y:157:ASP:C[1_556]   | 1.46                     | 0.74              |
| 4:1:160:THR:N   | 4:Y:180:LEU:CD1[1_556] | 1.46                     | 0.74              |
| 4:2:306:TYR:N   | 4:Z:255:PHE:CD1[1_556] | 1.46                     | 0.74              |
| 4:0:300:SER:CA  | 4:X:219:VAL:CB[1_556]  | 1.46                     | 0.74              |
| 4:2:168:GLY:N   | 4:Z:296:ASN:N[1_556]   | 1.46                     | 0.74              |
| 4:2:300:SER:CA  | 4:Z:219:VAL:CB[1_556]  | 1.46                     | 0.74              |
| 4:0:113:LYS:N   | 4:X:137:GLN:CA[1_556]  | 1.46                     | 0.74              |
| 4:0:104:LEU:CG  | 4:X:334:GLU:OE2[1_556] | 1.46                     | 0.74              |
| 4:3:233:SER:CB  | 4:Z:367:PRO:CA[1_556]  | 1.46                     | 0.74              |
| 4:2:167:GLU:OE2 | 4:Z:326:LYS:C[1_556]   | 1.46                     | 0.74              |
| 4:0:121:GLN:CD  | 4:X:20:GLY:O[1_556]    | 1.46                     | 0.74              |
| 4:1:292:ASP:CA  | 4:Y:321:ALA:O[1_556]   | 1.46                     | 0.74              |
| 4:1:116:ARG:CG  | 4:Y:339:VAL:CA[1_556]  | 1.46                     | 0.74              |
| 4:1:112:PRO:N   | 4:Y:137:GLN:OE1[1_556] | 1.46                     | 0.74              |
| 4:2:172:PRO:CG  | 4:Z:164:PRO:CG[1_556]  | 1.46                     | 0.74              |
| 4:0:307:PRO:O   | 4:X:227:MET:CB[1_556]  | 1.46                     | 0.74              |
| 4:1:365:ALA:CA  | 4:Y:349:LEU:CA[1_556]  | 1.46                     | 0.74              |
| 4:0:206:ARG:CZ  | 4:X:190:MET:CE[1_556]  | 1.46                     | 0.74              |
| 4:2:72:GLU:C    | 4:Z:157:ASP:C[1_556]   | 1.46                     | 0.74              |
| 4:1:174:ALA:O   | 4:Y:277:THR:O[1_556]   | 1.46                     | 0.74              |
| 4:0:126:THR:CG2 | 4:X:28:ARG:CB[1_556]   | 1.46                     | 0.74              |
| 4:2:307:PRO:CA  | 4:Z:227:MET:N[1_556]   | 1.46                     | 0.74              |
| 4:2:231:ALA:CB  | 4:Y:369:ILE:C[1_556]   | 1.46                     | 0.74              |
| 4:2:298:VAL:CA  | 4:Z:312:ARG:C[1_556]   | 1.46                     | 0.74              |
| 4:2:62:ARG:CG   | 4:Z:204:ALA:C[1_556]   | 1.47                     | 0.73              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:292:ASP:CA  | 4:X:321:ALA:O[1_556]   | 1.47                     | 0.73              |
| 4:0:365:ALA:CA  | 4:X:349:LEU:N[1_556]   | 1.47                     | 0.73              |
| 4:2:278:THR:O   | 4:Z:276:GLU:CB[1_556]  | 1.47                     | 0.73              |
| 4:2:206:ARG:CG  | 4:Z:200:PHE:CB[1_556]  | 1.47                     | 0.73              |
| 4:2:307:PRO:O   | 4:Z:227:MET:CB[1_556]  | 1.47                     | 0.73              |
| 4:2:365:ALA:CA  | 4:Z:349:LEU:N[1_556]   | 1.47                     | 0.73              |
| 4:2:142:LEU:CB  | 4:Z:329:ILE:CG1[1_556] | 1.47                     | 0.73              |
| 4:0:307:PRO:CA  | 4:X:227:MET:N[1_556]   | 1.47                     | 0.73              |
| 4:0:295:ALA:CA  | 4:X:319:ALA:CA[1_556]  | 1.47                     | 0.73              |
| 4:0:114:ALA:O   | 4:X:106:THR:CG2[1_556] | 1.47                     | 0.73              |
| 4:2:372:ARG:CZ  | 4:Z:145:SER:N[1_556]   | 1.47                     | 0.73              |
| 4:4:39:ARG:O    | 4:Z:166:TYR:CE2[1_556] | 1.47                     | 0.73              |
| 4:0:197:GLY:O   | 4:W:75:ILE:C[1_556]    | 1.47                     | 0.73              |
| 4:1:119:MET:CG  | 4:Y:340:TRP:CB[1_556]  | 1.47                     | 0.73              |
| 4:3:256:ARG:NH2 | 4:Z:111:ASN:O[1_556]   | 1.47                     | 0.73              |
| 4:2:37:ARG:CB   | 4:Z:60:SER:OG[1_556]   | 1.47                     | 0.73              |
| 4:0:159:VAL:CG1 | 4:X:181:ALA:N[1_556]   | 1.47                     | 0.73              |
| 4:1:267:ILE:N   | 4:X:173:HIS:N[1_556]   | 1.47                     | 0.73              |
| 4:1:303:THR:CA  | 4:Y:257:CYS:N[1_556]   | 1.47                     | 0.73              |
| 4:2:305:MET:CA  | 4:Z:255:PHE:CB[1_556]  | 1.47                     | 0.73              |
| 4:2:186:THR:C   | 4:Z:191:LYS:C[1_556]   | 1.47                     | 0.73              |
| 4:2:113:LYS:N   | 4:Z:137:GLN:CA[1_556]  | 1.47                     | 0.73              |
| 4:2:230:ALA:N   | 4:Y:368:SER:O[1_556]   | 1.47                     | 0.73              |
| 4:0:134:VAL:CG2 | 4:X:338:SER:CA[1_556]  | 1.47                     | 0.73              |
| 4:1:252:ASN:CA  | 4:X:113:LYS:CB[1_556]  | 1.47                     | 0.73              |
| 4:0:163:VAL:O   | 4:X:313:MET:CE[1_556]  | 1.47                     | 0.73              |
| 4:2:305:MET:C   | 4:Z:255:PHE:CG[1_556]  | 1.47                     | 0.73              |
| 4:1:290:ARG:CB  | 4:Y:279:TYR:OH[1_556]  | 1.47                     | 0.73              |
| 4:1:16:LEU:CG   | 4:Y:214:GLU:C[1_556]   | 1.47                     | 0.73              |
| 4:1:256:ARG:NH2 | 4:X:111:ASN:O[1_556]   | 1.47                     | 0.73              |
| 4:0:142:LEU:CB  | 4:X:329:ILE:CG1[1_556] | 1.47                     | 0.73              |
| 4:2:162:ASN:O   | 4:Z:274:ILE:O[1_556]   | 1.47                     | 0.73              |
| 4:0:297:ASN:OD1 | 4:X:316:GLU:OE1[1_556] | 1.47                     | 0.73              |
| 4:0:300:SER:N   | 4:X:219:VAL:CG1[1_556] | 1.47                     | 0.73              |
| 4:2:119:MET:CG  | 4:Z:340:TRP:CB[1_556]  | 1.47                     | 0.73              |
| 4:0:79:TRP:CG   | 4:X:17:VAL:CG1[1_556]  | 1.47                     | 0.73              |
| 4:2:116:ARG:O   | 4:Z:340:TRP:CA[1_556]  | 1.47                     | 0.73              |
| 4:2:112:PRO:CA  | 4:Z:137:GLN:CD[1_556]  | 1.47                     | 0.73              |
| 4:0:206:ARG:CG  | 4:X:200:PHE:CB[1_556]  | 1.47                     | 0.73              |
| 4:1:197:GLY:O   | 4:X:75:ILE:O[1_556]    | 1.47                     | 0.73              |
| 4:2:82:MET:N    | 4:Z:31:PHE:N[1_556]    | 1.47                     | 0.73              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:180:LEU:CD1 | 4:Z:267:ILE:CB[1_556]  | 1.47                     | 0.73              |
| 4:1:270:GLU:CD  | 4:X:286:ASP:CA[1_556]  | 1.47                     | 0.73              |
| 4:2:116:ARG:CA  | 4:Z:339:VAL:C[1_556]   | 1.47                     | 0.73              |
| 4:1:213:LYS:CD  | 4:Y:192:ILE:CB[1_556]  | 1.47                     | 0.73              |
| 4:0:164:PRO:CB  | 4:X:278:THR:C[1_556]   | 1.47                     | 0.73              |
| 4:0:12:ASN:O    | 4:X:302:GLY:CA[1_556]  | 1.47                     | 0.73              |
| 4:1:78:ASN:CB   | 4:Y:32:PRO:CA[1_556]   | 1.47                     | 0.73              |
| 4:1:76:ILE:O    | 4:Y:13:GLY:CA[1_556]   | 1.47                     | 0.73              |
| 4:1:214:GLU:OE1 | 4:Y:250:ILE:CB[1_556]  | 1.47                     | 0.73              |
| 4:0:299:MET:N   | 4:X:312:ARG:CD[1_556]  | 1.47                     | 0.73              |
| 4:2:114:ALA:O   | 4:Z:106:THR:CG2[1_556] | 1.47                     | 0.73              |
| 4:0:116:ARG:O   | 4:X:340:TRP:CA[1_556]  | 1.47                     | 0.73              |
| 4:0:63:GLY:CA   | 4:V:289:ILE:N[1_556]   | 1.47                     | 0.73              |
| 4:2:300:SER:N   | 4:Z:219:VAL:CG1[1_556] | 1.47                     | 0.73              |
| 4:2:163:VAL:O   | 4:Z:313:MET:CE[1_556]  | 1.47                     | 0.73              |
| 4:1:206:ARG:CG  | 4:Y:200:PHE:N[1_556]   | 1.47                     | 0.73              |
| 4:2:68:LYS:CG   | 4:Z:59:GLN:NE2[1_556]  | 1.47                     | 0.73              |
| 4:2:78:ASN:CG   | 4:Z:32:PRO:C[1_556]    | 1.47                     | 0.73              |
| 4:3:39:ARG:O    | 4:Y:166:TYR:CE2[1_556] | 1.47                     | 0.73              |
| 4:2:291:LYS:CE  | 4:Z:322:PRO:CA[1_556]  | 1.47                     | 0.73              |
| 4:2:112:PRO:N   | 4:Z:137:GLN:OE1[1_556] | 1.47                     | 0.73              |
| 4:2:267:ILE:N   | 4:Y:173:HIS:CG[1_556]  | 1.47                     | 0.73              |
| 4:0:68:LYS:CE   | 4:X:59:GLN:CB[1_556]   | 1.47                     | 0.73              |
| 4:3:197:GLY:O   | 4:Z:75:ILE:O[1_556]    | 1.47                     | 0.73              |
| 4:0:267:ILE:N   | 4:W:173:HIS:CA[1_556]  | 1.47                     | 0.73              |
| 4:1:30:VAL:O    | 4:Y:215:LYS:CE[1_556]  | 1.47                     | 0.73              |
| 4:0:122:ILE:CG1 | 4:X:19:ALA:CA[1_556]   | 1.47                     | 0.73              |
| 4:1:336:LYS:CB  | 4:Y:218:TYR:CB[1_556]  | 1.47                     | 0.73              |
| 4:2:233:SER:N   | 4:Y:367:PRO:N[1_556]   | 1.47                     | 0.73              |
| 4:0:169:TYR:CD1 | 4:X:150:GLY:CA[1_556]  | 1.47                     | 0.73              |
| 4:2:12:ASN:O    | 4:Z:302:GLY:CA[1_556]  | 1.47                     | 0.73              |
| 4:2:215:LYS:CE  | 4:Z:237:GLU:OE1[1_556] | 1.47                     | 0.73              |
| 4:0:230:ALA:C   | 4:W:367:PRO:O[1_556]   | 1.47                     | 0.73              |
| 4:0:180:LEU:CD1 | 4:X:267:ILE:CB[1_556]  | 1.47                     | 0.73              |
| 4:0:306:TYR:N   | 4:X:255:PHE:CD1[1_556] | 1.47                     | 0.73              |
| 4:2:122:ILE:CG1 | 4:Z:19:ALA:CA[1_556]   | 1.47                     | 0.73              |
| 4:0:267:ILE:N   | 4:W:173:HIS:CG[1_556]  | 1.47                     | 0.73              |
| 4:2:197:GLY:O   | 4:Y:75:ILE:C[1_556]    | 1.47                     | 0.73              |
| 4:1:277:THR:CB  | 4:Y:272:ALA:C[1_556]   | 1.47                     | 0.73              |
| 4:2:159:VAL:CG1 | 4:Z:181:ALA:N[1_556]   | 1.47                     | 0.73              |
| 4:1:149:THR:N   | 4:Y:327:ILE:CB[1_556]  | 1.47                     | 0.73              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:68:LYS:CD   | 4:Y:59:GLN:CB[1_556]   | 1.48                     | 0.72              |
| 4:1:68:LYS:CE   | 4:Y:59:GLN:CB[1_556]   | 1.48                     | 0.72              |
| 4:1:298:VAL:CA  | 4:Y:312:ARG:C[1_556]   | 1.48                     | 0.72              |
| 4:0:372:ARG:CZ  | 4:X:145:SER:N[1_556]   | 1.48                     | 0.72              |
| 4:0:30:VAL:O    | 4:X:215:LYS:CD[1_556]  | 1.48                     | 0.72              |
| 4:0:81:ASP:CG   | 4:X:32:PRO:CD[1_556]   | 1.48                     | 0.72              |
| 4:0:210:ARG:CD  | 4:X:193:LEU:CD2[1_556] | 1.48                     | 0.72              |
| 4:0:116:ARG:O   | 4:X:339:VAL:O[1_556]   | 1.48                     | 0.72              |
| 4:1:277:THR:CB  | 4:Y:272:ALA:CA[1_556]  | 1.48                     | 0.72              |
| 4:1:107:GLU:CG  | 4:Y:300:SER:OG[1_556]  | 1.48                     | 0.72              |
| 4:0:357:ILE:CB  | 4:X:345:ILE:CD1[1_556] | 1.48                     | 0.72              |
| 4:2:10:CYS:SG   | 4:Z:336:LYS:NZ[1_556]  | 1.48                     | 0.72              |
| 4:1:79:TRP:CD2  | 4:Y:17:VAL:C[1_556]    | 1.48                     | 0.72              |
| 4:0:277:THR:CB  | 4:X:272:ALA:C[1_556]   | 1.48                     | 0.72              |
| 4:2:125:GLU:CG  | 4:Z:21:PHE:C[1_556]    | 1.48                     | 0.72              |
| 4:2:126:THR:CG2 | 4:Z:28:ARG:CB[1_556]   | 1.48                     | 0.72              |
| 4:0:291:LYS:CE  | 4:X:322:PRO:CA[1_556]  | 1.48                     | 0.72              |
| 4:1:183:ARG:C   | 4:Y:187:ASP:O[1_556]   | 1.48                     | 0.72              |
| 4:2:292:ASP:CA  | 4:Z:321:ALA:O[1_556]   | 1.48                     | 0.72              |
| 4:0:10:CYS:SG   | 4:X:336:LYS:NZ[1_556]  | 1.48                     | 0.72              |
| 4:1:166:TYR:CZ  | 4:Y:325:MET:SD[1_556]  | 1.48                     | 0.72              |
| 4:1:307:PRO:CB  | 4:Y:227:MET:C[1_556]   | 1.48                     | 0.72              |
| 4:0:112:PRO:CA  | 4:X:137:GLN:CD[1_556]  | 1.48                     | 0.72              |
| 4:2:149:THR:N   | 4:Z:327:ILE:CB[1_556]  | 1.48                     | 0.72              |
| 4:1:206:ARG:N   | 4:Y:199:SER:C[1_556]   | 1.48                     | 0.72              |
| 4:1:337:TYR:CB  | 4:Y:307:PRO:CB[1_556]  | 1.48                     | 0.72              |
| 4:1:230:ALA:O   | 4:X:367:PRO:C[1_556]   | 1.48                     | 0.72              |
| 4:0:116:ARG:CA  | 4:X:339:VAL:C[1_556]   | 1.48                     | 0.72              |
| 4:0:168:GLY:N   | 4:X:296:ASN:N[1_556]   | 1.48                     | 0.72              |
| 4:2:106:THR:O   | 4:Z:336:LYS:CA[1_556]  | 1.48                     | 0.72              |
| 4:0:129:VAL:O   | 4:X:25:ASP:OD2[1_556]  | 1.48                     | 0.72              |
| 4:1:277:THR:OG1 | 4:Y:272:ALA:N[1_556]   | 1.48                     | 0.72              |
| 4:0:303:THR:OG1 | 4:X:257:CYS:C[1_556]   | 1.48                     | 0.72              |
| 4:2:81:ASP:OD1  | 4:Z:56:ASP:CG[1_556]   | 1.48                     | 0.72              |
| 4:0:136:ILE:C   | 4:X:299:MET:CA[1_556]  | 1.48                     | 0.72              |
| 4:0:140:LEU:CG  | 4:X:331:ALA:CB[1_556]  | 1.48                     | 0.72              |
| 4:0:233:SER:N   | 4:W:367:PRO:N[1_556]   | 1.48                     | 0.72              |
| 4:1:112:PRO:CA  | 4:Y:137:GLN:CD[1_556]  | 1.48                     | 0.72              |
| 4:0:72:GLU:O    | 4:X:158:GLY:N[1_556]   | 1.48                     | 0.72              |
| 4:0:251:GLY:N   | 4:W:114:ALA:CA[1_556]  | 1.48                     | 0.72              |
| 4:2:303:THR:OG1 | 4:Z:257:CYS:C[1_556]   | 1.48                     | 0.72              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:116:ARG:CG  | 4:X:339:VAL:CA[1_556]  | 1.48                     | 0.72              |
| 4:0:37:ARG:CB   | 4:X:60:SER:OG[1_556]   | 1.48                     | 0.72              |
| 4:1:125:GLU:CG  | 4:Y:21:PHE:C[1_556]    | 1.48                     | 0.72              |
| 4:1:78:ASN:OD1  | 4:Y:32:PRO:O[1_556]    | 1.48                     | 0.72              |
| 4:1:214:GLU:OE1 | 4:Y:250:ILE:CG1[1_556] | 1.48                     | 0.72              |
| 4:1:271:SER:OG  | 4:Y:269:MET:CA[1_556]  | 1.48                     | 0.72              |
| 4:1:261:LEU:CD1 | 4:Y:266:PHE:CG[1_556]  | 1.48                     | 0.72              |
| 4:2:196:ARG:N   | 4:Y:75:ILE:CD1[1_556]  | 1.48                     | 0.72              |
| 4:3:270:GLU:CD  | 4:Z:286:ASP:CA[1_556]  | 1.48                     | 0.72              |
| 4:2:154:ASP:O   | 4:Z:261:LEU:CG[1_556]  | 1.48                     | 0.72              |
| 4:1:81:ASP:CG   | 4:Y:32:PRO:CD[1_556]   | 1.48                     | 0.72              |
| 4:0:267:ILE:N   | 4:W:173:HIS:N[1_556]   | 1.48                     | 0.72              |
| 4:1:162:ASN:OD1 | 4:Y:274:ILE:N[1_556]   | 1.48                     | 0.72              |
| 4:1:114:ALA:O   | 4:Y:106:THR:CG2[1_556] | 1.48                     | 0.72              |
| 4:0:112:PRO:N   | 4:X:137:GLN:OE1[1_556] | 1.48                     | 0.72              |
| 4:2:119:MET:O   | 4:Z:340:TRP:CD2[1_556] | 1.48                     | 0.72              |
| 4:0:74:GLY:O    | 4:X:156:GLY:CA[1_556]  | 1.48                     | 0.72              |
| 4:1:211:ASP:N   | 4:Y:193:LEU:CD1[1_556] | 1.48                     | 0.72              |
| 4:1:185:LEU:CG  | 4:Y:188:TYR:CD1[1_556] | 1.48                     | 0.72              |
| 4:1:208:ILE:CG1 | 4:Y:198:TYR:CD1[1_556] | 1.48                     | 0.72              |
| 4:2:116:ARG:CG  | 4:Z:339:VAL:CA[1_556]  | 1.48                     | 0.72              |
| 4:0:106:THR:O   | 4:X:336:LYS:CA[1_556]  | 1.48                     | 0.72              |
| 4:2:136:ILE:C   | 4:Z:299:MET:CA[1_556]  | 1.48                     | 0.72              |
| 4:0:186:THR:CA  | 4:X:192:ILE:N[1_556]   | 1.48                     | 0.72              |
| 4:0:82:MET:N    | 4:X:31:PHE:N[1_556]    | 1.48                     | 0.72              |
| 4:0:154:ASP:O   | 4:X:261:LEU:CG[1_556]  | 1.48                     | 0.72              |
| 4:0:362:TYR:CE2 | 4:X:23:GLY:N[1_556]    | 1.48                     | 0.72              |
| 4:3:230:ALA:C   | 4:Z:367:PRO:O[1_556]   | 1.48                     | 0.72              |
| 4:1:300:SER:CA  | 4:Y:219:VAL:CB[1_556]  | 1.48                     | 0.72              |
| 4:2:114:ALA:CA  | 4:Z:106:THR:CG2[1_556] | 1.49                     | 0.71              |
| 4:0:278:THR:O   | 4:X:276:GLU:CB[1_556]  | 1.49                     | 0.71              |
| 4:0:303:THR:CA  | 4:X:257:CYS:N[1_556]   | 1.49                     | 0.71              |
| 4:0:136:ILE:CB  | 4:X:299:MET:CA[1_556]  | 1.49                     | 0.71              |
| 4:0:125:GLU:CB  | 4:X:21:PHE:N[1_556]    | 1.49                     | 0.71              |
| 4:0:78:ASN:OD1  | 4:X:32:PRO:O[1_556]    | 1.49                     | 0.71              |
| 4:2:230:ALA:C   | 4:Y:367:PRO:O[1_556]   | 1.49                     | 0.71              |
| 4:3:252:ASN:CA  | 4:Z:113:LYS:CB[1_556]  | 1.49                     | 0.71              |
| 4:2:195:GLU:C   | 4:Y:75:ILE:CD1[1_556]  | 1.49                     | 0.71              |
| 4:2:81:ASP:CG   | 4:Z:32:PRO:CD[1_556]   | 1.49                     | 0.71              |
| 4:0:298:VAL:CA  | 4:X:312:ARG:C[1_556]   | 1.49                     | 0.71              |
| 4:2:357:ILE:CB  | 4:Z:345:ILE:CD1[1_556] | 1.49                     | 0.71              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:253:GLU:OE1 | 4:Z:113:LYS:N[1_556]   | 1.49                     | 0.71              |
| 4:1:32:PRO:CG   | 4:Y:211:ASP:CG[1_556]  | 1.49                     | 0.71              |
| 4:0:364:GLU:CA  | 4:X:348:SER:O[1_556]   | 1.49                     | 0.71              |
| 4:1:281:SER:OG  | 4:Y:276:GLU:C[1_556]   | 1.49                     | 0.71              |
| 4:2:116:ARG:O   | 4:Z:339:VAL:O[1_556]   | 1.49                     | 0.71              |
| 4:1:206:ARG:CG  | 4:Y:200:PHE:CB[1_556]  | 1.49                     | 0.71              |
| 4:0:81:ASP:OD1  | 4:X:56:ASP:CG[1_556]   | 1.49                     | 0.71              |
| 4:1:116:ARG:O   | 4:Y:339:VAL:O[1_556]   | 1.49                     | 0.71              |
| 4:0:305:MET:CA  | 4:X:255:PHE:CB[1_556]  | 1.49                     | 0.71              |
| 4:2:362:TYR:CE2 | 4:Z:23:GLY:N[1_556]    | 1.49                     | 0.71              |
| 4:0:305:MET:C   | 4:X:255:PHE:CG[1_556]  | 1.49                     | 0.71              |
| 4:0:180:LEU:CB  | 4:X:267:ILE:CG1[1_556] | 1.49                     | 0.71              |
| 4:2:299:MET:N   | 4:Z:312:ARG:CD[1_556]  | 1.49                     | 0.71              |
| 4:1:171:LEU:C   | 4:Y:151:ILE:CD1[1_556] | 1.49                     | 0.71              |
| 4:0:72:GLU:N    | 4:X:157:ASP:OD2[1_556] | 1.49                     | 0.71              |
| 4:2:134:VAL:CG2 | 4:Z:338:SER:CA[1_556]  | 1.49                     | 0.71              |
| 4:0:119:MET:CG  | 4:X:340:TRP:CB[1_556]  | 1.49                     | 0.71              |
| 4:2:30:VAL:O    | 4:Z:215:LYS:CD[1_556]  | 1.49                     | 0.71              |
| 4:0:303:THR:C   | 4:X:255:PHE:O[1_556]   | 1.49                     | 0.71              |
| 4:1:253:GLU:OE1 | 4:X:113:LYS:N[1_556]   | 1.49                     | 0.71              |
| 4:2:335:ARG:NE  | 4:Z:220:ALA:CB[1_556]  | 1.49                     | 0.71              |
| 4:2:267:ILE:N   | 4:Y:173:HIS:N[1_556]   | 1.49                     | 0.71              |
| 4:0:104:LEU:O   | 4:X:334:GLU:CA[1_556]  | 1.49                     | 0.71              |
| 4:1:305:MET:CA  | 4:Y:255:PHE:CB[1_556]  | 1.49                     | 0.71              |
| 4:0:157:ASP:C   | 4:X:185:LEU:CB[1_556]  | 1.49                     | 0.71              |
| 4:0:107:GLU:CG  | 4:X:300:SER:OG[1_556]  | 1.49                     | 0.71              |
| 4:0:372:ARG:N   | 4:X:143:TYR:CB[1_556]  | 1.49                     | 0.71              |
| 4:2:109:PRO:C   | 4:Z:154:ASP:CA[1_556]  | 1.49                     | 0.71              |
| 4:1:39:ARG:O    | 4:W:166:TYR:CE2[1_556] | 1.49                     | 0.71              |
| 4:2:206:ARG:N   | 4:Z:199:SER:C[1_556]   | 1.49                     | 0.71              |
| 4:2:72:GLU:O    | 4:Z:158:GLY:N[1_556]   | 1.49                     | 0.71              |
| 4:0:214:GLU:N   | 4:X:253:GLU:OE1[1_556] | 1.49                     | 0.71              |
| 4:2:104:LEU:O   | 4:Z:334:GLU:CA[1_556]  | 1.49                     | 0.71              |
| 4:2:177:ARG:CB  | 4:Z:178:LEU:O[1_556]   | 1.49                     | 0.71              |
| 4:2:277:THR:CA  | 4:Z:272:ALA:CA[1_556]  | 1.49                     | 0.71              |
| 4:0:150:GLY:O   | 4:X:317:ILE:CG2[1_556] | 1.49                     | 0.71              |
| 4:1:62:ARG:CG   | 4:Y:204:ALA:C[1_556]   | 1.49                     | 0.71              |
| 4:1:169:TYR:N   | 4:Y:296:ASN:CA[1_556]  | 1.49                     | 0.71              |
| 4:2:166:TYR:C   | 4:Z:295:ALA:N[1_556]   | 1.49                     | 0.71              |
| 4:0:151:ILE:N   | 4:X:317:ILE:N[1_556]   | 1.49                     | 0.71              |
| 4:2:68:LYS:CE   | 4:Z:59:GLN:CB[1_556]   | 1.49                     | 0.71              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:196:ARG:N   | 4:W:75:ILE:CD1[1_556]  | 1.49                     | 0.71              |
| 4:0:281:SER:O   | 4:X:280:ASN:CG[1_556]  | 1.49                     | 0.71              |
| 4:1:157:ASP:C   | 4:Y:185:LEU:CB[1_556]  | 1.49                     | 0.71              |
| 4:2:251:GLY:N   | 4:Y:114:ALA:CA[1_556]  | 1.49                     | 0.71              |
| 4:2:208:ILE:CG2 | 4:Z:198:TYR:CD1[1_556] | 1.49                     | 0.71              |
| 4:1:306:TYR:CZ  | 4:Y:256:ARG:CB[1_556]  | 1.49                     | 0.71              |
| 4:1:125:GLU:OE2 | 4:Y:7:ALA:O[1_556]     | 1.49                     | 0.71              |
| 4:2:303:THR:C   | 4:Z:255:PHE:O[1_556]   | 1.49                     | 0.71              |
| 4:0:77:THR:OG1  | 4:X:14:SER:O[1_556]    | 1.49                     | 0.71              |
| 4:2:303:THR:CA  | 4:Z:257:CYS:N[1_556]   | 1.49                     | 0.71              |
| 4:1:300:SER:C   | 4:Y:219:VAL:CB[1_556]  | 1.49                     | 0.71              |
| 4:0:114:ALA:CA  | 4:X:106:THR:CG2[1_556] | 1.49                     | 0.71              |
| 4:1:166:TYR:CB  | 4:Y:294:TYR:CA[1_556]  | 1.49                     | 0.71              |
| 4:1:233:SER:CA  | 4:X:367:PRO:CB[1_556]  | 1.49                     | 0.71              |
| 4:2:113:LYS:CD  | 4:Z:136:ILE:N[1_556]   | 1.50                     | 0.70              |
| 4:0:119:MET:O   | 4:X:340:TRP:CD2[1_556] | 1.50                     | 0.70              |
| 4:2:210:ARG:CD  | 4:Z:193:LEU:CD2[1_556] | 1.50                     | 0.70              |
| 4:2:16:LEU:CD1  | 4:Z:211:ASP:O[1_556]   | 1.50                     | 0.70              |
| 4:1:372:ARG:CB  | 4:Y:143:TYR:N[1_556]   | 1.50                     | 0.70              |
| 4:0:109:PRO:C   | 4:X:154:ASP:CA[1_556]  | 1.50                     | 0.70              |
| 4:1:137:GLN:CD  | 4:Y:301:GLY:O[1_556]   | 1.50                     | 0.70              |
| 4:0:335:ARG:NE  | 4:X:220:ALA:CB[1_556]  | 1.50                     | 0.70              |
| 4:0:208:ILE:CG2 | 4:X:198:TYR:CD1[1_556] | 1.50                     | 0.70              |
| 4:1:169:TYR:O   | 4:Y:151:ILE:CG2[1_556] | 1.50                     | 0.70              |
| 4:2:129:VAL:O   | 4:Z:25:ASP:OD2[1_556]  | 1.50                     | 0.70              |
| 4:1:210:ARG:CD  | 4:Y:193:LEU:CD2[1_556] | 1.50                     | 0.70              |
| 4:1:281:SER:CB  | 4:Y:276:GLU:O[1_556]   | 1.50                     | 0.70              |
| 4:1:212:ILE:CG1 | 4:Y:196:ARG:C[1_556]   | 1.50                     | 0.70              |
| 4:0:289:ILE:CD1 | 4:X:294:TYR:OH[1_556]  | 1.50                     | 0.70              |
| 4:1:186:THR:CG2 | 4:Y:190:MET:C[1_556]   | 1.50                     | 0.70              |
| 4:1:367:PRO:C   | 4:Y:343:GLY:O[1_556]   | 1.50                     | 0.70              |
| 4:1:110:LEU:CD2 | 4:Y:162:ASN:N[1_556]   | 1.50                     | 0.70              |
| 4:1:163:VAL:O   | 4:Y:313:MET:CE[1_556]  | 1.50                     | 0.70              |
| 4:2:68:LYS:CG   | 4:Z:59:GLN:CB[1_556]   | 1.50                     | 0.70              |
| 4:1:113:LYS:CD  | 4:Y:136:ILE:N[1_556]   | 1.50                     | 0.70              |
| 4:2:126:THR:O   | 4:Z:28:ARG:NE[1_556]   | 1.50                     | 0.70              |
| 4:1:186:THR:CA  | 4:Y:191:LYS:N[1_556]   | 1.50                     | 0.70              |
| 4:1:286:ASP:O   | 4:Y:283:MET:CE[1_556]  | 1.50                     | 0.70              |
| 4:0:16:LEU:CD1  | 4:X:211:ASP:O[1_556]   | 1.50                     | 0.70              |
| 4:1:230:ALA:C   | 4:X:367:PRO:O[1_556]   | 1.50                     | 0.70              |
| 4:1:11:ASP:CG   | 4:Y:305:MET:CG[1_556]  | 1.50                     | 0.70              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:77:THR:OG1  | 4:Z:14:SER:O[1_556]    | 1.50                     | 0.70              |
| 4:0:110:LEU:CG  | 4:X:161:HIS:C[1_556]   | 1.50                     | 0.70              |
| 4:0:195:GLU:C   | 4:W:75:ILE:CD1[1_556]  | 1.50                     | 0.70              |
| 4:2:136:ILE:CB  | 4:Z:299:MET:CA[1_556]  | 1.50                     | 0.70              |
| 4:2:149:THR:N   | 4:Z:327:ILE:CA[1_556]  | 1.50                     | 0.70              |
| 4:2:148:THR:CG2 | 4:Z:328:LYS:CB[1_556]  | 1.50                     | 0.70              |
| 4:2:372:ARG:N   | 4:Z:143:TYR:CB[1_556]  | 1.50                     | 0.70              |
| 4:2:72:GLU:N    | 4:Z:157:ASP:OD2[1_556] | 1.50                     | 0.70              |
| 4:1:16:LEU:CD1  | 4:Y:211:ASP:O[1_556]   | 1.50                     | 0.70              |
| 4:1:366:GLY:N   | 4:Y:347:ALA:O[1_556]   | 1.50                     | 0.70              |
| 4:0:184:ASP:N   | 4:X:188:TYR:CA[1_556]  | 1.50                     | 0.70              |
| 4:1:140:LEU:CG  | 4:Y:331:ALA:CB[1_556]  | 1.50                     | 0.70              |
| 4:0:214:GLU:OE1 | 4:X:250:ILE:CG1[1_556] | 1.50                     | 0.70              |
| 4:2:157:ASP:C   | 4:Z:185:LEU:CB[1_556]  | 1.50                     | 0.70              |
| 4:2:233:SER:CA  | 4:Y:367:PRO:CB[1_556]  | 1.50                     | 0.70              |
| 4:1:300:SER:N   | 4:Y:219:VAL:CG1[1_556] | 1.50                     | 0.70              |
| 4:1:338:SER:CB  | 4:Y:308:GLY:C[1_556]   | 1.50                     | 0.70              |
| 4:2:151:ILE:CA  | 4:Z:317:ILE:CG2[1_556] | 1.50                     | 0.70              |
| 4:1:281:SER:CA  | 4:Y:280:ASN:OD1[1_556] | 1.50                     | 0.70              |
| 4:0:149:THR:N   | 4:X:327:ILE:CA[1_556]  | 1.50                     | 0.70              |
| 4:1:214:GLU:CA  | 4:Y:253:GLU:CG[1_556]  | 1.50                     | 0.70              |
| 4:2:140:LEU:CG  | 4:Z:331:ALA:CB[1_556]  | 1.50                     | 0.70              |
| 4:2:74:GLY:O    | 4:Z:156:GLY:CA[1_556]  | 1.50                     | 0.70              |
| 4:2:365:ALA:CB  | 4:Z:349:LEU:CA[1_556]  | 1.50                     | 0.70              |
| 4:0:126:THR:O   | 4:X:28:ARG:NE[1_556]   | 1.50                     | 0.70              |
| 4:1:215:LYS:CE  | 4:Y:237:GLU:OE1[1_556] | 1.50                     | 0.70              |
| 4:1:149:THR:N   | 4:Y:327:ILE:CA[1_556]  | 1.50                     | 0.70              |
| 4:2:138:ALA:C   | 4:Z:299:MET:CE[1_556]  | 1.50                     | 0.70              |
| 4:2:137:GLN:CD  | 4:Z:301:GLY:O[1_556]   | 1.50                     | 0.70              |
| 4:2:191:LYS:NZ  | 4:Y:110:LEU:CD2[1_556] | 1.50                     | 0.70              |
| 4:0:177:ARG:CB  | 4:X:178:LEU:O[1_556]   | 1.50                     | 0.70              |
| 4:1:303:THR:OG1 | 4:Y:257:CYS:C[1_556]   | 1.50                     | 0.70              |
| 4:2:364:GLU:CA  | 4:Z:348:SER:O[1_556]   | 1.50                     | 0.70              |
| 4:2:186:THR:CA  | 4:Z:192:ILE:N[1_556]   | 1.50                     | 0.70              |
| 4:1:337:TYR:CB  | 4:Y:307:PRO:CG[1_556]  | 1.50                     | 0.70              |
| 4:2:16:LEU:CD2  | 4:Z:214:GLU:N[1_556]   | 1.50                     | 0.70              |
| 4:1:159:VAL:CB  | 4:Y:181:ALA:CA[1_556]  | 1.50                     | 0.70              |
| 4:2:281:SER:O   | 4:Z:280:ASN:CG[1_556]  | 1.50                     | 0.70              |
| 4:1:108:ALA:CB  | 4:Y:155:SER:C[1_556]   | 1.50                     | 0.70              |
| 4:2:180:LEU:CB  | 4:Z:267:ILE:CG1[1_556] | 1.50                     | 0.70              |
| 4:1:227:MET:CA  | 4:X:372:ARG:C[1_556]   | 1.50                     | 0.70              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:161:HIS:C   | 4:Y:274:ILE:CD1[1_556] | 1.50                     | 0.70              |
| 4:1:302:GLY:O   | 4:Y:255:PHE:CA[1_556]  | 1.51                     | 0.69              |
| 4:2:107:GLU:CG  | 4:Z:300:SER:OG[1_556]  | 1.51                     | 0.69              |
| 4:2:164:PRO:N   | 4:Z:278:THR:CG2[1_556] | 1.51                     | 0.69              |
| 4:0:209:VAL:CG1 | 4:X:194:THR:N[1_556]   | 1.51                     | 0.69              |
| 4:0:272:ALA:O   | 4:X:269:MET:C[1_556]   | 1.51                     | 0.69              |
| 4:1:286:ASP:OD2 | 4:Y:290:ARG:NE[1_556]  | 1.51                     | 0.69              |
| 4:0:148:THR:CG2 | 4:X:328:LYS:CB[1_556]  | 1.51                     | 0.69              |
| 4:2:171:LEU:CA  | 4:Z:151:ILE:CG1[1_556] | 1.51                     | 0.69              |
| 4:2:207:GLU:CA  | 4:Z:200:PHE:CE1[1_556] | 1.51                     | 0.69              |
| 4:1:286:ASP:N   | 4:Y:283:MET:CB[1_556]  | 1.51                     | 0.69              |
| 4:0:213:LYS:CD  | 4:X:192:ILE:CB[1_556]  | 1.51                     | 0.69              |
| 4:2:213:LYS:C   | 4:Z:253:GLU:CD[1_556]  | 1.51                     | 0.69              |
| 4:0:206:ARG:N   | 4:X:199:SER:C[1_556]   | 1.51                     | 0.69              |
| 4:2:78:ASN:OD1  | 4:Z:32:PRO:O[1_556]    | 1.51                     | 0.69              |
| 4:0:166:TYR:C   | 4:X:295:ALA:N[1_556]   | 1.51                     | 0.69              |
| 4:2:125:GLU:CB  | 4:Z:21:PHE:N[1_556]    | 1.51                     | 0.69              |
| 4:3:227:MET:CA  | 4:Z:372:ARG:C[1_556]   | 1.51                     | 0.69              |
| 4:1:207:GLU:CA  | 4:Y:200:PHE:CE1[1_556] | 1.51                     | 0.69              |
| 4:1:140:LEU:CD2 | 4:Y:331:ALA:CA[1_556]  | 1.51                     | 0.69              |
| 4:2:272:ALA:O   | 4:Z:269:MET:C[1_556]   | 1.51                     | 0.69              |
| 4:0:277:THR:CA  | 4:X:272:ALA:CA[1_556]  | 1.51                     | 0.69              |
| 4:2:165:ILE:CB  | 4:Z:297:ASN:CG[1_556]  | 1.51                     | 0.69              |
| 4:0:166:TYR:O   | 4:X:295:ALA:N[1_556]   | 1.51                     | 0.69              |
| 4:0:113:LYS:CD  | 4:X:136:ILE:N[1_556]   | 1.51                     | 0.69              |
| 4:2:150:GLY:O   | 4:Z:317:ILE:CG2[1_556] | 1.51                     | 0.69              |
| 4:2:302:GLY:C   | 4:Z:258:PRO:CD[1_556]  | 1.51                     | 0.69              |
| 4:1:233:SER:O   | 4:X:367:PRO:CD[1_556]  | 1.51                     | 0.69              |
| 4:1:66:THR:OG1  | 4:Y:61:LYS:N[1_556]    | 1.51                     | 0.69              |
| 4:2:166:TYR:O   | 4:Z:295:ALA:N[1_556]   | 1.51                     | 0.69              |
| 4:0:151:ILE:CA  | 4:X:317:ILE:CG2[1_556] | 1.51                     | 0.69              |
| 4:1:213:LYS:CG  | 4:Y:192:ILE:CB[1_556]  | 1.51                     | 0.69              |
| 4:1:151:ILE:CA  | 4:Y:317:ILE:CG2[1_556] | 1.51                     | 0.69              |
| 4:1:214:GLU:N   | 4:Y:253:GLU:OE1[1_556] | 1.51                     | 0.69              |
| 4:1:37:ARG:NH1  | 4:Y:56:ASP:C[1_556]    | 1.51                     | 0.69              |
| 4:0:197:GLY:C   | 4:W:75:ILE:CA[1_556]   | 1.51                     | 0.69              |
| 4:2:151:ILE:N   | 4:Z:317:ILE:N[1_556]   | 1.51                     | 0.69              |
| 4:2:233:SER:O   | 4:Y:367:PRO:CD[1_556]  | 1.51                     | 0.69              |
| 4:2:214:GLU:OE1 | 4:Z:250:ILE:CG1[1_556] | 1.51                     | 0.69              |
| 4:1:122:ILE:CD1 | 4:Y:18:LYS:C[1_556]    | 1.51                     | 0.69              |
| 4:0:166:TYR:O   | 4:X:294:TYR:C[1_556]   | 1.51                     | 0.69              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:108:ALA:CB  | 4:X:155:SER:C[1_556]   | 1.51                     | 0.69              |
| 4:2:305:MET:O   | 4:Z:255:PHE:CD1[1_556] | 1.51                     | 0.69              |
| 4:1:62:ARG:NH1  | 4:Y:204:ALA:O[1_556]   | 1.51                     | 0.69              |
| 4:1:105:LEU:CD1 | 4:Y:337:TYR:CB[1_556]  | 1.51                     | 0.69              |
| 4:2:371:HIS:CG  | 4:Z:140:LEU:CD2[1_556] | 1.51                     | 0.69              |
| 4:1:178:LEU:C   | 4:Y:180:LEU:CG[1_556]  | 1.51                     | 0.69              |
| 4:3:233:SER:CA  | 4:Z:367:PRO:CB[1_556]  | 1.51                     | 0.69              |
| 4:2:369:ILE:O   | 4:Z:143:TYR:CZ[1_556]  | 1.51                     | 0.69              |
| 4:1:77:THR:CB   | 4:Y:15:GLY:N[1_556]    | 1.51                     | 0.69              |
| 4:1:148:THR:CA  | 4:Y:328:LYS:CA[1_556]  | 1.51                     | 0.69              |
| 4:1:154:ASP:CG  | 4:Y:309:ILE:CD1[1_556] | 1.51                     | 0.69              |
| 4:1:149:THR:CA  | 4:Y:327:ILE:CB[1_556]  | 1.51                     | 0.69              |
| 4:3:231:ALA:CB  | 4:Z:369:ILE:C[1_556]   | 1.51                     | 0.69              |
| 4:2:123:MET:CB  | 4:Z:26:ALA:N[1_556]    | 1.51                     | 0.69              |
| 4:0:68:LYS:CG   | 4:X:59:GLN:CB[1_556]   | 1.51                     | 0.69              |
| 4:1:106:THR:O   | 4:Y:336:LYS:CA[1_556]  | 1.51                     | 0.69              |
| 4:2:214:GLU:N   | 4:Z:253:GLU:OE1[1_556] | 1.51                     | 0.69              |
| 4:2:110:LEU:CG  | 4:Z:161:HIS:C[1_556]   | 1.51                     | 0.69              |
| 4:1:296:ASN:C   | 4:Y:315:LYS:C[1_556]   | 1.51                     | 0.69              |
| 4:2:195:GLU:OE1 | 4:Y:110:LEU:CA[1_556]  | 1.51                     | 0.69              |
| 4:1:107:GLU:C   | 4:Y:301:GLY:CA[1_556]  | 1.51                     | 0.69              |
| 4:0:369:ILE:O   | 4:X:143:TYR:CZ[1_556]  | 1.51                     | 0.69              |
| 4:0:136:ILE:C   | 4:X:299:MET:CB[1_556]  | 1.51                     | 0.69              |
| 4:1:116:ARG:O   | 4:Y:340:TRP:CA[1_556]  | 1.51                     | 0.69              |
| 4:0:181:ALA:O   | 4:X:188:TYR:CG[1_556]  | 1.51                     | 0.69              |
| 4:0:170:ALA:C   | 4:X:151:ILE:CG2[1_556] | 1.51                     | 0.69              |
| 4:0:138:ALA:C   | 4:X:299:MET:CE[1_556]  | 1.51                     | 0.69              |
| 4:1:301:GLY:O   | 4:Y:218:TYR:O[1_556]   | 1.52                     | 0.68              |
| 4:2:289:ILE:CD1 | 4:Z:294:TYR:OH[1_556]  | 1.52                     | 0.68              |
| 4:1:339:VAL:CG1 | 4:Y:335:ARG:NH2[1_556] | 1.52                     | 0.68              |
| 4:1:162:ASN:ND2 | 4:Y:273:GLY:C[1_556]   | 1.52                     | 0.68              |
| 4:2:197:GLY:C   | 4:Y:75:ILE:CA[1_556]   | 1.52                     | 0.68              |
| 4:0:207:GLU:CA  | 4:X:200:PHE:CE1[1_556] | 1.52                     | 0.68              |
| 4:2:125:GLU:O   | 4:Z:28:ARG:NH2[1_556]  | 1.52                     | 0.68              |
| 4:1:338:SER:CB  | 4:Y:309:ILE:N[1_556]   | 1.52                     | 0.68              |
| 4:1:109:PRO:N   | 4:Y:155:SER:N[1_556]   | 1.52                     | 0.68              |
| 4:0:164:PRO:N   | 4:X:278:THR:CG2[1_556] | 1.52                     | 0.68              |
| 4:1:154:ASP:C   | 4:Y:261:LEU:CB[1_556]  | 1.52                     | 0.68              |
| 4:3:196:ARG:NH2 | 4:Z:115:ASN:N[1_556]   | 1.52                     | 0.68              |
| 4:2:209:VAL:CG1 | 4:Z:194:THR:N[1_556]   | 1.52                     | 0.68              |
| 4:0:268:GLY:N   | 4:W:173:HIS:CD2[1_556] | 1.52                     | 0.68              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:372:ARG:CB  | 4:Y:143:TYR:CA[1_556]  | 1.52                     | 0.68              |
| 4:2:174:ALA:N   | 4:Z:281:SER:CB[1_556]  | 1.52                     | 0.68              |
| 4:2:184:ASP:N   | 4:Z:188:TYR:CA[1_556]  | 1.52                     | 0.68              |
| 4:2:170:ALA:C   | 4:Z:151:ILE:CG2[1_556] | 1.52                     | 0.68              |
| 4:2:271:SER:O   | 4:Z:270:GLU:N[1_556]   | 1.52                     | 0.68              |
| 4:0:233:SER:CA  | 4:W:367:PRO:CB[1_556]  | 1.52                     | 0.68              |
| 4:1:229:THR:C   | 4:X:368:SER:CB[1_556]  | 1.52                     | 0.68              |
| 4:1:196:ARG:NH2 | 4:X:115:ASN:N[1_556]   | 1.52                     | 0.68              |
| 4:0:307:PRO:N   | 4:X:227:MET:SD[1_556]  | 1.52                     | 0.68              |
| 4:0:125:GLU:O   | 4:X:28:ARG:NH2[1_556]  | 1.52                     | 0.68              |
| 4:1:295:ALA:N   | 4:Y:319:ALA:O[1_556]   | 1.52                     | 0.68              |
| 4:1:339:VAL:CA  | 4:Y:335:ARG:NH2[1_556] | 1.52                     | 0.68              |
| 4:3:229:THR:C   | 4:Z:368:SER:CB[1_556]  | 1.52                     | 0.68              |
| 4:0:213:LYS:C   | 4:X:253:GLU:CD[1_556]  | 1.52                     | 0.68              |
| 4:1:299:MET:SD  | 4:Y:312:ARG:NH1[1_556] | 1.52                     | 0.68              |
| 4:0:191:LYS:NZ  | 4:W:110:LEU:CD2[1_556] | 1.52                     | 0.68              |
| 4:1:286:ASP:O   | 4:Y:283:MET:CG[1_556]  | 1.52                     | 0.68              |
| 4:0:302:GLY:C   | 4:X:258:PRO:CD[1_556]  | 1.52                     | 0.68              |
| 4:0:33:SER:OG   | 4:X:214:GLU:OE2[1_556] | 1.52                     | 0.68              |
| 4:0:169:TYR:CE1 | 4:X:150:GLY:C[1_556]   | 1.52                     | 0.68              |
| 4:2:211:ASP:N   | 4:Z:193:LEU:CD1[1_556] | 1.52                     | 0.68              |
| 4:1:205:GLU:C   | 4:Y:199:SER:N[1_556]   | 1.52                     | 0.68              |
| 4:2:252:ASN:C   | 4:Y:113:LYS:CG[1_556]  | 1.52                     | 0.68              |
| 4:0:123:MET:CB  | 4:X:26:ALA:N[1_556]    | 1.52                     | 0.68              |
| 4:2:178:LEU:O   | 4:Z:180:LEU:CD1[1_556] | 1.52                     | 0.68              |
| 4:0:16:LEU:CD2  | 4:X:214:GLU:N[1_556]   | 1.52                     | 0.68              |
| 4:1:165:ILE:CD1 | 4:Y:297:ASN:ND2[1_556] | 1.52                     | 0.68              |
| 4:0:31:PHE:CB   | 4:X:215:LYS:NZ[1_556]  | 1.52                     | 0.68              |
| 4:0:365:ALA:CB  | 4:X:349:LEU:CA[1_556]  | 1.52                     | 0.68              |
| 4:2:169:TYR:CE1 | 4:Z:150:GLY:C[1_556]   | 1.52                     | 0.68              |
| 4:1:332:PRO:CD  | 4:Y:221:LEU:CG[1_556]  | 1.52                     | 0.68              |
| 4:2:79:TRP:CD1  | 4:Z:17:VAL:CG1[1_556]  | 1.52                     | 0.68              |
| 4:1:149:THR:C   | 4:Y:327:ILE:CG2[1_556] | 1.52                     | 0.68              |
| 4:1:231:ALA:CB  | 4:X:369:ILE:C[1_556]   | 1.52                     | 0.68              |
| 4:0:137:GLN:CD  | 4:X:301:GLY:O[1_556]   | 1.52                     | 0.68              |
| 4:0:174:ALA:N   | 4:X:281:SER:CB[1_556]  | 1.52                     | 0.68              |
| 4:0:252:ASN:C   | 4:W:113:LYS:CG[1_556]  | 1.52                     | 0.68              |
| 4:0:305:MET:O   | 4:X:255:PHE:CD1[1_556] | 1.52                     | 0.68              |
| 4:1:267:ILE:CA  | 4:X:173:HIS:C[1_556]   | 1.52                     | 0.68              |
| 4:1:214:GLU:CD  | 4:Y:250:ILE:CG2[1_556] | 1.52                     | 0.68              |
| 4:0:165:ILE:CB  | 4:X:297:ASN:CG[1_556]  | 1.52                     | 0.68              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:268:GLY:N   | 4:Y:173:HIS:CD2[1_556] | 1.52                     | 0.68              |
| 4:0:178:LEU:O   | 4:X:180:LEU:CD1[1_556] | 1.52                     | 0.68              |
| 4:1:208:ILE:O   | 4:Y:198:TYR:CG[1_556]  | 1.52                     | 0.68              |
| 4:2:307:PRO:N   | 4:Z:227:MET:SD[1_556]  | 1.52                     | 0.68              |
| 4:0:205:GLU:C   | 4:X:199:SER:N[1_556]   | 1.52                     | 0.68              |
| 4:2:108:ALA:CB  | 4:Z:155:SER:C[1_556]   | 1.53                     | 0.67              |
| 4:2:213:LYS:CD  | 4:Z:192:ILE:CB[1_556]  | 1.53                     | 0.67              |
| 4:1:215:LYS:CB  | 4:Y:196:ARG:NH2[1_556] | 1.53                     | 0.67              |
| 4:1:153:LEU:C   | 4:Y:262:PHE:CZ[1_556]  | 1.53                     | 0.67              |
| 4:2:290:ARG:CB  | 4:Z:279:TYR:OH[1_556]  | 1.53                     | 0.67              |
| 4:1:151:ILE:N   | 4:Y:317:ILE:CG2[1_556] | 1.53                     | 0.67              |
| 4:2:30:VAL:O    | 4:Z:215:LYS:CE[1_556]  | 1.53                     | 0.67              |
| 4:1:305:MET:C   | 4:Y:255:PHE:CG[1_556]  | 1.53                     | 0.67              |
| 4:2:166:TYR:O   | 4:Z:294:TYR:C[1_556]   | 1.53                     | 0.67              |
| 4:0:171:LEU:CA  | 4:X:151:ILE:CG1[1_556] | 1.53                     | 0.67              |
| 4:2:277:THR:CB  | 4:Z:272:ALA:CA[1_556]  | 1.53                     | 0.67              |
| 4:1:369:ILE:O   | 4:Y:143:TYR:CZ[1_556]  | 1.53                     | 0.67              |
| 4:2:277:THR:OG1 | 4:Z:272:ALA:N[1_556]   | 1.53                     | 0.67              |
| 4:0:211:ASP:N   | 4:X:193:LEU:CD1[1_556] | 1.53                     | 0.67              |
| 4:3:267:ILE:CA  | 4:Z:173:HIS:C[1_556]   | 1.53                     | 0.67              |
| 4:0:78:ASN:CB   | 4:X:33:SER:N[1_556]    | 1.53                     | 0.67              |
| 4:3:233:SER:O   | 4:Z:367:PRO:CD[1_556]  | 1.53                     | 0.67              |
| 4:0:338:SER:CB  | 4:X:308:GLY:C[1_556]   | 1.53                     | 0.67              |
| 4:1:68:LYS:CG   | 4:Y:59:GLN:CG[1_556]   | 1.53                     | 0.67              |
| 4:1:121:GLN:CD  | 4:Y:20:GLY:O[1_556]    | 1.53                     | 0.67              |
| 4:0:160:THR:N   | 4:X:180:LEU:CD1[1_556] | 1.53                     | 0.67              |
| 4:1:162:ASN:O   | 4:Y:274:ILE:O[1_556]   | 1.53                     | 0.67              |
| 4:2:205:GLU:C   | 4:Z:199:SER:N[1_556]   | 1.53                     | 0.67              |
| 4:2:180:LEU:CD1 | 4:Z:267:ILE:CG2[1_556] | 1.53                     | 0.67              |
| 4:2:186:THR:CB  | 4:Z:189:LEU:O[1_556]   | 1.53                     | 0.67              |
| 4:1:180:LEU:CD1 | 4:Y:267:ILE:CG2[1_556] | 1.53                     | 0.67              |
| 4:0:371:HIS:CG  | 4:X:140:LEU:CD2[1_556] | 1.53                     | 0.67              |
| 4:1:110:LEU:CB  | 4:Y:161:HIS:CG[1_556]  | 1.53                     | 0.67              |
| 4:1:297:ASN:OD1 | 4:Y:316:GLU:OE1[1_556] | 1.53                     | 0.67              |
| 4:1:252:ASN:O   | 4:X:113:LYS:CG[1_556]  | 1.53                     | 0.67              |
| 4:0:233:SER:O   | 4:W:367:PRO:CD[1_556]  | 1.53                     | 0.67              |
| 4:2:305:MET:O   | 4:Z:255:PHE:CE2[1_556] | 1.53                     | 0.67              |
| 4:1:113:LYS:CA  | 4:Y:136:ILE:C[1_556]   | 1.53                     | 0.67              |
| 4:1:180:LEU:CB  | 4:Y:267:ILE:CG1[1_556] | 1.53                     | 0.67              |
| 4:0:277:THR:CB  | 4:X:272:ALA:CA[1_556]  | 1.53                     | 0.67              |
| 4:1:261:LEU:C   | 4:Y:265:SER:C[1_556]   | 1.53                     | 0.67              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:271:SER:O   | 4:X:270:GLU:N[1_556]   | 1.53                     | 0.67              |
| 4:0:169:TYR:CE2 | 4:X:293:LEU:CG[1_556]  | 1.53                     | 0.67              |
| 4:2:252:ASN:CA  | 4:Y:113:LYS:CB[1_556]  | 1.53                     | 0.67              |
| 4:0:186:THR:CB  | 4:X:189:LEU:O[1_556]   | 1.53                     | 0.67              |
| 4:0:107:GLU:C   | 4:X:301:GLY:CA[1_556]  | 1.53                     | 0.67              |
| 4:2:125:GLU:N   | 4:Z:24:ASP:CG[1_556]   | 1.53                     | 0.67              |
| 4:0:371:HIS:ND1 | 4:X:140:LEU:N[1_556]   | 1.53                     | 0.67              |
| 4:0:125:GLU:C   | 4:X:24:ASP:OD2[1_556]  | 1.53                     | 0.67              |
| 4:0:116:ARG:NE  | 4:X:141:SER:CB[1_556]  | 1.53                     | 0.67              |
| 4:1:372:ARG:CZ  | 4:Y:145:SER:N[1_556]   | 1.53                     | 0.67              |
| 4:1:369:ILE:CB  | 4:Y:346:LEU:N[1_556]   | 1.53                     | 0.67              |
| 4:1:186:THR:C   | 4:Y:191:LYS:C[1_556]   | 1.53                     | 0.67              |
| 4:0:30:VAL:O    | 4:X:215:LYS:CE[1_556]  | 1.53                     | 0.67              |
| 4:2:215:LYS:CB  | 4:Z:196:ARG:NH2[1_556] | 1.53                     | 0.67              |
| 4:1:123:MET:SD  | 4:Y:26:ALA:CA[1_556]   | 1.53                     | 0.67              |
| 4:2:31:PHE:CB   | 4:Z:215:LYS:NZ[1_556]  | 1.53                     | 0.67              |
| 4:2:107:GLU:C   | 4:Z:301:GLY:CA[1_556]  | 1.53                     | 0.67              |
| 4:1:33:SER:CA   | 4:Y:210:ARG:NH2[1_556] | 1.53                     | 0.67              |
| 4:1:195:GLU:C   | 4:X:75:ILE:CD1[1_556]  | 1.53                     | 0.67              |
| 4:1:365:ALA:CA  | 4:Y:349:LEU:N[1_556]   | 1.53                     | 0.67              |
| 4:2:136:ILE:C   | 4:Z:299:MET:CB[1_556]  | 1.53                     | 0.67              |
| 4:2:66:THR:OG1  | 4:Z:61:LYS:N[1_556]    | 1.53                     | 0.67              |
| 4:0:104:LEU:C   | 4:X:334:GLU:N[1_556]   | 1.53                     | 0.67              |
| 4:0:183:ARG:C   | 4:X:187:ASP:O[1_556]   | 1.53                     | 0.67              |
| 4:0:195:GLU:OE1 | 4:W:110:LEU:CA[1_556]  | 1.53                     | 0.67              |
| 4:3:233:SER:OG  | 4:Z:367:PRO:CB[1_556]  | 1.54                     | 0.66              |
| 4:3:252:ASN:O   | 4:Z:113:LYS:CG[1_556]  | 1.54                     | 0.66              |
| 4:0:336:LYS:CB  | 4:X:218:TYR:CG[1_556]  | 1.54                     | 0.66              |
| 4:2:206:ARG:CB  | 4:Z:200:PHE:CA[1_556]  | 1.54                     | 0.66              |
| 4:0:107:GLU:OE1 | 4:X:141:SER:OG[1_556]  | 1.54                     | 0.66              |
| 4:2:371:HIS:ND1 | 4:Z:140:LEU:CG[1_556]  | 1.54                     | 0.66              |
| 4:0:305:MET:O   | 4:X:255:PHE:CE2[1_556] | 1.54                     | 0.66              |
| 4:2:196:ARG:CD  | 4:Y:115:ASN:OD1[1_556] | 1.54                     | 0.66              |
| 4:2:107:GLU:OE1 | 4:Z:141:SER:OG[1_556]  | 1.54                     | 0.66              |
| 4:1:12:ASN:OD1  | 4:Y:336:LYS:CD[1_556]  | 1.54                     | 0.66              |
| 4:2:181:ALA:O   | 4:Z:188:TYR:CG[1_556]  | 1.54                     | 0.66              |
| 4:2:33:SER:OG   | 4:Z:214:GLU:OE2[1_556] | 1.54                     | 0.66              |
| 4:1:164:PRO:CG  | 4:Y:278:THR:N[1_556]   | 1.54                     | 0.66              |
| 4:0:125:GLU:N   | 4:X:24:ASP:CG[1_556]   | 1.54                     | 0.66              |
| 4:1:79:TRP:CZ3  | 4:Y:18:LYS:CB[1_556]   | 1.54                     | 0.66              |
| 4:1:297:ASN:N   | 4:Y:315:LYS:O[1_556]   | 1.54                     | 0.66              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:277:THR:OG1 | 4:X:272:ALA:N[1_556]   | 1.54                     | 0.66              |
| 4:0:180:LEU:CD1 | 4:X:267:ILE:CG2[1_556] | 1.54                     | 0.66              |
| 4:0:37:ARG:CZ   | 4:X:56:ASP:CB[1_556]   | 1.54                     | 0.66              |
| 4:1:171:LEU:CA  | 4:Y:151:ILE:CG1[1_556] | 1.54                     | 0.66              |
| 4:0:337:TYR:CB  | 4:X:307:PRO:CB[1_556]  | 1.54                     | 0.66              |
| 4:0:76:ILE:O    | 4:X:13:GLY:CA[1_556]   | 1.54                     | 0.66              |
| 4:1:335:ARG:CG  | 4:Y:219:VAL:C[1_556]   | 1.54                     | 0.66              |
| 4:1:362:TYR:OH  | 4:Y:22:ALA:CA[1_556]   | 1.54                     | 0.66              |
| 4:2:78:ASN:CB   | 4:Z:33:SER:N[1_556]    | 1.54                     | 0.66              |
| 4:1:337:TYR:CA  | 4:Y:307:PRO:CA[1_556]  | 1.54                     | 0.66              |
| 4:1:233:SER:OG  | 4:X:367:PRO:CB[1_556]  | 1.54                     | 0.66              |
| 4:1:195:GLU:OE1 | 4:X:110:LEU:N[1_556]   | 1.54                     | 0.66              |
| 4:2:123:MET:SD  | 4:Z:26:ALA:CA[1_556]   | 1.54                     | 0.66              |
| 4:2:172:PRO:CB  | 4:Z:164:PRO:N[1_556]   | 1.54                     | 0.66              |
| 4:2:160:THR:N   | 4:Z:180:LEU:CD1[1_556] | 1.54                     | 0.66              |
| 4:2:76:ILE:O    | 4:Z:13:GLY:CA[1_556]   | 1.54                     | 0.66              |
| 4:1:186:THR:CA  | 4:Y:192:ILE:N[1_556]   | 1.54                     | 0.66              |
| 4:0:290:ARG:CB  | 4:X:279:TYR:OH[1_556]  | 1.54                     | 0.66              |
| 4:1:209:VAL:O   | 4:Y:193:LEU:C[1_556]   | 1.54                     | 0.66              |
| 4:0:214:GLU:OE1 | 4:X:250:ILE:CG2[1_556] | 1.54                     | 0.66              |
| 4:1:117:GLU:OE2 | 4:Y:135:ALA:CB[1_556]  | 1.54                     | 0.66              |
| 4:1:175:ILE:CD1 | 4:Y:162:ASN:CA[1_556]  | 1.54                     | 0.66              |
| 4:1:139:VAL:CG1 | 4:Y:297:ASN:O[1_556]   | 1.54                     | 0.66              |
| 4:2:336:LYS:CB  | 4:Z:218:TYR:CG[1_556]  | 1.54                     | 0.66              |
| 4:1:372:ARG:NE  | 4:Y:142:LEU:C[1_556]   | 1.54                     | 0.66              |
| 4:0:79:TRP:CD1  | 4:X:17:VAL:CG1[1_556]  | 1.54                     | 0.66              |
| 4:1:371:HIS:ND1 | 4:Y:140:LEU:CG[1_556]  | 1.54                     | 0.66              |
| 4:1:209:VAL:CG1 | 4:Y:194:THR:N[1_556]   | 1.54                     | 0.66              |
| 4:0:114:ALA:CB  | 4:X:106:THR:CB[1_556]  | 1.54                     | 0.66              |
| 4:1:144:ALA:C   | 4:Y:311:ASP:OD1[1_556] | 1.54                     | 0.66              |
| 4:2:183:ARG:C   | 4:Z:187:ASP:O[1_556]   | 1.54                     | 0.66              |
| 4:2:125:GLU:C   | 4:Z:24:ASP:OD2[1_556]  | 1.54                     | 0.66              |
| 4:3:64:ILE:N    | 4:Y:289:ILE:N[1_556]   | 1.54                     | 0.66              |
| 4:1:116:ARG:NE  | 4:Y:141:SER:CB[1_556]  | 1.54                     | 0.66              |
| 4:0:364:GLU:C   | 4:X:348:SER:O[1_556]   | 1.54                     | 0.66              |
| 4:0:113:LYS:CE  | 4:X:136:ILE:N[1_556]   | 1.54                     | 0.66              |
| 4:1:311:ASP:OD1 | 4:Y:224:GLU:CD[1_556]  | 1.55                     | 0.65              |
| 4:1:371:HIS:CG  | 4:Y:140:LEU:CD2[1_556] | 1.55                     | 0.65              |
| 4:2:215:LYS:O   | 4:Z:252:ASN:CG[1_556]  | 1.55                     | 0.65              |
| 4:0:252:ASN:CA  | 4:W:113:LYS:CB[1_556]  | 1.55                     | 0.65              |
| 4:1:279:TYR:CA  | 4:Y:276:GLU:OE1[1_556] | 1.55                     | 0.65              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:195:GLU:C   | 4:Z:75:ILE:CD1[1_556]  | 1.55                     | 0.65              |
| 4:1:306:TYR:N   | 4:Y:255:PHE:CD1[1_556] | 1.55                     | 0.65              |
| 4:1:212:ILE:CD1 | 4:Y:196:ARG:C[1_556]   | 1.55                     | 0.65              |
| 4:1:208:ILE:CG2 | 4:Y:198:TYR:CD1[1_556] | 1.55                     | 0.65              |
| 4:2:203:THR:OG1 | 4:Z:205:GLU:CD[1_556]  | 1.55                     | 0.65              |
| 4:0:289:ILE:O   | 4:X:321:ALA:CA[1_556]  | 1.55                     | 0.65              |
| 4:2:169:TYR:CE2 | 4:Z:293:LEU:CG[1_556]  | 1.55                     | 0.65              |
| 4:1:236:LEU:CD1 | 4:X:117:GLU:OE2[1_556] | 1.55                     | 0.65              |
| 4:1:104:LEU:O   | 4:Y:334:GLU:N[1_556]   | 1.55                     | 0.65              |
| 4:2:337:TYR:CB  | 4:Z:307:PRO:CB[1_556]  | 1.55                     | 0.65              |
| 4:1:79:TRP:C    | 4:Y:31:PHE:CD1[1_556]  | 1.55                     | 0.65              |
| 4:2:114:ALA:CB  | 4:Z:106:THR:CB[1_556]  | 1.55                     | 0.65              |
| 4:2:66:THR:OG1  | 4:Z:60:SER:O[1_556]    | 1.55                     | 0.65              |
| 4:2:229:THR:O   | 4:Y:368:SER:C[1_556]   | 1.55                     | 0.65              |
| 4:2:113:LYS:CE  | 4:Z:136:ILE:N[1_556]   | 1.55                     | 0.65              |
| 4:1:81:ASP:OD1  | 4:Y:56:ASP:CG[1_556]   | 1.55                     | 0.65              |
| 4:1:195:GLU:OE1 | 4:X:109:PRO:O[1_556]   | 1.55                     | 0.65              |
| 4:0:288:ASP:CG  | 4:Z:205:GLU:OE2[1_556] | 1.55                     | 0.65              |
| 4:3:268:GLY:N   | 4:Z:173:HIS:CD2[1_556] | 1.55                     | 0.65              |
| 4:2:364:GLU:C   | 4:Z:348:SER:O[1_556]   | 1.55                     | 0.65              |
| 4:1:126:THR:CG2 | 4:Y:28:ARG:CB[1_556]   | 1.55                     | 0.65              |
| 4:0:229:THR:O   | 4:W:368:SER:C[1_556]   | 1.55                     | 0.65              |
| 4:0:113:LYS:CA  | 4:X:136:ILE:C[1_556]   | 1.55                     | 0.65              |
| 4:1:31:PHE:CB   | 4:Y:215:LYS:NZ[1_556]  | 1.55                     | 0.65              |
| 4:3:236:LEU:CD1 | 4:Z:117:GLU:OE2[1_556] | 1.55                     | 0.65              |
| 4:0:116:ARG:CB  | 4:X:339:VAL:CA[1_556]  | 1.55                     | 0.65              |
| 4:1:175:ILE:CG2 | 4:Y:162:ASN:OD1[1_556] | 1.55                     | 0.65              |
| 4:1:206:ARG:CB  | 4:Y:200:PHE:CA[1_556]  | 1.55                     | 0.65              |
| 4:2:311:ASP:OD1 | 4:Z:224:GLU:CD[1_556]  | 1.55                     | 0.65              |
| 4:0:196:ARG:CD  | 4:W:115:ASN:OD1[1_556] | 1.55                     | 0.65              |
| 4:1:232:SER:OG  | 4:X:369:ILE:CB[1_556]  | 1.55                     | 0.65              |
| 4:3:195:GLU:OE1 | 4:Z:109:PRO:O[1_556]   | 1.55                     | 0.65              |
| 4:2:37:ARG:CZ   | 4:Z:56:ASP:CB[1_556]   | 1.55                     | 0.65              |
| 4:1:285:CYS:CB  | 4:Y:279:TYR:O[1_556]   | 1.55                     | 0.65              |
| 4:2:371:HIS:ND1 | 4:Z:140:LEU:N[1_556]   | 1.55                     | 0.65              |
| 4:2:289:ILE:O   | 4:Z:321:ALA:CA[1_556]  | 1.55                     | 0.65              |
| 4:2:338:SER:CB  | 4:Z:308:GLY:C[1_556]   | 1.55                     | 0.65              |
| 4:2:154:ASP:OD1 | 4:Z:309:ILE:CD1[1_556] | 1.55                     | 0.65              |
| 4:2:148:THR:CA  | 4:Z:328:LYS:CA[1_556]  | 1.55                     | 0.65              |
| 4:2:339:VAL:CA  | 4:Z:335:ARG:NH2[1_556] | 1.55                     | 0.65              |
| 4:2:366:GLY:N   | 4:Z:347:ALA:O[1_556]   | 1.55                     | 0.65              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:79:TRP:CD1  | 4:Y:17:VAL:CG1[1_556]  | 1.55                     | 0.65              |
| 4:1:105:LEU:CA  | 4:Y:334:GLU:CA[1_556]  | 1.55                     | 0.65              |
| 4:1:210:ARG:CB  | 4:Y:193:LEU:CB[1_556]  | 1.55                     | 0.65              |
| 4:1:365:ALA:CB  | 4:Y:349:LEU:CA[1_556]  | 1.55                     | 0.65              |
| 4:1:169:TYR:CD1 | 4:Y:150:GLY:CA[1_556]  | 1.55                     | 0.65              |
| 4:2:295:ALA:O   | 4:Z:315:LYS:NZ[1_556]  | 1.55                     | 0.65              |
| 4:2:285:CYS:CB  | 4:Z:279:TYR:O[1_556]   | 1.55                     | 0.65              |
| 4:2:116:ARG:CD  | 4:Z:140:LEU:C[1_556]   | 1.55                     | 0.65              |
| 4:0:172:PRO:CB  | 4:X:164:PRO:N[1_556]   | 1.55                     | 0.65              |
| 4:1:215:LYS:O   | 4:Y:252:ASN:CG[1_556]  | 1.55                     | 0.65              |
| 4:0:203:THR:OG1 | 4:X:205:GLU:CD[1_556]  | 1.55                     | 0.65              |
| 4:2:185:LEU:CG  | 4:Z:188:TYR:CD1[1_556] | 1.55                     | 0.65              |
| 4:0:371:HIS:ND1 | 4:X:140:LEU:CG[1_556]  | 1.55                     | 0.65              |
| 4:1:129:VAL:O   | 4:Y:25:ASP:OD2[1_556]  | 1.55                     | 0.65              |
| 4:0:215:LYS:CB  | 4:X:196:ARG:NH2[1_556] | 1.55                     | 0.65              |
| 4:1:181:ALA:O   | 4:Y:188:TYR:CG[1_556]  | 1.55                     | 0.65              |
| 4:2:109:PRO:N   | 4:Z:155:SER:N[1_556]   | 1.55                     | 0.65              |
| 4:1:133:TYR:OH  | 4:Y:145:SER:CA[1_556]  | 1.55                     | 0.65              |
| 4:1:195:GLU:OE1 | 4:X:110:LEU:CA[1_556]  | 1.55                     | 0.65              |
| 4:0:104:LEU:O   | 4:X:334:GLU:N[1_556]   | 1.55                     | 0.65              |
| 4:2:309:ILE:CG2 | 4:Z:223:PHE:CB[1_556]  | 1.55                     | 0.65              |
| 4:0:206:ARG:CB  | 4:X:200:PHE:CA[1_556]  | 1.55                     | 0.65              |
| 4:2:113:LYS:CA  | 4:Z:136:ILE:C[1_556]   | 1.55                     | 0.65              |
| 4:0:66:THR:OG1  | 4:X:60:SER:O[1_556]    | 1.55                     | 0.65              |
| 4:1:136:ILE:C   | 4:Y:299:MET:CB[1_556]  | 1.55                     | 0.65              |
| 4:2:62:ARG:NH1  | 4:Z:204:ALA:O[1_556]   | 1.55                     | 0.65              |
| 4:1:335:ARG:CA  | 4:Y:219:VAL:O[1_556]   | 1.55                     | 0.65              |
| 4:2:116:ARG:CB  | 4:Z:339:VAL:CA[1_556]  | 1.55                     | 0.65              |
| 4:0:144:ALA:C   | 4:X:311:ASP:OD1[1_556] | 1.55                     | 0.65              |
| 4:1:268:GLY:N   | 4:X:173:HIS:CD2[1_556] | 1.55                     | 0.65              |
| 4:0:123:MET:SD  | 4:X:26:ALA:CA[1_556]   | 1.56                     | 0.64              |
| 4:1:68:LYS:CG   | 4:Y:59:GLN:CB[1_556]   | 1.56                     | 0.64              |
| 4:2:139:VAL:CG1 | 4:Z:330:ILE:O[1_556]   | 1.56                     | 0.64              |
| 4:0:178:LEU:CD2 | 4:X:264:PRO:CA[1_556]  | 1.56                     | 0.64              |
| 4:2:116:ARG:NE  | 4:Z:141:SER:CB[1_556]  | 1.56                     | 0.64              |
| 4:2:197:GLY:O   | 4:Y:75:ILE:O[1_556]    | 1.56                     | 0.64              |
| 4:0:66:THR:OG1  | 4:X:61:LYS:N[1_556]    | 1.56                     | 0.64              |
| 4:0:109:PRO:N   | 4:X:155:SER:N[1_556]   | 1.56                     | 0.64              |
| 4:2:104:LEU:C   | 4:Z:334:GLU:N[1_556]   | 1.56                     | 0.64              |
| 4:2:214:GLU:OE1 | 4:Z:250:ILE:CG2[1_556] | 1.56                     | 0.64              |
| 4:1:141:SER:OG  | 4:Y:309:ILE:CB[1_556]  | 1.56                     | 0.64              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:122:ILE:CD1 | 4:X:18:LYS:C[1_556]    | 1.56                     | 0.64              |
| 4:1:307:PRO:CA  | 4:Y:227:MET:N[1_556]   | 1.56                     | 0.64              |
| 4:2:331:ALA:CB  | 4:Z:221:LEU:C[1_556]   | 1.56                     | 0.64              |
| 4:0:197:GLY:O   | 4:W:75:ILE:O[1_556]    | 1.56                     | 0.64              |
| 4:0:142:LEU:N   | 4:X:310:ALA:CA[1_556]  | 1.56                     | 0.64              |
| 4:0:215:LYS:O   | 4:X:252:ASN:CG[1_556]  | 1.56                     | 0.64              |
| 4:2:185:LEU:N   | 4:Z:188:TYR:CA[1_556]  | 1.56                     | 0.64              |
| 4:0:233:SER:N   | 4:W:366:GLY:O[1_556]   | 1.56                     | 0.64              |
| 4:2:70:PRO:O    | 4:Z:15:GLY:C[1_556]    | 1.56                     | 0.64              |
| 4:1:116:ARG:CD  | 4:Y:140:LEU:C[1_556]   | 1.56                     | 0.64              |
| 4:2:180:LEU:CD2 | 4:Z:267:ILE:CG1[1_556] | 1.56                     | 0.64              |
| 4:2:336:LYS:CB  | 4:Z:218:TYR:CD1[1_556] | 1.56                     | 0.64              |
| 4:3:63:GLY:CA   | 4:Y:288:ASP:N[1_556]   | 1.56                     | 0.64              |
| 4:0:286:ASP:N   | 4:X:283:MET:CB[1_556]  | 1.56                     | 0.64              |
| 4:0:295:ALA:O   | 4:X:315:LYS:NZ[1_556]  | 1.56                     | 0.64              |
| 4:1:296:ASN:N   | 4:Y:319:ALA:N[1_556]   | 1.56                     | 0.64              |
| 4:0:116:ARG:CD  | 4:X:140:LEU:C[1_556]   | 1.56                     | 0.64              |
| 4:3:270:GLU:OE1 | 4:Z:286:ASP:CG[1_556]  | 1.56                     | 0.64              |
| 4:2:107:GLU:OE2 | 4:Z:141:SER:OG[1_556]  | 1.56                     | 0.64              |
| 4:2:296:ASN:N   | 4:Z:319:ALA:N[1_556]   | 1.56                     | 0.64              |
| 4:0:70:PRO:O    | 4:X:15:GLY:C[1_556]    | 1.56                     | 0.64              |
| 4:2:270:GLU:CD  | 4:Y:286:ASP:CA[1_556]  | 1.56                     | 0.64              |
| 4:1:109:PRO:C   | 4:Y:154:ASP:CA[1_556]  | 1.56                     | 0.64              |
| 4:1:164:PRO:N   | 4:Y:278:THR:CG2[1_556] | 1.56                     | 0.64              |
| 4:0:261:LEU:CD1 | 4:X:266:PHE:CG[1_556]  | 1.56                     | 0.64              |
| 4:1:142:LEU:N   | 4:Y:310:ALA:CA[1_556]  | 1.56                     | 0.64              |
| 4:1:104:LEU:C   | 4:Y:334:GLU:N[1_556]   | 1.56                     | 0.64              |
| 4:2:142:LEU:N   | 4:Z:310:ALA:CA[1_556]  | 1.56                     | 0.64              |
| 4:2:79:TRP:C    | 4:Z:31:PHE:CD1[1_556]  | 1.56                     | 0.64              |
| 4:3:195:GLU:OE1 | 4:Z:110:LEU:N[1_556]   | 1.56                     | 0.64              |
| 4:1:309:ILE:CB  | 4:Y:259:GLU:CD[1_556]  | 1.56                     | 0.64              |
| 4:2:280:ASN:C   | 4:Z:280:ASN:OD1[1_556] | 1.56                     | 0.64              |
| 4:1:113:LYS:N   | 4:Y:137:GLN:CA[1_556]  | 1.56                     | 0.64              |
| 4:1:142:LEU:CA  | 4:Y:310:ALA:O[1_556]   | 1.56                     | 0.64              |
| 4:0:162:ASN:N   | 4:X:274:ILE:CB[1_556]  | 1.56                     | 0.64              |
| 4:2:162:ASN:N   | 4:Z:274:ILE:CB[1_556]  | 1.56                     | 0.64              |
| 4:1:59:GLN:CD   | 4:Y:208:ILE:N[1_556]   | 1.56                     | 0.64              |
| 4:1:119:MET:CA  | 4:Y:340:TRP:CD1[1_556] | 1.56                     | 0.64              |
| 4:1:151:ILE:CD1 | 4:Y:276:GLU:N[1_556]   | 1.56                     | 0.64              |
| 4:1:163:VAL:N   | 4:Y:274:ILE:O[1_556]   | 1.56                     | 0.64              |
| 4:1:278:THR:C   | 4:Y:276:GLU:OE2[1_556] | 1.56                     | 0.64              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:78:ASN:ND2  | 4:Y:32:PRO:O[1_556]    | 1.56                     | 0.64              |
| 4:0:272:ALA:N   | 4:X:270:GLU:C[1_556]   | 1.56                     | 0.64              |
| 4:1:64:ILE:N    | 4:W:289:ILE:N[1_556]   | 1.56                     | 0.64              |
| 4:3:232:SER:OG  | 4:Z:369:ILE:CB[1_556]  | 1.56                     | 0.64              |
| 4:2:272:ALA:N   | 4:Z:270:GLU:C[1_556]   | 1.56                     | 0.64              |
| 4:1:151:ILE:N   | 4:Y:317:ILE:N[1_556]   | 1.56                     | 0.64              |
| 4:1:270:GLU:OE1 | 4:X:286:ASP:CG[1_556]  | 1.56                     | 0.64              |
| 4:2:161:HIS:C   | 4:Z:274:ILE:CD1[1_556] | 1.56                     | 0.64              |
| 4:0:366:GLY:N   | 4:X:347:ALA:O[1_556]   | 1.56                     | 0.64              |
| 4:1:307:PRO:O   | 4:Y:227:MET:CB[1_556]  | 1.56                     | 0.64              |
| 4:0:212:ILE:CD1 | 4:X:196:ARG:C[1_556]   | 1.56                     | 0.64              |
| 4:1:166:TYR:C   | 4:Y:295:ALA:N[1_556]   | 1.56                     | 0.64              |
| 4:1:261:LEU:CB  | 4:Y:266:PHE:CB[1_556]  | 1.56                     | 0.64              |
| 4:1:289:ILE:CD1 | 4:Y:294:TYR:OH[1_556]  | 1.56                     | 0.64              |
| 4:2:212:ILE:CD1 | 4:Z:196:ARG:C[1_556]   | 1.56                     | 0.64              |
| 4:2:369:ILE:CB  | 4:Z:345:ILE:C[1_556]   | 1.56                     | 0.64              |
| 4:0:16:LEU:CD2  | 4:X:213:LYS:O[1_556]   | 1.56                     | 0.64              |
| 4:2:120:THR:CG2 | 4:Z:344:SER:CB[1_556]  | 1.57                     | 0.63              |
| 4:0:139:VAL:CG1 | 4:X:330:ILE:O[1_556]   | 1.57                     | 0.63              |
| 4:1:136:ILE:CB  | 4:Y:299:MET:CA[1_556]  | 1.57                     | 0.63              |
| 4:2:104:LEU:O   | 4:Z:334:GLU:N[1_556]   | 1.57                     | 0.63              |
| 4:1:169:TYR:CE2 | 4:Y:293:LEU:CG[1_556]  | 1.57                     | 0.63              |
| 4:0:166:TYR:C   | 4:X:294:TYR:O[1_556]   | 1.57                     | 0.63              |
| 4:1:138:ALA:C   | 4:Y:299:MET:CE[1_556]  | 1.57                     | 0.63              |
| 4:0:185:LEU:CG  | 4:X:188:TYR:CD1[1_556] | 1.57                     | 0.63              |
| 4:0:72:GLU:O    | 4:X:157:ASP:CA[1_556]  | 1.57                     | 0.63              |
| 4:0:296:ASN:N   | 4:X:319:ALA:N[1_556]   | 1.57                     | 0.63              |
| 4:2:208:ILE:O   | 4:Z:198:TYR:CG[1_556]  | 1.57                     | 0.63              |
| 4:0:154:ASP:OD1 | 4:X:309:ILE:CD1[1_556] | 1.57                     | 0.63              |
| 4:0:142:LEU:CA  | 4:X:310:ALA:O[1_556]   | 1.57                     | 0.63              |
| 4:0:270:GLU:CD  | 4:W:286:ASP:CA[1_556]  | 1.57                     | 0.63              |
| 4:1:63:GLY:CA   | 4:W:288:ASP:N[1_556]   | 1.57                     | 0.63              |
| 4:0:311:ASP:OD1 | 4:X:224:GLU:CD[1_556]  | 1.57                     | 0.63              |
| 4:0:208:ILE:CB  | 4:X:198:TYR:CE1[1_556] | 1.57                     | 0.63              |
| 4:0:148:THR:CA  | 4:X:328:LYS:CA[1_556]  | 1.57                     | 0.63              |
| 4:1:62:ARG:NH2  | 4:Y:205:GLU:CB[1_556]  | 1.57                     | 0.63              |
| 4:0:285:CYS:CB  | 4:X:279:TYR:O[1_556]   | 1.57                     | 0.63              |
| 4:0:331:ALA:CB  | 4:X:221:LEU:C[1_556]   | 1.57                     | 0.63              |
| 4:0:339:VAL:CA  | 4:X:335:ARG:NH2[1_556] | 1.57                     | 0.63              |
| 4:1:11:ASP:OD2  | 4:Y:305:MET:CA[1_556]  | 1.57                     | 0.63              |
| 4:0:336:LYS:CB  | 4:X:218:TYR:CD1[1_556] | 1.57                     | 0.63              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:369:ILE:CB  | 4:Y:345:ILE:C[1_556]   | 1.57                     | 0.63              |
| 4:1:16:LEU:CD2  | 4:Y:213:LYS:O[1_556]   | 1.57                     | 0.63              |
| 4:0:309:ILE:CG2 | 4:X:223:PHE:CB[1_556]  | 1.57                     | 0.63              |
| 4:3:233:SER:N   | 4:Z:367:PRO:N[1_556]   | 1.57                     | 0.63              |
| 4:1:367:PRO:O   | 4:Y:343:GLY:CA[1_556]  | 1.57                     | 0.63              |
| 4:3:62:ARG:O    | 4:Y:288:ASP:CG[1_556]  | 1.57                     | 0.63              |
| 4:1:233:SER:N   | 4:X:367:PRO:N[1_556]   | 1.57                     | 0.63              |
| 4:1:116:ARG:CA  | 4:Y:339:VAL:C[1_556]   | 1.57                     | 0.63              |
| 4:0:369:ILE:CB  | 4:X:345:ILE:C[1_556]   | 1.57                     | 0.63              |
| 4:2:72:GLU:O    | 4:Z:157:ASP:CA[1_556]  | 1.57                     | 0.63              |
| 4:2:186:THR:CA  | 4:Z:191:LYS:N[1_556]   | 1.57                     | 0.63              |
| 4:2:178:LEU:CD2 | 4:Z:264:PRO:CA[1_556]  | 1.57                     | 0.63              |
| 4:1:134:VAL:CB  | 4:Y:338:SER:CB[1_556]  | 1.57                     | 0.63              |
| 4:0:62:ARG:NH1  | 4:X:204:ALA:O[1_556]   | 1.57                     | 0.63              |
| 4:2:233:SER:N   | 4:Y:366:GLY:O[1_556]   | 1.57                     | 0.63              |
| 4:2:215:LYS:CD  | 4:Z:237:GLU:OE1[1_556] | 1.57                     | 0.63              |
| 4:2:299:MET:SD  | 4:Z:312:ARG:NH1[1_556] | 1.57                     | 0.63              |
| 4:1:191:LYS:NZ  | 4:X:110:LEU:CD2[1_556] | 1.57                     | 0.63              |
| 4:0:281:SER:CA  | 4:X:280:ASN:OD1[1_556] | 1.57                     | 0.63              |
| 4:2:122:ILE:CD1 | 4:Z:18:LYS:C[1_556]    | 1.57                     | 0.63              |
| 4:2:166:TYR:C   | 4:Z:294:TYR:O[1_556]   | 1.57                     | 0.63              |
| 4:0:215:LYS:CD  | 4:X:237:GLU:OE1[1_556] | 1.57                     | 0.63              |
| 4:2:261:LEU:CD1 | 4:Z:266:PHE:CG[1_556]  | 1.57                     | 0.63              |
| 4:2:108:ALA:N   | 4:Z:301:GLY:CA[1_556]  | 1.57                     | 0.63              |
| 4:0:364:GLU:O   | 4:X:349:LEU:C[1_556]   | 1.57                     | 0.63              |
| 4:1:148:THR:CG2 | 4:Y:328:LYS:CG[1_556]  | 1.57                     | 0.63              |
| 4:1:62:ARG:O    | 4:W:288:ASP:CG[1_556]  | 1.57                     | 0.63              |
| 4:3:195:GLU:OE1 | 4:Z:110:LEU:CA[1_556]  | 1.57                     | 0.63              |
| 4:3:63:GLY:N    | 4:Y:288:ASP:N[1_556]   | 1.57                     | 0.63              |
| 4:2:16:LEU:CD2  | 4:Z:213:LYS:O[1_556]   | 1.57                     | 0.63              |
| 4:1:150:GLY:C   | 4:Y:317:ILE:CG2[1_556] | 1.57                     | 0.63              |
| 4:2:306:TYR:CG  | 4:Z:256:ARG:CG[1_556]  | 1.57                     | 0.63              |
| 4:3:267:ILE:CB  | 4:Z:173:HIS:CB[1_556]  | 1.57                     | 0.63              |
| 4:0:366:GLY:N   | 4:X:348:SER:N[1_556]   | 1.57                     | 0.63              |
| 4:2:286:ASP:N   | 4:Z:283:MET:CB[1_556]  | 1.57                     | 0.63              |
| 4:1:33:SER:OG   | 4:Y:214:GLU:OE2[1_556] | 1.58                     | 0.62              |
| 4:0:180:LEU:CD2 | 4:X:267:ILE:CG1[1_556] | 1.58                     | 0.62              |
| 4:2:159:VAL:CB  | 4:Z:181:ALA:CA[1_556]  | 1.58                     | 0.62              |
| 4:2:144:ALA:C   | 4:Z:311:ASP:OD1[1_556] | 1.58                     | 0.62              |
| 4:0:108:ALA:N   | 4:X:301:GLY:CA[1_556]  | 1.58                     | 0.62              |
| 4:0:140:LEU:CD2 | 4:X:331:ALA:CA[1_556]  | 1.58                     | 0.62              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:79:TRP:C    | 4:X:31:PHE:CD1[1_556]  | 1.58                     | 0.62              |
| 4:0:228:ALA:O   | 4:W:369:ILE:CA[1_556]  | 1.58                     | 0.62              |
| 4:1:171:LEU:CB  | 4:Y:151:ILE:CD1[1_556] | 1.58                     | 0.62              |
| 4:0:175:ILE:CG2 | 4:X:162:ASN:OD1[1_556] | 1.58                     | 0.62              |
| 4:0:59:GLN:CG   | 4:X:208:ILE:CG1[1_556] | 1.58                     | 0.62              |
| 4:0:40:HIS:NE2  | 4:V:166:TYR:CG[1_556]  | 1.58                     | 0.62              |
| 4:2:195:GLU:OE1 | 4:Y:110:LEU:N[1_556]   | 1.58                     | 0.62              |
| 4:1:139:VAL:CG1 | 4:Y:330:ILE:O[1_556]   | 1.58                     | 0.62              |
| 4:0:161:HIS:C   | 4:X:274:ILE:CD1[1_556] | 1.58                     | 0.62              |
| 4:0:125:GLU:OE2 | 4:X:7:ALA:O[1_556]     | 1.58                     | 0.62              |
| 4:1:105:LEU:O   | 4:Y:335:ARG:CA[1_556]  | 1.58                     | 0.62              |
| 4:2:335:ARG:CG  | 4:Z:219:VAL:C[1_556]   | 1.58                     | 0.62              |
| 4:1:108:ALA:O   | 4:Y:154:ASP:CG[1_556]  | 1.58                     | 0.62              |
| 4:1:184:ASP:N   | 4:Y:188:TYR:CA[1_556]  | 1.58                     | 0.62              |
| 4:1:148:THR:CA  | 4:Y:328:LYS:N[1_556]   | 1.58                     | 0.62              |
| 4:0:208:ILE:O   | 4:X:198:TYR:CG[1_556]  | 1.58                     | 0.62              |
| 4:1:114:ALA:CA  | 4:Y:106:THR:CG2[1_556] | 1.58                     | 0.62              |
| 4:0:274:ILE:CB  | 4:X:263:GLN:CB[1_556]  | 1.58                     | 0.62              |
| 4:0:185:LEU:N   | 4:X:188:TYR:CA[1_556]  | 1.58                     | 0.62              |
| 4:1:77:THR:CB   | 4:Y:14:SER:C[1_556]    | 1.58                     | 0.62              |
| 4:2:300:SER:CB  | 4:Z:309:ILE:CA[1_556]  | 1.58                     | 0.62              |
| 4:2:162:ASN:ND2 | 4:Z:273:GLY:C[1_556]   | 1.58                     | 0.62              |
| 4:0:210:ARG:CB  | 4:X:193:LEU:CB[1_556]  | 1.58                     | 0.62              |
| 4:1:208:ILE:C   | 4:Y:198:TYR:CB[1_556]  | 1.58                     | 0.62              |
| 4:0:16:LEU:CA   | 4:X:214:GLU:CA[1_556]  | 1.58                     | 0.62              |
| 4:2:281:SER:CA  | 4:Z:280:ASN:OD1[1_556] | 1.58                     | 0.62              |
| 4:2:366:GLY:N   | 4:Z:348:SER:N[1_556]   | 1.58                     | 0.62              |
| 4:1:307:PRO:CA  | 4:Y:227:MET:CG[1_556]  | 1.58                     | 0.62              |
| 4:0:166:TYR:CE1 | 4:X:325:MET:CG[1_556]  | 1.58                     | 0.62              |
| 4:1:33:SER:CA   | 4:Y:210:ARG:NH1[1_556] | 1.58                     | 0.62              |
| 4:1:306:TYR:CD1 | 4:Y:256:ARG:CB[1_556]  | 1.58                     | 0.62              |
| 4:0:63:GLY:CA   | 4:V:288:ASP:N[1_556]   | 1.58                     | 0.62              |
| 4:2:208:ILE:CB  | 4:Z:198:TYR:CE1[1_556] | 1.58                     | 0.62              |
| 4:1:372:ARG:N   | 4:Y:143:TYR:CB[1_556]  | 1.58                     | 0.62              |
| 4:2:169:TYR:O   | 4:Z:151:ILE:CG2[1_556] | 1.58                     | 0.62              |
| 4:2:11:ASP:CG   | 4:Z:305:MET:CG[1_556]  | 1.58                     | 0.62              |
| 4:2:299:MET:SD  | 4:Z:312:ARG:NE[1_556]  | 1.58                     | 0.62              |
| 4:0:107:GLU:OE2 | 4:X:141:SER:OG[1_556]  | 1.58                     | 0.62              |
| 4:1:108:ALA:C   | 4:Y:154:ASP:CA[1_556]  | 1.58                     | 0.62              |
| 4:1:63:GLY:N    | 4:W:288:ASP:N[1_556]   | 1.58                     | 0.62              |
| 4:2:40:HIS:NE2  | 4:X:166:TYR:CG[1_556]  | 1.58                     | 0.62              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:171:LEU:CB  | 4:Z:151:ILE:CD1[1_556] | 1.58                     | 0.62              |
| 4:1:108:ALA:C   | 4:Y:155:SER:N[1_556]   | 1.58                     | 0.62              |
| 4:0:120:THR:CA  | 4:X:340:TRP:CE3[1_556] | 1.58                     | 0.62              |
| 4:2:59:GLN:CG   | 4:Z:208:ILE:CG1[1_556] | 1.58                     | 0.62              |
| 4:2:120:THR:CA  | 4:Z:340:TRP:CE3[1_556] | 1.58                     | 0.62              |
| 4:1:364:GLU:C   | 4:Y:348:SER:O[1_556]   | 1.58                     | 0.62              |
| 4:0:280:ASN:C   | 4:X:280:ASN:OD1[1_556] | 1.58                     | 0.62              |
| 4:1:40:HIS:ND1  | 4:W:166:TYR:CD2[1_556] | 1.58                     | 0.62              |
| 4:2:208:ILE:CG1 | 4:Z:198:TYR:CD1[1_556] | 1.58                     | 0.62              |
| 4:0:169:TYR:O   | 4:X:151:ILE:CG2[1_556] | 1.58                     | 0.62              |
| 4:1:185:LEU:N   | 4:Y:188:TYR:CA[1_556]  | 1.58                     | 0.62              |
| 4:2:175:ILE:CG2 | 4:Z:162:ASN:OD1[1_556] | 1.58                     | 0.62              |
| 4:0:186:THR:CA  | 4:X:191:LYS:N[1_556]   | 1.58                     | 0.62              |
| 4:0:299:MET:SD  | 4:X:312:ARG:NH1[1_556] | 1.58                     | 0.62              |
| 4:2:125:GLU:OE2 | 4:Z:7:ALA:O[1_556]     | 1.58                     | 0.62              |
| 4:2:181:ALA:CB  | 4:Z:185:LEU:CD1[1_556] | 1.58                     | 0.62              |
| 4:2:142:LEU:CA  | 4:Z:310:ALA:O[1_556]   | 1.58                     | 0.62              |
| 4:0:367:PRO:O   | 4:X:343:GLY:CA[1_556]  | 1.58                     | 0.62              |
| 4:1:110:LEU:CG  | 4:Y:161:HIS:C[1_556]   | 1.58                     | 0.62              |
| 4:0:208:ILE:CG1 | 4:X:198:TYR:CD1[1_556] | 1.58                     | 0.62              |
| 4:1:192:ILE:O   | 4:X:110:LEU:O[1_556]   | 1.58                     | 0.62              |
| 4:2:274:ILE:CB  | 4:Z:263:GLN:CB[1_556]  | 1.58                     | 0.62              |
| 4:0:159:VAL:CB  | 4:X:181:ALA:CA[1_556]  | 1.58                     | 0.62              |
| 4:1:335:ARG:NE  | 4:Y:220:ALA:CB[1_556]  | 1.58                     | 0.62              |
| 4:1:281:SER:N   | 4:Y:280:ASN:OD1[1_556] | 1.58                     | 0.62              |
| 4:1:271:SER:O   | 4:Y:270:GLU:N[1_556]   | 1.58                     | 0.62              |
| 4:1:63:GLY:N    | 4:W:288:ASP:C[1_556]   | 1.58                     | 0.62              |
| 4:1:362:TYR:CE2 | 4:Y:23:GLY:N[1_556]    | 1.58                     | 0.62              |
| 4:1:166:TYR:O   | 4:Y:294:TYR:C[1_556]   | 1.59                     | 0.61              |
| 4:0:212:ILE:CG1 | 4:X:196:ARG:C[1_556]   | 1.59                     | 0.61              |
| 4:1:125:GLU:C   | 4:Y:24:ASP:OD2[1_556]  | 1.59                     | 0.61              |
| 4:3:233:SER:N   | 4:Z:366:GLY:O[1_556]   | 1.59                     | 0.61              |
| 4:3:191:LYS:NZ  | 4:Z:110:LEU:CD2[1_556] | 1.59                     | 0.61              |
| 4:2:162:ASN:CB  | 4:Z:274:ILE:C[1_556]   | 1.59                     | 0.61              |
| 4:2:279:TYR:CA  | 4:Z:276:GLU:OE1[1_556] | 1.59                     | 0.61              |
| 4:2:186:THR:CG2 | 4:Z:190:MET:C[1_556]   | 1.59                     | 0.61              |
| 4:1:40:HIS:CA   | 4:W:167:GLU:CG[1_556]  | 1.59                     | 0.61              |
| 4:0:306:TYR:CG  | 4:X:256:ARG:CG[1_556]  | 1.59                     | 0.61              |
| 4:0:186:THR:CG2 | 4:X:190:MET:C[1_556]   | 1.59                     | 0.61              |
| 4:1:70:PRO:O    | 4:Y:16:LEU:N[1_556]    | 1.59                     | 0.61              |
| 4:1:369:ILE:O   | 4:Y:143:TYR:CD2[1_556] | 1.59                     | 0.61              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:267:ILE:CB  | 4:X:173:HIS:CB[1_556]  | 1.59                     | 0.61              |
| 4:0:296:ASN:O   | 4:X:316:GLU:N[1_556]   | 1.59                     | 0.61              |
| 4:1:78:ASN:O    | 4:Y:31:PHE:C[1_556]    | 1.59                     | 0.61              |
| 4:1:170:ALA:C   | 4:Y:151:ILE:CG2[1_556] | 1.59                     | 0.61              |
| 4:0:120:THR:CG2 | 4:X:344:SER:CB[1_556]  | 1.59                     | 0.61              |
| 4:0:253:GLU:OE2 | 4:W:114:ALA:N[1_556]   | 1.59                     | 0.61              |
| 4:3:228:ALA:O   | 4:Z:369:ILE:CA[1_556]  | 1.59                     | 0.61              |
| 4:1:214:GLU:OE1 | 4:Y:250:ILE:CG2[1_556] | 1.59                     | 0.61              |
| 4:2:140:LEU:CD2 | 4:Z:331:ALA:CA[1_556]  | 1.59                     | 0.61              |
| 4:0:266:PHE:CA  | 4:W:172:PRO:CG[1_556]  | 1.59                     | 0.61              |
| 4:1:215:LYS:CB  | 4:Y:196:ARG:NH1[1_556] | 1.59                     | 0.61              |
| 4:0:86:TRP:CZ2  | 4:X:337:TYR:CZ[1_556]  | 1.59                     | 0.61              |
| 4:0:183:ARG:N   | 4:X:189:LEU:N[1_556]   | 1.59                     | 0.61              |
| 4:2:166:TYR:CE1 | 4:Z:325:MET:CG[1_556]  | 1.59                     | 0.61              |
| 4:0:11:ASP:CG   | 4:X:305:MET:CG[1_556]  | 1.59                     | 0.61              |
| 4:0:212:ILE:N   | 4:X:196:ARG:CG[1_556]  | 1.59                     | 0.61              |
| 4:0:139:VAL:CG1 | 4:X:297:ASN:O[1_556]   | 1.59                     | 0.61              |
| 4:1:303:THR:C   | 4:Y:255:PHE:O[1_556]   | 1.59                     | 0.61              |
| 4:2:212:ILE:CG1 | 4:Z:196:ARG:C[1_556]   | 1.59                     | 0.61              |
| 4:2:228:ALA:O   | 4:Y:369:ILE:CA[1_556]  | 1.59                     | 0.61              |
| 4:2:296:ASN:O   | 4:Z:316:GLU:N[1_556]   | 1.59                     | 0.61              |
| 4:1:71:ILE:C    | 4:Y:157:ASP:CG[1_556]  | 1.59                     | 0.61              |
| 4:0:337:TYR:CE2 | 4:X:218:TYR:OH[1_556]  | 1.59                     | 0.61              |
| 4:2:367:PRO:O   | 4:Z:343:GLY:CA[1_556]  | 1.59                     | 0.61              |
| 4:0:337:TYR:CA  | 4:X:307:PRO:CA[1_556]  | 1.59                     | 0.61              |
| 4:1:174:ALA:N   | 4:Y:281:SER:CB[1_556]  | 1.59                     | 0.61              |
| 4:0:62:ARG:O    | 4:V:288:ASP:CG[1_556]  | 1.59                     | 0.61              |
| 4:1:197:GLY:N   | 4:X:75:ILE:CA[1_556]   | 1.59                     | 0.61              |
| 4:0:119:MET:CA  | 4:X:340:TRP:CB[1_556]  | 1.59                     | 0.61              |
| 4:1:366:GLY:C   | 4:Y:347:ALA:CB[1_556]  | 1.59                     | 0.61              |
| 4:2:39:ARG:CA   | 4:X:166:TYR:OH[1_556]  | 1.59                     | 0.61              |
| 4:1:107:GLU:OE1 | 4:Y:141:SER:OG[1_556]  | 1.59                     | 0.61              |
| 4:1:362:TYR:O   | 4:Y:348:SER:C[1_556]   | 1.59                     | 0.61              |
| 4:2:86:TRP:CZ2  | 4:Z:337:TYR:CZ[1_556]  | 1.59                     | 0.61              |
| 4:1:165:ILE:CG1 | 4:Y:297:ASN:OD1[1_556] | 1.59                     | 0.61              |
| 4:0:64:ILE:N    | 4:V:289:ILE:N[1_556]   | 1.59                     | 0.61              |
| 4:2:33:SER:CA   | 4:Z:210:ARG:NH2[1_556] | 1.59                     | 0.61              |
| 4:1:253:GLU:OE1 | 4:X:112:PRO:CA[1_556]  | 1.59                     | 0.61              |
| 4:1:86:TRP:CE2  | 4:Y:337:TYR:CE1[1_556] | 1.59                     | 0.61              |
| 4:2:337:TYR:N   | 4:Z:307:PRO:CB[1_556]  | 1.59                     | 0.61              |
| 4:0:369:ILE:CB  | 4:X:346:LEU:N[1_556]   | 1.59                     | 0.61              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:214:GLU:CA  | 4:Z:253:GLU:CG[1_556]  | 1.59                     | 0.61              |
| 4:2:278:THR:CG2 | 4:Z:275:HIS:NE2[1_556] | 1.59                     | 0.61              |
| 4:1:309:ILE:CG2 | 4:Y:223:PHE:CB[1_556]  | 1.59                     | 0.61              |
| 4:2:337:TYR:CA  | 4:Z:307:PRO:CA[1_556]  | 1.59                     | 0.61              |
| 4:2:78:ASN:O    | 4:Z:31:PHE:C[1_556]    | 1.59                     | 0.61              |
| 4:1:116:ARG:NH2 | 4:Y:141:SER:C[1_556]   | 1.59                     | 0.61              |
| 4:1:181:ALA:CB  | 4:Y:185:LEU:CD1[1_556] | 1.59                     | 0.61              |
| 4:4:40:HIS:NE2  | 4:Z:166:TYR:CG[1_556]  | 1.59                     | 0.61              |
| 4:0:134:VAL:CB  | 4:X:338:SER:CB[1_556]  | 1.59                     | 0.61              |
| 4:0:39:ARG:CA   | 4:V:166:TYR:OH[1_556]  | 1.59                     | 0.61              |
| 4:2:286:ASP:CB  | 4:Z:290:ARG:CD[1_556]  | 1.59                     | 0.61              |
| 4:0:117:GLU:OE2 | 4:X:135:ALA:CB[1_556]  | 1.59                     | 0.61              |
| 4:2:164:PRO:CG  | 4:Z:278:THR:N[1_556]   | 1.59                     | 0.61              |
| 4:3:266:PHE:CA  | 4:Z:172:PRO:CG[1_556]  | 1.59                     | 0.61              |
| 4:2:106:THR:CB  | 4:Z:335:ARG:CB[1_556]  | 1.59                     | 0.61              |
| 4:0:306:TYR:N   | 4:X:255:PHE:CE1[1_556] | 1.59                     | 0.61              |
| 4:0:286:ASP:OD2 | 4:X:290:ARG:NE[1_556]  | 1.59                     | 0.61              |
| 4:0:33:SER:CA   | 4:X:210:ARG:NH2[1_556] | 1.59                     | 0.61              |
| 4:1:155:SER:OG  | 4:Y:261:LEU:N[1_556]   | 1.59                     | 0.61              |
| 4:1:371:HIS:ND1 | 4:Y:140:LEU:N[1_556]   | 1.59                     | 0.61              |
| 4:0:195:GLU:OE1 | 4:W:110:LEU:N[1_556]   | 1.59                     | 0.61              |
| 4:0:335:ARG:CG  | 4:X:219:VAL:C[1_556]   | 1.59                     | 0.61              |
| 4:0:186:THR:O   | 4:X:191:LYS:O[1_556]   | 1.59                     | 0.61              |
| 4:2:63:GLY:CA   | 4:X:288:ASP:N[1_556]   | 1.59                     | 0.61              |
| 4:1:136:ILE:N   | 4:Y:299:MET:C[1_556]   | 1.59                     | 0.61              |
| 4:2:364:GLU:O   | 4:Z:349:LEU:C[1_556]   | 1.59                     | 0.61              |
| 4:2:165:ILE:CD1 | 4:Z:297:ASN:ND2[1_556] | 1.59                     | 0.61              |
| 4:0:162:ASN:ND2 | 4:X:273:GLY:C[1_556]   | 1.59                     | 0.61              |
| 4:2:174:ALA:O   | 4:Z:277:THR:C[1_556]   | 1.60                     | 0.60              |
| 4:1:62:ARG:C    | 4:W:288:ASP:CB[1_556]  | 1.60                     | 0.60              |
| 4:2:337:TYR:CB  | 4:Z:307:PRO:CG[1_556]  | 1.60                     | 0.60              |
| 4:1:289:ILE:CB  | 4:Y:294:TYR:OH[1_556]  | 1.60                     | 0.60              |
| 4:2:151:ILE:N   | 4:Z:317:ILE:CG2[1_556] | 1.60                     | 0.60              |
| 4:1:77:THR:OG1  | 4:Y:14:SER:CA[1_556]   | 1.60                     | 0.60              |
| 4:2:157:ASP:CG  | 4:Z:213:LYS:CD[1_556]  | 1.60                     | 0.60              |
| 4:2:116:ARG:NH2 | 4:Z:141:SER:C[1_556]   | 1.60                     | 0.60              |
| 4:0:174:ALA:O   | 4:X:277:THR:C[1_556]   | 1.60                     | 0.60              |
| 4:3:192:ILE:O   | 4:Z:110:LEU:O[1_556]   | 1.60                     | 0.60              |
| 4:2:253:GLU:OE1 | 4:Y:112:PRO:CA[1_556]  | 1.60                     | 0.60              |
| 4:0:154:ASP:C   | 4:X:261:LEU:CB[1_556]  | 1.60                     | 0.60              |
| 4:2:148:THR:CG2 | 4:Z:328:LYS:CG[1_556]  | 1.60                     | 0.60              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:181:ALA:CB  | 4:X:185:LEU:CD1[1_556] | 1.60                     | 0.60              |
| 4:2:210:ARG:CB  | 4:Z:193:LEU:CB[1_556]  | 1.60                     | 0.60              |
| 4:1:131:ALA:CA  | 4:Y:25:ASP:OD1[1_556]  | 1.60                     | 0.60              |
| 4:0:164:PRO:CG  | 4:X:278:THR:N[1_556]   | 1.60                     | 0.60              |
| 4:4:63:GLY:C    | 4:Z:289:ILE:CA[1_556]  | 1.60                     | 0.60              |
| 4:1:280:ASN:C   | 4:Y:280:ASN:OD1[1_556] | 1.60                     | 0.60              |
| 4:1:168:GLY:CA  | 4:Y:296:ASN:N[1_556]   | 1.60                     | 0.60              |
| 4:0:78:ASN:O    | 4:X:31:PHE:C[1_556]    | 1.60                     | 0.60              |
| 4:1:172:PRO:CB  | 4:Y:164:PRO:N[1_556]   | 1.60                     | 0.60              |
| 4:0:106:THR:CA  | 4:X:335:ARG:CB[1_556]  | 1.60                     | 0.60              |
| 4:0:171:LEU:CB  | 4:X:151:ILE:CD1[1_556] | 1.60                     | 0.60              |
| 4:2:67:LEU:CB   | 4:Z:207:GLU:OE2[1_556] | 1.60                     | 0.60              |
| 4:2:16:LEU:CA   | 4:Z:214:GLU:CA[1_556]  | 1.60                     | 0.60              |
| 4:3:40:HIS:ND1  | 4:Y:166:TYR:CD2[1_556] | 1.60                     | 0.60              |
| 4:2:369:ILE:CB  | 4:Z:346:LEU:N[1_556]   | 1.60                     | 0.60              |
| 4:1:281:SER:C   | 4:Y:280:ASN:CG[1_556]  | 1.60                     | 0.60              |
| 4:2:119:MET:CA  | 4:Z:340:TRP:CB[1_556]  | 1.60                     | 0.60              |
| 4:2:286:ASP:OD2 | 4:Z:290:ARG:NE[1_556]  | 1.60                     | 0.60              |
| 4:2:139:VAL:CG1 | 4:Z:297:ASN:O[1_556]   | 1.60                     | 0.60              |
| 4:2:62:ARG:O    | 4:X:288:ASP:CG[1_556]  | 1.60                     | 0.60              |
| 4:0:300:SER:CB  | 4:X:309:ILE:CA[1_556]  | 1.60                     | 0.60              |
| 4:1:213:LYS:C   | 4:Y:253:GLU:CD[1_556]  | 1.60                     | 0.60              |
| 4:2:362:TYR:O   | 4:Z:348:SER:C[1_556]   | 1.60                     | 0.60              |
| 4:0:77:THR:CB   | 4:X:14:SER:C[1_556]    | 1.60                     | 0.60              |
| 4:2:369:ILE:CG2 | 4:Z:345:ILE:O[1_556]   | 1.60                     | 0.60              |
| 4:0:214:GLU:CA  | 4:X:253:GLU:CG[1_556]  | 1.60                     | 0.60              |
| 4:1:163:VAL:C   | 4:Y:278:THR:CB[1_556]  | 1.60                     | 0.60              |
| 4:0:162:ASN:CB  | 4:X:274:ILE:C[1_556]   | 1.60                     | 0.60              |
| 4:4:39:ARG:CA   | 4:Z:166:TYR:OH[1_556]  | 1.60                     | 0.60              |
| 4:1:205:GLU:O   | 4:Y:198:TYR:C[1_556]   | 1.60                     | 0.60              |
| 4:1:113:LYS:CB  | 4:Y:136:ILE:N[1_556]   | 1.60                     | 0.60              |
| 4:0:299:MET:SD  | 4:X:312:ARG:NE[1_556]  | 1.60                     | 0.60              |
| 4:2:264:PRO:CB  | 4:Z:269:MET:N[1_556]   | 1.60                     | 0.60              |
| 4:0:185:LEU:CD2 | 4:X:188:TYR:OH[1_556]  | 1.60                     | 0.60              |
| 4:1:332:PRO:N   | 4:Y:221:LEU:CA[1_556]  | 1.60                     | 0.60              |
| 4:1:154:ASP:OD1 | 4:Y:309:ILE:CD1[1_556] | 1.60                     | 0.60              |
| 4:1:37:ARG:CZ   | 4:Y:56:ASP:CB[1_556]   | 1.60                     | 0.60              |
| 4:3:197:GLY:N   | 4:Z:75:ILE:CA[1_556]   | 1.60                     | 0.60              |
| 4:0:149:THR:CA  | 4:X:327:ILE:CG1[1_556] | 1.60                     | 0.60              |
| 4:1:233:SER:N   | 4:X:366:GLY:O[1_556]   | 1.60                     | 0.60              |
| 4:2:306:TYR:CD1 | 4:Z:256:ARG:CB[1_556]  | 1.60                     | 0.60              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:62:ARG:O    | 4:Z:288:ASP:CG[1_556]  | 1.60                     | 0.60              |
| 4:1:66:THR:OG1  | 4:Y:60:SER:O[1_556]    | 1.60                     | 0.60              |
| 4:2:291:LYS:NZ  | 4:Z:322:PRO:O[1_556]   | 1.60                     | 0.60              |
| 4:4:63:GLY:CA   | 4:Z:288:ASP:N[1_556]   | 1.60                     | 0.60              |
| 4:0:106:THR:CB  | 4:X:335:ARG:CB[1_556]  | 1.60                     | 0.60              |
| 4:0:362:TYR:O   | 4:X:348:SER:C[1_556]   | 1.60                     | 0.60              |
| 4:0:337:TYR:CB  | 4:X:307:PRO:CG[1_556]  | 1.60                     | 0.60              |
| 4:0:105:LEU:CD1 | 4:X:337:TYR:CB[1_556]  | 1.60                     | 0.60              |
| 4:2:306:TYR:N   | 4:Z:255:PHE:CE1[1_556] | 1.60                     | 0.60              |
| 4:4:63:GLY:N    | 4:Z:288:ASP:C[1_556]   | 1.60                     | 0.60              |
| 4:1:228:ALA:O   | 4:X:369:ILE:CA[1_556]  | 1.60                     | 0.60              |
| 4:0:196:ARG:NH2 | 4:W:115:ASN:N[1_556]   | 1.60                     | 0.60              |
| 4:2:261:LEU:CB  | 4:Z:266:PHE:CB[1_556]  | 1.60                     | 0.60              |
| 4:0:77:THR:CG2  | 4:X:14:SER:O[1_556]    | 1.60                     | 0.60              |
| 4:1:32:PRO:CD   | 4:Y:211:ASP:CB[1_556]  | 1.60                     | 0.60              |
| 4:2:12:ASN:CG   | 4:Z:336:LYS:CD[1_556]  | 1.60                     | 0.60              |
| 4:1:296:ASN:OD1 | 4:Y:318:THR:CB[1_556]  | 1.60                     | 0.60              |
| 4:2:82:MET:N    | 4:Z:30:VAL:C[1_556]    | 1.60                     | 0.60              |
| 4:0:165:ILE:CD1 | 4:X:297:ASN:ND2[1_556] | 1.60                     | 0.60              |
| 4:2:73:HIS:C    | 4:Z:156:GLY:O[1_556]   | 1.60                     | 0.60              |
| 4:1:270:GLU:OE1 | 4:X:286:ASP:CA[1_556]  | 1.60                     | 0.60              |
| 4:1:67:LEU:C    | 4:Y:62:ARG:NH1[1_556]  | 1.60                     | 0.60              |
| 4:2:37:ARG:NH1  | 4:Z:56:ASP:C[1_556]    | 1.60                     | 0.60              |
| 4:2:209:VAL:N   | 4:Z:198:TYR:CG[1_556]  | 1.60                     | 0.60              |
| 4:2:183:ARG:N   | 4:Z:189:LEU:N[1_556]   | 1.60                     | 0.60              |
| 4:2:63:GLY:C    | 4:X:289:ILE:CA[1_556]  | 1.60                     | 0.60              |
| 4:3:63:GLY:N    | 4:Y:288:ASP:C[1_556]   | 1.60                     | 0.60              |
| 4:0:213:LYS:CG  | 4:X:192:ILE:CB[1_556]  | 1.60                     | 0.60              |
| 4:2:213:LYS:CG  | 4:Z:192:ILE:CB[1_556]  | 1.60                     | 0.60              |
| 4:1:121:GLN:CB  | 4:Y:9:VAL:CB[1_556]    | 1.60                     | 0.60              |
| 4:0:279:TYR:CA  | 4:X:276:GLU:OE1[1_556] | 1.60                     | 0.60              |
| 4:0:227:MET:CA  | 4:W:372:ARG:C[1_556]   | 1.60                     | 0.60              |
| 4:0:37:ARG:NH1  | 4:X:56:ASP:C[1_556]    | 1.60                     | 0.60              |
| 4:1:166:TYR:O   | 4:Y:295:ALA:N[1_556]   | 1.60                     | 0.60              |
| 4:1:123:MET:C   | 4:Y:26:ALA:O[1_556]    | 1.60                     | 0.60              |
| 4:0:157:ASP:CG  | 4:X:213:LYS:CD[1_556]  | 1.60                     | 0.60              |
| 4:0:209:VAL:N   | 4:X:198:TYR:CG[1_556]  | 1.60                     | 0.60              |
| 4:0:72:GLU:N    | 4:X:157:ASP:CB[1_556]  | 1.61                     | 0.59              |
| 4:2:227:MET:CA  | 4:Y:372:ARG:C[1_556]   | 1.61                     | 0.59              |
| 4:2:161:HIS:CA  | 4:Z:274:ILE:CG1[1_556] | 1.61                     | 0.59              |
| 4:2:267:ILE:CA  | 4:Y:173:HIS:C[1_556]   | 1.61                     | 0.59              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:305:MET:O   | 4:Y:255:PHE:CE2[1_556] | 1.61                     | 0.59              |
| 4:3:40:HIS:CA   | 4:Y:167:GLU:CG[1_556]  | 1.61                     | 0.59              |
| 4:0:295:ALA:N   | 4:X:319:ALA:O[1_556]   | 1.61                     | 0.59              |
| 4:0:151:ILE:N   | 4:X:317:ILE:CG2[1_556] | 1.61                     | 0.59              |
| 4:2:163:VAL:CG2 | 4:Z:153:LEU:CG[1_556]  | 1.61                     | 0.59              |
| 4:3:234:SER:N   | 4:Z:367:PRO:N[1_556]   | 1.61                     | 0.59              |
| 4:2:105:LEU:CD1 | 4:Z:337:TYR:CB[1_556]  | 1.61                     | 0.59              |
| 4:2:154:ASP:C   | 4:Z:261:LEU:CB[1_556]  | 1.61                     | 0.59              |
| 4:1:166:TYR:O   | 4:Y:294:TYR:N[1_556]   | 1.61                     | 0.59              |
| 4:0:64:ILE:CD1  | 4:V:291:LYS:NZ[1_556]  | 1.61                     | 0.59              |
| 4:2:266:PHE:CA  | 4:Y:172:PRO:CG[1_556]  | 1.61                     | 0.59              |
| 4:0:278:THR:C   | 4:X:276:GLU:OE2[1_556] | 1.61                     | 0.59              |
| 4:2:253:GLU:OE2 | 4:Y:114:ALA:N[1_556]   | 1.61                     | 0.59              |
| 4:2:118:LYS:C   | 4:Z:340:TRP:NE1[1_556] | 1.61                     | 0.59              |
| 4:1:107:GLU:OE2 | 4:Y:141:SER:OG[1_556]  | 1.61                     | 0.59              |
| 4:0:12:ASN:CG   | 4:X:336:LYS:CD[1_556]  | 1.61                     | 0.59              |
| 4:2:186:THR:O   | 4:Z:191:LYS:O[1_556]   | 1.61                     | 0.59              |
| 4:0:338:SER:CB  | 4:X:309:ILE:N[1_556]   | 1.61                     | 0.59              |
| 4:3:62:ARG:C    | 4:Y:288:ASP:CB[1_556]  | 1.61                     | 0.59              |
| 4:0:267:ILE:CA  | 4:W:173:HIS:C[1_556]   | 1.61                     | 0.59              |
| 4:1:16:LEU:C    | 4:Y:214:GLU:CG[1_556]  | 1.61                     | 0.59              |
| 4:1:123:MET:CB  | 4:Y:26:ALA:N[1_556]    | 1.61                     | 0.59              |
| 4:2:212:ILE:N   | 4:Z:196:ARG:CG[1_556]  | 1.61                     | 0.59              |
| 4:2:294:TYR:CB  | 4:Z:319:ALA:O[1_556]   | 1.61                     | 0.59              |
| 4:1:120:THR:CG2 | 4:Y:344:SER:CB[1_556]  | 1.61                     | 0.59              |
| 4:1:212:ILE:N   | 4:Y:196:ARG:CG[1_556]  | 1.61                     | 0.59              |
| 4:2:299:MET:CB  | 4:Z:312:ARG:CG[1_556]  | 1.61                     | 0.59              |
| 4:2:196:ARG:NH2 | 4:Y:115:ASN:N[1_556]   | 1.61                     | 0.59              |
| 4:1:125:GLU:O   | 4:Y:28:ARG:NH2[1_556]  | 1.61                     | 0.59              |
| 4:2:133:TYR:OH  | 4:Z:145:SER:CA[1_556]  | 1.61                     | 0.59              |
| 4:2:337:TYR:CE2 | 4:Z:218:TYR:OH[1_556]  | 1.61                     | 0.59              |
| 4:0:337:TYR:N   | 4:X:307:PRO:CB[1_556]  | 1.61                     | 0.59              |
| 4:1:116:ARG:NH2 | 4:Y:141:SER:CB[1_556]  | 1.61                     | 0.59              |
| 4:1:169:TYR:CE1 | 4:Y:150:GLY:C[1_556]   | 1.61                     | 0.59              |
| 4:0:291:LYS:NZ  | 4:X:322:PRO:O[1_556]   | 1.61                     | 0.59              |
| 4:0:286:ASP:CB  | 4:X:290:ARG:CD[1_556]  | 1.61                     | 0.59              |
| 4:0:372:ARG:NE  | 4:X:142:LEU:C[1_556]   | 1.61                     | 0.59              |
| 4:0:67:LEU:CB   | 4:X:207:GLU:OE2[1_556] | 1.61                     | 0.59              |
| 4:2:117:GLU:OE2 | 4:Z:135:ALA:CB[1_556]  | 1.61                     | 0.59              |
| 4:0:161:HIS:CA  | 4:X:274:ILE:CG1[1_556] | 1.61                     | 0.59              |
| 4:3:64:ILE:CD1  | 4:Y:291:LYS:NZ[1_556]  | 1.61                     | 0.59              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:116:ARG:NH2 | 4:X:141:SER:C[1_556]   | 1.61                     | 0.59              |
| 4:2:106:THR:CA  | 4:Z:335:ARG:CB[1_556]  | 1.61                     | 0.59              |
| 4:1:369:ILE:CG2 | 4:Y:345:ILE:O[1_556]   | 1.61                     | 0.59              |
| 4:2:309:ILE:CB  | 4:Z:259:GLU:CD[1_556]  | 1.61                     | 0.59              |
| 4:1:108:ALA:O   | 4:Y:154:ASP:CA[1_556]  | 1.61                     | 0.59              |
| 4:1:364:GLU:O   | 4:Y:349:LEU:C[1_556]   | 1.61                     | 0.59              |
| 4:2:64:ILE:N    | 4:X:289:ILE:N[1_556]   | 1.61                     | 0.59              |
| 4:0:73:HIS:C    | 4:X:156:GLY:O[1_556]   | 1.61                     | 0.59              |
| 4:0:278:THR:CG2 | 4:X:275:HIS:NE2[1_556] | 1.61                     | 0.59              |
| 4:2:339:VAL:CG1 | 4:Z:335:ARG:CZ[1_556]  | 1.61                     | 0.59              |
| 4:2:72:GLU:N    | 4:Z:157:ASP:CB[1_556]  | 1.61                     | 0.59              |
| 4:1:68:LYS:CB   | 4:Y:59:GLN:CD[1_556]   | 1.61                     | 0.59              |
| 4:1:163:VAL:CG2 | 4:Y:153:LEU:CG[1_556]  | 1.61                     | 0.59              |
| 4:1:266:PHE:CA  | 4:X:172:PRO:CG[1_556]  | 1.61                     | 0.59              |
| 4:0:174:ALA:O   | 4:X:277:THR:CA[1_556]  | 1.61                     | 0.59              |
| 4:2:338:SER:CB  | 4:Z:309:ILE:N[1_556]   | 1.61                     | 0.59              |
| 4:2:134:VAL:CB  | 4:Z:338:SER:CB[1_556]  | 1.61                     | 0.59              |
| 4:0:62:ARG:CB   | 4:X:204:ALA:CB[1_556]  | 1.61                     | 0.59              |
| 4:1:77:THR:CG2  | 4:Y:14:SER:O[1_556]    | 1.61                     | 0.59              |
| 4:2:209:VAL:O   | 4:Z:193:LEU:C[1_556]   | 1.61                     | 0.59              |
| 4:0:63:GLY:C    | 4:V:289:ILE:CA[1_556]  | 1.61                     | 0.59              |
| 4:2:119:MET:N   | 4:Z:340:TRP:CG[1_556]  | 1.61                     | 0.59              |
| 4:2:77:THR:CB   | 4:Z:14:SER:C[1_556]    | 1.61                     | 0.59              |
| 4:2:295:ALA:N   | 4:Z:319:ALA:O[1_556]   | 1.61                     | 0.59              |
| 4:3:253:GLU:OE1 | 4:Z:112:PRO:CA[1_556]  | 1.61                     | 0.59              |
| 4:1:63:GLY:C    | 4:W:289:ILE:CA[1_556]  | 1.61                     | 0.59              |
| 4:2:281:SER:N   | 4:Z:280:ASN:OD1[1_556] | 1.61                     | 0.59              |
| 4:0:59:GLN:CD   | 4:X:208:ILE:N[1_556]   | 1.61                     | 0.59              |
| 4:1:195:GLU:OE1 | 4:X:109:PRO:C[1_556]   | 1.62                     | 0.58              |
| 4:1:336:LYS:CD  | 4:Y:218:TYR:CD1[1_556] | 1.62                     | 0.58              |
| 4:2:291:LYS:CD  | 4:Z:322:PRO:CA[1_556]  | 1.62                     | 0.58              |
| 4:1:362:TYR:CA  | 4:Y:348:SER:CB[1_556]  | 1.62                     | 0.58              |
| 4:3:40:HIS:N    | 4:Y:166:TYR:CZ[1_556]  | 1.62                     | 0.58              |
| 4:1:149:THR:CA  | 4:Y:327:ILE:CG1[1_556] | 1.62                     | 0.58              |
| 4:0:261:LEU:CB  | 4:X:266:PHE:CB[1_556]  | 1.62                     | 0.58              |
| 4:1:234:SER:N   | 4:X:367:PRO:N[1_556]   | 1.62                     | 0.58              |
| 4:0:72:GLU:OE1  | 4:X:183:ARG:NE[1_556]  | 1.62                     | 0.58              |
| 4:0:86:TRP:CE2  | 4:X:337:TYR:CE1[1_556] | 1.62                     | 0.58              |
| 4:1:300:SER:CB  | 4:Y:309:ILE:CA[1_556]  | 1.62                     | 0.58              |
| 4:2:286:ASP:O   | 4:Z:283:MET:CG[1_556]  | 1.62                     | 0.58              |
| 4:0:294:TYR:N   | 4:X:319:ALA:C[1_556]   | 1.62                     | 0.58              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:148:THR:CG2 | 4:X:328:LYS:CG[1_556]  | 1.62                     | 0.58              |
| 4:2:294:TYR:CA  | 4:Z:319:ALA:C[1_556]   | 1.62                     | 0.58              |
| 4:1:122:ILE:CD1 | 4:Y:19:ALA:CA[1_556]   | 1.62                     | 0.58              |
| 4:2:59:GLN:CD   | 4:Z:208:ILE:N[1_556]   | 1.62                     | 0.58              |
| 4:1:127:PHE:CD2 | 4:Y:27:PRO:O[1_556]    | 1.62                     | 0.58              |
| 4:1:159:VAL:N   | 4:Y:181:ALA:C[1_556]   | 1.62                     | 0.58              |
| 4:0:108:ALA:C   | 4:X:154:ASP:CA[1_556]  | 1.62                     | 0.58              |
| 4:1:186:THR:CB  | 4:Y:189:LEU:O[1_556]   | 1.62                     | 0.58              |
| 4:0:264:PRO:CB  | 4:X:269:MET:N[1_556]   | 1.62                     | 0.58              |
| 4:0:155:SER:OG  | 4:X:261:LEU:N[1_556]   | 1.62                     | 0.58              |
| 4:1:62:ARG:CZ   | 4:Y:205:GLU:N[1_556]   | 1.62                     | 0.58              |
| 4:1:159:VAL:CG1 | 4:Y:180:LEU:O[1_556]   | 1.62                     | 0.58              |
| 4:0:335:ARG:CA  | 4:X:219:VAL:O[1_556]   | 1.62                     | 0.58              |
| 4:2:69:TYR:CD2  | 4:Z:210:ARG:CD[1_556]  | 1.62                     | 0.58              |
| 4:0:286:ASP:O   | 4:X:283:MET:CG[1_556]  | 1.62                     | 0.58              |
| 4:2:197:GLY:N   | 4:Y:75:ILE:CA[1_556]   | 1.62                     | 0.58              |
| 4:1:140:LEU:O   | 4:Y:310:ALA:CB[1_556]  | 1.62                     | 0.58              |
| 4:1:166:TYR:CG  | 4:Y:294:TYR:CD2[1_556] | 1.62                     | 0.58              |
| 4:0:108:ALA:C   | 4:X:155:SER:N[1_556]   | 1.62                     | 0.58              |
| 4:0:253:GLU:OE1 | 4:W:112:PRO:CA[1_556]  | 1.62                     | 0.58              |
| 4:2:155:SER:OG  | 4:Z:261:LEU:N[1_556]   | 1.62                     | 0.58              |
| 4:1:83:GLU:N    | 4:Y:30:VAL:C[1_556]    | 1.62                     | 0.58              |
| 4:1:178:LEU:O   | 4:Y:180:LEU:CD1[1_556] | 1.62                     | 0.58              |
| 4:0:294:TYR:CB  | 4:X:319:ALA:O[1_556]   | 1.62                     | 0.58              |
| 4:2:149:THR:CA  | 4:Z:327:ILE:CG1[1_556] | 1.62                     | 0.58              |
| 4:2:185:LEU:CD2 | 4:Z:188:TYR:OH[1_556]  | 1.62                     | 0.58              |
| 4:0:165:ILE:CG1 | 4:X:297:ASN:OD1[1_556] | 1.62                     | 0.58              |
| 4:2:119:MET:CA  | 4:Z:340:TRP:CD1[1_556] | 1.62                     | 0.58              |
| 4:0:369:ILE:CG2 | 4:X:345:ILE:O[1_556]   | 1.62                     | 0.58              |
| 4:2:161:HIS:CE1 | 4:Z:155:SER:OG[1_556]  | 1.62                     | 0.58              |
| 4:0:306:TYR:CD1 | 4:X:256:ARG:CB[1_556]  | 1.62                     | 0.58              |
| 4:2:109:PRO:C   | 4:Z:154:ASP:CB[1_556]  | 1.62                     | 0.58              |
| 4:1:113:LYS:CE  | 4:Y:136:ILE:N[1_556]   | 1.62                     | 0.58              |
| 4:2:77:THR:CG2  | 4:Z:14:SER:O[1_556]    | 1.62                     | 0.58              |
| 4:1:120:THR:CA  | 4:Y:340:TRP:CE3[1_556] | 1.62                     | 0.58              |
| 4:3:63:GLY:C    | 4:Y:289:ILE:CA[1_556]  | 1.62                     | 0.58              |
| 4:1:104:LEU:CB  | 4:Y:334:GLU:OE2[1_556] | 1.62                     | 0.58              |
| 4:2:131:ALA:CA  | 4:Z:25:ASP:OD1[1_556]  | 1.62                     | 0.58              |
| 4:3:270:GLU:OE1 | 4:Z:286:ASP:CA[1_556]  | 1.62                     | 0.58              |
| 4:0:110:LEU:CB  | 4:X:161:HIS:CG[1_556]  | 1.62                     | 0.58              |
| 4:2:63:GLY:N    | 4:X:288:ASP:C[1_556]   | 1.62                     | 0.58              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:270:GLU:OE1 | 4:W:286:ASP:CG[1_556]  | 1.62                     | 0.58              |
| 4:2:80:ASP:OD2  | 4:Z:93:GLU:OE2[1_556]  | 1.62                     | 0.58              |
| 4:1:106:THR:CB  | 4:Y:335:ARG:CB[1_556]  | 1.62                     | 0.58              |
| 4:0:370:VAL:CG1 | 4:X:342:GLY:N[1_556]   | 1.62                     | 0.58              |
| 4:2:336:LYS:O   | 4:Z:307:PRO:CD[1_556]  | 1.62                     | 0.58              |
| 4:2:278:THR:C   | 4:Z:276:GLU:OE2[1_556] | 1.62                     | 0.58              |
| 4:0:131:ALA:CA  | 4:X:25:ASP:OD1[1_556]  | 1.62                     | 0.58              |
| 4:0:141:SER:OG  | 4:X:309:ILE:CB[1_556]  | 1.62                     | 0.58              |
| 4:0:118:LYS:C   | 4:X:340:TRP:NE1[1_556] | 1.62                     | 0.58              |
| 4:1:125:GLU:N   | 4:Y:24:ASP:CG[1_556]   | 1.62                     | 0.58              |
| 4:0:11:ASP:OD2  | 4:X:305:MET:CA[1_556]  | 1.62                     | 0.58              |
| 4:1:68:LYS:NZ   | 4:Y:59:GLN:CB[1_556]   | 1.62                     | 0.58              |
| 4:2:108:ALA:C   | 4:Z:154:ASP:CA[1_556]  | 1.62                     | 0.58              |
| 4:3:253:GLU:OE2 | 4:Z:114:ALA:N[1_556]   | 1.62                     | 0.58              |
| 4:2:64:ILE:CD1  | 4:X:291:LYS:NZ[1_556]  | 1.62                     | 0.58              |
| 4:0:299:MET:CB  | 4:X:312:ARG:CG[1_556]  | 1.62                     | 0.58              |
| 4:1:268:GLY:C   | 4:X:284:LYS:O[1_556]   | 1.62                     | 0.58              |
| 4:2:165:ILE:CG1 | 4:Z:297:ASN:OD1[1_556] | 1.62                     | 0.58              |
| 4:4:40:HIS:CA   | 4:Z:167:GLU:CG[1_556]  | 1.62                     | 0.58              |
| 4:1:107:GLU:OE1 | 4:Y:339:VAL:CG2[1_556] | 1.62                     | 0.58              |
| 4:0:69:TYR:CD2  | 4:X:210:ARG:CD[1_556]  | 1.62                     | 0.58              |
| 4:4:64:ILE:N    | 4:Z:289:ILE:N[1_556]   | 1.62                     | 0.58              |
| 4:2:289:ILE:CB  | 4:Z:294:TYR:OH[1_556]  | 1.62                     | 0.58              |
| 4:0:15:GLY:N    | 4:X:213:LYS:CE[1_556]  | 1.62                     | 0.58              |
| 4:2:368:SER:CA  | 4:Z:346:LEU:CB[1_556]  | 1.62                     | 0.58              |
| 4:2:62:ARG:CB   | 4:Z:204:ALA:CB[1_556]  | 1.62                     | 0.58              |
| 4:1:261:LEU:O   | 4:Y:265:SER:CA[1_556]  | 1.62                     | 0.58              |
| 4:2:294:TYR:N   | 4:Z:319:ALA:C[1_556]   | 1.62                     | 0.58              |
| 4:2:372:ARG:NE  | 4:Z:142:LEU:C[1_556]   | 1.62                     | 0.58              |
| 4:2:172:PRO:CG  | 4:Z:164:PRO:CA[1_556]  | 1.63                     | 0.57              |
| 4:0:119:MET:N   | 4:X:340:TRP:CG[1_556]  | 1.63                     | 0.57              |
| 4:0:281:SER:N   | 4:X:280:ASN:OD1[1_556] | 1.63                     | 0.57              |
| 4:3:195:GLU:OE1 | 4:Z:109:PRO:C[1_556]   | 1.63                     | 0.57              |
| 4:0:82:MET:N    | 4:X:30:VAL:C[1_556]    | 1.63                     | 0.57              |
| 4:2:177:ARG:CD  | 4:Z:160:THR:N[1_556]   | 1.63                     | 0.57              |
| 4:0:267:ILE:CB  | 4:W:173:HIS:CB[1_556]  | 1.63                     | 0.57              |
| 4:0:133:TYR:OH  | 4:X:145:SER:CA[1_556]  | 1.63                     | 0.57              |
| 4:1:64:ILE:CD1  | 4:W:292:ASP:OD2[1_556] | 1.63                     | 0.57              |
| 4:2:174:ALA:O   | 4:Z:277:THR:CA[1_556]  | 1.63                     | 0.57              |
| 4:1:73:HIS:CA   | 4:Y:157:ASP:C[1_556]   | 1.63                     | 0.57              |
| 4:1:37:ARG:CZ   | 4:Y:56:ASP:C[1_556]    | 1.63                     | 0.57              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:179:ASP:OD1 | 4:X:180:LEU:N[1_556]   | 1.63                     | 0.57              |
| 4:2:175:ILE:CD1 | 4:Z:162:ASN:CA[1_556]  | 1.63                     | 0.57              |
| 4:0:121:GLN:CB  | 4:X:9:VAL:CB[1_556]    | 1.63                     | 0.57              |
| 4:0:339:VAL:CG1 | 4:X:335:ARG:CZ[1_556]  | 1.63                     | 0.57              |
| 4:0:289:ILE:CB  | 4:X:294:TYR:OH[1_556]  | 1.63                     | 0.57              |
| 4:1:116:ARG:CB  | 4:Y:339:VAL:CA[1_556]  | 1.63                     | 0.57              |
| 4:0:123:MET:C   | 4:X:26:ALA:O[1_556]    | 1.63                     | 0.57              |
| 4:0:294:TYR:CA  | 4:X:319:ALA:C[1_556]   | 1.63                     | 0.57              |
| 4:0:209:VAL:O   | 4:X:193:LEU:C[1_556]   | 1.63                     | 0.57              |
| 4:2:86:TRP:CE2  | 4:Z:337:TYR:CE1[1_556] | 1.63                     | 0.57              |
| 4:2:261:LEU:C   | 4:Z:265:SER:C[1_556]   | 1.63                     | 0.57              |
| 4:2:72:GLU:OE1  | 4:Z:183:ARG:NE[1_556]  | 1.63                     | 0.57              |
| 4:2:232:SER:OG  | 4:Y:369:ILE:CB[1_556]  | 1.63                     | 0.57              |
| 4:2:151:ILE:CD1 | 4:Z:276:GLU:N[1_556]   | 1.63                     | 0.57              |
| 4:1:119:MET:CA  | 4:Y:340:TRP:CB[1_556]  | 1.63                     | 0.57              |
| 4:0:369:ILE:O   | 4:X:143:TYR:CD2[1_556] | 1.63                     | 0.57              |
| 4:2:110:LEU:CB  | 4:Z:161:HIS:CG[1_556]  | 1.63                     | 0.57              |
| 4:1:82:MET:N    | 4:Y:30:VAL:C[1_556]    | 1.63                     | 0.57              |
| 4:1:64:ILE:CD1  | 4:W:291:LYS:NZ[1_556]  | 1.63                     | 0.57              |
| 4:1:364:GLU:C   | 4:Y:349:LEU:C[1_556]   | 1.63                     | 0.57              |
| 4:1:196:ARG:CD  | 4:X:115:ASN:OD1[1_556] | 1.63                     | 0.57              |
| 4:2:70:PRO:O    | 4:Z:16:LEU:N[1_556]    | 1.63                     | 0.57              |
| 4:1:272:ALA:N   | 4:Y:270:GLU:C[1_556]   | 1.63                     | 0.57              |
| 4:0:368:SER:CA  | 4:X:346:LEU:CB[1_556]  | 1.63                     | 0.57              |
| 4:2:141:SER:OG  | 4:Z:309:ILE:CB[1_556]  | 1.63                     | 0.57              |
| 4:2:188:TYR:N   | 4:Z:191:LYS:CB[1_556]  | 1.63                     | 0.57              |
| 4:1:210:ARG:C   | 4:Y:193:LEU:CG[1_556]  | 1.63                     | 0.57              |
| 4:0:163:VAL:N   | 4:X:274:ILE:O[1_556]   | 1.63                     | 0.57              |
| 4:1:296:ASN:O   | 4:Y:316:GLU:CA[1_556]  | 1.63                     | 0.57              |
| 4:2:335:ARG:CA  | 4:Z:219:VAL:O[1_556]   | 1.63                     | 0.57              |
| 4:1:73:HIS:N    | 4:Y:157:ASP:C[1_556]   | 1.63                     | 0.57              |
| 4:0:309:ILE:CB  | 4:X:259:GLU:CD[1_556]  | 1.63                     | 0.57              |
| 4:1:296:ASN:O   | 4:Y:316:GLU:N[1_556]   | 1.63                     | 0.57              |
| 4:0:151:ILE:CD1 | 4:X:276:GLU:N[1_556]   | 1.63                     | 0.57              |
| 4:0:236:LEU:CD1 | 4:W:117:GLU:OE2[1_556] | 1.63                     | 0.57              |
| 4:0:126:THR:CA  | 4:X:28:ARG:CD[1_556]   | 1.63                     | 0.57              |
| 4:0:108:ALA:O   | 4:X:154:ASP:CA[1_556]  | 1.63                     | 0.57              |
| 4:0:163:VAL:CG2 | 4:X:153:LEU:CG[1_556]  | 1.63                     | 0.57              |
| 4:0:252:ASN:O   | 4:W:113:LYS:CG[1_556]  | 1.63                     | 0.57              |
| 4:0:192:ILE:O   | 4:W:112:PRO:CD[1_556]  | 1.63                     | 0.57              |
| 4:0:197:GLY:N   | 4:W:75:ILE:CA[1_556]   | 1.63                     | 0.57              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:336:LYS:CD  | 4:Z:218:TYR:CD1[1_556] | 1.63                     | 0.57              |
| 4:1:330:ILE:CD1 | 4:Y:315:LYS:CB[1_556]  | 1.63                     | 0.57              |
| 4:0:274:ILE:CD1 | 4:X:263:GLN:O[1_556]   | 1.63                     | 0.57              |
| 4:2:236:LEU:CD1 | 4:Y:117:GLU:OE2[1_556] | 1.63                     | 0.57              |
| 4:1:147:ARG:CB  | 4:Y:314:GLN:CD[1_556]  | 1.63                     | 0.57              |
| 4:1:306:TYR:CG  | 4:Y:256:ARG:CG[1_556]  | 1.63                     | 0.57              |
| 4:0:112:PRO:O   | 4:X:137:GLN:CB[1_556]  | 1.63                     | 0.57              |
| 4:3:266:PHE:O   | 4:Z:172:PRO:CA[1_556]  | 1.63                     | 0.57              |
| 4:0:108:ALA:CB  | 4:X:155:SER:N[1_556]   | 1.63                     | 0.57              |
| 4:0:159:VAL:CG1 | 4:X:180:LEU:O[1_556]   | 1.63                     | 0.57              |
| 4:2:11:ASP:OD2  | 4:Z:305:MET:CA[1_556]  | 1.63                     | 0.57              |
| 4:0:105:LEU:O   | 4:X:335:ARG:CA[1_556]  | 1.63                     | 0.57              |
| 4:1:180:LEU:CD2 | 4:Y:267:ILE:CG1[1_556] | 1.63                     | 0.57              |
| 4:1:298:VAL:CG1 | 4:Y:313:MET:N[1_556]   | 1.63                     | 0.57              |
| 4:0:78:ASN:ND2  | 4:X:32:PRO:O[1_556]    | 1.63                     | 0.57              |
| 4:1:278:THR:CG2 | 4:Y:275:HIS:NE2[1_556] | 1.63                     | 0.57              |
| 4:1:72:GLU:N    | 4:Y:157:ASP:CB[1_556]  | 1.63                     | 0.57              |
| 4:2:252:ASN:O   | 4:Y:113:LYS:CG[1_556]  | 1.63                     | 0.57              |
| 4:0:195:GLU:OE1 | 4:W:109:PRO:O[1_556]   | 1.63                     | 0.57              |
| 4:0:261:LEU:C   | 4:X:265:SER:C[1_556]   | 1.63                     | 0.57              |
| 4:1:272:ALA:N   | 4:Y:270:GLU:CB[1_556]  | 1.63                     | 0.57              |
| 4:2:270:GLU:OE1 | 4:Y:286:ASP:CG[1_556]  | 1.63                     | 0.57              |
| 4:0:40:HIS:N    | 4:V:166:TYR:CZ[1_556]  | 1.63                     | 0.57              |
| 4:0:161:HIS:CE1 | 4:X:155:SER:OG[1_556]  | 1.63                     | 0.57              |
| 4:1:183:ARG:N   | 4:Y:189:LEU:N[1_556]   | 1.63                     | 0.57              |
| 4:1:33:SER:CA   | 4:Y:210:ARG:CZ[1_556]  | 1.63                     | 0.57              |
| 4:0:284:LYS:CB  | 4:X:280:ASN:CB[1_556]  | 1.63                     | 0.57              |
| 4:0:67:LEU:C    | 4:X:62:ARG:NH1[1_556]  | 1.63                     | 0.57              |
| 4:4:40:HIS:ND1  | 4:Z:166:TYR:CD2[1_556] | 1.63                     | 0.57              |
| 4:0:39:ARG:C    | 4:V:166:TYR:CZ[1_556]  | 1.63                     | 0.57              |
| 4:0:136:ILE:CA  | 4:X:299:MET:CA[1_556]  | 1.63                     | 0.57              |
| 4:2:108:ALA:C   | 4:Z:155:SER:N[1_556]   | 1.63                     | 0.57              |
| 4:1:336:LYS:CB  | 4:Y:218:TYR:CG[1_556]  | 1.63                     | 0.57              |
| 4:1:371:HIS:O   | 4:Y:140:LEU:CA[1_556]  | 1.63                     | 0.57              |
| 4:1:177:ARG:NH1 | 4:Y:159:VAL:N[1_556]   | 1.63                     | 0.57              |
| 4:0:205:GLU:O   | 4:X:198:TYR:C[1_556]   | 1.63                     | 0.57              |
| 4:2:126:THR:CA  | 4:Z:28:ARG:CD[1_556]   | 1.63                     | 0.57              |
| 4:1:108:ALA:N   | 4:Y:301:GLY:CA[1_556]  | 1.63                     | 0.57              |
| 4:3:64:ILE:CD1  | 4:Y:292:ASP:OD2[1_556] | 1.63                     | 0.57              |
| 4:2:195:GLU:OE1 | 4:Y:109:PRO:O[1_556]   | 1.63                     | 0.57              |
| 4:0:175:ILE:CD1 | 4:X:162:ASN:CA[1_556]  | 1.63                     | 0.57              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:230:ALA:N   | 4:Z:368:SER:C[1_556]   | 1.63                     | 0.57              |
| 4:2:192:ILE:O   | 4:Y:112:PRO:CD[1_556]  | 1.63                     | 0.57              |
| 4:2:105:LEU:O   | 4:Z:334:GLU:C[1_556]   | 1.63                     | 0.57              |
| 4:2:82:MET:CA   | 4:Z:30:VAL:CG1[1_556]  | 1.63                     | 0.57              |
| 4:2:136:ILE:CB  | 4:Z:299:MET:C[1_556]   | 1.63                     | 0.57              |
| 4:2:284:LYS:CB  | 4:Z:280:ASN:CB[1_556]  | 1.63                     | 0.57              |
| 4:2:121:GLN:CB  | 4:Z:9:VAL:CB[1_556]    | 1.64                     | 0.56              |
| 4:2:112:PRO:CA  | 4:Z:137:GLN:CG[1_556]  | 1.64                     | 0.56              |
| 4:3:196:ARG:CD  | 4:Z:115:ASN:OD1[1_556] | 1.64                     | 0.56              |
| 4:2:79:TRP:CD1  | 4:Z:17:VAL:CB[1_556]   | 1.64                     | 0.56              |
| 4:1:210:ARG:N   | 4:Y:193:LEU:C[1_556]   | 1.64                     | 0.56              |
| 4:0:119:MET:CA  | 4:X:340:TRP:CD1[1_556] | 1.64                     | 0.56              |
| 4:1:162:ASN:CB  | 4:Y:273:GLY:C[1_556]   | 1.64                     | 0.56              |
| 4:0:291:LYS:CD  | 4:X:322:PRO:CA[1_556]  | 1.64                     | 0.56              |
| 4:1:337:TYR:N   | 4:Y:307:PRO:CB[1_556]  | 1.64                     | 0.56              |
| 4:0:113:LYS:CB  | 4:X:136:ILE:O[1_556]   | 1.64                     | 0.56              |
| 4:1:264:PRO:CB  | 4:Y:269:MET:N[1_556]   | 1.64                     | 0.56              |
| 4:2:115:ASN:CG  | 4:Z:11:ASP:OD1[1_556]  | 1.64                     | 0.56              |
| 4:2:78:ASN:ND2  | 4:Z:32:PRO:O[1_556]    | 1.64                     | 0.56              |
| 4:0:169:TYR:CD1 | 4:X:151:ILE:N[1_556]   | 1.64                     | 0.56              |
| 4:0:82:MET:CA   | 4:X:30:VAL:CG1[1_556]  | 1.64                     | 0.56              |
| 4:1:185:LEU:CD2 | 4:Y:188:TYR:OH[1_556]  | 1.64                     | 0.56              |
| 4:2:210:ARG:CA  | 4:Z:193:LEU:CD1[1_556] | 1.64                     | 0.56              |
| 4:0:70:PRO:O    | 4:X:16:LEU:N[1_556]    | 1.64                     | 0.56              |
| 4:0:232:SER:OG  | 4:W:369:ILE:CB[1_556]  | 1.64                     | 0.56              |
| 4:1:178:LEU:CD2 | 4:Y:264:PRO:CA[1_556]  | 1.64                     | 0.56              |
| 4:2:67:LEU:C    | 4:Z:62:ARG:NH1[1_556]  | 1.64                     | 0.56              |
| 4:1:124:PHE:CD1 | 4:Y:24:ASP:O[1_556]    | 1.64                     | 0.56              |
| 4:1:371:HIS:CG  | 4:Y:140:LEU:CG[1_556]  | 1.64                     | 0.56              |
| 4:1:105:LEU:C   | 4:Y:335:ARG:CA[1_556]  | 1.64                     | 0.56              |
| 4:1:289:ILE:O   | 4:Y:321:ALA:CA[1_556]  | 1.64                     | 0.56              |
| 4:1:292:ASP:C   | 4:Y:321:ALA:N[1_556]   | 1.64                     | 0.56              |
| 4:1:366:GLY:N   | 4:Y:348:SER:N[1_556]   | 1.64                     | 0.56              |
| 4:1:40:HIS:N    | 4:W:166:TYR:CZ[1_556]  | 1.64                     | 0.56              |
| 4:0:172:PRO:CG  | 4:X:164:PRO:CA[1_556]  | 1.64                     | 0.56              |
| 4:2:179:ASP:OD1 | 4:Z:180:LEU:N[1_556]   | 1.64                     | 0.56              |
| 4:1:203:THR:CA  | 4:Y:201:VAL:CG2[1_556] | 1.64                     | 0.56              |
| 4:2:293:LEU:CA  | 4:Z:317:ILE:O[1_556]   | 1.64                     | 0.56              |
| 4:0:336:LYS:CD  | 4:X:218:TYR:CD1[1_556] | 1.64                     | 0.56              |
| 4:0:136:ILE:CB  | 4:X:299:MET:C[1_556]   | 1.64                     | 0.56              |
| 4:0:210:ARG:CA  | 4:X:193:LEU:CD1[1_556] | 1.64                     | 0.56              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:371:HIS:CG  | 4:X:140:LEU:CG[1_556]  | 1.64                     | 0.56              |
| 4:0:211:ASP:CB  | 4:X:249:THR:O[1_556]   | 1.64                     | 0.56              |
| 4:0:186:THR:O   | 4:X:191:LYS:C[1_556]   | 1.64                     | 0.56              |
| 4:3:197:GLY:C   | 4:Z:75:ILE:O[1_556]    | 1.64                     | 0.56              |
| 4:2:274:ILE:CD1 | 4:Z:263:GLN:O[1_556]   | 1.64                     | 0.56              |
| 4:1:166:TYR:C   | 4:Y:294:TYR:O[1_556]   | 1.64                     | 0.56              |
| 4:2:113:LYS:CB  | 4:Z:136:ILE:N[1_556]   | 1.64                     | 0.56              |
| 4:2:371:HIS:CG  | 4:Z:140:LEU:CG[1_556]  | 1.64                     | 0.56              |
| 4:0:80:ASP:OD2  | 4:X:93:GLU:OE2[1_556]  | 1.64                     | 0.56              |
| 4:1:159:VAL:CG1 | 4:Y:180:LEU:C[1_556]   | 1.64                     | 0.56              |
| 4:3:268:GLY:C   | 4:Z:284:LYS:O[1_556]   | 1.64                     | 0.56              |
| 4:0:63:GLY:N    | 4:V:288:ASP:C[1_556]   | 1.64                     | 0.56              |
| 4:3:40:HIS:CG   | 4:Y:166:TYR:CD2[1_556] | 1.64                     | 0.56              |
| 4:1:274:ILE:CG2 | 4:Y:263:GLN:CA[1_556]  | 1.64                     | 0.56              |
| 4:1:108:ALA:CB  | 4:Y:155:SER:N[1_556]   | 1.64                     | 0.56              |
| 4:1:109:PRO:C   | 4:Y:154:ASP:CB[1_556]  | 1.64                     | 0.56              |
| 4:0:79:TRP:CD1  | 4:X:17:VAL:CB[1_556]   | 1.64                     | 0.56              |
| 4:0:365:ALA:C   | 4:X:346:LEU:O[1_556]   | 1.64                     | 0.56              |
| 4:0:124:PHE:CA  | 4:X:24:ASP:C[1_556]    | 1.64                     | 0.56              |
| 4:1:122:ILE:CG1 | 4:Y:19:ALA:N[1_556]    | 1.64                     | 0.56              |
| 4:4:64:ILE:CD1  | 4:Z:291:LYS:NZ[1_556]  | 1.64                     | 0.56              |
| 4:2:279:TYR:CA  | 4:Z:276:GLU:CD[1_556]  | 1.64                     | 0.56              |
| 4:0:109:PRO:C   | 4:X:154:ASP:CB[1_556]  | 1.64                     | 0.56              |
| 4:2:267:ILE:CB  | 4:Y:173:HIS:CB[1_556]  | 1.64                     | 0.56              |
| 4:0:118:LYS:CG  | 4:X:18:LYS:O[1_556]    | 1.64                     | 0.56              |
| 4:2:330:ILE:CD1 | 4:Z:315:LYS:CB[1_556]  | 1.64                     | 0.56              |
| 4:0:136:ILE:N   | 4:X:299:MET:C[1_556]   | 1.64                     | 0.56              |
| 4:2:123:MET:C   | 4:Z:26:ALA:O[1_556]    | 1.64                     | 0.56              |
| 4:0:288:ASP:C   | 4:X:322:PRO:CG[1_556]  | 1.64                     | 0.56              |
| 4:1:16:LEU:CA   | 4:Y:214:GLU:CA[1_556]  | 1.64                     | 0.56              |
| 4:1:336:LYS:CB  | 4:Y:218:TYR:CD1[1_556] | 1.64                     | 0.56              |
| 4:2:163:VAL:N   | 4:Z:274:ILE:O[1_556]   | 1.64                     | 0.56              |
| 4:2:370:VAL:CG1 | 4:Z:342:GLY:N[1_556]   | 1.64                     | 0.56              |
| 4:2:122:ILE:CG2 | 4:Z:28:ARG:N[1_556]    | 1.64                     | 0.56              |
| 4:1:295:ALA:O   | 4:Y:315:LYS:NZ[1_556]  | 1.64                     | 0.56              |
| 4:2:33:SER:O    | 4:Z:210:ARG:NH2[1_556] | 1.64                     | 0.56              |
| 4:1:197:GLY:C   | 4:X:75:ILE:O[1_556]    | 1.64                     | 0.56              |
| 4:0:105:LEU:O   | 4:X:334:GLU:C[1_556]   | 1.64                     | 0.56              |
| 4:1:331:ALA:N   | 4:Y:222:ASP:N[1_556]   | 1.64                     | 0.56              |
| 4:0:77:THR:OG1  | 4:X:14:SER:CA[1_556]   | 1.64                     | 0.56              |
| 4:2:108:ALA:CB  | 4:Z:155:SER:N[1_556]   | 1.64                     | 0.56              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:40:HIS:CG   | 4:W:166:TYR:CD2[1_556] | 1.64                     | 0.56              |
| 4:0:336:LYS:O   | 4:X:307:PRO:CD[1_556]  | 1.64                     | 0.56              |
| 4:0:163:VAL:C   | 4:X:278:THR:CB[1_556]  | 1.64                     | 0.56              |
| 4:0:188:TYR:N   | 4:X:191:LYS:CB[1_556]  | 1.64                     | 0.56              |
| 4:2:186:THR:O   | 4:Z:191:LYS:C[1_556]   | 1.64                     | 0.56              |
| 4:2:270:GLU:OE1 | 4:Y:286:ASP:CA[1_556]  | 1.64                     | 0.56              |
| 4:1:15:GLY:N    | 4:Y:213:LYS:CE[1_556]  | 1.64                     | 0.56              |
| 4:1:253:GLU:OE2 | 4:X:114:ALA:N[1_556]   | 1.64                     | 0.56              |
| 4:2:113:LYS:CB  | 4:Z:136:ILE:O[1_556]   | 1.64                     | 0.56              |
| 4:2:177:ARG:NH2 | 4:Z:159:VAL:N[1_556]   | 1.64                     | 0.56              |
| 4:2:168:GLY:CA  | 4:Z:296:ASN:N[1_556]   | 1.65                     | 0.55              |
| 4:2:77:THR:OG1  | 4:Z:14:SER:CA[1_556]   | 1.65                     | 0.55              |
| 4:2:118:LYS:CG  | 4:Z:18:LYS:O[1_556]    | 1.65                     | 0.55              |
| 4:1:365:ALA:C   | 4:Y:346:LEU:O[1_556]   | 1.65                     | 0.55              |
| 4:2:369:ILE:O   | 4:Z:143:TYR:CD2[1_556] | 1.65                     | 0.55              |
| 4:0:137:GLN:OE1 | 4:X:304:THR:CA[1_556]  | 1.65                     | 0.55              |
| 4:2:159:VAL:CG1 | 4:Z:180:LEU:O[1_556]   | 1.65                     | 0.55              |
| 4:2:169:TYR:CD1 | 4:Z:151:ILE:N[1_556]   | 1.65                     | 0.55              |
| 4:0:364:GLU:C   | 4:X:349:LEU:C[1_556]   | 1.65                     | 0.55              |
| 4:2:15:GLY:N    | 4:Z:213:LYS:CE[1_556]  | 1.65                     | 0.55              |
| 4:1:203:THR:OG1 | 4:Y:205:GLU:CD[1_556]  | 1.65                     | 0.55              |
| 4:1:68:LYS:CA   | 4:Y:59:GLN:CD[1_556]   | 1.65                     | 0.55              |
| 4:1:208:ILE:CB  | 4:Y:198:TYR:CE1[1_556] | 1.65                     | 0.55              |
| 4:1:114:ALA:CB  | 4:Y:106:THR:CB[1_556]  | 1.65                     | 0.55              |
| 4:1:212:ILE:CD1 | 4:Y:197:GLY:CA[1_556]  | 1.65                     | 0.55              |
| 4:2:205:GLU:O   | 4:Z:198:TYR:C[1_556]   | 1.65                     | 0.55              |
| 4:0:168:GLY:CA  | 4:X:296:ASN:N[1_556]   | 1.65                     | 0.55              |
| 4:2:112:PRO:O   | 4:Z:137:GLN:CB[1_556]  | 1.65                     | 0.55              |
| 4:0:177:ARG:CD  | 4:X:160:THR:N[1_556]   | 1.65                     | 0.55              |
| 4:0:33:SER:O    | 4:X:210:ARG:NH2[1_556] | 1.65                     | 0.55              |
| 4:2:40:HIS:CA   | 4:X:167:GLU:CG[1_556]  | 1.65                     | 0.55              |
| 4:2:108:ALA:O   | 4:Z:154:ASP:CA[1_556]  | 1.65                     | 0.55              |
| 4:0:62:ARG:NH2  | 4:X:205:GLU:CB[1_556]  | 1.65                     | 0.55              |
| 4:1:331:ALA:CB  | 4:Y:221:LEU:C[1_556]   | 1.65                     | 0.55              |
| 4:0:165:ILE:O   | 4:X:317:ILE:CD1[1_556] | 1.65                     | 0.55              |
| 4:2:306:TYR:CE2 | 4:Z:256:ARG:CB[1_556]  | 1.65                     | 0.55              |
| 4:0:166:TYR:CG  | 4:X:294:TYR:CD2[1_556] | 1.65                     | 0.55              |
| 4:2:288:ASP:C   | 4:Z:322:PRO:CG[1_556]  | 1.65                     | 0.55              |
| 4:0:331:ALA:N   | 4:X:222:ASP:N[1_556]   | 1.65                     | 0.55              |
| 4:1:212:ILE:CD1 | 4:Y:197:GLY:N[1_556]   | 1.65                     | 0.55              |
| 4:1:67:LEU:CB   | 4:Y:207:GLU:OE2[1_556] | 1.65                     | 0.55              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:299:MET:SD  | 4:Y:312:ARG:NE[1_556]  | 1.65                     | 0.55              |
| 4:2:105:LEU:O   | 4:Z:335:ARG:CA[1_556]  | 1.65                     | 0.55              |
| 4:1:266:PHE:O   | 4:X:172:PRO:CA[1_556]  | 1.65                     | 0.55              |
| 4:2:211:ASP:CB  | 4:Z:249:THR:O[1_556]   | 1.65                     | 0.55              |
| 4:2:39:ARG:C    | 4:X:166:TYR:CZ[1_556]  | 1.65                     | 0.55              |
| 4:2:163:VAL:C   | 4:Z:278:THR:CB[1_556]  | 1.65                     | 0.55              |
| 4:1:177:ARG:NH1 | 4:Y:159:VAL:CB[1_556]  | 1.65                     | 0.55              |
| 4:0:306:TYR:CE2 | 4:X:256:ARG:CB[1_556]  | 1.65                     | 0.55              |
| 4:0:230:ALA:N   | 4:W:368:SER:C[1_556]   | 1.65                     | 0.55              |
| 4:0:140:LEU:O   | 4:X:310:ALA:CB[1_556]  | 1.65                     | 0.55              |
| 4:1:16:LEU:CG   | 4:Y:214:GLU:N[1_556]   | 1.65                     | 0.55              |
| 4:0:113:LYS:CB  | 4:X:136:ILE:N[1_556]   | 1.65                     | 0.55              |
| 4:1:291:LYS:CD  | 4:Y:322:PRO:CA[1_556]  | 1.65                     | 0.55              |
| 4:2:40:HIS:ND1  | 4:X:166:TYR:CD2[1_556] | 1.65                     | 0.55              |
| 4:1:337:TYR:CE2 | 4:Y:218:TYR:OH[1_556]  | 1.65                     | 0.55              |
| 4:1:296:ASN:ND2 | 4:Y:318:THR:CA[1_556]  | 1.65                     | 0.55              |
| 4:2:108:ALA:O   | 4:Z:154:ASP:CG[1_556]  | 1.65                     | 0.55              |
| 4:1:78:ASN:CB   | 4:Y:32:PRO:O[1_556]    | 1.65                     | 0.55              |
| 4:2:117:GLU:OE1 | 4:Z:104:LEU:CD2[1_556] | 1.65                     | 0.55              |
| 4:2:124:PHE:CA  | 4:Z:24:ASP:C[1_556]    | 1.65                     | 0.55              |
| 4:2:62:ARG:NH2  | 4:Z:205:GLU:CB[1_556]  | 1.65                     | 0.55              |
| 4:0:299:MET:C   | 4:X:312:ARG:CG[1_556]  | 1.65                     | 0.55              |
| 4:0:293:LEU:CA  | 4:X:317:ILE:O[1_556]   | 1.65                     | 0.55              |
| 4:1:162:ASN:N   | 4:Y:274:ILE:CB[1_556]  | 1.65                     | 0.55              |
| 4:1:303:THR:CA  | 4:Y:257:CYS:C[1_556]   | 1.65                     | 0.55              |
| 4:1:180:LEU:CD1 | 4:Y:267:ILE:CG1[1_556] | 1.65                     | 0.55              |
| 4:0:296:ASN:N   | 4:X:319:ALA:CB[1_556]  | 1.65                     | 0.55              |
| 4:2:192:ILE:O   | 4:Y:110:LEU:O[1_556]   | 1.65                     | 0.55              |
| 4:2:147:ARG:CD  | 4:Z:314:GLN:OE1[1_556] | 1.65                     | 0.55              |
| 4:2:122:ILE:CD1 | 4:Z:19:ALA:CA[1_556]   | 1.65                     | 0.55              |
| 4:1:206:ARG:C   | 4:Y:199:SER:C[1_556]   | 1.65                     | 0.55              |
| 4:1:286:ASP:OD2 | 4:Y:290:ARG:CD[1_556]  | 1.65                     | 0.55              |
| 4:1:230:ALA:N   | 4:X:368:SER:C[1_556]   | 1.65                     | 0.55              |
| 4:2:149:THR:N   | 4:Z:327:ILE:C[1_556]   | 1.65                     | 0.55              |
| 4:2:106:THR:N   | 4:Z:335:ARG:N[1_556]   | 1.65                     | 0.55              |
| 4:0:33:SER:CA   | 4:X:210:ARG:NH1[1_556] | 1.65                     | 0.55              |
| 4:2:136:ILE:CA  | 4:Z:299:MET:CA[1_556]  | 1.65                     | 0.55              |
| 4:1:370:VAL:CG1 | 4:Y:342:GLY:N[1_556]   | 1.65                     | 0.55              |
| 4:0:115:ASN:CG  | 4:X:11:ASP:OD1[1_556]  | 1.65                     | 0.55              |
| 4:1:274:ILE:CB  | 4:Y:263:GLN:CB[1_556]  | 1.65                     | 0.55              |
| 4:0:112:PRO:CA  | 4:X:137:GLN:CG[1_556]  | 1.66                     | 0.54              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:169:TYR:CD1 | 4:Y:151:ILE:N[1_556]   | 1.66                     | 0.54              |
| 4:1:112:PRO:O   | 4:Y:137:GLN:CB[1_556]  | 1.66                     | 0.54              |
| 4:1:297:ASN:N   | 4:Y:316:GLU:CA[1_556]  | 1.66                     | 0.54              |
| 4:0:106:THR:N   | 4:X:335:ARG:N[1_556]   | 1.66                     | 0.54              |
| 4:0:166:TYR:CB  | 4:X:294:TYR:CB[1_556]  | 1.66                     | 0.54              |
| 4:2:40:HIS:N    | 4:X:166:TYR:CZ[1_556]  | 1.66                     | 0.54              |
| 4:1:59:GLN:CG   | 4:Y:208:ILE:CG1[1_556] | 1.66                     | 0.54              |
| 4:0:292:ASP:C   | 4:X:318:THR:O[1_556]   | 1.66                     | 0.54              |
| 4:0:71:ILE:C    | 4:X:157:ASP:CG[1_556]  | 1.66                     | 0.54              |
| 4:0:141:SER:N   | 4:X:310:ALA:CB[1_556]  | 1.66                     | 0.54              |
| 4:2:298:VAL:CG2 | 4:Z:311:ASP:O[1_556]   | 1.66                     | 0.54              |
| 4:0:173:HIS:NE2 | 4:X:281:SER:C[1_556]   | 1.66                     | 0.54              |
| 4:2:303:THR:CG2 | 4:Z:257:CYS:O[1_556]   | 1.66                     | 0.54              |
| 4:0:63:GLY:N    | 4:V:288:ASP:N[1_556]   | 1.66                     | 0.54              |
| 4:2:137:GLN:OE1 | 4:Z:304:THR:CA[1_556]  | 1.66                     | 0.54              |
| 4:1:296:ASN:N   | 4:Y:319:ALA:CB[1_556]  | 1.66                     | 0.54              |
| 4:1:305:MET:N   | 4:Y:255:PHE:O[1_556]   | 1.66                     | 0.54              |
| 4:0:192:ILE:O   | 4:W:110:LEU:O[1_556]   | 1.66                     | 0.54              |
| 4:0:68:LYS:CB   | 4:X:59:GLN:CD[1_556]   | 1.66                     | 0.54              |
| 4:2:104:LEU:CB  | 4:Z:334:GLU:OE2[1_556] | 1.66                     | 0.54              |
| 4:1:279:TYR:CA  | 4:Y:276:GLU:CD[1_556]  | 1.66                     | 0.54              |
| 4:1:106:THR:CA  | 4:Y:335:ARG:CB[1_556]  | 1.66                     | 0.54              |
| 4:0:279:TYR:CA  | 4:X:276:GLU:CD[1_556]  | 1.66                     | 0.54              |
| 4:0:122:ILE:CG2 | 4:X:28:ARG:N[1_556]    | 1.66                     | 0.54              |
| 4:2:364:GLU:C   | 4:Z:349:LEU:C[1_556]   | 1.66                     | 0.54              |
| 4:2:116:ARG:CZ  | 4:Z:141:SER:O[1_556]   | 1.66                     | 0.54              |
| 4:0:270:GLU:OE1 | 4:W:286:ASP:CA[1_556]  | 1.66                     | 0.54              |
| 4:1:189:LEU:CG  | 4:Y:195:GLU:CG[1_556]  | 1.66                     | 0.54              |
| 4:2:172:PRO:CB  | 4:Z:163:VAL:CA[1_556]  | 1.66                     | 0.54              |
| 4:0:167:GLU:O   | 4:X:295:ALA:CA[1_556]  | 1.66                     | 0.54              |
| 4:2:136:ILE:N   | 4:Z:299:MET:C[1_556]   | 1.66                     | 0.54              |
| 4:1:369:ILE:CA  | 4:Y:346:LEU:CA[1_556]  | 1.66                     | 0.54              |
| 4:2:177:ARG:NH1 | 4:Z:159:VAL:N[1_556]   | 1.66                     | 0.54              |
| 4:1:137:GLN:CG  | 4:Y:304:THR:CB[1_556]  | 1.66                     | 0.54              |
| 4:0:162:ASN:N   | 4:X:274:ILE:N[1_556]   | 1.66                     | 0.54              |
| 4:3:270:GLU:CG  | 4:Z:286:ASP:CA[1_556]  | 1.66                     | 0.54              |
| 4:1:157:ASP:CG  | 4:Y:213:LYS:CD[1_556]  | 1.66                     | 0.54              |
| 4:2:331:ALA:N   | 4:Z:222:ASP:N[1_556]   | 1.66                     | 0.54              |
| 4:2:73:HIS:N    | 4:Z:157:ASP:C[1_556]   | 1.66                     | 0.54              |
| 4:0:40:HIS:ND1  | 4:V:166:TYR:CD2[1_556] | 1.66                     | 0.54              |
| 4:0:68:LYS:NZ   | 4:X:59:GLN:CB[1_556]   | 1.66                     | 0.54              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:266:PHE:O   | 4:W:172:PRO:CA[1_556]  | 1.66                     | 0.54              |
| 4:1:133:TYR:CD1 | 4:Y:144:ALA:O[1_556]   | 1.66                     | 0.54              |
| 4:2:148:THR:CA  | 4:Z:328:LYS:N[1_556]   | 1.66                     | 0.54              |
| 4:1:134:VAL:CG2 | 4:Y:338:SER:C[1_556]   | 1.66                     | 0.54              |
| 4:2:122:ILE:CG2 | 4:Z:27:PRO:C[1_556]    | 1.66                     | 0.54              |
| 4:1:62:ARG:CB   | 4:Y:204:ALA:CB[1_556]  | 1.66                     | 0.54              |
| 4:2:33:SER:CA   | 4:Z:210:ARG:NH1[1_556] | 1.66                     | 0.54              |
| 4:0:301:GLY:CA  | 4:X:219:VAL:CG2[1_556] | 1.66                     | 0.54              |
| 4:4:62:ARG:C    | 4:Z:288:ASP:CB[1_556]  | 1.66                     | 0.54              |
| 4:2:166:TYR:CB  | 4:Z:294:TYR:CB[1_556]  | 1.66                     | 0.54              |
| 4:1:153:LEU:O   | 4:Y:262:PHE:CE1[1_556] | 1.66                     | 0.54              |
| 4:1:186:THR:CA  | 4:Y:191:LYS:CA[1_556]  | 1.66                     | 0.54              |
| 4:0:117:GLU:OE1 | 4:X:104:LEU:CD2[1_556] | 1.66                     | 0.54              |
| 4:0:116:ARG:CZ  | 4:X:141:SER:O[1_556]   | 1.66                     | 0.54              |
| 4:1:210:ARG:CA  | 4:Y:193:LEU:CA[1_556]  | 1.66                     | 0.54              |
| 4:1:336:LYS:O   | 4:Y:307:PRO:CD[1_556]  | 1.66                     | 0.54              |
| 4:1:185:LEU:C   | 4:Y:191:LYS:CG[1_556]  | 1.66                     | 0.54              |
| 4:1:30:VAL:C    | 4:Y:215:LYS:CG[1_556]  | 1.66                     | 0.54              |
| 4:1:142:LEU:CB  | 4:Y:329:ILE:CB[1_556]  | 1.66                     | 0.54              |
| 4:0:122:ILE:CG2 | 4:X:27:PRO:C[1_556]    | 1.66                     | 0.54              |
| 4:0:40:HIS:CA   | 4:V:167:GLU:CG[1_556]  | 1.66                     | 0.54              |
| 4:0:330:ILE:CD1 | 4:X:315:LYS:CB[1_556]  | 1.66                     | 0.54              |
| 4:1:140:LEU:CD2 | 4:Y:332:PRO:N[1_556]   | 1.66                     | 0.54              |
| 4:2:214:GLU:CG  | 4:Z:250:ILE:CG2[1_556] | 1.66                     | 0.54              |
| 4:1:210:ARG:N   | 4:Y:193:LEU:O[1_556]   | 1.66                     | 0.54              |
| 4:2:165:ILE:O   | 4:Z:317:ILE:CD1[1_556] | 1.66                     | 0.54              |
| 4:0:296:ASN:O   | 4:X:316:GLU:CA[1_556]  | 1.66                     | 0.54              |
| 4:2:301:GLY:CA  | 4:Z:219:VAL:CG2[1_556] | 1.66                     | 0.54              |
| 4:1:124:PHE:CD1 | 4:Y:23:GLY:O[1_556]    | 1.66                     | 0.54              |
| 4:2:365:ALA:C   | 4:Z:346:LEU:O[1_556]   | 1.66                     | 0.54              |
| 4:0:169:TYR:CA  | 4:X:296:ASN:C[1_556]   | 1.66                     | 0.54              |
| 4:0:108:ALA:O   | 4:X:154:ASP:CG[1_556]  | 1.66                     | 0.54              |
| 4:1:217:CYS:CB  | 4:Y:256:ARG:CZ[1_556]  | 1.66                     | 0.54              |
| 4:0:177:ARG:NH2 | 4:X:159:VAL:N[1_556]   | 1.66                     | 0.54              |
| 4:1:11:ASP:CA   | 4:Y:305:MET:SD[1_556]  | 1.66                     | 0.54              |
| 4:0:148:THR:CA  | 4:X:328:LYS:N[1_556]   | 1.66                     | 0.54              |
| 4:1:274:ILE:CD1 | 4:Y:263:GLN:O[1_556]   | 1.66                     | 0.54              |
| 4:2:362:TYR:OH  | 4:Z:22:ALA:N[1_556]    | 1.66                     | 0.54              |
| 4:2:169:TYR:CA  | 4:Z:296:ASN:C[1_556]   | 1.66                     | 0.54              |
| 4:1:162:ASN:N   | 4:Y:274:ILE:N[1_556]   | 1.66                     | 0.54              |
| 4:0:104:LEU:CB  | 4:X:334:GLU:OE2[1_556] | 1.66                     | 0.54              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:366:GLY:C   | 4:Z:347:ALA:CB[1_556]  | 1.66                     | 0.54              |
| 4:1:286:ASP:CB  | 4:Y:290:ARG:CD[1_556]  | 1.66                     | 0.54              |
| 4:1:179:ASP:OD1 | 4:Y:180:LEU:N[1_556]   | 1.66                     | 0.54              |
| 4:2:292:ASP:C   | 4:Z:318:THR:O[1_556]   | 1.66                     | 0.54              |
| 4:2:119:MET:CB  | 4:Z:340:TRP:CB[1_556]  | 1.66                     | 0.54              |
| 4:3:40:HIS:NE2  | 4:Y:166:TYR:CG[1_556]  | 1.66                     | 0.54              |
| 4:1:105:LEU:O   | 4:Y:334:GLU:C[1_556]   | 1.66                     | 0.54              |
| 4:1:253:GLU:CD  | 4:X:112:PRO:CA[1_556]  | 1.66                     | 0.54              |
| 4:2:264:PRO:CA  | 4:Z:268:GLY:N[1_556]   | 1.66                     | 0.54              |
| 4:2:73:HIS:CA   | 4:Z:157:ASP:C[1_556]   | 1.66                     | 0.54              |
| 4:1:339:VAL:CG1 | 4:Y:335:ARG:CZ[1_556]  | 1.67                     | 0.53              |
| 4:2:142:LEU:CB  | 4:Z:329:ILE:CB[1_556]  | 1.67                     | 0.53              |
| 4:0:149:THR:CB  | 4:X:327:ILE:CB[1_556]  | 1.67                     | 0.53              |
| 4:2:149:THR:CB  | 4:Z:327:ILE:CB[1_556]  | 1.67                     | 0.53              |
| 4:0:298:VAL:CG2 | 4:X:311:ASP:O[1_556]   | 1.67                     | 0.53              |
| 4:1:126:THR:CA  | 4:Y:28:ARG:CD[1_556]   | 1.67                     | 0.53              |
| 4:0:177:ARG:NH1 | 4:X:159:VAL:N[1_556]   | 1.67                     | 0.53              |
| 4:1:136:ILE:O   | 4:Y:299:MET:CA[1_556]  | 1.67                     | 0.53              |
| 4:0:162:ASN:CB  | 4:X:273:GLY:C[1_556]   | 1.67                     | 0.53              |
| 4:0:332:PRO:CG  | 4:X:221:LEU:CD1[1_556] | 1.67                     | 0.53              |
| 4:1:215:LYS:CD  | 4:Y:237:GLU:OE1[1_556] | 1.67                     | 0.53              |
| 4:4:63:GLY:O    | 4:Z:289:ILE:CA[1_556]  | 1.67                     | 0.53              |
| 4:1:129:VAL:CB  | 4:Y:25:ASP:CB[1_556]   | 1.67                     | 0.53              |
| 4:0:137:GLN:CG  | 4:X:304:THR:CB[1_556]  | 1.67                     | 0.53              |
| 4:1:74:GLY:C    | 4:Y:157:ASP:N[1_556]   | 1.67                     | 0.53              |
| 4:2:159:VAL:N   | 4:Z:181:ALA:C[1_556]   | 1.67                     | 0.53              |
| 4:2:166:TYR:CG  | 4:Z:294:TYR:CD2[1_556] | 1.67                     | 0.53              |
| 4:4:40:HIS:CE1  | 4:Z:166:TYR:CD2[1_556] | 1.67                     | 0.53              |
| 4:0:105:LEU:C   | 4:X:335:ARG:CA[1_556]  | 1.67                     | 0.53              |
| 4:2:63:GLY:O    | 4:X:289:ILE:CA[1_556]  | 1.67                     | 0.53              |
| 4:1:136:ILE:CA  | 4:Y:299:MET:CA[1_556]  | 1.67                     | 0.53              |
| 4:2:371:HIS:O   | 4:Z:140:LEU:CA[1_556]  | 1.67                     | 0.53              |
| 4:1:72:GLU:O    | 4:Y:157:ASP:CA[1_556]  | 1.67                     | 0.53              |
| 4:0:73:HIS:N    | 4:X:157:ASP:C[1_556]   | 1.67                     | 0.53              |
| 4:2:81:ASP:OD2  | 4:Z:32:PRO:CD[1_556]   | 1.67                     | 0.53              |
| 4:1:303:THR:CG2 | 4:Y:257:CYS:O[1_556]   | 1.67                     | 0.53              |
| 4:2:124:PHE:CD1 | 4:Z:23:GLY:O[1_556]    | 1.67                     | 0.53              |
| 4:2:71:ILE:C    | 4:Z:157:ASP:CG[1_556]  | 1.67                     | 0.53              |
| 4:3:253:GLU:N   | 4:Z:113:LYS:CG[1_556]  | 1.67                     | 0.53              |
| 4:2:208:ILE:C   | 4:Z:198:TYR:CB[1_556]  | 1.67                     | 0.53              |
| 4:4:39:ARG:C    | 4:Z:166:TYR:CZ[1_556]  | 1.67                     | 0.53              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:371:HIS:CE1 | 4:X:140:LEU:N[1_556]   | 1.67                     | 0.53              |
| 4:1:113:LYS:CD  | 4:Y:136:ILE:CB[1_556]  | 1.67                     | 0.53              |
| 4:0:366:GLY:C   | 4:X:347:ALA:CB[1_556]  | 1.67                     | 0.53              |
| 4:0:81:ASP:OD2  | 4:X:32:PRO:CD[1_556]   | 1.67                     | 0.53              |
| 4:2:299:MET:C   | 4:Z:312:ARG:CG[1_556]  | 1.67                     | 0.53              |
| 4:1:165:ILE:O   | 4:Y:317:ILE:CD1[1_556] | 1.67                     | 0.53              |
| 4:2:298:VAL:CG1 | 4:Z:311:ASP:C[1_556]   | 1.67                     | 0.53              |
| 4:0:208:ILE:C   | 4:X:198:TYR:CB[1_556]  | 1.67                     | 0.53              |
| 4:0:169:TYR:N   | 4:X:296:ASN:N[1_556]   | 1.67                     | 0.53              |
| 4:2:174:ALA:N   | 4:Z:281:SER:OG[1_556]  | 1.67                     | 0.53              |
| 4:1:162:ASN:CB  | 4:Y:274:ILE:C[1_556]   | 1.67                     | 0.53              |
| 4:0:149:THR:C   | 4:X:327:ILE:CG1[1_556] | 1.67                     | 0.53              |
| 4:1:339:VAL:C   | 4:Y:335:ARG:NH2[1_556] | 1.67                     | 0.53              |
| 4:0:197:GLY:C   | 4:W:75:ILE:O[1_556]    | 1.67                     | 0.53              |
| 4:0:214:GLU:CG  | 4:X:250:ILE:CG2[1_556] | 1.67                     | 0.53              |
| 4:1:270:GLU:CG  | 4:X:286:ASP:CA[1_556]  | 1.67                     | 0.53              |
| 4:2:141:SER:N   | 4:Z:310:ALA:CB[1_556]  | 1.67                     | 0.53              |
| 4:2:230:ALA:N   | 4:Y:368:SER:C[1_556]   | 1.67                     | 0.53              |
| 4:1:149:THR:C   | 4:Y:327:ILE:CG1[1_556] | 1.67                     | 0.53              |
| 4:1:167:GLU:O   | 4:Y:295:ALA:CA[1_556]  | 1.67                     | 0.53              |
| 4:0:116:ARG:O   | 4:X:339:VAL:C[1_556]   | 1.67                     | 0.53              |
| 4:0:210:ARG:N   | 4:X:193:LEU:O[1_556]   | 1.67                     | 0.53              |
| 4:2:68:LYS:CB   | 4:Z:59:GLN:CD[1_556]   | 1.67                     | 0.53              |
| 4:2:296:ASN:OD1 | 4:Z:318:THR:CB[1_556]  | 1.67                     | 0.53              |
| 4:0:116:ARG:O   | 4:X:340:TRP:N[1_556]   | 1.67                     | 0.53              |
| 4:0:371:HIS:O   | 4:X:140:LEU:CA[1_556]  | 1.67                     | 0.53              |
| 4:1:82:MET:CA   | 4:Y:30:VAL:CG1[1_556]  | 1.67                     | 0.53              |
| 4:0:149:THR:N   | 4:X:327:ILE:C[1_556]   | 1.67                     | 0.53              |
| 4:0:116:ARG:C   | 4:X:339:VAL:C[1_556]   | 1.67                     | 0.53              |
| 4:2:63:GLY:N    | 4:X:288:ASP:N[1_556]   | 1.67                     | 0.53              |
| 4:1:172:PRO:CB  | 4:Y:163:VAL:CA[1_556]  | 1.67                     | 0.53              |
| 4:0:122:ILE:CD1 | 4:X:19:ALA:CA[1_556]   | 1.67                     | 0.53              |
| 4:2:147:ARG:CB  | 4:Z:314:GLN:CD[1_556]  | 1.67                     | 0.53              |
| 4:1:77:THR:C    | 4:Y:33:SER:CB[1_556]   | 1.67                     | 0.53              |
| 4:0:272:ALA:N   | 4:X:270:GLU:CB[1_556]  | 1.67                     | 0.53              |
| 4:1:80:ASP:OD2  | 4:Y:93:GLU:OE2[1_556]  | 1.67                     | 0.53              |
| 4:2:140:LEU:O   | 4:Z:310:ALA:CB[1_556]  | 1.67                     | 0.53              |
| 4:0:296:ASN:OD1 | 4:X:318:THR:CB[1_556]  | 1.67                     | 0.53              |
| 4:2:296:ASN:O   | 4:Z:316:GLU:CA[1_556]  | 1.67                     | 0.53              |
| 4:0:33:SER:O    | 4:X:210:ARG:NE[1_556]  | 1.67                     | 0.53              |
| 4:1:166:TYR:CE1 | 4:Y:325:MET:CG[1_556]  | 1.67                     | 0.53              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:298:VAL:CG1 | 4:X:311:ASP:C[1_556]   | 1.67                     | 0.53              |
| 4:1:40:HIS:NE2  | 4:W:166:TYR:CG[1_556]  | 1.67                     | 0.53              |
| 4:1:299:MET:CB  | 4:Y:312:ARG:CG[1_556]  | 1.67                     | 0.53              |
| 4:2:149:THR:C   | 4:Z:327:ILE:CG1[1_556] | 1.67                     | 0.53              |
| 4:1:118:LYS:C   | 4:Y:340:TRP:NE1[1_556] | 1.67                     | 0.53              |
| 4:0:307:PRO:CA  | 4:X:227:MET:CG[1_556]  | 1.67                     | 0.53              |
| 4:1:253:GLU:N   | 4:X:113:LYS:CG[1_556]  | 1.67                     | 0.53              |
| 4:1:114:ALA:N   | 4:Y:106:THR:CB[1_556]  | 1.67                     | 0.53              |
| 4:1:79:TRP:CD1  | 4:Y:17:VAL:CB[1_556]   | 1.67                     | 0.53              |
| 4:0:166:TYR:O   | 4:X:294:TYR:N[1_556]   | 1.67                     | 0.53              |
| 4:2:114:ALA:N   | 4:Z:106:THR:CB[1_556]  | 1.67                     | 0.53              |
| 4:2:169:TYR:N   | 4:Z:296:ASN:N[1_556]   | 1.67                     | 0.53              |
| 4:2:150:GLY:C   | 4:Z:317:ILE:CG2[1_556] | 1.67                     | 0.53              |
| 4:0:304:THR:O   | 4:X:223:PHE:CG[1_556]  | 1.67                     | 0.53              |
| 4:0:150:GLY:C   | 4:X:317:ILE:CG2[1_556] | 1.67                     | 0.53              |
| 4:4:63:GLY:N    | 4:Z:288:ASP:N[1_556]   | 1.67                     | 0.53              |
| 4:3:39:ARG:CA   | 4:Y:166:TYR:OH[1_556]  | 1.67                     | 0.53              |
| 4:0:137:GLN:O   | 4:X:299:MET:CE[1_556]  | 1.67                     | 0.53              |
| 4:1:197:GLY:C   | 4:X:75:ILE:CB[1_556]   | 1.67                     | 0.53              |
| 4:1:180:LEU:CD2 | 4:Y:267:ILE:C[1_556]   | 1.67                     | 0.53              |
| 4:0:172:PRO:CB  | 4:X:163:VAL:CA[1_556]  | 1.67                     | 0.53              |
| 4:4:40:HIS:N    | 4:Z:166:TYR:CZ[1_556]  | 1.67                     | 0.53              |
| 4:0:119:MET:CB  | 4:X:340:TRP:CB[1_556]  | 1.67                     | 0.53              |
| 4:0:362:TYR:OH  | 4:X:22:ALA:N[1_556]    | 1.68                     | 0.52              |
| 4:2:295:ALA:N   | 4:Z:319:ALA:CB[1_556]  | 1.68                     | 0.52              |
| 4:2:296:ASN:N   | 4:Z:319:ALA:CB[1_556]  | 1.68                     | 0.52              |
| 4:0:298:VAL:CG2 | 4:X:315:LYS:N[1_556]   | 1.68                     | 0.52              |
| 4:2:197:GLY:C   | 4:Y:75:ILE:O[1_556]    | 1.68                     | 0.52              |
| 4:1:119:MET:CB  | 4:Y:340:TRP:CB[1_556]  | 1.68                     | 0.52              |
| 4:2:173:HIS:NE2 | 4:Z:281:SER:C[1_556]   | 1.68                     | 0.52              |
| 4:2:68:LYS:NZ   | 4:Z:59:GLN:CB[1_556]   | 1.68                     | 0.52              |
| 4:0:31:PHE:N    | 4:X:215:LYS:CG[1_556]  | 1.68                     | 0.52              |
| 4:1:174:ALA:O   | 4:Y:277:THR:CA[1_556]  | 1.68                     | 0.52              |
| 4:0:147:ARG:CD  | 4:X:314:GLN:OE1[1_556] | 1.68                     | 0.52              |
| 4:1:134:VAL:CA  | 4:Y:338:SER:OG[1_556]  | 1.68                     | 0.52              |
| 4:1:147:ARG:CD  | 4:Y:314:GLN:OE1[1_556] | 1.68                     | 0.52              |
| 4:2:371:HIS:CE1 | 4:Z:140:LEU:N[1_556]   | 1.68                     | 0.52              |
| 4:2:307:PRO:CA  | 4:Z:227:MET:CG[1_556]  | 1.68                     | 0.52              |
| 4:1:72:GLU:CD   | 4:Y:183:ARG:CZ[1_556]  | 1.68                     | 0.52              |
| 4:2:72:GLU:C    | 4:Z:157:ASP:CG[1_556]  | 1.68                     | 0.52              |
| 4:0:63:GLY:O    | 4:V:289:ILE:CA[1_556]  | 1.68                     | 0.52              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:125:GLU:CD  | 4:X:21:PHE:CA[1_556]   | 1.68                     | 0.52              |
| 4:0:79:TRP:CG   | 4:X:17:VAL:C[1_556]    | 1.68                     | 0.52              |
| 4:2:72:GLU:C    | 4:Z:157:ASP:CA[1_556]  | 1.68                     | 0.52              |
| 4:0:285:CYS:O   | 4:X:283:MET:CG[1_556]  | 1.68                     | 0.52              |
| 4:1:304:THR:O   | 4:Y:223:PHE:CG[1_556]  | 1.68                     | 0.52              |
| 4:2:62:ARG:C    | 4:X:288:ASP:CB[1_556]  | 1.68                     | 0.52              |
| 4:0:303:THR:CG2 | 4:X:257:CYS:O[1_556]   | 1.68                     | 0.52              |
| 4:0:295:ALA:N   | 4:X:319:ALA:CB[1_556]  | 1.68                     | 0.52              |
| 4:2:298:VAL:CG2 | 4:Z:315:LYS:N[1_556]   | 1.68                     | 0.52              |
| 4:1:281:SER:O   | 4:Y:280:ASN:CB[1_556]  | 1.68                     | 0.52              |
| 4:0:137:GLN:CD  | 4:X:304:THR:N[1_556]   | 1.68                     | 0.52              |
| 4:2:285:CYS:O   | 4:Z:283:MET:CG[1_556]  | 1.68                     | 0.52              |
| 4:3:39:ARG:C    | 4:Y:166:TYR:CZ[1_556]  | 1.68                     | 0.52              |
| 4:2:162:ASN:CB  | 4:Z:273:GLY:C[1_556]   | 1.68                     | 0.52              |
| 4:1:39:ARG:CA   | 4:W:166:TYR:OH[1_556]  | 1.68                     | 0.52              |
| 4:0:215:LYS:CB  | 4:X:196:ARG:NH1[1_556] | 1.68                     | 0.52              |
| 4:1:83:GLU:N    | 4:Y:30:VAL:N[1_556]    | 1.68                     | 0.52              |
| 4:2:304:THR:O   | 4:Z:223:PHE:CG[1_556]  | 1.68                     | 0.52              |
| 4:1:40:HIS:C    | 4:W:167:GLU:CD[1_556]  | 1.68                     | 0.52              |
| 4:0:301:GLY:C   | 4:X:218:TYR:O[1_556]   | 1.68                     | 0.52              |
| 4:1:336:LYS:CB  | 4:Y:218:TYR:N[1_556]   | 1.68                     | 0.52              |
| 4:2:362:TYR:CA  | 4:Z:348:SER:CB[1_556]  | 1.68                     | 0.52              |
| 4:0:233:SER:N   | 4:W:366:GLY:C[1_556]   | 1.68                     | 0.52              |
| 4:3:253:GLU:CD  | 4:Z:112:PRO:CA[1_556]  | 1.68                     | 0.52              |
| 4:0:72:GLU:C    | 4:X:157:ASP:CA[1_556]  | 1.68                     | 0.52              |
| 4:2:266:PHE:O   | 4:Y:172:PRO:CA[1_556]  | 1.68                     | 0.52              |
| 4:1:161:HIS:CA  | 4:Y:274:ILE:CG1[1_556] | 1.68                     | 0.52              |
| 4:1:227:MET:O   | 4:X:372:ARG:N[1_556]   | 1.68                     | 0.52              |
| 4:0:178:LEU:O   | 4:X:180:LEU:CD2[1_556] | 1.68                     | 0.52              |
| 4:2:131:ALA:C   | 4:Z:25:ASP:OD1[1_556]  | 1.68                     | 0.52              |
| 4:0:147:ARG:CB  | 4:X:314:GLN:CD[1_556]  | 1.68                     | 0.52              |
| 4:1:79:TRP:CB   | 4:Y:17:VAL:CG1[1_556]  | 1.68                     | 0.52              |
| 4:0:189:LEU:CG  | 4:X:195:GLU:CG[1_556]  | 1.68                     | 0.52              |
| 4:2:285:CYS:CA  | 4:Z:283:MET:N[1_556]   | 1.68                     | 0.52              |
| 4:2:293:LEU:O   | 4:Z:316:GLU:O[1_556]   | 1.68                     | 0.52              |
| 4:2:167:GLU:O   | 4:Z:295:ALA:CA[1_556]  | 1.68                     | 0.52              |
| 4:0:153:LEU:O   | 4:X:262:PHE:CE1[1_556] | 1.68                     | 0.52              |
| 4:0:264:PRO:CA  | 4:X:268:GLY:N[1_556]   | 1.68                     | 0.52              |
| 4:2:332:PRO:CG  | 4:Z:221:LEU:CD1[1_556] | 1.68                     | 0.52              |
| 4:0:73:HIS:CA   | 4:X:157:ASP:C[1_556]   | 1.68                     | 0.52              |
| 4:0:114:ALA:N   | 4:X:106:THR:CB[1_556]  | 1.68                     | 0.52              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:162:ASN:N   | 4:Z:274:ILE:N[1_556]   | 1.68                     | 0.52              |
| 4:1:233:SER:C   | 4:X:367:PRO:CG[1_556]  | 1.68                     | 0.52              |
| 4:2:137:GLN:O   | 4:Z:299:MET:CE[1_556]  | 1.68                     | 0.52              |
| 4:1:86:TRP:CZ2  | 4:Y:337:TYR:CZ[1_556]  | 1.68                     | 0.52              |
| 4:1:169:TYR:CG  | 4:Y:150:GLY:C[1_556]   | 1.68                     | 0.52              |
| 4:2:153:LEU:O   | 4:Z:262:PHE:CE1[1_556] | 1.68                     | 0.52              |
| 4:0:159:VAL:N   | 4:X:181:ALA:C[1_556]   | 1.68                     | 0.52              |
| 4:2:282:ILE:O   | 4:Z:279:TYR:CE2[1_556] | 1.68                     | 0.52              |
| 4:2:166:TYR:O   | 4:Z:294:TYR:N[1_556]   | 1.68                     | 0.52              |
| 4:2:210:ARG:C   | 4:Z:193:LEU:CG[1_556]  | 1.68                     | 0.52              |
| 4:2:274:ILE:CG2 | 4:Z:263:GLN:CA[1_556]  | 1.68                     | 0.52              |
| 4:2:40:HIS:CE1  | 4:X:166:TYR:CD2[1_556] | 1.68                     | 0.52              |
| 4:2:81:ASP:OD1  | 4:Z:56:ASP:OD1[1_556]  | 1.68                     | 0.52              |
| 4:1:298:VAL:CG2 | 4:Y:315:LYS:N[1_556]   | 1.69                     | 0.51              |
| 4:2:365:ALA:N   | 4:Z:348:SER:O[1_556]   | 1.69                     | 0.51              |
| 4:2:79:TRP:CG   | 4:Z:17:VAL:C[1_556]    | 1.69                     | 0.51              |
| 4:0:11:ASP:CA   | 4:X:305:MET:SD[1_556]  | 1.69                     | 0.51              |
| 4:1:33:SER:O    | 4:Y:210:ARG:NE[1_556]  | 1.69                     | 0.51              |
| 4:2:116:ARG:C   | 4:Z:339:VAL:C[1_556]   | 1.69                     | 0.51              |
| 4:3:197:GLY:C   | 4:Z:75:ILE:CB[1_556]   | 1.69                     | 0.51              |
| 4:0:253:GLU:N   | 4:W:113:LYS:CG[1_556]  | 1.69                     | 0.51              |
| 4:0:142:LEU:CB  | 4:X:329:ILE:CB[1_556]  | 1.69                     | 0.51              |
| 4:2:116:ARG:O   | 4:Z:340:TRP:N[1_556]   | 1.69                     | 0.51              |
| 4:1:186:THR:O   | 4:Y:191:LYS:O[1_556]   | 1.69                     | 0.51              |
| 4:2:281:SER:O   | 4:Z:280:ASN:N[1_556]   | 1.69                     | 0.51              |
| 4:1:278:THR:O   | 4:Y:276:GLU:CD[1_556]  | 1.69                     | 0.51              |
| 4:0:230:ALA:N   | 4:W:368:SER:CA[1_556]  | 1.69                     | 0.51              |
| 4:0:113:LYS:CD  | 4:X:136:ILE:CB[1_556]  | 1.69                     | 0.51              |
| 4:0:282:ILE:O   | 4:X:279:TYR:CE2[1_556] | 1.69                     | 0.51              |
| 4:1:105:LEU:N   | 4:Y:334:GLU:C[1_556]   | 1.69                     | 0.51              |
| 4:3:196:ARG:NE  | 4:Z:115:ASN:CB[1_556]  | 1.69                     | 0.51              |
| 4:0:62:ARG:C    | 4:V:288:ASP:CB[1_556]  | 1.69                     | 0.51              |
| 4:1:136:ILE:CB  | 4:Y:299:MET:C[1_556]   | 1.69                     | 0.51              |
| 4:1:137:GLN:CD  | 4:Y:304:THR:N[1_556]   | 1.69                     | 0.51              |
| 4:1:16:LEU:CG   | 4:Y:214:GLU:CA[1_556]  | 1.69                     | 0.51              |
| 4:0:77:THR:CB   | 4:X:15:GLY:CA[1_556]   | 1.69                     | 0.51              |
| 4:1:291:LYS:NZ  | 4:Y:322:PRO:O[1_556]   | 1.69                     | 0.51              |
| 4:1:142:LEU:O   | 4:Y:314:GLN:CG[1_556]  | 1.69                     | 0.51              |
| 4:1:173:HIS:NE2 | 4:Y:281:SER:C[1_556]   | 1.69                     | 0.51              |
| 4:2:137:GLN:CG  | 4:Z:304:THR:CB[1_556]  | 1.69                     | 0.51              |
| 4:2:105:LEU:C   | 4:Z:335:ARG:CA[1_556]  | 1.69                     | 0.51              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:215:LYS:CB  | 4:Z:196:ARG:NH1[1_556] | 1.69                     | 0.51              |
| 4:0:32:PRO:CD   | 4:X:211:ASP:CB[1_556]  | 1.69                     | 0.51              |
| 4:2:339:VAL:CB  | 4:Z:335:ARG:NH2[1_556] | 1.69                     | 0.51              |
| 4:0:124:PHE:CD1 | 4:X:23:GLY:O[1_556]    | 1.69                     | 0.51              |
| 4:0:203:THR:CG2 | 4:X:205:GLU:OE2[1_556] | 1.69                     | 0.51              |
| 4:2:233:SER:N   | 4:Y:366:GLY:C[1_556]   | 1.69                     | 0.51              |
| 4:2:286:ASP:OD2 | 4:Z:290:ARG:CD[1_556]  | 1.69                     | 0.51              |
| 4:1:299:MET:C   | 4:Y:312:ARG:CG[1_556]  | 1.69                     | 0.51              |
| 4:0:332:PRO:N   | 4:X:221:LEU:CA[1_556]  | 1.69                     | 0.51              |
| 4:1:177:ARG:CD  | 4:Y:160:THR:N[1_556]   | 1.69                     | 0.51              |
| 4:2:301:GLY:C   | 4:Z:218:TYR:O[1_556]   | 1.69                     | 0.51              |
| 4:2:281:SER:C   | 4:Z:280:ASN:CG[1_556]  | 1.69                     | 0.51              |
| 4:3:227:MET:O   | 4:Z:372:ARG:N[1_556]   | 1.69                     | 0.51              |
| 4:2:299:MET:C   | 4:Z:312:ARG:CB[1_556]  | 1.69                     | 0.51              |
| 4:0:210:ARG:N   | 4:X:193:LEU:C[1_556]   | 1.69                     | 0.51              |
| 4:1:293:LEU:O   | 4:Y:316:GLU:O[1_556]   | 1.69                     | 0.51              |
| 4:0:281:SER:C   | 4:X:280:ASN:CG[1_556]  | 1.69                     | 0.51              |
| 4:0:174:ALA:N   | 4:X:281:SER:OG[1_556]  | 1.69                     | 0.51              |
| 4:2:72:GLU:C    | 4:Z:157:ASP:CB[1_556]  | 1.69                     | 0.51              |
| 4:0:299:MET:C   | 4:X:312:ARG:CB[1_556]  | 1.69                     | 0.51              |
| 4:3:192:ILE:O   | 4:Z:112:PRO:CD[1_556]  | 1.69                     | 0.51              |
| 4:0:72:GLU:C    | 4:X:157:ASP:CG[1_556]  | 1.69                     | 0.51              |
| 4:0:122:ILE:CG1 | 4:X:19:ALA:N[1_556]    | 1.69                     | 0.51              |
| 4:2:190:MET:SD  | 4:Z:194:THR:CB[1_556]  | 1.69                     | 0.51              |
| 4:1:40:HIS:CE1  | 4:W:166:TYR:CD2[1_556] | 1.69                     | 0.51              |
| 4:1:209:VAL:N   | 4:Y:198:TYR:CG[1_556]  | 1.69                     | 0.51              |
| 4:1:357:ILE:CB  | 4:Y:345:ILE:CG1[1_556] | 1.69                     | 0.51              |
| 4:1:161:HIS:CE1 | 4:Y:155:SER:OG[1_556]  | 1.69                     | 0.51              |
| 4:1:370:VAL:CB  | 4:Y:342:GLY:CA[1_556]  | 1.69                     | 0.51              |
| 4:0:16:LEU:C    | 4:X:214:GLU:CG[1_556]  | 1.69                     | 0.51              |
| 4:0:234:SER:N   | 4:W:367:PRO:N[1_556]   | 1.69                     | 0.51              |
| 4:0:190:MET:SD  | 4:X:194:THR:CB[1_556]  | 1.69                     | 0.51              |
| 4:2:210:ARG:N   | 4:Z:193:LEU:O[1_556]   | 1.69                     | 0.51              |
| 4:2:290:ARG:O   | 4:Z:320:LEU:C[1_556]   | 1.69                     | 0.51              |
| 4:1:148:THR:CB  | 4:Y:328:LYS:CA[1_556]  | 1.69                     | 0.51              |
| 4:0:293:LEU:O   | 4:X:316:GLU:O[1_556]   | 1.69                     | 0.51              |
| 4:0:133:TYR:C   | 4:X:334:GLU:OE1[1_556] | 1.69                     | 0.51              |
| 4:2:11:ASP:CA   | 4:Z:305:MET:SD[1_556]  | 1.69                     | 0.51              |
| 4:1:372:ARG:NH1 | 4:Y:142:LEU:O[1_556]   | 1.69                     | 0.51              |
| 4:1:306:TYR:N   | 4:Y:255:PHE:CE1[1_556] | 1.69                     | 0.51              |
| 4:2:116:ARG:O   | 4:Z:339:VAL:C[1_556]   | 1.69                     | 0.51              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:272:ALA:N   | 4:Z:270:GLU:CB[1_556]  | 1.69                     | 0.51              |
| 4:0:37:ARG:CZ   | 4:X:56:ASP:C[1_556]    | 1.69                     | 0.51              |
| 4:2:253:GLU:N   | 4:Y:113:LYS:CG[1_556]  | 1.69                     | 0.51              |
| 4:1:131:ALA:C   | 4:Y:25:ASP:OD1[1_556]  | 1.69                     | 0.51              |
| 4:2:125:GLU:CD  | 4:Z:21:PHE:CA[1_556]   | 1.69                     | 0.51              |
| 4:1:196:ARG:NE  | 4:X:115:ASN:CB[1_556]  | 1.69                     | 0.51              |
| 4:0:159:VAL:CG1 | 4:X:180:LEU:C[1_556]   | 1.69                     | 0.51              |
| 4:2:107:GLU:OE1 | 4:Z:339:VAL:CG2[1_556] | 1.69                     | 0.51              |
| 4:1:212:ILE:C   | 4:Y:196:ARG:CB[1_556]  | 1.69                     | 0.51              |
| 4:1:153:LEU:N   | 4:Y:262:PHE:CD1[1_556] | 1.69                     | 0.51              |
| 4:2:230:ALA:N   | 4:Y:368:SER:CA[1_556]  | 1.69                     | 0.51              |
| 4:2:33:SER:O    | 4:Z:210:ARG:NE[1_556]  | 1.69                     | 0.51              |
| 4:0:362:TYR:CA  | 4:X:348:SER:CB[1_556]  | 1.69                     | 0.51              |
| 4:2:232:SER:C   | 4:Y:366:GLY:C[1_556]   | 1.69                     | 0.51              |
| 4:2:110:LEU:CD1 | 4:Z:161:HIS:CB[1_556]  | 1.69                     | 0.51              |
| 4:2:332:PRO:N   | 4:Z:221:LEU:CA[1_556]  | 1.69                     | 0.51              |
| 4:2:67:LEU:O    | 4:Z:62:ARG:NH1[1_556]  | 1.69                     | 0.51              |
| 4:2:124:PHE:CB  | 4:Z:24:ASP:CA[1_556]   | 1.69                     | 0.51              |
| 4:1:174:ALA:O   | 4:Y:277:THR:C[1_556]   | 1.69                     | 0.51              |
| 4:1:174:ALA:N   | 4:Y:281:SER:OG[1_556]  | 1.69                     | 0.51              |
| 4:1:294:TYR:CB  | 4:Y:319:ALA:O[1_556]   | 1.70                     | 0.50              |
| 4:3:233:SER:C   | 4:Z:367:PRO:CG[1_556]  | 1.70                     | 0.50              |
| 4:2:229:THR:O   | 4:Y:368:SER:N[1_556]   | 1.70                     | 0.50              |
| 4:2:197:GLY:C   | 4:Y:75:ILE:CB[1_556]   | 1.70                     | 0.50              |
| 4:0:368:SER:CB  | 4:X:346:LEU:CD2[1_556] | 1.70                     | 0.50              |
| 4:1:116:ARG:NH1 | 4:Y:141:SER:CA[1_556]  | 1.70                     | 0.50              |
| 4:2:281:SER:C   | 4:Z:276:GLU:O[1_556]   | 1.70                     | 0.50              |
| 4:0:113:LYS:NZ  | 4:X:136:ILE:CG1[1_556] | 1.70                     | 0.50              |
| 4:1:112:PRO:CA  | 4:Y:137:GLN:CG[1_556]  | 1.70                     | 0.50              |
| 4:0:106:THR:O   | 4:X:335:ARG:C[1_556]   | 1.70                     | 0.50              |
| 4:1:157:ASP:C   | 4:Y:185:LEU:C[1_556]   | 1.70                     | 0.50              |
| 4:0:286:ASP:OD2 | 4:X:290:ARG:CD[1_556]  | 1.70                     | 0.50              |
| 4:2:32:PRO:CD   | 4:Z:211:ASP:CB[1_556]  | 1.70                     | 0.50              |
| 4:2:106:THR:O   | 4:Z:335:ARG:C[1_556]   | 1.70                     | 0.50              |
| 4:1:311:ASP:OD1 | 4:Y:224:GLU:CG[1_556]  | 1.70                     | 0.50              |
| 4:0:149:THR:CA  | 4:X:327:ILE:CG2[1_556] | 1.70                     | 0.50              |
| 4:1:301:GLY:CA  | 4:Y:219:VAL:CG2[1_556] | 1.70                     | 0.50              |
| 4:2:31:PHE:N    | 4:Z:215:LYS:CG[1_556]  | 1.70                     | 0.50              |
| 4:1:178:LEU:O   | 4:Y:180:LEU:CD2[1_556] | 1.70                     | 0.50              |
| 4:0:67:LEU:O    | 4:X:62:ARG:NH1[1_556]  | 1.70                     | 0.50              |
| 4:3:253:GLU:CG  | 4:Z:112:PRO:CA[1_556]  | 1.70                     | 0.50              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:109:PRO:CA  | 4:Y:154:ASP:C[1_556]   | 1.70                     | 0.50              |
| 4:1:119:MET:C   | 4:Y:340:TRP:CB[1_556]  | 1.70                     | 0.50              |
| 4:2:233:SER:C   | 4:Y:367:PRO:CG[1_556]  | 1.70                     | 0.50              |
| 4:2:140:LEU:CD2 | 4:Z:332:PRO:N[1_556]   | 1.70                     | 0.50              |
| 4:1:162:ASN:CG  | 4:Y:273:GLY:CA[1_556]  | 1.70                     | 0.50              |
| 4:2:203:THR:CG2 | 4:Z:205:GLU:OE2[1_556] | 1.70                     | 0.50              |
| 4:1:172:PRO:CG  | 4:Y:164:PRO:CA[1_556]  | 1.70                     | 0.50              |
| 4:1:39:ARG:C    | 4:W:166:TYR:CZ[1_556]  | 1.70                     | 0.50              |
| 4:1:115:ASN:CG  | 4:Y:11:ASP:OD1[1_556]  | 1.70                     | 0.50              |
| 4:0:129:VAL:CB  | 4:X:25:ASP:CB[1_556]   | 1.70                     | 0.50              |
| 4:0:40:HIS:CG   | 4:V:166:TYR:CD2[1_556] | 1.70                     | 0.50              |
| 4:2:77:THR:CB   | 4:Z:15:GLY:CA[1_556]   | 1.70                     | 0.50              |
| 4:1:215:LYS:CB  | 4:Y:196:ARG:CZ[1_556]  | 1.70                     | 0.50              |
| 4:1:192:ILE:O   | 4:X:112:PRO:CD[1_556]  | 1.70                     | 0.50              |
| 4:1:77:THR:CB   | 4:Y:14:SER:O[1_556]    | 1.70                     | 0.50              |
| 4:4:64:ILE:CD1  | 4:Z:292:ASP:OD2[1_556] | 1.70                     | 0.50              |
| 4:0:124:PHE:CB  | 4:X:24:ASP:CA[1_556]   | 1.70                     | 0.50              |
| 4:2:137:GLN:CD  | 4:Z:304:THR:N[1_556]   | 1.70                     | 0.50              |
| 4:3:40:HIS:C    | 4:Y:167:GLU:CD[1_556]  | 1.70                     | 0.50              |
| 4:1:261:LEU:CD2 | 4:Y:266:PHE:CB[1_556]  | 1.70                     | 0.50              |
| 4:1:253:GLU:CG  | 4:X:112:PRO:CA[1_556]  | 1.70                     | 0.50              |
| 4:2:189:LEU:CG  | 4:Z:195:GLU:CG[1_556]  | 1.70                     | 0.50              |
| 4:1:73:HIS:ND1  | 4:Y:184:ASP:OD1[1_556] | 1.70                     | 0.50              |
| 4:2:16:LEU:C    | 4:Z:214:GLU:CG[1_556]  | 1.70                     | 0.50              |
| 4:0:365:ALA:N   | 4:X:348:SER:O[1_556]   | 1.70                     | 0.50              |
| 4:0:158:GLY:N   | 4:X:185:LEU:CB[1_556]  | 1.70                     | 0.50              |
| 4:1:137:GLN:O   | 4:Y:299:MET:CE[1_556]  | 1.70                     | 0.50              |
| 4:1:73:HIS:C    | 4:Y:156:GLY:O[1_556]   | 1.70                     | 0.50              |
| 4:0:113:LYS:CA  | 4:X:137:GLN:CA[1_556]  | 1.70                     | 0.50              |
| 4:0:131:ALA:C   | 4:X:25:ASP:OD1[1_556]  | 1.70                     | 0.50              |
| 4:0:86:TRP:CZ2  | 4:X:337:TYR:CD1[1_556] | 1.70                     | 0.50              |
| 4:2:149:THR:CA  | 4:Z:327:ILE:CG2[1_556] | 1.70                     | 0.50              |
| 4:1:286:ASP:CB  | 4:Y:290:ARG:CZ[1_556]  | 1.70                     | 0.50              |
| 4:2:178:LEU:O   | 4:Z:180:LEU:CD2[1_556] | 1.70                     | 0.50              |
| 4:2:133:TYR:C   | 4:Z:334:GLU:OE1[1_556] | 1.70                     | 0.50              |
| 4:1:268:GLY:O   | 4:X:284:LYS:C[1_556]   | 1.70                     | 0.50              |
| 4:0:210:ARG:C   | 4:X:193:LEU:CG[1_556]  | 1.70                     | 0.50              |
| 4:1:180:LEU:CA  | 4:Y:267:ILE:CD1[1_556] | 1.70                     | 0.50              |
| 4:0:229:THR:O   | 4:W:368:SER:N[1_556]   | 1.70                     | 0.50              |
| 4:2:129:VAL:CB  | 4:Z:25:ASP:CB[1_556]   | 1.70                     | 0.50              |
| 4:0:285:CYS:CA  | 4:X:283:MET:N[1_556]   | 1.70                     | 0.50              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:297:ASN:N   | 4:Z:316:GLU:CA[1_556]  | 1.70                     | 0.50              |
| 4:0:40:HIS:CE1  | 4:V:166:TYR:CD2[1_556] | 1.70                     | 0.50              |
| 4:2:206:ARG:CD  | 4:Z:200:PHE:CA[1_556]  | 1.70                     | 0.50              |
| 4:1:12:ASN:CG   | 4:Y:336:LYS:CD[1_556]  | 1.70                     | 0.50              |
| 4:1:141:SER:O   | 4:Y:310:ALA:CA[1_556]  | 1.70                     | 0.50              |
| 4:2:78:ASN:CB   | 4:Z:32:PRO:O[1_556]    | 1.70                     | 0.50              |
| 4:2:116:ARG:NH2 | 4:Z:141:SER:CB[1_556]  | 1.70                     | 0.50              |
| 4:2:371:HIS:ND1 | 4:Z:140:LEU:CB[1_556]  | 1.70                     | 0.50              |
| 4:0:274:ILE:CG2 | 4:X:263:GLN:CA[1_556]  | 1.70                     | 0.50              |
| 4:0:116:ARG:NH2 | 4:X:141:SER:CB[1_556]  | 1.70                     | 0.50              |
| 4:2:234:SER:N   | 4:Y:367:PRO:N[1_556]   | 1.70                     | 0.50              |
| 4:1:116:ARG:O   | 4:Y:339:VAL:C[1_556]   | 1.70                     | 0.50              |
| 4:2:62:ARG:CZ   | 4:Z:205:GLU:N[1_556]   | 1.70                     | 0.50              |
| 4:0:15:GLY:C    | 4:X:210:ARG:O[1_556]   | 1.70                     | 0.50              |
| 4:1:72:GLU:OE1  | 4:Y:183:ARG:NE[1_556]  | 1.70                     | 0.50              |
| 4:0:339:VAL:CB  | 4:X:335:ARG:NH2[1_556] | 1.70                     | 0.50              |
| 4:0:127:PHE:CD2 | 4:X:27:PRO:O[1_556]    | 1.70                     | 0.50              |
| 4:1:186:THR:O   | 4:Y:191:LYS:C[1_556]   | 1.70                     | 0.50              |
| 4:0:124:PHE:CD1 | 4:X:24:ASP:O[1_556]    | 1.70                     | 0.50              |
| 4:0:107:GLU:OE1 | 4:X:339:VAL:CG2[1_556] | 1.70                     | 0.50              |
| 4:1:137:GLN:OE1 | 4:Y:303:THR:C[1_556]   | 1.70                     | 0.50              |
| 4:1:149:THR:N   | 4:Y:327:ILE:C[1_556]   | 1.70                     | 0.50              |
| 4:0:212:ILE:CB  | 4:X:196:ARG:O[1_556]   | 1.70                     | 0.50              |
| 4:0:81:ASP:OD1  | 4:X:56:ASP:OD1[1_556]  | 1.70                     | 0.50              |
| 4:1:365:ALA:N   | 4:Y:349:LEU:C[1_556]   | 1.70                     | 0.50              |
| 4:1:285:CYS:CA  | 4:Y:283:MET:N[1_556]   | 1.70                     | 0.50              |
| 4:2:336:LYS:CE  | 4:Z:254:ARG:NH2[1_556] | 1.70                     | 0.50              |
| 4:1:116:ARG:CZ  | 4:Y:141:SER:CB[1_556]  | 1.70                     | 0.50              |
| 4:0:62:ARG:CD   | 4:X:204:ALA:O[1_556]   | 1.70                     | 0.50              |
| 4:0:232:SER:C   | 4:W:366:GLY:C[1_556]   | 1.70                     | 0.50              |
| 4:2:160:THR:CA  | 4:Z:261:LEU:CD2[1_556] | 1.70                     | 0.50              |
| 4:0:281:SER:O   | 4:X:280:ASN:N[1_556]   | 1.71                     | 0.49              |
| 4:2:210:ARG:N   | 4:Z:193:LEU:C[1_556]   | 1.71                     | 0.49              |
| 4:2:86:TRP:CZ2  | 4:Z:337:TYR:CD1[1_556] | 1.71                     | 0.49              |
| 4:2:268:GLY:C   | 4:Y:284:LYS:O[1_556]   | 1.71                     | 0.49              |
| 4:2:62:ARG:CD   | 4:Z:204:ALA:O[1_556]   | 1.71                     | 0.49              |
| 4:2:277:THR:OG1 | 4:Z:272:ALA:CA[1_556]  | 1.71                     | 0.49              |
| 4:1:124:PHE:C   | 4:Y:24:ASP:OD2[1_556]  | 1.71                     | 0.49              |
| 4:2:299:MET:CA  | 4:Z:312:ARG:CB[1_556]  | 1.71                     | 0.49              |
| 4:2:83:GLU:N    | 4:Z:30:VAL:N[1_556]    | 1.71                     | 0.49              |
| 4:2:278:THR:OG1 | 4:Z:275:HIS:CE1[1_556] | 1.71                     | 0.49              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:281:SER:C   | 4:X:276:GLU:O[1_556]   | 1.71                     | 0.49              |
| 4:1:229:THR:O   | 4:X:368:SER:N[1_556]   | 1.71                     | 0.49              |
| 4:4:40:HIS:CG   | 4:Z:166:TYR:CD2[1_556] | 1.71                     | 0.49              |
| 4:2:40:HIS:CG   | 4:X:166:TYR:CD2[1_556] | 1.71                     | 0.49              |
| 4:1:294:TYR:CA  | 4:Y:319:ALA:C[1_556]   | 1.71                     | 0.49              |
| 4:0:371:HIS:ND1 | 4:X:140:LEU:CB[1_556]  | 1.71                     | 0.49              |
| 4:0:197:GLY:C   | 4:W:75:ILE:CB[1_556]   | 1.71                     | 0.49              |
| 4:0:335:ARG:CD  | 4:X:220:ALA:CB[1_556]  | 1.71                     | 0.49              |
| 4:1:31:PHE:N    | 4:Y:215:LYS:CG[1_556]  | 1.71                     | 0.49              |
| 4:2:37:ARG:CZ   | 4:Z:56:ASP:C[1_556]    | 1.71                     | 0.49              |
| 4:0:206:ARG:CD  | 4:X:200:PHE:CA[1_556]  | 1.71                     | 0.49              |
| 4:1:145:SER:CA  | 4:Y:311:ASP:OD1[1_556] | 1.71                     | 0.49              |
| 4:1:79:TRP:CE3  | 4:Y:17:VAL:C[1_556]    | 1.71                     | 0.49              |
| 4:1:148:THR:CA  | 4:Y:327:ILE:C[1_556]   | 1.71                     | 0.49              |
| 4:2:150:GLY:O   | 4:Z:317:ILE:CD1[1_556] | 1.71                     | 0.49              |
| 4:0:141:SER:OG  | 4:X:309:ILE:CA[1_556]  | 1.71                     | 0.49              |
| 4:2:122:ILE:CG1 | 4:Z:19:ALA:N[1_556]    | 1.71                     | 0.49              |
| 4:2:106:THR:O   | 4:Z:336:LYS:N[1_556]   | 1.71                     | 0.49              |
| 4:1:180:LEU:CG  | 4:Y:267:ILE:CD1[1_556] | 1.71                     | 0.49              |
| 4:1:172:PRO:CD  | 4:Y:164:PRO:N[1_556]   | 1.71                     | 0.49              |
| 4:0:72:GLU:C    | 4:X:157:ASP:CB[1_556]  | 1.71                     | 0.49              |
| 4:0:233:SER:C   | 4:W:367:PRO:CG[1_556]  | 1.71                     | 0.49              |
| 4:2:113:LYS:CD  | 4:Z:136:ILE:CB[1_556]  | 1.71                     | 0.49              |
| 4:2:64:ILE:CD1  | 4:X:292:ASP:OD2[1_556] | 1.71                     | 0.49              |
| 4:1:86:TRP:CE3  | 4:Y:30:VAL:CG2[1_556]  | 1.71                     | 0.49              |
| 4:0:290:ARG:O   | 4:X:320:LEU:C[1_556]   | 1.71                     | 0.49              |
| 4:0:336:LYS:CE  | 4:X:254:ARG:NH2[1_556] | 1.71                     | 0.49              |
| 4:3:40:HIS:CE1  | 4:Y:166:TYR:CD2[1_556] | 1.71                     | 0.49              |
| 4:1:119:MET:N   | 4:Y:340:TRP:CG[1_556]  | 1.71                     | 0.49              |
| 4:2:159:VAL:CG1 | 4:Z:180:LEU:C[1_556]   | 1.71                     | 0.49              |
| 4:1:81:ASP:CA   | 4:Y:31:PHE:CA[1_556]   | 1.71                     | 0.49              |
| 4:0:180:LEU:CD2 | 4:X:267:ILE:C[1_556]   | 1.71                     | 0.49              |
| 4:2:145:SER:CA  | 4:Z:311:ASP:OD1[1_556] | 1.71                     | 0.49              |
| 4:0:106:THR:O   | 4:X:336:LYS:N[1_556]   | 1.71                     | 0.49              |
| 4:0:142:LEU:O   | 4:X:314:GLN:CG[1_556]  | 1.71                     | 0.49              |
| 4:0:180:LEU:CA  | 4:X:267:ILE:CD1[1_556] | 1.71                     | 0.49              |
| 4:0:196:ARG:CG  | 4:W:115:ASN:CG[1_556]  | 1.71                     | 0.49              |
| 4:1:141:SER:OG  | 4:Y:309:ILE:CA[1_556]  | 1.71                     | 0.49              |
| 4:0:30:VAL:C    | 4:X:215:LYS:CG[1_556]  | 1.71                     | 0.49              |
| 4:0:134:VAL:CA  | 4:X:338:SER:OG[1_556]  | 1.71                     | 0.49              |
| 4:2:195:GLU:OE1 | 4:Y:109:PRO:C[1_556]   | 1.71                     | 0.49              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:117:GLU:OE1 | 4:Y:104:LEU:CD2[1_556] | 1.71                     | 0.49              |
| 4:2:217:CYS:CB  | 4:Z:256:ARG:CZ[1_556]  | 1.71                     | 0.49              |
| 4:3:229:THR:O   | 4:Z:368:SER:N[1_556]   | 1.71                     | 0.49              |
| 4:0:83:GLU:N    | 4:X:30:VAL:C[1_556]    | 1.71                     | 0.49              |
| 4:2:169:TYR:CG  | 4:Z:150:GLY:C[1_556]   | 1.71                     | 0.49              |
| 4:0:210:ARG:CA  | 4:X:193:LEU:CA[1_556]  | 1.71                     | 0.49              |
| 4:3:268:GLY:O   | 4:Z:284:LYS:C[1_556]   | 1.71                     | 0.49              |
| 4:2:127:PHE:CD2 | 4:Z:27:PRO:O[1_556]    | 1.71                     | 0.49              |
| 4:0:173:HIS:CD2 | 4:X:281:SER:C[1_556]   | 1.71                     | 0.49              |
| 4:1:118:LYS:CG  | 4:Y:18:LYS:O[1_556]    | 1.71                     | 0.49              |
| 4:0:62:ARG:CZ   | 4:X:205:GLU:N[1_556]   | 1.71                     | 0.49              |
| 4:0:104:LEU:CD2 | 4:X:332:PRO:C[1_556]   | 1.71                     | 0.49              |
| 4:0:64:ILE:CD1  | 4:V:292:ASP:OD2[1_556] | 1.71                     | 0.49              |
| 4:2:206:ARG:C   | 4:Z:199:SER:C[1_556]   | 1.71                     | 0.49              |
| 4:1:362:TYR:N   | 4:Y:348:SER:OG[1_556]  | 1.71                     | 0.49              |
| 4:1:137:GLN:C   | 4:Y:299:MET:CG[1_556]  | 1.71                     | 0.49              |
| 4:1:362:TYR:OH  | 4:Y:22:ALA:N[1_556]    | 1.71                     | 0.49              |
| 4:1:203:THR:N   | 4:Y:201:VAL:CG2[1_556] | 1.71                     | 0.49              |
| 4:3:195:GLU:OE2 | 4:Z:109:PRO:CA[1_556]  | 1.71                     | 0.49              |
| 4:2:306:TYR:OH  | 4:Z:192:ILE:CD1[1_556] | 1.71                     | 0.49              |
| 4:0:177:ARG:O   | 4:X:178:LEU:CD1[1_556] | 1.71                     | 0.49              |
| 4:0:277:THR:OG1 | 4:X:272:ALA:CA[1_556]  | 1.71                     | 0.49              |
| 4:0:76:ILE:CG2  | 4:X:16:LEU:CB[1_556]   | 1.71                     | 0.49              |
| 4:2:15:GLY:C    | 4:Z:210:ARG:O[1_556]   | 1.71                     | 0.49              |
| 4:0:203:THR:CA  | 4:X:201:VAL:CG2[1_556] | 1.71                     | 0.49              |
| 4:0:72:GLU:OE2  | 4:X:183:ARG:CG[1_556]  | 1.71                     | 0.49              |
| 4:2:212:ILE:CB  | 4:Z:196:ARG:O[1_556]   | 1.71                     | 0.49              |
| 4:1:132:MET:SD  | 4:Y:341:ILE:CB[1_556]  | 1.71                     | 0.49              |
| 4:1:306:TYR:OH  | 4:Y:192:ILE:CD1[1_556] | 1.71                     | 0.49              |
| 4:2:232:SER:CA  | 4:Y:366:GLY:O[1_556]   | 1.71                     | 0.49              |
| 4:0:67:LEU:CA   | 4:X:207:GLU:OE2[1_556] | 1.71                     | 0.49              |
| 4:1:209:VAL:CG2 | 4:Y:195:GLU:N[1_556]   | 1.71                     | 0.49              |
| 4:2:369:ILE:CA  | 4:Z:346:LEU:CA[1_556]  | 1.71                     | 0.49              |
| 4:0:257:CYS:SG  | 4:X:195:GLU:OE1[1_556] | 1.71                     | 0.49              |
| 4:1:177:ARG:NH2 | 4:Y:159:VAL:N[1_556]   | 1.71                     | 0.49              |
| 4:1:108:ALA:CB  | 4:Y:155:SER:CA[1_556]  | 1.71                     | 0.49              |
| 4:2:284:LYS:C   | 4:Z:280:ASN:O[1_556]   | 1.72                     | 0.48              |
| 4:0:195:GLU:OE1 | 4:W:109:PRO:C[1_556]   | 1.72                     | 0.48              |
| 4:0:268:GLY:C   | 4:W:284:LYS:O[1_556]   | 1.72                     | 0.48              |
| 4:0:137:GLN:OE1 | 4:X:303:THR:C[1_556]   | 1.72                     | 0.48              |
| 4:2:83:GLU:N    | 4:Z:30:VAL:C[1_556]    | 1.72                     | 0.48              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:369:ILE:CG1 | 4:X:345:ILE:CG2[1_556] | 1.72                     | 0.48              |
| 4:1:261:LEU:O   | 4:Y:265:SER:N[1_556]   | 1.72                     | 0.48              |
| 4:0:124:PHE:O   | 4:X:24:ASP:CB[1_556]   | 1.72                     | 0.48              |
| 4:1:143:TYR:CB  | 4:Y:329:ILE:O[1_556]   | 1.72                     | 0.48              |
| 4:2:177:ARG:NH1 | 4:Z:159:VAL:CB[1_556]  | 1.72                     | 0.48              |
| 4:1:188:TYR:N   | 4:Y:191:LYS:CB[1_556]  | 1.72                     | 0.48              |
| 4:0:110:LEU:CD1 | 4:X:161:HIS:CB[1_556]  | 1.72                     | 0.48              |
| 4:0:33:SER:CA   | 4:X:210:ARG:CZ[1_556]  | 1.72                     | 0.48              |
| 4:1:368:SER:CB  | 4:Y:346:LEU:CD2[1_556] | 1.72                     | 0.48              |
| 4:0:206:ARG:C   | 4:X:199:SER:C[1_556]   | 1.72                     | 0.48              |
| 4:2:180:LEU:CD1 | 4:Z:267:ILE:CG1[1_556] | 1.72                     | 0.48              |
| 4:4:40:HIS:C    | 4:Z:167:GLU:CD[1_556]  | 1.72                     | 0.48              |
| 4:1:15:GLY:C    | 4:Y:210:ARG:O[1_556]   | 1.72                     | 0.48              |
| 4:1:81:ASP:OD2  | 4:Y:32:PRO:CD[1_556]   | 1.72                     | 0.48              |
| 4:1:166:TYR:O   | 4:Y:293:LEU:C[1_556]   | 1.72                     | 0.48              |
| 4:1:284:LYS:CB  | 4:Y:280:ASN:CB[1_556]  | 1.72                     | 0.48              |
| 4:1:294:TYR:N   | 4:Y:319:ALA:C[1_556]   | 1.72                     | 0.48              |
| 4:2:196:ARG:CG  | 4:Y:115:ASN:CG[1_556]  | 1.72                     | 0.48              |
| 4:2:124:PHE:CD1 | 4:Z:24:ASP:O[1_556]    | 1.72                     | 0.48              |
| 4:2:113:LYS:NZ  | 4:Z:136:ILE:CG1[1_556] | 1.72                     | 0.48              |
| 4:1:122:ILE:CG2 | 4:Y:28:ARG:N[1_556]    | 1.72                     | 0.48              |
| 4:2:303:THR:CB  | 4:Z:258:PRO:N[1_556]   | 1.72                     | 0.48              |
| 4:2:368:SER:CB  | 4:Z:346:LEU:CD2[1_556] | 1.72                     | 0.48              |
| 4:0:140:LEU:CD2 | 4:X:332:PRO:N[1_556]   | 1.72                     | 0.48              |
| 4:0:209:VAL:CG2 | 4:X:195:GLU:N[1_556]   | 1.72                     | 0.48              |
| 4:0:78:ASN:CB   | 4:X:32:PRO:O[1_556]    | 1.72                     | 0.48              |
| 4:1:83:GLU:CA   | 4:Y:30:VAL:N[1_556]    | 1.72                     | 0.48              |
| 4:1:168:GLY:CA  | 4:Y:296:ASN:CA[1_556]  | 1.72                     | 0.48              |
| 4:1:212:ILE:CB  | 4:Y:196:ARG:O[1_556]   | 1.72                     | 0.48              |
| 4:1:336:LYS:CE  | 4:Y:254:ARG:NH2[1_556] | 1.72                     | 0.48              |
| 4:0:80:ASP:CA   | 4:X:31:PHE:CB[1_556]   | 1.72                     | 0.48              |
| 4:0:145:SER:CA  | 4:X:311:ASP:OD1[1_556] | 1.72                     | 0.48              |
| 4:2:311:ASP:CG  | 4:Z:224:GLU:CG[1_556]  | 1.72                     | 0.48              |
| 4:1:69:TYR:CD2  | 4:Y:210:ARG:CD[1_556]  | 1.72                     | 0.48              |
| 4:2:72:GLU:CD   | 4:Z:183:ARG:CZ[1_556]  | 1.72                     | 0.48              |
| 4:2:298:VAL:CG1 | 4:Z:313:MET:N[1_556]   | 1.72                     | 0.48              |
| 4:1:124:PHE:O   | 4:Y:24:ASP:CB[1_556]   | 1.72                     | 0.48              |
| 4:0:304:THR:C   | 4:X:223:PHE:CD1[1_556] | 1.72                     | 0.48              |
| 4:1:113:LYS:CG  | 4:Y:136:ILE:N[1_556]   | 1.72                     | 0.48              |
| 4:0:261:LEU:CD2 | 4:X:266:PHE:CB[1_556]  | 1.72                     | 0.48              |
| 4:2:296:ASN:ND2 | 4:Z:318:THR:CA[1_556]  | 1.72                     | 0.48              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:160:THR:CG2 | 4:Z:261:LEU:CA[1_556]  | 1.72                     | 0.48              |
| 4:2:172:PRO:CB  | 4:Z:163:VAL:C[1_556]   | 1.72                     | 0.48              |
| 4:2:335:ARG:CD  | 4:Z:220:ALA:CB[1_556]  | 1.72                     | 0.48              |
| 4:0:297:ASN:N   | 4:X:316:GLU:CA[1_556]  | 1.72                     | 0.48              |
| 4:0:180:LEU:CB  | 4:X:267:ILE:CB[1_556]  | 1.72                     | 0.48              |
| 4:2:362:TYR:OH  | 4:Z:22:ALA:CB[1_556]   | 1.72                     | 0.48              |
| 4:1:272:ALA:C   | 4:Y:270:GLU:CA[1_556]  | 1.72                     | 0.48              |
| 4:2:180:LEU:CG  | 4:Z:267:ILE:CD1[1_556] | 1.72                     | 0.48              |
| 4:2:113:LYS:CA  | 4:Z:137:GLN:CA[1_556]  | 1.72                     | 0.48              |
| 4:2:142:LEU:O   | 4:Z:314:GLN:CG[1_556]  | 1.72                     | 0.48              |
| 4:1:62:ARG:CG   | 4:Y:204:ALA:N[1_556]   | 1.72                     | 0.48              |
| 4:1:108:ALA:O   | 4:Y:154:ASP:CB[1_556]  | 1.72                     | 0.48              |
| 4:2:365:ALA:N   | 4:Z:349:LEU:C[1_556]   | 1.72                     | 0.48              |
| 4:1:108:ALA:CA  | 4:Y:155:SER:N[1_556]   | 1.72                     | 0.48              |
| 4:1:72:GLU:C    | 4:Y:157:ASP:CG[1_556]  | 1.72                     | 0.48              |
| 4:0:119:MET:C   | 4:X:340:TRP:CB[1_556]  | 1.72                     | 0.48              |
| 4:0:261:LEU:O   | 4:X:265:SER:CA[1_556]  | 1.72                     | 0.48              |
| 4:1:270:GLU:CD  | 4:X:286:ASP:N[1_556]   | 1.72                     | 0.48              |
| 4:0:150:GLY:O   | 4:X:317:ILE:CD1[1_556] | 1.72                     | 0.48              |
| 4:0:299:MET:CA  | 4:X:312:ARG:CB[1_556]  | 1.72                     | 0.48              |
| 4:2:158:GLY:N   | 4:Z:185:LEU:CB[1_556]  | 1.72                     | 0.48              |
| 4:2:67:LEU:CA   | 4:Z:207:GLU:OE2[1_556] | 1.72                     | 0.48              |
| 4:0:160:THR:CA  | 4:X:261:LEU:CD2[1_556] | 1.72                     | 0.48              |
| 4:3:195:GLU:CD  | 4:Z:109:PRO:O[1_556]   | 1.72                     | 0.48              |
| 4:1:137:GLN:OE1 | 4:Y:304:THR:CA[1_556]  | 1.72                     | 0.48              |
| 4:1:175:ILE:CG1 | 4:Y:162:ASN:CB[1_556]  | 1.72                     | 0.48              |
| 4:0:157:ASP:C   | 4:X:185:LEU:C[1_556]   | 1.72                     | 0.48              |
| 4:1:299:MET:C   | 4:Y:312:ARG:CB[1_556]  | 1.72                     | 0.48              |
| 4:2:173:HIS:CD2 | 4:Z:281:SER:C[1_556]   | 1.72                     | 0.48              |
| 4:1:335:ARG:CB  | 4:Y:220:ALA:N[1_556]   | 1.72                     | 0.48              |
| 4:0:72:GLU:CD   | 4:X:183:ARG:CZ[1_556]  | 1.72                     | 0.48              |
| 4:0:286:ASP:CA  | 4:X:283:MET:CG[1_556]  | 1.72                     | 0.48              |
| 4:1:368:SER:CA  | 4:Y:346:LEU:CB[1_556]  | 1.72                     | 0.48              |
| 4:1:124:PHE:CA  | 4:Y:24:ASP:C[1_556]    | 1.72                     | 0.48              |
| 4:0:306:TYR:OH  | 4:X:192:ILE:CD1[1_556] | 1.72                     | 0.48              |
| 4:1:296:ASN:ND2 | 4:Y:318:THR:C[1_556]   | 1.72                     | 0.48              |
| 4:1:116:ARG:O   | 4:Y:340:TRP:N[1_556]   | 1.72                     | 0.48              |
| 4:0:278:THR:OG1 | 4:X:275:HIS:CE1[1_556] | 1.72                     | 0.48              |
| 4:0:166:TYR:CB  | 4:X:294:TYR:CG[1_556]  | 1.72                     | 0.48              |
| 4:1:195:GLU:OE2 | 4:X:109:PRO:CA[1_556]  | 1.72                     | 0.48              |
| 4:2:180:LEU:CA  | 4:Z:267:ILE:CD1[1_556] | 1.72                     | 0.48              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:153:LEU:N   | 4:X:262:PHE:CD1[1_556] | 1.72                     | 0.48              |
| 4:1:211:ASP:CB  | 4:Y:249:THR:O[1_556]   | 1.72                     | 0.48              |
| 4:2:149:THR:OG1 | 4:Z:327:ILE:N[1_556]   | 1.72                     | 0.48              |
| 4:0:153:LEU:CD1 | 4:X:262:PHE:CB[1_556]  | 1.72                     | 0.48              |
| 4:1:147:ARG:CA  | 4:Y:314:GLN:CD[1_556]  | 1.72                     | 0.48              |
| 4:0:83:GLU:N    | 4:X:30:VAL:N[1_556]    | 1.72                     | 0.48              |
| 4:0:179:ASP:CB  | 4:X:184:ASP:OD2[1_556] | 1.72                     | 0.48              |
| 4:0:149:THR:OG1 | 4:X:327:ILE:N[1_556]   | 1.72                     | 0.48              |
| 4:1:296:ASN:CB  | 4:Y:318:THR:N[1_556]   | 1.72                     | 0.48              |
| 4:2:76:ILE:CG2  | 4:Z:16:LEU:CB[1_556]   | 1.72                     | 0.48              |
| 4:1:295:ALA:N   | 4:Y:319:ALA:CB[1_556]  | 1.72                     | 0.48              |
| 4:2:180:LEU:CD2 | 4:Z:267:ILE:CB[1_556]  | 1.72                     | 0.48              |
| 4:2:177:ARG:O   | 4:Z:178:LEU:CD1[1_556] | 1.72                     | 0.48              |
| 4:1:108:ALA:C   | 4:Y:154:ASP:C[1_556]   | 1.72                     | 0.48              |
| 4:2:203:THR:CA  | 4:Z:201:VAL:CG2[1_556] | 1.72                     | 0.48              |
| 4:2:67:LEU:CG   | 4:Z:207:GLU:OE1[1_556] | 1.72                     | 0.48              |
| 4:0:135:ALA:O   | 4:X:299:MET:O[1_556]   | 1.72                     | 0.48              |
| 4:3:232:SER:O   | 4:Z:362:TYR:CD1[1_556] | 1.72                     | 0.48              |
| 4:2:311:ASP:OD1 | 4:Z:224:GLU:CG[1_556]  | 1.72                     | 0.48              |
| 4:2:33:SER:CA   | 4:Z:210:ARG:CZ[1_556]  | 1.72                     | 0.48              |
| 4:0:108:ALA:CB  | 4:X:155:SER:CA[1_556]  | 1.72                     | 0.48              |
| 4:1:230:ALA:CB  | 4:X:371:HIS:CG[1_556]  | 1.72                     | 0.48              |
| 4:1:293:LEU:CA  | 4:Y:317:ILE:O[1_556]   | 1.73                     | 0.47              |
| 4:2:180:LEU:CD2 | 4:Z:267:ILE:C[1_556]   | 1.73                     | 0.47              |
| 4:2:187:ASP:OD1 | 4:Z:190:MET:CG[1_556]  | 1.73                     | 0.47              |
| 4:0:365:ALA:N   | 4:X:349:LEU:C[1_556]   | 1.73                     | 0.47              |
| 4:2:261:LEU:O   | 4:Z:265:SER:CA[1_556]  | 1.73                     | 0.47              |
| 4:1:116:ARG:NH2 | 4:Y:141:SER:CA[1_556]  | 1.73                     | 0.47              |
| 4:0:177:ARG:NH1 | 4:X:159:VAL:CB[1_556]  | 1.73                     | 0.47              |
| 4:0:217:CYS:CB  | 4:X:256:ARG:CZ[1_556]  | 1.73                     | 0.47              |
| 4:0:160:THR:CG2 | 4:X:261:LEU:CA[1_556]  | 1.73                     | 0.47              |
| 4:1:113:LYS:CB  | 4:Y:136:ILE:O[1_556]   | 1.73                     | 0.47              |
| 4:1:80:ASP:N    | 4:Y:31:PHE:CD2[1_556]  | 1.73                     | 0.47              |
| 4:0:298:VAL:CG1 | 4:X:313:MET:N[1_556]   | 1.73                     | 0.47              |
| 4:2:210:ARG:CA  | 4:Z:193:LEU:CA[1_556]  | 1.73                     | 0.47              |
| 4:2:303:THR:CA  | 4:Z:257:CYS:C[1_556]   | 1.73                     | 0.47              |
| 4:1:298:VAL:CG2 | 4:Y:311:ASP:O[1_556]   | 1.73                     | 0.47              |
| 4:2:179:ASP:CB  | 4:Z:184:ASP:OD2[1_556] | 1.73                     | 0.47              |
| 4:2:153:LEU:CD1 | 4:Z:262:PHE:CB[1_556]  | 1.73                     | 0.47              |
| 4:0:40:HIS:N    | 4:V:166:TYR:OH[1_556]  | 1.73                     | 0.47              |
| 4:2:30:VAL:C    | 4:Z:215:LYS:CG[1_556]  | 1.73                     | 0.47              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:126:THR:CB  | 4:Z:28:ARG:CD[1_556]   | 1.73                     | 0.47              |
| 4:0:180:LEU:CD1 | 4:X:267:ILE:CG1[1_556] | 1.73                     | 0.47              |
| 4:0:232:SER:CA  | 4:W:366:GLY:O[1_556]   | 1.73                     | 0.47              |
| 4:0:169:TYR:CG  | 4:X:150:GLY:C[1_556]   | 1.73                     | 0.47              |
| 4:2:292:ASP:C   | 4:Z:321:ALA:N[1_556]   | 1.73                     | 0.47              |
| 4:1:37:ARG:CB   | 4:Y:60:SER:CA[1_556]   | 1.73                     | 0.47              |
| 4:1:86:TRP:CZ2  | 4:Y:337:TYR:CD1[1_556] | 1.73                     | 0.47              |
| 4:0:292:ASP:C   | 4:X:321:ALA:N[1_556]   | 1.73                     | 0.47              |
| 4:1:16:LEU:CB   | 4:Y:214:GLU:N[1_556]   | 1.73                     | 0.47              |
| 4:2:209:VAL:CG2 | 4:Z:195:GLU:N[1_556]   | 1.73                     | 0.47              |
| 4:2:304:THR:C   | 4:Z:223:PHE:CD1[1_556] | 1.73                     | 0.47              |
| 4:3:270:GLU:CD  | 4:Z:286:ASP:N[1_556]   | 1.73                     | 0.47              |
| 4:1:303:THR:O   | 4:Y:256:ARG:C[1_556]   | 1.73                     | 0.47              |
| 4:2:134:VAL:CA  | 4:Z:338:SER:OG[1_556]  | 1.73                     | 0.47              |
| 4:2:257:CYS:SG  | 4:Z:195:GLU:OE1[1_556] | 1.73                     | 0.47              |
| 4:1:118:LYS:CB  | 4:Y:10:CYS:C[1_556]    | 1.73                     | 0.47              |
| 4:1:71:ILE:CG1  | 4:Y:16:LEU:CD2[1_556]  | 1.73                     | 0.47              |
| 4:1:195:GLU:CD  | 4:X:109:PRO:O[1_556]   | 1.73                     | 0.47              |
| 4:0:105:LEU:N   | 4:X:334:GLU:C[1_556]   | 1.73                     | 0.47              |
| 4:1:107:GLU:C   | 4:Y:300:SER:O[1_556]   | 1.73                     | 0.47              |
| 4:1:33:SER:O    | 4:Y:210:ARG:NH2[1_556] | 1.73                     | 0.47              |
| 4:1:144:ALA:O   | 4:Y:311:ASP:OD1[1_556] | 1.73                     | 0.47              |
| 4:2:183:ARG:CA  | 4:Z:186:THR:O[1_556]   | 1.73                     | 0.47              |
| 4:0:75:ILE:N    | 4:X:156:GLY:C[1_556]   | 1.73                     | 0.47              |
| 4:0:109:PRO:CA  | 4:X:153:LEU:C[1_556]   | 1.73                     | 0.47              |
| 4:0:369:ILE:CA  | 4:X:346:LEU:CA[1_556]  | 1.73                     | 0.47              |
| 4:2:16:LEU:CG   | 4:Z:214:GLU:CA[1_556]  | 1.73                     | 0.47              |
| 4:1:365:ALA:N   | 4:Y:348:SER:O[1_556]   | 1.73                     | 0.47              |
| 4:2:291:LYS:C   | 4:Z:321:ALA:O[1_556]   | 1.73                     | 0.47              |
| 4:2:137:GLN:OE1 | 4:Z:303:THR:C[1_556]   | 1.73                     | 0.47              |
| 4:1:233:SER:N   | 4:X:367:PRO:C[1_556]   | 1.73                     | 0.47              |
| 4:2:141:SER:OG  | 4:Z:309:ILE:CA[1_556]  | 1.73                     | 0.47              |
| 4:2:104:LEU:CD2 | 4:Z:332:PRO:C[1_556]   | 1.73                     | 0.47              |
| 4:1:232:SER:O   | 4:X:362:TYR:CD1[1_556] | 1.73                     | 0.47              |
| 4:1:124:PHE:CD2 | 4:Y:344:SER:OG[1_556]  | 1.73                     | 0.47              |
| 4:1:74:GLY:CA   | 4:Y:156:GLY:CA[1_556]  | 1.73                     | 0.47              |
| 4:1:264:PRO:CA  | 4:Y:268:GLY:N[1_556]   | 1.73                     | 0.47              |
| 4:1:104:LEU:CD2 | 4:Y:332:PRO:C[1_556]   | 1.73                     | 0.47              |
| 4:2:369:ILE:CG1 | 4:Z:345:ILE:CG2[1_556] | 1.73                     | 0.47              |
| 4:2:109:PRO:CA  | 4:Z:153:LEU:C[1_556]   | 1.73                     | 0.47              |
| 4:0:288:ASP:O   | 4:X:322:PRO:CB[1_556]  | 1.73                     | 0.47              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:293:LEU:C   | 4:Y:320:LEU:CA[1_556]  | 1.73                     | 0.47              |
| 4:1:164:PRO:N   | 4:Y:278:THR:CA[1_556]  | 1.73                     | 0.47              |
| 4:1:125:GLU:CD  | 4:Y:21:PHE:CA[1_556]   | 1.73                     | 0.47              |
| 4:1:288:ASP:C   | 4:Y:322:PRO:CG[1_556]  | 1.73                     | 0.47              |
| 4:3:253:GLU:CD  | 4:Z:112:PRO:O[1_556]   | 1.73                     | 0.47              |
| 4:1:37:ARG:O    | 4:Y:60:SER:O[1_556]    | 1.73                     | 0.47              |
| 4:1:284:LYS:C   | 4:Y:280:ASN:O[1_556]   | 1.73                     | 0.47              |
| 4:0:362:TYR:OH  | 4:X:22:ALA:CB[1_556]   | 1.73                     | 0.47              |
| 4:2:212:ILE:CD1 | 4:Z:197:GLY:N[1_556]   | 1.73                     | 0.47              |
| 4:0:296:ASN:ND2 | 4:X:318:THR:CA[1_556]  | 1.73                     | 0.47              |
| 4:2:72:GLU:OE2  | 4:Z:183:ARG:CG[1_556]  | 1.73                     | 0.47              |
| 4:1:67:LEU:O    | 4:Y:62:ARG:NH1[1_556]  | 1.73                     | 0.47              |
| 4:1:135:ALA:O   | 4:Y:299:MET:O[1_556]   | 1.73                     | 0.47              |
| 4:1:311:ASP:CG  | 4:Y:224:GLU:CG[1_556]  | 1.73                     | 0.47              |
| 4:0:141:SER:OG  | 4:X:310:ALA:N[1_556]   | 1.73                     | 0.47              |
| 4:1:306:TYR:CE2 | 4:Y:256:ARG:CB[1_556]  | 1.73                     | 0.47              |
| 4:0:126:THR:CB  | 4:X:28:ARG:CD[1_556]   | 1.73                     | 0.47              |
| 4:1:76:ILE:CG2  | 4:Y:16:LEU:CB[1_556]   | 1.73                     | 0.47              |
| 4:0:212:ILE:CD1 | 4:X:197:GLY:N[1_556]   | 1.73                     | 0.47              |
| 4:0:303:THR:CB  | 4:X:258:PRO:N[1_556]   | 1.73                     | 0.47              |
| 4:0:180:LEU:CD2 | 4:X:267:ILE:CB[1_556]  | 1.73                     | 0.47              |
| 4:1:339:VAL:CB  | 4:Y:335:ARG:NH2[1_556] | 1.73                     | 0.47              |
| 4:0:116:ARG:CA  | 4:X:339:VAL:CB[1_556]  | 1.73                     | 0.47              |
| 4:2:32:PRO:CG   | 4:Z:211:ASP:OD2[1_556] | 1.73                     | 0.47              |
| 4:1:185:LEU:CB  | 4:Y:188:TYR:CD1[1_556] | 1.73                     | 0.47              |
| 4:2:68:LYS:CA   | 4:Z:59:GLN:CD[1_556]   | 1.73                     | 0.47              |
| 4:1:183:ARG:CD  | 4:Y:187:ASP:OD1[1_556] | 1.73                     | 0.47              |
| 4:2:206:ARG:NH1 | 4:Z:190:MET:CE[1_556]  | 1.73                     | 0.47              |
| 4:1:286:ASP:CA  | 4:Y:283:MET:CG[1_556]  | 1.73                     | 0.47              |
| 4:1:332:PRO:CG  | 4:Y:221:LEU:CD1[1_556] | 1.73                     | 0.47              |
| 4:1:203:THR:CG2 | 4:Y:205:GLU:OE2[1_556] | 1.74                     | 0.46              |
| 4:0:107:GLU:C   | 4:X:300:SER:O[1_556]   | 1.74                     | 0.46              |
| 4:1:185:LEU:CD2 | 4:Y:188:TYR:CE1[1_556] | 1.74                     | 0.46              |
| 4:1:210:ARG:CA  | 4:Y:193:LEU:CD1[1_556] | 1.74                     | 0.46              |
| 4:0:172:PRO:CB  | 4:X:163:VAL:C[1_556]   | 1.74                     | 0.46              |
| 4:2:124:PHE:O   | 4:Z:24:ASP:CB[1_556]   | 1.74                     | 0.46              |
| 4:1:106:THR:N   | 4:Y:335:ARG:N[1_556]   | 1.74                     | 0.46              |
| 4:1:279:TYR:N   | 4:Y:276:GLU:OE1[1_556] | 1.74                     | 0.46              |
| 4:4:63:GLY:CA   | 4:Z:288:ASP:CA[1_556]  | 1.74                     | 0.46              |
| 4:2:153:LEU:N   | 4:Z:262:PHE:CD1[1_556] | 1.74                     | 0.46              |
| 4:0:284:LYS:C   | 4:X:280:ASN:O[1_556]   | 1.74                     | 0.46              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:152:VAL:CB  | 4:Y:313:MET:SD[1_556]  | 1.74                     | 0.46              |
| 4:2:253:GLU:CD  | 4:Y:112:PRO:CA[1_556]  | 1.74                     | 0.46              |
| 4:1:179:ASP:CB  | 4:Y:184:ASP:OD2[1_556] | 1.74                     | 0.46              |
| 4:2:119:MET:C   | 4:Z:340:TRP:CB[1_556]  | 1.74                     | 0.46              |
| 4:2:157:ASP:C   | 4:Z:185:LEU:C[1_556]   | 1.74                     | 0.46              |
| 4:2:40:HIS:C    | 4:X:167:GLU:CD[1_556]  | 1.74                     | 0.46              |
| 4:0:16:LEU:CG   | 4:X:214:GLU:N[1_556]   | 1.74                     | 0.46              |
| 4:2:109:PRO:CA  | 4:Z:154:ASP:C[1_556]   | 1.74                     | 0.46              |
| 4:0:16:LEU:CG   | 4:X:214:GLU:CA[1_556]  | 1.74                     | 0.46              |
| 4:2:153:LEU:CD2 | 4:Z:262:PHE:CG[1_556]  | 1.74                     | 0.46              |
| 4:0:212:ILE:CD1 | 4:X:197:GLY:CA[1_556]  | 1.74                     | 0.46              |
| 4:2:113:LYS:O   | 4:Z:140:LEU:CD1[1_556] | 1.74                     | 0.46              |
| 4:0:289:ILE:CD1 | 4:X:294:TYR:CZ[1_556]  | 1.74                     | 0.46              |
| 4:2:288:ASP:O   | 4:Z:322:PRO:CB[1_556]  | 1.74                     | 0.46              |
| 4:4:40:HIS:NE2  | 4:Z:166:TYR:CD2[1_556] | 1.74                     | 0.46              |
| 4:2:113:LYS:CG  | 4:Z:136:ILE:N[1_556]   | 1.74                     | 0.46              |
| 4:0:68:LYS:CA   | 4:X:59:GLN:CD[1_556]   | 1.74                     | 0.46              |
| 4:1:212:ILE:CG2 | 4:Y:196:ARG:C[1_556]   | 1.74                     | 0.46              |
| 4:0:134:VAL:CG2 | 4:X:338:SER:C[1_556]   | 1.74                     | 0.46              |
| 4:2:74:GLY:CA   | 4:Z:156:GLY:CA[1_556]  | 1.74                     | 0.46              |
| 4:0:311:ASP:CG  | 4:X:224:GLU:CG[1_556]  | 1.74                     | 0.46              |
| 4:2:108:ALA:CA  | 4:Z:300:SER:O[1_556]   | 1.74                     | 0.46              |
| 4:0:303:THR:CA  | 4:X:257:CYS:C[1_556]   | 1.74                     | 0.46              |
| 4:2:298:VAL:C   | 4:Z:312:ARG:C[1_556]   | 1.74                     | 0.46              |
| 4:0:180:LEU:CG  | 4:X:267:ILE:CD1[1_556] | 1.74                     | 0.46              |
| 4:2:212:ILE:CD1 | 4:Z:197:GLY:CA[1_556]  | 1.74                     | 0.46              |
| 4:2:135:ALA:O   | 4:Z:299:MET:O[1_556]   | 1.74                     | 0.46              |
| 4:1:120:THR:CG2 | 4:Y:344:SER:N[1_556]   | 1.74                     | 0.46              |
| 4:1:281:SER:O   | 4:Y:280:ASN:N[1_556]   | 1.74                     | 0.46              |
| 4:3:230:ALA:N   | 4:Z:368:SER:CA[1_556]  | 1.74                     | 0.46              |
| 4:2:261:LEU:CD2 | 4:Z:266:PHE:CB[1_556]  | 1.74                     | 0.46              |
| 4:2:286:ASP:CA  | 4:Z:283:MET:CG[1_556]  | 1.74                     | 0.46              |
| 4:2:180:LEU:CB  | 4:Z:267:ILE:CB[1_556]  | 1.74                     | 0.46              |
| 4:2:372:ARG:NH1 | 4:Z:142:LEU:O[1_556]   | 1.74                     | 0.46              |
| 4:0:33:SER:O    | 4:X:210:ARG:NH1[1_556] | 1.74                     | 0.46              |
| 4:1:169:TYR:C   | 4:Y:151:ILE:CG2[1_556] | 1.74                     | 0.46              |
| 4:1:167:GLU:CB  | 4:Y:295:ALA:N[1_556]   | 1.74                     | 0.46              |
| 4:2:214:GLU:O   | 4:Z:252:ASN:CA[1_556]  | 1.74                     | 0.46              |
| 4:2:80:ASP:CA   | 4:Z:31:PHE:CB[1_556]   | 1.74                     | 0.46              |
| 4:0:72:GLU:C    | 4:X:157:ASP:O[1_556]   | 1.74                     | 0.46              |
| 4:2:81:ASP:CA   | 4:Z:31:PHE:CA[1_556]   | 1.74                     | 0.46              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:277:THR:OG1 | 4:Y:272:ALA:CA[1_556]  | 1.74                     | 0.46              |
| 4:2:133:TYR:CD1 | 4:Z:144:ALA:O[1_556]   | 1.74                     | 0.46              |
| 4:2:166:TYR:CB  | 4:Z:294:TYR:CG[1_556]  | 1.74                     | 0.46              |
| 4:0:300:SER:C   | 4:X:219:VAL:CG1[1_556] | 1.74                     | 0.46              |
| 4:2:305:MET:N   | 4:Z:255:PHE:O[1_556]   | 1.74                     | 0.46              |
| 4:0:108:ALA:CA  | 4:X:300:SER:O[1_556]   | 1.74                     | 0.46              |
| 4:0:148:THR:CA  | 4:X:327:ILE:C[1_556]   | 1.74                     | 0.46              |
| 4:1:158:GLY:N   | 4:Y:185:LEU:CB[1_556]  | 1.74                     | 0.46              |
| 4:2:167:GLU:C   | 4:Z:295:ALA:O[1_556]   | 1.74                     | 0.46              |
| 4:2:289:ILE:CD1 | 4:Z:294:TYR:CZ[1_556]  | 1.74                     | 0.46              |
| 4:0:187:ASP:OD1 | 4:X:190:MET:CG[1_556]  | 1.74                     | 0.46              |
| 4:2:63:GLY:CA   | 4:X:288:ASP:CA[1_556]  | 1.74                     | 0.46              |
| 4:0:109:PRO:CA  | 4:X:154:ASP:C[1_556]   | 1.74                     | 0.46              |
| 4:0:214:GLU:O   | 4:X:252:ASN:CA[1_556]  | 1.74                     | 0.46              |
| 4:1:63:GLY:O    | 4:W:289:ILE:CA[1_556]  | 1.74                     | 0.46              |
| 4:1:153:LEU:CB  | 4:Y:262:PHE:CB[1_556]  | 1.74                     | 0.46              |
| 4:0:183:ARG:CB  | 4:X:186:THR:O[1_556]   | 1.74                     | 0.46              |
| 4:2:183:ARG:CB  | 4:Z:186:THR:O[1_556]   | 1.74                     | 0.46              |
| 4:2:16:LEU:CG   | 4:Z:214:GLU:N[1_556]   | 1.74                     | 0.46              |
| 4:2:40:HIS:NE2  | 4:X:166:TYR:CD2[1_556] | 1.74                     | 0.46              |
| 4:2:141:SER:OG  | 4:Z:310:ALA:N[1_556]   | 1.74                     | 0.46              |
| 4:0:67:LEU:CG   | 4:X:207:GLU:OE1[1_556] | 1.74                     | 0.46              |
| 4:1:257:CYS:SG  | 4:Y:195:GLU:OE1[1_556] | 1.74                     | 0.46              |
| 4:3:230:ALA:CB  | 4:Z:371:HIS:CG[1_556]  | 1.74                     | 0.46              |
| 4:0:270:GLU:CG  | 4:W:286:ASP:CA[1_556]  | 1.74                     | 0.46              |
| 4:0:121:GLN:NE2 | 4:X:20:GLY:C[1_556]    | 1.74                     | 0.46              |
| 4:0:278:THR:O   | 4:X:276:GLU:CD[1_556]  | 1.74                     | 0.46              |
| 4:0:186:THR:CA  | 4:X:191:LYS:CA[1_556]  | 1.74                     | 0.46              |
| 4:2:40:HIS:N    | 4:X:166:TYR:OH[1_556]  | 1.74                     | 0.46              |
| 4:1:149:THR:CB  | 4:Y:327:ILE:CB[1_556]  | 1.74                     | 0.46              |
| 4:0:311:ASP:OD1 | 4:X:224:GLU:CG[1_556]  | 1.74                     | 0.46              |
| 4:0:81:ASP:CA   | 4:X:31:PHE:CA[1_556]   | 1.74                     | 0.46              |
| 4:1:81:ASP:OD1  | 4:Y:56:ASP:OD1[1_556]  | 1.74                     | 0.46              |
| 4:2:257:CYS:CB  | 4:Z:195:GLU:OE1[1_556] | 1.74                     | 0.46              |
| 4:1:113:LYS:NZ  | 4:Y:136:ILE:CG1[1_556] | 1.74                     | 0.46              |
| 4:1:110:LEU:CD1 | 4:Y:161:HIS:CB[1_556]  | 1.74                     | 0.46              |
| 4:1:141:SER:N   | 4:Y:310:ALA:CB[1_556]  | 1.75                     | 0.45              |
| 4:2:118:LYS:NZ  | 4:Z:19:ALA:CB[1_556]   | 1.75                     | 0.45              |
| 4:2:190:MET:CB  | 4:Z:194:THR:OG1[1_556] | 1.75                     | 0.45              |
| 4:0:371:HIS:ND1 | 4:X:140:LEU:CA[1_556]  | 1.75                     | 0.45              |
| 4:1:253:GLU:CD  | 4:X:112:PRO:O[1_556]   | 1.75                     | 0.45              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:183:ARG:CA  | 4:X:186:THR:O[1_556]   | 1.75                     | 0.45              |
| 4:0:59:GLN:CD   | 4:X:208:ILE:CA[1_556]  | 1.75                     | 0.45              |
| 4:2:108:ALA:CB  | 4:Z:155:SER:CA[1_556]  | 1.75                     | 0.45              |
| 4:1:122:ILE:CG2 | 4:Y:19:ALA:O[1_556]    | 1.75                     | 0.45              |
| 4:3:39:ARG:NH1  | 4:Y:286:ASP:OD2[1_556] | 1.75                     | 0.45              |
| 4:2:121:GLN:NE2 | 4:Z:20:GLY:C[1_556]    | 1.75                     | 0.45              |
| 4:1:372:ARG:CD  | 4:Y:143:TYR:N[1_556]   | 1.75                     | 0.45              |
| 4:0:32:PRO:CG   | 4:X:211:ASP:OD2[1_556] | 1.75                     | 0.45              |
| 4:2:195:GLU:CG  | 4:Y:110:LEU:N[1_556]   | 1.75                     | 0.45              |
| 4:0:63:GLY:CA   | 4:V:288:ASP:CA[1_556]  | 1.75                     | 0.45              |
| 4:3:63:GLY:O    | 4:Y:289:ILE:CA[1_556]  | 1.75                     | 0.45              |
| 4:1:206:ARG:NH2 | 4:Y:190:MET:CG[1_556]  | 1.75                     | 0.45              |
| 4:2:71:ILE:CG1  | 4:Z:16:LEU:CD2[1_556]  | 1.75                     | 0.45              |
| 4:0:40:HIS:NE2  | 4:V:166:TYR:CD2[1_556] | 1.75                     | 0.45              |
| 4:1:290:ARG:O   | 4:Y:320:LEU:C[1_556]   | 1.75                     | 0.45              |
| 4:2:336:LYS:CG  | 4:Z:218:TYR:CE1[1_556] | 1.75                     | 0.45              |
| 4:0:162:ASN:CG  | 4:X:273:GLY:CA[1_556]  | 1.75                     | 0.45              |
| 4:0:368:SER:OG  | 4:X:346:LEU:CD2[1_556] | 1.75                     | 0.45              |
| 4:0:73:HIS:ND1  | 4:X:184:ASP:OD1[1_556] | 1.75                     | 0.45              |
| 4:2:148:THR:CA  | 4:Z:327:ILE:C[1_556]   | 1.75                     | 0.45              |
| 4:2:33:SER:O    | 4:Z:210:ARG:NH1[1_556] | 1.75                     | 0.45              |
| 4:0:74:GLY:C    | 4:X:157:ASP:N[1_556]   | 1.75                     | 0.45              |
| 4:0:79:TRP:CE3  | 4:X:17:VAL:C[1_556]    | 1.75                     | 0.45              |
| 4:0:120:THR:OG1 | 4:X:341:ILE:CA[1_556]  | 1.75                     | 0.45              |
| 4:2:123:MET:N   | 4:Z:26:ALA:O[1_556]    | 1.75                     | 0.45              |
| 4:1:116:ARG:CZ  | 4:Y:141:SER:O[1_556]   | 1.75                     | 0.45              |
| 4:2:134:VAL:CG2 | 4:Z:338:SER:C[1_556]   | 1.75                     | 0.45              |
| 4:1:80:ASP:CA   | 4:Y:31:PHE:CB[1_556]   | 1.75                     | 0.45              |
| 4:1:134:VAL:CB  | 4:Y:338:SER:C[1_556]   | 1.75                     | 0.45              |
| 4:0:271:SER:C   | 4:X:270:GLU:CA[1_556]  | 1.75                     | 0.45              |
| 4:0:291:LYS:C   | 4:X:321:ALA:O[1_556]   | 1.75                     | 0.45              |
| 4:2:105:LEU:N   | 4:Z:334:GLU:C[1_556]   | 1.75                     | 0.45              |
| 4:2:113:LYS:CG  | 4:Z:136:ILE:O[1_556]   | 1.75                     | 0.45              |
| 4:0:190:MET:CB  | 4:X:194:THR:OG1[1_556] | 1.75                     | 0.45              |
| 4:0:196:ARG:NH2 | 4:W:114:ALA:O[1_556]   | 1.75                     | 0.45              |
| 4:1:169:TYR:CA  | 4:Y:296:ASN:C[1_556]   | 1.75                     | 0.45              |
| 4:2:371:HIS:ND1 | 4:Z:140:LEU:CA[1_556]  | 1.75                     | 0.45              |
| 4:1:183:ARG:CA  | 4:Y:186:THR:O[1_556]   | 1.75                     | 0.45              |
| 4:0:133:TYR:CD1 | 4:X:144:ALA:O[1_556]   | 1.75                     | 0.45              |
| 4:1:190:MET:SD  | 4:Y:194:THR:CB[1_556]  | 1.75                     | 0.45              |
| 4:2:141:SER:CB  | 4:Z:310:ALA:CA[1_556]  | 1.75                     | 0.45              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:141:SER:CB  | 4:X:310:ALA:CA[1_556]  | 1.75                     | 0.45              |
| 4:1:80:ASP:CB   | 4:Y:31:PHE:CD2[1_556]  | 1.75                     | 0.45              |
| 4:1:335:ARG:O   | 4:Y:219:VAL:N[1_556]   | 1.75                     | 0.45              |
| 4:2:75:ILE:N    | 4:Z:156:GLY:C[1_556]   | 1.75                     | 0.45              |
| 4:0:72:GLU:N    | 4:X:157:ASP:OD1[1_556] | 1.75                     | 0.45              |
| 4:2:152:VAL:CA  | 4:Z:313:MET:CG[1_556]  | 1.75                     | 0.45              |
| 4:2:177:ARG:O   | 4:Z:178:LEU:CG[1_556]  | 1.75                     | 0.45              |
| 4:3:40:HIS:N    | 4:Y:166:TYR:OH[1_556]  | 1.75                     | 0.45              |
| 4:1:72:GLU:C    | 4:Y:157:ASP:O[1_556]   | 1.75                     | 0.45              |
| 4:0:206:ARG:NH1 | 4:X:190:MET:CE[1_556]  | 1.75                     | 0.45              |
| 4:2:59:GLN:CD   | 4:Z:208:ILE:CA[1_556]  | 1.75                     | 0.45              |
| 4:0:152:VAL:CG2 | 4:X:313:MET:CA[1_556]  | 1.75                     | 0.45              |
| 4:2:186:THR:CA  | 4:Z:191:LYS:CA[1_556]  | 1.75                     | 0.45              |
| 4:0:305:MET:N   | 4:X:255:PHE:O[1_556]   | 1.75                     | 0.45              |
| 4:0:253:GLU:CD  | 4:W:112:PRO:CA[1_556]  | 1.75                     | 0.45              |
| 4:0:372:ARG:NH1 | 4:X:142:LEU:O[1_556]   | 1.75                     | 0.45              |
| 4:1:166:TYR:CB  | 4:Y:294:TYR:CB[1_556]  | 1.75                     | 0.45              |
| 4:0:211:ASP:O   | 4:X:196:ARG:CZ[1_556]  | 1.75                     | 0.45              |
| 4:2:170:ALA:CB  | 4:Z:151:ILE:O[1_556]   | 1.75                     | 0.45              |
| 4:0:113:LYS:CG  | 4:X:136:ILE:O[1_556]   | 1.75                     | 0.45              |
| 4:0:195:GLU:CD  | 4:W:109:PRO:O[1_556]   | 1.75                     | 0.45              |
| 4:2:67:LEU:CD1  | 4:Z:207:GLU:CG[1_556]  | 1.75                     | 0.45              |
| 4:0:177:ARG:O   | 4:X:178:LEU:CG[1_556]  | 1.75                     | 0.45              |
| 4:0:74:GLY:CA   | 4:X:156:GLY:CA[1_556]  | 1.75                     | 0.45              |
| 4:2:79:TRP:CE3  | 4:Z:17:VAL:C[1_556]    | 1.75                     | 0.45              |
| 4:0:185:LEU:C   | 4:X:191:LYS:CG[1_556]  | 1.75                     | 0.45              |
| 4:0:118:LYS:NZ  | 4:X:19:ALA:CB[1_556]   | 1.75                     | 0.45              |
| 4:1:167:GLU:C   | 4:Y:296:ASN:N[1_556]   | 1.75                     | 0.45              |
| 4:1:72:GLU:C    | 4:Y:157:ASP:CA[1_556]  | 1.75                     | 0.45              |
| 4:2:136:ILE:O   | 4:Z:299:MET:CA[1_556]  | 1.75                     | 0.45              |
| 4:2:120:THR:OG1 | 4:Z:341:ILE:CA[1_556]  | 1.75                     | 0.45              |
| 4:1:180:LEU:CB  | 4:Y:267:ILE:CB[1_556]  | 1.75                     | 0.45              |
| 4:0:40:HIS:C    | 4:V:167:GLU:CD[1_556]  | 1.75                     | 0.45              |
| 4:0:113:LYS:O   | 4:X:140:LEU:CD1[1_556] | 1.75                     | 0.45              |
| 4:2:79:TRP:CB   | 4:Z:17:VAL:CG1[1_556]  | 1.75                     | 0.45              |
| 4:2:107:GLU:C   | 4:Z:300:SER:O[1_556]   | 1.75                     | 0.45              |
| 4:3:233:SER:N   | 4:Z:367:PRO:C[1_556]   | 1.75                     | 0.45              |
| 4:1:63:GLY:O    | 4:W:289:ILE:CG2[1_556] | 1.75                     | 0.45              |
| 4:0:367:PRO:CA  | 4:X:343:GLY:C[1_556]   | 1.75                     | 0.45              |
| 4:0:136:ILE:O   | 4:X:299:MET:CA[1_556]  | 1.75                     | 0.45              |
| 4:1:230:ALA:N   | 4:X:368:SER:CA[1_556]  | 1.75                     | 0.45              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:167:GLU:CA  | 4:Z:295:ALA:CB[1_556]  | 1.75                     | 0.45              |
| 4:2:212:ILE:C   | 4:Z:196:ARG:CB[1_556]  | 1.75                     | 0.45              |
| 4:0:123:MET:N   | 4:X:26:ALA:O[1_556]    | 1.75                     | 0.45              |
| 4:2:74:GLY:C    | 4:Z:157:ASP:N[1_556]   | 1.75                     | 0.45              |
| 4:1:72:GLU:C    | 4:Y:157:ASP:CB[1_556]  | 1.75                     | 0.45              |
| 4:2:286:ASP:CB  | 4:Z:290:ARG:CZ[1_556]  | 1.75                     | 0.45              |
| 4:0:257:CYS:CB  | 4:X:195:GLU:OE1[1_556] | 1.75                     | 0.45              |
| 4:1:173:HIS:CB  | 4:Y:174:ALA:CA[1_556]  | 1.75                     | 0.45              |
| 4:1:83:GLU:CD   | 4:Y:29:ALA:CA[1_556]   | 1.75                     | 0.45              |
| 4:2:365:ALA:CA  | 4:Z:349:LEU:C[1_556]   | 1.76                     | 0.44              |
| 4:1:177:ARG:O   | 4:Y:178:LEU:CD1[1_556] | 1.76                     | 0.44              |
| 4:0:79:TRP:CB   | 4:X:17:VAL:CG1[1_556]  | 1.76                     | 0.44              |
| 4:2:261:LEU:CA  | 4:Z:266:PHE:CB[1_556]  | 1.76                     | 0.44              |
| 4:2:270:GLU:CG  | 4:Y:286:ASP:CA[1_556]  | 1.76                     | 0.44              |
| 4:1:214:GLU:CG  | 4:Y:250:ILE:CG2[1_556] | 1.76                     | 0.44              |
| 4:2:233:SER:CA  | 4:Y:367:PRO:CD[1_556]  | 1.76                     | 0.44              |
| 4:0:116:ARG:CA  | 4:X:339:VAL:CA[1_556]  | 1.76                     | 0.44              |
| 4:1:292:ASP:C   | 4:Y:318:THR:O[1_556]   | 1.76                     | 0.44              |
| 4:0:116:ARG:CZ  | 4:X:141:SER:CB[1_556]  | 1.76                     | 0.44              |
| 4:2:116:ARG:CA  | 4:Z:339:VAL:CB[1_556]  | 1.76                     | 0.44              |
| 4:2:126:THR:CA  | 4:Z:28:ARG:CZ[1_556]   | 1.76                     | 0.44              |
| 4:2:271:SER:C   | 4:Z:270:GLU:CA[1_556]  | 1.76                     | 0.44              |
| 4:1:116:ARG:C   | 4:Y:339:VAL:C[1_556]   | 1.76                     | 0.44              |
| 4:2:185:LEU:C   | 4:Z:191:LYS:CG[1_556]  | 1.76                     | 0.44              |
| 4:0:116:ARG:NH1 | 4:X:141:SER:CA[1_556]  | 1.76                     | 0.44              |
| 4:0:153:LEU:CD2 | 4:X:262:PHE:CG[1_556]  | 1.76                     | 0.44              |
| 4:1:113:LYS:CA  | 4:Y:137:GLN:CA[1_556]  | 1.76                     | 0.44              |
| 4:0:132:MET:SD  | 4:X:341:ILE:CB[1_556]  | 1.76                     | 0.44              |
| 4:0:298:VAL:C   | 4:X:312:ARG:C[1_556]   | 1.76                     | 0.44              |
| 4:0:195:GLU:CG  | 4:W:110:LEU:N[1_556]   | 1.76                     | 0.44              |
| 4:2:278:THR:O   | 4:Z:276:GLU:CD[1_556]  | 1.76                     | 0.44              |
| 4:2:233:SER:N   | 4:Y:367:PRO:C[1_556]   | 1.76                     | 0.44              |
| 4:1:63:GLY:CA   | 4:W:288:ASP:CA[1_556]  | 1.76                     | 0.44              |
| 4:1:64:ILE:CD1  | 4:W:292:ASP:CG[1_556]  | 1.76                     | 0.44              |
| 4:2:148:THR:CB  | 4:Z:328:LYS:CA[1_556]  | 1.76                     | 0.44              |
| 4:1:189:LEU:CD1 | 4:Y:195:GLU:CB[1_556]  | 1.76                     | 0.44              |
| 4:0:233:SER:CA  | 4:W:367:PRO:CD[1_556]  | 1.76                     | 0.44              |
| 4:2:300:SER:C   | 4:Z:219:VAL:CG1[1_556] | 1.76                     | 0.44              |
| 4:0:370:VAL:CB  | 4:X:342:GLY:CA[1_556]  | 1.76                     | 0.44              |
| 4:1:303:THR:CA  | 4:Y:257:CYS:CA[1_556]  | 1.76                     | 0.44              |
| 4:2:167:GLU:CB  | 4:Z:295:ALA:CA[1_556]  | 1.76                     | 0.44              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:296:ASN:C   | 4:Z:316:GLU:N[1_556]   | 1.76                     | 0.44              |
| 4:2:212:ILE:CG2 | 4:Z:196:ARG:C[1_556]   | 1.76                     | 0.44              |
| 4:1:183:ARG:CG  | 4:Y:187:ASP:CA[1_556]  | 1.76                     | 0.44              |
| 4:1:362:TYR:OH  | 4:Y:22:ALA:CB[1_556]   | 1.76                     | 0.44              |
| 4:0:212:ILE:C   | 4:X:196:ARG:CB[1_556]  | 1.76                     | 0.44              |
| 4:1:169:TYR:N   | 4:Y:296:ASN:N[1_556]   | 1.76                     | 0.44              |
| 4:2:368:SER:OG  | 4:Z:346:LEU:CD2[1_556] | 1.76                     | 0.44              |
| 4:1:150:GLY:O   | 4:Y:317:ILE:CD1[1_556] | 1.76                     | 0.44              |
| 4:3:233:SER:N   | 4:Z:366:GLY:C[1_556]   | 1.76                     | 0.44              |
| 4:1:167:GLU:CB  | 4:Y:295:ALA:CA[1_556]  | 1.76                     | 0.44              |
| 4:1:195:GLU:CG  | 4:X:110:LEU:N[1_556]   | 1.76                     | 0.44              |
| 4:0:167:GLU:C   | 4:X:295:ALA:O[1_556]   | 1.76                     | 0.44              |
| 4:0:183:ARG:NH2 | 4:X:186:THR:OG1[1_556] | 1.76                     | 0.44              |
| 4:0:286:ASP:CB  | 4:X:290:ARG:CZ[1_556]  | 1.76                     | 0.44              |
| 4:1:15:GLY:N    | 4:Y:213:LYS:NZ[1_556]  | 1.76                     | 0.44              |
| 4:4:40:HIS:N    | 4:Z:166:TYR:OH[1_556]  | 1.76                     | 0.44              |
| 4:0:109:PRO:O   | 4:X:154:ASP:N[1_556]   | 1.76                     | 0.44              |
| 4:1:274:ILE:CB  | 4:Y:263:GLN:C[1_556]   | 1.76                     | 0.44              |
| 4:2:339:VAL:C   | 4:Z:335:ARG:NH2[1_556] | 1.76                     | 0.44              |
| 4:0:203:THR:N   | 4:X:201:VAL:CG2[1_556] | 1.76                     | 0.44              |
| 4:2:162:ASN:CG  | 4:Z:273:GLY:CA[1_556]  | 1.76                     | 0.44              |
| 4:0:67:LEU:CD1  | 4:X:207:GLU:CG[1_556]  | 1.76                     | 0.44              |
| 4:1:153:LEU:CG  | 4:Y:262:PHE:N[1_556]   | 1.76                     | 0.44              |
| 4:1:213:LYS:CE  | 4:Y:192:ILE:CG1[1_556] | 1.76                     | 0.44              |
| 4:1:240:TYR:OH  | 4:Y:198:TYR:OH[1_556]  | 1.76                     | 0.44              |
| 4:1:369:ILE:CG1 | 4:Y:345:ILE:CG2[1_556] | 1.76                     | 0.44              |
| 4:2:195:GLU:CD  | 4:Y:109:PRO:O[1_556]   | 1.76                     | 0.44              |
| 4:0:113:LYS:CG  | 4:X:136:ILE:N[1_556]   | 1.76                     | 0.44              |
| 4:2:300:SER:OG  | 4:Z:309:ILE:CA[1_556]  | 1.76                     | 0.44              |
| 4:2:303:THR:O   | 4:Z:256:ARG:C[1_556]   | 1.76                     | 0.44              |
| 4:1:215:LYS:NZ  | 4:Y:249:THR:CG2[1_556] | 1.76                     | 0.44              |
| 4:1:298:VAL:CB  | 4:Y:313:MET:N[1_556]   | 1.76                     | 0.44              |
| 4:2:172:PRO:CD  | 4:Z:164:PRO:N[1_556]   | 1.76                     | 0.44              |
| 4:1:106:THR:CA  | 4:Y:335:ARG:O[1_556]   | 1.76                     | 0.44              |
| 4:3:64:ILE:CD1  | 4:Y:292:ASP:CG[1_556]  | 1.76                     | 0.44              |
| 4:0:153:LEU:CB  | 4:X:262:PHE:CB[1_556]  | 1.76                     | 0.44              |
| 4:2:114:ALA:CB  | 4:Z:106:THR:N[1_556]   | 1.76                     | 0.44              |
| 4:2:77:THR:C    | 4:Z:33:SER:CB[1_556]   | 1.76                     | 0.44              |
| 4:0:39:ARG:C    | 4:V:166:TYR:OH[1_556]  | 1.76                     | 0.44              |
| 4:2:281:SER:O   | 4:Z:280:ASN:CB[1_556]  | 1.76                     | 0.44              |
| 4:1:122:ILE:CG2 | 4:Y:27:PRO:C[1_556]    | 1.76                     | 0.44              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:72:GLU:C    | 4:Z:157:ASP:O[1_556]   | 1.76                     | 0.44              |
| 4:1:166:TYR:O   | 4:Y:294:TYR:CA[1_556]  | 1.76                     | 0.44              |
| 4:0:37:ARG:CB   | 4:X:60:SER:CA[1_556]   | 1.76                     | 0.44              |
| 4:0:77:THR:CB   | 4:X:14:SER:O[1_556]    | 1.76                     | 0.44              |
| 4:0:339:VAL:C   | 4:X:335:ARG:NH2[1_556] | 1.76                     | 0.44              |
| 4:1:116:ARG:CA  | 4:Y:339:VAL:CB[1_556]  | 1.76                     | 0.44              |
| 4:0:77:THR:C    | 4:X:33:SER:CB[1_556]   | 1.76                     | 0.44              |
| 4:2:115:ASN:CB  | 4:Z:11:ASP:CG[1_556]   | 1.76                     | 0.44              |
| 4:0:166:TYR:O   | 4:X:294:TYR:CA[1_556]  | 1.76                     | 0.44              |
| 4:1:39:ARG:NH1  | 4:W:286:ASP:OD2[1_556] | 1.76                     | 0.44              |
| 4:1:281:SER:C   | 4:Y:276:GLU:O[1_556]   | 1.76                     | 0.44              |
| 4:3:196:ARG:CG  | 4:Z:115:ASN:CG[1_556]  | 1.76                     | 0.44              |
| 4:2:137:GLN:C   | 4:Z:299:MET:CG[1_556]  | 1.76                     | 0.44              |
| 4:3:63:GLY:CA   | 4:Y:288:ASP:CA[1_556]  | 1.76                     | 0.44              |
| 4:1:124:PHE:CB  | 4:Y:24:ASP:CA[1_556]   | 1.76                     | 0.44              |
| 4:2:203:THR:N   | 4:Z:201:VAL:CG2[1_556] | 1.76                     | 0.44              |
| 4:0:148:THR:CB  | 4:X:328:LYS:CA[1_556]  | 1.76                     | 0.44              |
| 4:1:206:ARG:CD  | 4:Y:200:PHE:CA[1_556]  | 1.76                     | 0.44              |
| 4:0:137:GLN:C   | 4:X:299:MET:CG[1_556]  | 1.76                     | 0.44              |
| 4:3:196:ARG:NH2 | 4:Z:114:ALA:O[1_556]   | 1.76                     | 0.44              |
| 4:0:167:GLU:CB  | 4:X:295:ALA:CA[1_556]  | 1.76                     | 0.44              |
| 4:1:148:THR:CB  | 4:Y:328:LYS:CB[1_556]  | 1.76                     | 0.44              |
| 4:0:71:ILE:CG1  | 4:X:16:LEU:CD2[1_556]  | 1.76                     | 0.44              |
| 4:2:73:HIS:ND1  | 4:Z:184:ASP:OD1[1_556] | 1.76                     | 0.44              |
| 4:2:124:PHE:C   | 4:Z:24:ASP:OD2[1_556]  | 1.76                     | 0.44              |
| 4:0:303:THR:O   | 4:X:256:ARG:C[1_556]   | 1.77                     | 0.43              |
| 4:0:336:LYS:CG  | 4:X:218:TYR:CE1[1_556] | 1.77                     | 0.43              |
| 4:1:40:HIS:N    | 4:W:166:TYR:OH[1_556]  | 1.77                     | 0.43              |
| 4:1:157:ASP:C   | 4:Y:185:LEU:CA[1_556]  | 1.77                     | 0.43              |
| 4:2:166:TYR:CB  | 4:Z:294:TYR:N[1_556]   | 1.77                     | 0.43              |
| 4:1:281:SER:O   | 4:Y:280:ASN:CA[1_556]  | 1.77                     | 0.43              |
| 4:0:293:LEU:C   | 4:X:320:LEU:CA[1_556]  | 1.77                     | 0.43              |
| 4:0:83:GLU:CD   | 4:X:29:ALA:CA[1_556]   | 1.77                     | 0.43              |
| 4:1:301:GLY:C   | 4:Y:218:TYR:O[1_556]   | 1.77                     | 0.43              |
| 4:2:116:ARG:NH1 | 4:Z:141:SER:CA[1_556]  | 1.77                     | 0.43              |
| 4:2:272:ALA:C   | 4:Z:269:MET:O[1_556]   | 1.77                     | 0.43              |
| 4:1:285:CYS:O   | 4:Y:283:MET:CG[1_556]  | 1.77                     | 0.43              |
| 4:2:72:GLU:N    | 4:Z:157:ASP:OD1[1_556] | 1.77                     | 0.43              |
| 4:2:107:GLU:O   | 4:Z:300:SER:CA[1_556]  | 1.77                     | 0.43              |
| 4:1:166:TYR:CB  | 4:Y:294:TYR:CG[1_556]  | 1.77                     | 0.43              |
| 4:1:161:HIS:CD2 | 4:Y:160:THR:CB[1_556]  | 1.77                     | 0.43              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:111:ASN:N   | 4:X:154:ASP:CG[1_556]  | 1.77                     | 0.43              |
| 4:0:170:ALA:CB  | 4:X:151:ILE:O[1_556]   | 1.77                     | 0.43              |
| 4:2:211:ASP:O   | 4:Z:196:ARG:CZ[1_556]  | 1.77                     | 0.43              |
| 4:1:281:SER:C   | 4:Y:280:ASN:OD1[1_556] | 1.77                     | 0.43              |
| 4:2:231:ALA:N   | 4:Y:368:SER:O[1_556]   | 1.77                     | 0.43              |
| 4:2:111:ASN:N   | 4:Z:154:ASP:CG[1_556]  | 1.77                     | 0.43              |
| 4:2:111:ASN:ND2 | 4:Z:339:VAL:CG2[1_556] | 1.77                     | 0.43              |
| 4:0:212:ILE:CG2 | 4:X:196:ARG:C[1_556]   | 1.77                     | 0.43              |
| 4:1:371:HIS:CE1 | 4:Y:140:LEU:N[1_556]   | 1.77                     | 0.43              |
| 4:2:152:VAL:CG2 | 4:Z:313:MET:CA[1_556]  | 1.77                     | 0.43              |
| 4:0:300:SER:OG  | 4:X:309:ILE:CA[1_556]  | 1.77                     | 0.43              |
| 4:2:196:ARG:NH2 | 4:Y:114:ALA:O[1_556]   | 1.77                     | 0.43              |
| 4:0:139:VAL:N   | 4:X:299:MET:CE[1_556]  | 1.77                     | 0.43              |
| 4:0:124:PHE:C   | 4:X:24:ASP:OD2[1_556]  | 1.77                     | 0.43              |
| 4:0:167:GLU:CA  | 4:X:295:ALA:CB[1_556]  | 1.77                     | 0.43              |
| 4:0:11:ASP:OD2  | 4:X:305:MET:C[1_556]   | 1.77                     | 0.43              |
| 4:2:367:PRO:CA  | 4:Z:343:GLY:C[1_556]   | 1.77                     | 0.43              |
| 4:2:116:ARG:CA  | 4:Z:339:VAL:CA[1_556]  | 1.77                     | 0.43              |
| 4:0:232:SER:O   | 4:W:362:TYR:CD1[1_556] | 1.77                     | 0.43              |
| 4:1:370:VAL:N   | 4:Y:342:GLY:O[1_556]   | 1.77                     | 0.43              |
| 4:1:295:ALA:C   | 4:Y:319:ALA:CA[1_556]  | 1.77                     | 0.43              |
| 4:0:302:GLY:O   | 4:X:255:PHE:C[1_556]   | 1.77                     | 0.43              |
| 4:2:370:VAL:CB  | 4:Z:342:GLY:CA[1_556]  | 1.77                     | 0.43              |
| 4:1:79:TRP:CG   | 4:Y:17:VAL:C[1_556]    | 1.77                     | 0.43              |
| 4:0:152:VAL:CA  | 4:X:313:MET:CG[1_556]  | 1.77                     | 0.43              |
| 4:0:272:ALA:C   | 4:X:269:MET:O[1_556]   | 1.77                     | 0.43              |
| 4:1:298:VAL:CG1 | 4:Y:311:ASP:C[1_556]   | 1.77                     | 0.43              |
| 4:3:195:GLU:CG  | 4:Z:110:LEU:N[1_556]   | 1.77                     | 0.43              |
| 4:0:296:ASN:C   | 4:X:316:GLU:N[1_556]   | 1.77                     | 0.43              |
| 4:3:253:GLU:N   | 4:Z:113:LYS:CA[1_556]  | 1.77                     | 0.43              |
| 4:1:296:ASN:C   | 4:Y:316:GLU:N[1_556]   | 1.77                     | 0.43              |
| 4:0:180:LEU:CD2 | 4:X:267:ILE:CA[1_556]  | 1.77                     | 0.43              |
| 4:0:196:ARG:NE  | 4:W:115:ASN:CB[1_556]  | 1.77                     | 0.43              |
| 4:1:289:ILE:N   | 4:Y:283:MET:CE[1_556]  | 1.77                     | 0.43              |
| 4:2:152:VAL:CB  | 4:Z:313:MET:CB[1_556]  | 1.77                     | 0.43              |
| 4:2:39:ARG:C    | 4:X:166:TYR:OH[1_556]  | 1.77                     | 0.43              |
| 4:1:371:HIS:ND1 | 4:Y:140:LEU:CB[1_556]  | 1.77                     | 0.43              |
| 4:2:116:ARG:CZ  | 4:Z:141:SER:CB[1_556]  | 1.77                     | 0.43              |
| 4:0:120:THR:C   | 4:X:340:TRP:CZ3[1_556] | 1.77                     | 0.43              |
| 4:1:335:ARG:CD  | 4:Y:220:ALA:CB[1_556]  | 1.77                     | 0.43              |
| 4:0:231:ALA:N   | 4:W:368:SER:O[1_556]   | 1.77                     | 0.43              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:365:ALA:CA  | 4:X:349:LEU:C[1_556]   | 1.77                     | 0.43              |
| 4:1:233:SER:N   | 4:X:366:GLY:C[1_556]   | 1.77                     | 0.43              |
| 4:0:86:TRP:CE3  | 4:X:30:VAL:CG2[1_556]  | 1.77                     | 0.43              |
| 4:2:109:PRO:O   | 4:Z:154:ASP:N[1_556]   | 1.77                     | 0.43              |
| 4:2:139:VAL:N   | 4:Z:299:MET:CE[1_556]  | 1.77                     | 0.43              |
| 4:1:196:ARG:CG  | 4:X:115:ASN:CG[1_556]  | 1.77                     | 0.43              |
| 4:3:63:GLY:O    | 4:Y:289:ILE:CG2[1_556] | 1.77                     | 0.43              |
| 4:2:120:THR:C   | 4:Z:340:TRP:CZ3[1_556] | 1.77                     | 0.43              |
| 4:1:149:THR:CA  | 4:Y:327:ILE:CG2[1_556] | 1.77                     | 0.43              |
| 4:1:169:TYR:CD2 | 4:Y:293:LEU:CG[1_556]  | 1.77                     | 0.43              |
| 4:2:86:TRP:CE3  | 4:Z:30:VAL:CG2[1_556]  | 1.77                     | 0.43              |
| 4:0:261:LEU:CA  | 4:X:266:PHE:CB[1_556]  | 1.77                     | 0.43              |
| 4:1:124:PHE:CD1 | 4:Y:24:ASP:C[1_556]    | 1.77                     | 0.43              |
| 4:1:123:MET:CB  | 4:Y:26:ALA:C[1_556]    | 1.77                     | 0.43              |
| 4:1:11:ASP:OD2  | 4:Y:305:MET:C[1_556]   | 1.77                     | 0.43              |
| 4:1:152:VAL:CG1 | 4:Y:313:MET:CG[1_556]  | 1.77                     | 0.43              |
| 4:0:157:ASP:O   | 4:X:185:LEU:O[1_556]   | 1.77                     | 0.43              |
| 4:0:124:PHE:CD2 | 4:X:24:ASP:O[1_556]    | 1.77                     | 0.43              |
| 4:0:152:VAL:CB  | 4:X:313:MET:CB[1_556]  | 1.77                     | 0.43              |
| 4:0:281:SER:O   | 4:X:280:ASN:CB[1_556]  | 1.77                     | 0.43              |
| 4:2:270:GLU:CD  | 4:Y:286:ASP:N[1_556]   | 1.77                     | 0.43              |
| 4:1:77:THR:CB   | 4:Y:15:GLY:CA[1_556]   | 1.77                     | 0.43              |
| 4:1:162:ASN:ND2 | 4:Y:273:GLY:O[1_556]   | 1.77                     | 0.43              |
| 4:2:227:MET:O   | 4:Y:372:ARG:N[1_556]   | 1.77                     | 0.43              |
| 4:2:152:VAL:CG1 | 4:Z:313:MET:CG[1_556]  | 1.78                     | 0.42              |
| 4:0:336:LYS:CB  | 4:X:218:TYR:N[1_556]   | 1.78                     | 0.42              |
| 4:1:371:HIS:CE1 | 4:Y:136:ILE:O[1_556]   | 1.78                     | 0.42              |
| 4:1:154:ASP:C   | 4:Y:261:LEU:CD1[1_556] | 1.78                     | 0.42              |
| 4:2:215:LYS:CB  | 4:Z:196:ARG:CZ[1_556]  | 1.78                     | 0.42              |
| 4:2:153:LEU:CB  | 4:Z:262:PHE:CB[1_556]  | 1.78                     | 0.42              |
| 4:2:124:PHE:CD2 | 4:Z:24:ASP:O[1_556]    | 1.78                     | 0.42              |
| 4:1:278:THR:OG1 | 4:Y:275:HIS:CE1[1_556] | 1.78                     | 0.42              |
| 4:2:168:GLY:CA  | 4:Z:296:ASN:CA[1_556]  | 1.78                     | 0.42              |
| 4:0:175:ILE:CB  | 4:X:162:ASN:ND2[1_556] | 1.78                     | 0.42              |
| 4:0:195:GLU:OE2 | 4:W:109:PRO:O[1_556]   | 1.78                     | 0.42              |
| 4:0:195:GLU:OE2 | 4:W:109:PRO:CA[1_556]  | 1.78                     | 0.42              |
| 4:2:132:MET:SD  | 4:Z:341:ILE:CB[1_556]  | 1.78                     | 0.42              |
| 4:1:153:LEU:CD2 | 4:Y:262:PHE:CG[1_556]  | 1.78                     | 0.42              |
| 4:0:152:VAL:CG1 | 4:X:313:MET:CG[1_556]  | 1.78                     | 0.42              |
| 4:1:299:MET:CA  | 4:Y:312:ARG:CB[1_556]  | 1.78                     | 0.42              |
| 4:1:257:CYS:CB  | 4:Y:195:GLU:OE1[1_556] | 1.78                     | 0.42              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:173:HIS:N   | 4:Y:174:ALA:O[1_556]   | 1.78                     | 0.42              |
| 4:2:293:LEU:C   | 4:Z:320:LEU:CA[1_556]  | 1.78                     | 0.42              |
| 4:1:366:GLY:O   | 4:Y:347:ALA:CA[1_556]  | 1.78                     | 0.42              |
| 4:1:302:GLY:O   | 4:Y:255:PHE:C[1_556]   | 1.78                     | 0.42              |
| 4:4:64:ILE:CD1  | 4:Z:292:ASP:CG[1_556]  | 1.78                     | 0.42              |
| 4:0:253:GLU:CG  | 4:W:112:PRO:CA[1_556]  | 1.78                     | 0.42              |
| 4:2:357:ILE:CB  | 4:Z:345:ILE:CG1[1_556] | 1.78                     | 0.42              |
| 4:0:16:LEU:CB   | 4:X:214:GLU:N[1_556]   | 1.78                     | 0.42              |
| 4:1:72:GLU:OE2  | 4:Y:183:ARG:CG[1_556]  | 1.78                     | 0.42              |
| 4:0:79:TRP:CD1  | 4:X:17:VAL:CA[1_556]   | 1.78                     | 0.42              |
| 4:1:40:HIS:CD2  | 4:W:166:TYR:O[1_556]   | 1.78                     | 0.42              |
| 4:0:172:PRO:CD  | 4:X:164:PRO:N[1_556]   | 1.78                     | 0.42              |
| 4:1:133:TYR:CZ  | 4:Y:145:SER:CA[1_556]  | 1.78                     | 0.42              |
| 4:0:108:ALA:CA  | 4:X:155:SER:N[1_556]   | 1.78                     | 0.42              |
| 4:0:206:ARG:NH2 | 4:X:190:MET:CG[1_556]  | 1.78                     | 0.42              |
| 4:1:59:GLN:CD   | 4:Y:208:ILE:CA[1_556]  | 1.78                     | 0.42              |
| 4:2:336:LYS:CB  | 4:Z:218:TYR:N[1_556]   | 1.78                     | 0.42              |
| 4:0:233:SER:N   | 4:W:367:PRO:C[1_556]   | 1.78                     | 0.42              |
| 4:1:141:SER:O   | 4:Y:310:ALA:CB[1_556]  | 1.78                     | 0.42              |
| 4:2:175:ILE:CB  | 4:Z:162:ASN:ND2[1_556] | 1.78                     | 0.42              |
| 4:1:215:LYS:CD  | 4:Y:196:ARG:NH2[1_556] | 1.78                     | 0.42              |
| 4:0:291:LYS:CE  | 4:Z:244:ASP:OD2[1_556] | 1.78                     | 0.42              |
| 4:1:83:GLU:N    | 4:Y:30:VAL:O[1_556]    | 1.78                     | 0.42              |
| 4:2:77:THR:CB   | 4:Z:14:SER:O[1_556]    | 1.78                     | 0.42              |
| 4:1:180:LEU:CD2 | 4:Y:267:ILE:CB[1_556]  | 1.78                     | 0.42              |
| 4:0:335:ARG:CB  | 4:X:220:ALA:N[1_556]   | 1.78                     | 0.42              |
| 4:2:183:ARG:NH2 | 4:Z:186:THR:OG1[1_556] | 1.78                     | 0.42              |
| 4:2:72:GLU:O    | 4:Z:157:ASP:CB[1_556]  | 1.78                     | 0.42              |
| 4:0:126:THR:CA  | 4:X:28:ARG:CZ[1_556]   | 1.78                     | 0.42              |
| 4:1:136:ILE:CG2 | 4:Y:153:LEU:O[1_556]   | 1.78                     | 0.42              |
| 4:0:107:GLU:O   | 4:X:300:SER:CA[1_556]  | 1.78                     | 0.42              |
| 4:2:232:SER:O   | 4:Y:362:TYR:CD1[1_556] | 1.78                     | 0.42              |
| 4:0:227:MET:O   | 4:W:372:ARG:N[1_556]   | 1.78                     | 0.42              |
| 4:1:262:PHE:CA  | 4:Y:265:SER:CB[1_556]  | 1.78                     | 0.42              |
| 4:1:282:ILE:O   | 4:Y:279:TYR:CE2[1_556] | 1.78                     | 0.42              |
| 4:1:114:ALA:CB  | 4:Y:106:THR:O[1_556]   | 1.78                     | 0.42              |
| 4:2:189:LEU:CD1 | 4:Z:195:GLU:CB[1_556]  | 1.78                     | 0.42              |
| 4:1:179:ASP:OD1 | 4:Y:179:ASP:C[1_556]   | 1.78                     | 0.42              |
| 4:2:140:LEU:N   | 4:Z:331:ALA:CB[1_556]  | 1.78                     | 0.42              |
| 4:1:170:ALA:N   | 4:Y:151:ILE:O[1_556]   | 1.78                     | 0.42              |
| 4:1:114:ALA:CB  | 4:Y:106:THR:N[1_556]   | 1.78                     | 0.42              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:80:ASP:CB   | 4:X:31:PHE:CD2[1_556]  | 1.78                     | 0.42              |
| 4:2:261:LEU:O   | 4:Z:265:SER:N[1_556]   | 1.78                     | 0.42              |
| 4:0:63:GLY:CA   | 4:V:287:ILE:C[1_556]   | 1.78                     | 0.42              |
| 4:2:162:ASN:CB  | 4:Z:274:ILE:CA[1_556]  | 1.78                     | 0.42              |
| 4:0:270:GLU:CD  | 4:W:286:ASP:N[1_556]   | 1.78                     | 0.42              |
| 4:2:177:ARG:CZ  | 4:Z:159:VAL:N[1_556]   | 1.78                     | 0.42              |
| 4:2:37:ARG:CB   | 4:Z:60:SER:CA[1_556]   | 1.78                     | 0.42              |
| 4:2:264:PRO:C   | 4:Z:268:GLY:CA[1_556]  | 1.78                     | 0.42              |
| 4:0:111:ASN:ND2 | 4:X:339:VAL:CG2[1_556] | 1.78                     | 0.42              |
| 4:2:214:GLU:O   | 4:Z:252:ASN:N[1_556]   | 1.78                     | 0.42              |
| 4:2:230:ALA:CB  | 4:Y:371:HIS:CG[1_556]  | 1.78                     | 0.42              |
| 4:1:304:THR:N   | 4:Y:259:GLU:N[1_556]   | 1.78                     | 0.42              |
| 4:1:160:THR:CA  | 4:Y:261:LEU:CD2[1_556] | 1.78                     | 0.42              |
| 4:2:180:LEU:CD2 | 4:Z:267:ILE:CA[1_556]  | 1.78                     | 0.42              |
| 4:0:215:LYS:CB  | 4:X:196:ARG:CZ[1_556]  | 1.78                     | 0.42              |
| 4:2:116:ARG:NH2 | 4:Z:141:SER:CA[1_556]  | 1.78                     | 0.42              |
| 4:1:133:TYR:C   | 4:Y:334:GLU:OE1[1_556] | 1.78                     | 0.42              |
| 4:1:178:LEU:CD1 | 4:Y:269:MET:SD[1_556]  | 1.78                     | 0.42              |
| 4:2:83:GLU:CD   | 4:Z:29:ALA:CA[1_556]   | 1.78                     | 0.42              |
| 4:1:158:GLY:N   | 4:Y:182:GLY:O[1_556]   | 1.78                     | 0.42              |
| 4:0:115:ASN:CB  | 4:X:11:ASP:CG[1_556]   | 1.78                     | 0.42              |
| 4:2:64:ILE:CD1  | 4:X:292:ASP:CG[1_556]  | 1.78                     | 0.42              |
| 4:3:64:ILE:N    | 4:Y:289:ILE:CA[1_556]  | 1.78                     | 0.42              |
| 4:2:196:ARG:NE  | 4:Y:115:ASN:CB[1_556]  | 1.78                     | 0.42              |
| 4:2:253:GLU:CG  | 4:Y:112:PRO:CA[1_556]  | 1.78                     | 0.42              |
| 4:1:152:VAL:O   | 4:Y:274:ILE:CG2[1_556] | 1.78                     | 0.42              |
| 4:1:291:LYS:C   | 4:Y:321:ALA:O[1_556]   | 1.78                     | 0.42              |
| 4:0:152:VAL:CB  | 4:X:313:MET:SD[1_556]  | 1.78                     | 0.42              |
| 4:3:197:GLY:O   | 4:Z:76:ILE:N[1_556]    | 1.78                     | 0.42              |
| 4:1:170:ALA:CB  | 4:Y:151:ILE:O[1_556]   | 1.78                     | 0.42              |
| 4:1:76:ILE:CG2  | 4:Y:16:LEU:C[1_556]    | 1.78                     | 0.42              |
| 4:1:177:ARG:CB  | 4:Y:178:LEU:CB[1_556]  | 1.78                     | 0.42              |
| 4:1:106:THR:O   | 4:Y:335:ARG:C[1_556]   | 1.78                     | 0.42              |
| 4:0:114:ALA:CB  | 4:X:106:THR:N[1_556]   | 1.78                     | 0.42              |
| 4:2:281:SER:O   | 4:Z:280:ASN:CA[1_556]  | 1.78                     | 0.42              |
| 4:1:272:ALA:C   | 4:Y:269:MET:O[1_556]   | 1.78                     | 0.42              |
| 4:1:253:GLU:N   | 4:X:113:LYS:CA[1_556]  | 1.78                     | 0.42              |
| 4:2:296:ASN:CB  | 4:Z:318:THR:N[1_556]   | 1.79                     | 0.41              |
| 4:1:153:LEU:O   | 4:Y:262:PHE:CD2[1_556] | 1.79                     | 0.41              |
| 4:0:253:GLU:CD  | 4:W:112:PRO:O[1_556]   | 1.79                     | 0.41              |
| 4:1:187:ASP:OD1 | 4:Y:190:MET:CG[1_556]  | 1.79                     | 0.41              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:266:PHE:O   | 4:X:172:PRO:O[1_556]   | 1.79                     | 0.41              |
| 4:0:357:ILE:CB  | 4:X:345:ILE:CG1[1_556] | 1.79                     | 0.41              |
| 4:2:175:ILE:CG1 | 4:Z:162:ASN:CB[1_556]  | 1.79                     | 0.41              |
| 4:1:196:ARG:NH2 | 4:X:114:ALA:O[1_556]   | 1.79                     | 0.41              |
| 4:0:166:TYR:CB  | 4:X:294:TYR:N[1_556]   | 1.79                     | 0.41              |
| 4:2:166:TYR:O   | 4:Z:294:TYR:CA[1_556]  | 1.79                     | 0.41              |
| 4:1:172:PRO:CB  | 4:Y:163:VAL:C[1_556]   | 1.79                     | 0.41              |
| 4:1:166:TYR:O   | 4:Y:293:LEU:O[1_556]   | 1.79                     | 0.41              |
| 4:1:162:ASN:CA  | 4:Y:274:ILE:N[1_556]   | 1.79                     | 0.41              |
| 4:2:175:ILE:CA  | 4:Z:162:ASN:CG[1_556]  | 1.79                     | 0.41              |
| 4:0:64:ILE:CD1  | 4:V:292:ASP:CG[1_556]  | 1.79                     | 0.41              |
| 4:1:232:SER:C   | 4:X:366:GLY:C[1_556]   | 1.79                     | 0.41              |
| 4:4:39:ARG:C    | 4:Z:166:TYR:OH[1_556]  | 1.79                     | 0.41              |
| 4:1:67:LEU:CD1  | 4:Y:207:GLU:CG[1_556]  | 1.79                     | 0.41              |
| 4:0:39:ARG:NH1  | 4:V:286:ASP:OD2[1_556] | 1.79                     | 0.41              |
| 4:1:64:ILE:N    | 4:W:289:ILE:CA[1_556]  | 1.79                     | 0.41              |
| 4:4:63:GLY:O    | 4:Z:289:ILE:CG2[1_556] | 1.79                     | 0.41              |
| 4:2:79:TRP:CD1  | 4:Z:17:VAL:CA[1_556]   | 1.79                     | 0.41              |
| 4:2:274:ILE:CB  | 4:Z:263:GLN:C[1_556]   | 1.79                     | 0.41              |
| 4:2:157:ASP:O   | 4:Z:185:LEU:O[1_556]   | 1.79                     | 0.41              |
| 4:1:104:LEU:CD2 | 4:Y:334:GLU:N[1_556]   | 1.79                     | 0.41              |
| 4:3:40:HIS:CD2  | 4:Y:166:TYR:O[1_556]   | 1.79                     | 0.41              |
| 4:0:153:LEU:C   | 4:X:262:PHE:CD1[1_556] | 1.79                     | 0.41              |
| 4:1:75:ILE:N    | 4:Y:156:GLY:C[1_556]   | 1.79                     | 0.41              |
| 4:1:40:HIS:O    | 4:W:167:GLU:OE2[1_556] | 1.79                     | 0.41              |
| 4:1:371:HIS:O   | 4:Y:139:VAL:C[1_556]   | 1.79                     | 0.41              |
| 4:3:252:ASN:CB  | 4:Z:113:LYS:O[1_556]   | 1.79                     | 0.41              |
| 4:0:335:ARG:O   | 4:X:219:VAL:N[1_556]   | 1.79                     | 0.41              |
| 4:1:166:TYR:CB  | 4:Y:294:TYR:N[1_556]   | 1.79                     | 0.41              |
| 4:1:303:THR:CA  | 4:Y:258:PRO:N[1_556]   | 1.79                     | 0.41              |
| 4:2:206:ARG:NH2 | 4:Z:190:MET:CG[1_556]  | 1.79                     | 0.41              |
| 4:0:362:TYR:CD1 | 4:X:344:SER:C[1_556]   | 1.79                     | 0.41              |
| 4:1:157:ASP:OD2 | 4:Y:186:THR:CB[1_556]  | 1.79                     | 0.41              |
| 4:1:214:GLU:C   | 4:Y:253:GLU:CD[1_556]  | 1.79                     | 0.41              |
| 4:1:304:THR:C   | 4:Y:223:PHE:CD1[1_556] | 1.79                     | 0.41              |
| 4:0:177:ARG:CB  | 4:X:178:LEU:CB[1_556]  | 1.79                     | 0.41              |
| 4:1:306:TYR:CG  | 4:Y:256:ARG:CB[1_556]  | 1.79                     | 0.41              |
| 4:0:80:ASP:CB   | 4:X:31:PHE:CG[1_556]   | 1.79                     | 0.41              |
| 4:0:252:ASN:CB  | 4:W:113:LYS:O[1_556]   | 1.79                     | 0.41              |
| 4:0:214:GLU:O   | 4:X:252:ASN:N[1_556]   | 1.79                     | 0.41              |
| 4:1:303:THR:CB  | 4:Y:258:PRO:N[1_556]   | 1.79                     | 0.41              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:168:GLY:CA  | 4:X:296:ASN:CA[1_556]  | 1.79                     | 0.41              |
| 4:1:40:HIS:NE2  | 4:W:166:TYR:CD2[1_556] | 1.79                     | 0.41              |
| 4:2:11:ASP:OD2  | 4:Z:305:MET:C[1_556]   | 1.79                     | 0.41              |
| 4:3:63:GLY:CA   | 4:Y:287:ILE:C[1_556]   | 1.79                     | 0.41              |
| 4:0:72:GLU:O    | 4:X:157:ASP:CB[1_556]  | 1.79                     | 0.41              |
| 4:0:142:LEU:N   | 4:X:310:ALA:C[1_556]   | 1.79                     | 0.41              |
| 4:2:195:GLU:OE2 | 4:Y:109:PRO:CA[1_556]  | 1.79                     | 0.41              |
| 4:0:108:ALA:C   | 4:X:154:ASP:C[1_556]   | 1.79                     | 0.41              |
| 4:1:76:ILE:CD1  | 4:Y:18:LYS:CD[1_556]   | 1.79                     | 0.41              |
| 4:1:141:SER:OG  | 4:Y:310:ALA:N[1_556]   | 1.79                     | 0.41              |
| 4:2:166:TYR:CA  | 4:Z:294:TYR:C[1_556]   | 1.79                     | 0.41              |
| 4:2:108:ALA:CA  | 4:Z:155:SER:N[1_556]   | 1.79                     | 0.41              |
| 4:2:252:ASN:CB  | 4:Y:113:LYS:O[1_556]   | 1.79                     | 0.41              |
| 4:0:72:GLU:CA   | 4:X:157:ASP:OD1[1_556] | 1.79                     | 0.41              |
| 4:1:296:ASN:C   | 4:Y:316:GLU:CA[1_556]  | 1.79                     | 0.41              |
| 4:1:152:VAL:CA  | 4:Y:313:MET:CG[1_556]  | 1.79                     | 0.41              |
| 4:1:207:GLU:C   | 4:Y:200:PHE:CZ[1_556]  | 1.79                     | 0.41              |
| 4:1:60:SER:CA   | 4:Y:243:PRO:CG[1_556]  | 1.79                     | 0.41              |
| 4:3:232:SER:C   | 4:Z:366:GLY:C[1_556]   | 1.79                     | 0.41              |
| 4:3:195:GLU:OE2 | 4:Z:109:PRO:O[1_556]   | 1.79                     | 0.41              |
| 4:1:363:ASP:N   | 4:Y:348:SER:CB[1_556]  | 1.79                     | 0.41              |
| 4:2:148:THR:CB  | 4:Z:328:LYS:CB[1_556]  | 1.79                     | 0.41              |
| 4:0:214:GLU:N   | 4:X:253:GLU:OE2[1_556] | 1.79                     | 0.41              |
| 4:0:261:LEU:O   | 4:X:265:SER:N[1_556]   | 1.79                     | 0.41              |
| 4:1:183:ARG:CB  | 4:Y:186:THR:O[1_556]   | 1.79                     | 0.41              |
| 4:2:152:VAL:CB  | 4:Z:313:MET:SD[1_556]  | 1.79                     | 0.41              |
| 4:2:195:GLU:OE2 | 4:Y:109:PRO:O[1_556]   | 1.79                     | 0.41              |
| 4:1:67:LEU:CA   | 4:Y:207:GLU:OE2[1_556] | 1.79                     | 0.41              |
| 4:1:67:LEU:CG   | 4:Y:207:GLU:OE1[1_556] | 1.79                     | 0.41              |
| 4:0:108:ALA:O   | 4:X:154:ASP:CB[1_556]  | 1.79                     | 0.41              |
| 4:2:214:GLU:N   | 4:Z:253:GLU:OE2[1_556] | 1.79                     | 0.41              |
| 4:0:153:LEU:O   | 4:X:262:PHE:CD2[1_556] | 1.79                     | 0.41              |
| 4:0:140:LEU:N   | 4:X:331:ALA:CB[1_556]  | 1.79                     | 0.41              |
| 4:1:74:GLY:N    | 4:Y:157:ASP:CA[1_556]  | 1.79                     | 0.41              |
| 4:0:289:ILE:CA  | 4:X:322:PRO:CD[1_556]  | 1.79                     | 0.41              |
| 4:2:302:GLY:O   | 4:Z:255:PHE:C[1_556]   | 1.79                     | 0.41              |
| 4:1:252:ASN:CB  | 4:X:113:LYS:O[1_556]   | 1.79                     | 0.41              |
| 4:2:72:GLU:CA   | 4:Z:157:ASP:OD1[1_556] | 1.79                     | 0.41              |
| 4:2:16:LEU:CB   | 4:Z:214:GLU:N[1_556]   | 1.79                     | 0.41              |
| 4:1:205:GLU:C   | 4:Y:199:SER:CA[1_556]  | 1.79                     | 0.41              |
| 4:1:167:GLU:C   | 4:Y:295:ALA:O[1_556]   | 1.79                     | 0.41              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:296:ASN:C   | 4:Y:316:GLU:C[1_556]   | 1.79                     | 0.41              |
| 4:2:154:ASP:C   | 4:Z:261:LEU:CD1[1_556] | 1.79                     | 0.41              |
| 4:2:281:SER:CA  | 4:Z:276:GLU:O[1_556]   | 1.79                     | 0.41              |
| 4:1:153:LEU:C   | 4:Y:262:PHE:CD1[1_556] | 1.79                     | 0.41              |
| 4:1:118:LYS:CE  | 4:Y:10:CYS:CB[1_556]   | 1.79                     | 0.41              |
| 4:0:142:LEU:N   | 4:X:310:ALA:O[1_556]   | 1.79                     | 0.41              |
| 4:0:40:HIS:CD2  | 4:V:166:TYR:CD2[1_556] | 1.79                     | 0.41              |
| 4:1:182:GLY:C   | 4:Y:188:TYR:C[1_556]   | 1.79                     | 0.41              |
| 4:0:372:ARG:NH2 | 4:X:145:SER:CA[1_556]  | 1.79                     | 0.41              |
| 4:2:108:ALA:O   | 4:Z:154:ASP:CB[1_556]  | 1.79                     | 0.41              |
| 4:1:137:GLN:CA  | 4:Y:304:THR:OG1[1_556] | 1.79                     | 0.41              |
| 4:0:285:CYS:C   | 4:X:283:MET:CG[1_556]  | 1.79                     | 0.41              |
| 4:2:335:ARG:CB  | 4:Z:220:ALA:N[1_556]   | 1.79                     | 0.41              |
| 4:3:41:GLN:CG   | 4:Y:167:GLU:OE1[1_556] | 1.79                     | 0.41              |
| 4:0:148:THR:CA  | 4:X:327:ILE:O[1_556]   | 1.79                     | 0.41              |
| 4:0:175:ILE:CG1 | 4:X:162:ASN:CB[1_556]  | 1.79                     | 0.41              |
| 4:0:189:LEU:CB  | 4:X:195:GLU:CG[1_556]  | 1.80                     | 0.40              |
| 4:2:80:ASP:CB   | 4:Z:31:PHE:CD2[1_556]  | 1.80                     | 0.40              |
| 4:3:40:HIS:NE2  | 4:Y:166:TYR:CD2[1_556] | 1.80                     | 0.40              |
| 4:0:162:ASN:CB  | 4:X:274:ILE:CA[1_556]  | 1.80                     | 0.40              |
| 4:2:124:PHE:CA  | 4:Z:24:ASP:N[1_556]    | 1.80                     | 0.40              |
| 4:0:296:ASN:CB  | 4:X:318:THR:N[1_556]   | 1.80                     | 0.40              |
| 4:3:266:PHE:O   | 4:Z:172:PRO:O[1_556]   | 1.80                     | 0.40              |
| 4:2:268:GLY:O   | 4:Y:284:LYS:C[1_556]   | 1.80                     | 0.40              |
| 4:1:134:VAL:CG2 | 4:Y:338:SER:O[1_556]   | 1.80                     | 0.40              |
| 4:0:121:GLN:CA  | 4:X:340:TRP:CZ2[1_556] | 1.80                     | 0.40              |
| 4:2:279:TYR:N   | 4:Z:276:GLU:OE1[1_556] | 1.80                     | 0.40              |
| 4:0:183:ARG:CG  | 4:X:187:ASP:CA[1_556]  | 1.80                     | 0.40              |
| 4:1:300:SER:OG  | 4:Y:309:ILE:CG1[1_556] | 1.80                     | 0.40              |
| 4:0:306:TYR:CE1 | 4:X:256:ARG:CG[1_556]  | 1.80                     | 0.40              |
| 4:0:147:ARG:CA  | 4:X:314:GLN:CD[1_556]  | 1.80                     | 0.40              |
| 4:2:303:THR:CA  | 4:Z:258:PRO:N[1_556]   | 1.80                     | 0.40              |
| 4:0:116:ARG:NH2 | 4:X:141:SER:CA[1_556]  | 1.80                     | 0.40              |
| 4:2:148:THR:CA  | 4:Z:327:ILE:O[1_556]   | 1.80                     | 0.40              |
| 4:2:306:TYR:CE1 | 4:Z:256:ARG:CG[1_556]  | 1.80                     | 0.40              |
| 4:2:141:SER:O   | 4:Z:310:ALA:CA[1_556]  | 1.80                     | 0.40              |
| 4:0:230:ALA:CB  | 4:W:371:HIS:CG[1_556]  | 1.80                     | 0.40              |
| 4:0:267:ILE:C   | 4:W:173:HIS:CB[1_556]  | 1.80                     | 0.40              |
| 4:2:123:MET:CB  | 4:Z:26:ALA:C[1_556]    | 1.80                     | 0.40              |
| 4:1:286:ASP:OD1 | 4:Y:290:ARG:NE[1_556]  | 1.80                     | 0.40              |
| 4:1:173:HIS:CD2 | 4:Y:281:SER:C[1_556]   | 1.80                     | 0.40              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:167:GLU:OE1 | 4:X:326:LYS:CG[1_556]  | 1.80                     | 0.40              |
| 4:0:268:GLY:O   | 4:W:284:LYS:C[1_556]   | 1.80                     | 0.40              |
| 4:2:158:GLY:CA  | 4:Z:182:GLY:C[1_556]   | 1.80                     | 0.40              |
| 4:1:298:VAL:C   | 4:Y:312:ARG:C[1_556]   | 1.80                     | 0.40              |
| 4:0:264:PRO:C   | 4:X:268:GLY:CA[1_556]  | 1.80                     | 0.40              |
| 4:0:123:MET:CB  | 4:X:26:ALA:C[1_556]    | 1.80                     | 0.40              |
| 4:0:336:LYS:CG  | 4:X:218:TYR:CD2[1_556] | 1.80                     | 0.40              |
| 4:2:300:SER:O   | 4:Z:219:VAL:CG2[1_556] | 1.80                     | 0.40              |
| 4:0:189:LEU:CD1 | 4:X:195:GLU:CB[1_556]  | 1.80                     | 0.40              |
| 4:0:210:ARG:CG  | 4:X:193:LEU:CG[1_556]  | 1.80                     | 0.40              |
| 4:1:76:ILE:CG1  | 4:Y:18:LYS:NZ[1_556]   | 1.80                     | 0.40              |
| 4:2:253:GLU:CD  | 4:Y:112:PRO:O[1_556]   | 1.80                     | 0.40              |
| 4:0:177:ARG:CZ  | 4:X:159:VAL:N[1_556]   | 1.80                     | 0.40              |
| 4:1:365:ALA:CA  | 4:Y:349:LEU:C[1_556]   | 1.80                     | 0.40              |
| 4:0:281:SER:CA  | 4:X:276:GLU:O[1_556]   | 1.80                     | 0.40              |
| 4:3:232:SER:N   | 4:Z:369:ILE:CB[1_556]  | 1.80                     | 0.40              |
| 4:0:178:LEU:CA  | 4:X:180:LEU:CD2[1_556] | 1.80                     | 0.40              |
| 4:2:311:ASP:N   | 4:Z:224:GLU:CB[1_556]  | 1.80                     | 0.40              |
| 4:0:281:SER:O   | 4:X:280:ASN:CA[1_556]  | 1.80                     | 0.40              |
| 4:1:142:LEU:CD1 | 4:Y:313:MET:C[1_556]   | 1.80                     | 0.40              |
| 4:0:309:ILE:CD1 | 4:X:259:GLU:OE1[1_556] | 1.80                     | 0.40              |
| 4:1:336:LYS:CG  | 4:Y:218:TYR:CE1[1_556] | 1.80                     | 0.40              |
| 4:3:40:HIS:O    | 4:Y:167:GLU:OE2[1_556] | 1.80                     | 0.40              |
| 4:1:106:THR:CA  | 4:Y:336:LYS:N[1_556]   | 1.80                     | 0.40              |
| 4:2:169:TYR:CZ  | 4:Z:150:GLY:O[1_556]   | 1.80                     | 0.40              |
| 4:0:144:ALA:O   | 4:X:311:ASP:OD1[1_556] | 1.80                     | 0.40              |
| 4:1:167:GLU:CA  | 4:Y:295:ALA:CB[1_556]  | 1.80                     | 0.40              |
| 4:2:369:ILE:N   | 4:Z:346:LEU:N[1_556]   | 1.80                     | 0.40              |
| 4:1:231:ALA:N   | 4:X:368:SER:O[1_556]   | 1.80                     | 0.40              |
| 4:1:186:THR:C   | 4:Y:191:LYS:CB[1_556]  | 1.80                     | 0.40              |
| 4:1:197:GLY:O   | 4:X:76:ILE:N[1_556]    | 1.80                     | 0.40              |
| 4:0:141:SER:O   | 4:X:310:ALA:CA[1_556]  | 1.80                     | 0.40              |
| 4:1:301:GLY:C   | 4:Y:258:PRO:CB[1_556]  | 1.80                     | 0.40              |
| 4:2:233:SER:CB  | 4:Y:367:PRO:CG[1_556]  | 1.80                     | 0.40              |
| 4:2:286:ASP:OD1 | 4:Z:290:ARG:NE[1_556]  | 1.80                     | 0.40              |
| 4:1:106:THR:O   | 4:Y:336:LYS:N[1_556]   | 1.80                     | 0.40              |
| 4:3:254:ARG:C   | 4:Z:113:LYS:NZ[1_556]  | 1.80                     | 0.40              |
| 4:1:206:ARG:NH1 | 4:Y:190:MET:CE[1_556]  | 1.80                     | 0.40              |
| 4:2:40:HIS:CD2  | 4:X:166:TYR:CD2[1_556] | 1.80                     | 0.40              |
| 4:2:104:LEU:CD2 | 4:Z:334:GLU:N[1_556]   | 1.80                     | 0.40              |
| 4:1:214:GLU:O   | 4:Y:252:ASN:CA[1_556]  | 1.80                     | 0.40              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:63:GLY:CA   | 4:X:287:ILE:C[1_556]   | 1.80                     | 0.40              |
| 4:1:177:ARG:CZ  | 4:Y:159:VAL:N[1_556]   | 1.80                     | 0.40              |
| 4:2:139:VAL:CB  | 4:Z:330:ILE:O[1_556]   | 1.80                     | 0.40              |
| 4:3:267:ILE:N   | 4:Z:173:HIS:ND1[1_556] | 1.80                     | 0.40              |
| 4:1:264:PRO:CG  | 4:Y:269:MET:N[1_556]   | 1.80                     | 0.40              |
| 4:0:305:MET:CB  | 4:X:255:PHE:CD2[1_556] | 1.80                     | 0.40              |
| 4:1:32:PRO:CG   | 4:Y:211:ASP:OD2[1_556] | 1.80                     | 0.40              |
| 4:2:108:ALA:C   | 4:Z:154:ASP:C[1_556]   | 1.80                     | 0.40              |
| 4:2:306:TYR:CG  | 4:Z:256:ARG:CB[1_556]  | 1.80                     | 0.40              |
| 4:2:83:GLU:CA   | 4:Z:30:VAL:N[1_556]    | 1.80                     | 0.40              |
| 4:1:232:SER:CA  | 4:X:366:GLY:O[1_556]   | 1.80                     | 0.40              |
| 4:1:281:SER:O   | 4:Y:280:ASN:ND2[1_556] | 1.80                     | 0.40              |
| 4:0:274:ILE:CB  | 4:X:263:GLN:C[1_556]   | 1.80                     | 0.40              |
| 4:1:67:LEU:CB   | 4:Y:62:ARG:NH2[1_556]  | 1.80                     | 0.40              |
| 4:2:372:ARG:CD  | 4:Z:143:TYR:N[1_556]   | 1.80                     | 0.40              |
| 4:2:147:ARG:CA  | 4:Z:314:GLN:CD[1_556]  | 1.80                     | 0.40              |
| 4:2:173:HIS:CB  | 4:Z:174:ALA:CA[1_556]  | 1.81                     | 0.39              |
| 4:2:335:ARG:O   | 4:Z:219:VAL:N[1_556]   | 1.81                     | 0.39              |
| 4:1:261:LEU:CA  | 4:Y:266:PHE:CB[1_556]  | 1.81                     | 0.39              |
| 4:2:177:ARG:CB  | 4:Z:178:LEU:CB[1_556]  | 1.81                     | 0.39              |
| 4:2:289:ILE:CA  | 4:Z:322:PRO:CD[1_556]  | 1.81                     | 0.39              |
| 4:1:261:LEU:O   | 4:Y:266:PHE:N[1_556]   | 1.81                     | 0.39              |
| 4:3:231:ALA:N   | 4:Z:368:SER:O[1_556]   | 1.81                     | 0.39              |
| 4:1:62:ARG:CD   | 4:Y:204:ALA:O[1_556]   | 1.81                     | 0.39              |
| 4:1:169:TYR:N   | 4:Y:296:ASN:O[1_556]   | 1.81                     | 0.39              |
| 4:0:11:ASP:CA   | 4:X:305:MET:CE[1_556]  | 1.81                     | 0.39              |
| 4:2:80:ASP:CB   | 4:Z:31:PHE:CG[1_556]   | 1.81                     | 0.39              |
| 4:1:126:THR:CA  | 4:Y:28:ARG:CZ[1_556]   | 1.81                     | 0.39              |
| 4:0:166:TYR:CA  | 4:X:294:TYR:C[1_556]   | 1.81                     | 0.39              |
| 4:0:279:TYR:N   | 4:X:276:GLU:OE1[1_556] | 1.81                     | 0.39              |
| 4:0:192:ILE:O   | 4:W:112:PRO:N[1_556]   | 1.81                     | 0.39              |
| 4:0:83:GLU:CA   | 4:X:30:VAL:N[1_556]    | 1.81                     | 0.39              |
| 4:1:9:VAL:CG2   | 4:Y:333:PRO:CB[1_556]  | 1.81                     | 0.39              |
| 4:1:362:TYR:C   | 4:Y:348:SER:CA[1_556]  | 1.81                     | 0.39              |
| 4:2:372:ARG:NH2 | 4:Z:145:SER:CA[1_556]  | 1.81                     | 0.39              |
| 4:1:115:ASN:CB  | 4:Y:11:ASP:CG[1_556]   | 1.81                     | 0.39              |
| 4:2:120:THR:CG2 | 4:Z:344:SER:N[1_556]   | 1.81                     | 0.39              |
| 4:1:106:THR:CG2 | 4:Y:335:ARG:CB[1_556]  | 1.81                     | 0.39              |
| 4:1:205:GLU:C   | 4:Y:199:SER:CB[1_556]  | 1.81                     | 0.39              |
| 4:0:215:LYS:NZ  | 4:X:249:THR:CG2[1_556] | 1.81                     | 0.39              |
| 4:2:309:ILE:CD1 | 4:Z:259:GLU:OE1[1_556] | 1.81                     | 0.39              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:166:TYR:CD1 | 4:Z:294:TYR:CB[1_556]  | 1.81                     | 0.39              |
| 4:0:67:LEU:O    | 4:X:62:ARG:CZ[1_556]   | 1.81                     | 0.39              |
| 4:2:362:TYR:N   | 4:Z:348:SER:OG[1_556]  | 1.81                     | 0.39              |
| 4:1:33:SER:O    | 4:Y:210:ARG:NH1[1_556] | 1.81                     | 0.39              |
| 4:2:267:ILE:C   | 4:Y:173:HIS:CB[1_556]  | 1.81                     | 0.39              |
| 4:1:107:GLU:O   | 4:Y:300:SER:CA[1_556]  | 1.81                     | 0.39              |
| 4:2:195:GLU:CD  | 4:Y:110:LEU:CA[1_556]  | 1.81                     | 0.39              |
| 4:2:39:ARG:NH1  | 4:X:286:ASP:OD2[1_556] | 1.81                     | 0.39              |
| 4:0:185:LEU:CB  | 4:X:188:TYR:CD1[1_556] | 1.81                     | 0.39              |
| 4:1:152:VAL:CG2 | 4:Y:313:MET:CA[1_556]  | 1.81                     | 0.39              |
| 4:0:60:SER:CA   | 4:X:243:PRO:CG[1_556]  | 1.81                     | 0.39              |
| 4:1:300:SER:C   | 4:Y:219:VAL:CG1[1_556] | 1.81                     | 0.39              |
| 4:2:121:GLN:CA  | 4:Z:340:TRP:CZ2[1_556] | 1.81                     | 0.39              |
| 4:0:140:LEU:C   | 4:X:310:ALA:CB[1_556]  | 1.81                     | 0.39              |
| 4:2:63:GLY:O    | 4:X:289:ILE:CG2[1_556] | 1.81                     | 0.39              |
| 4:2:206:ARG:N   | 4:Z:199:SER:O[1_556]   | 1.81                     | 0.39              |
| 4:1:109:PRO:CA  | 4:Y:153:LEU:C[1_556]   | 1.81                     | 0.39              |
| 4:2:285:CYS:C   | 4:Z:283:MET:CG[1_556]  | 1.81                     | 0.39              |
| 4:3:40:HIS:CD2  | 4:Y:166:TYR:CD2[1_556] | 1.81                     | 0.39              |
| 4:0:369:ILE:N   | 4:X:346:LEU:N[1_556]   | 1.81                     | 0.39              |
| 4:0:11:ASP:OD2  | 4:X:305:MET:O[1_556]   | 1.81                     | 0.39              |
| 4:0:175:ILE:CA  | 4:X:162:ASN:CG[1_556]  | 1.81                     | 0.39              |
| 4:2:153:LEU:C   | 4:Z:262:PHE:CD1[1_556] | 1.81                     | 0.39              |
| 4:2:185:LEU:CB  | 4:Z:188:TYR:CD1[1_556] | 1.81                     | 0.39              |
| 4:2:136:ILE:C   | 4:Z:299:MET:O[1_556]   | 1.81                     | 0.39              |
| 4:1:124:PHE:CA  | 4:Y:24:ASP:N[1_556]    | 1.81                     | 0.39              |
| 4:0:124:PHE:CD1 | 4:X:24:ASP:C[1_556]    | 1.81                     | 0.39              |
| 4:2:304:THR:CA  | 4:Z:223:PHE:CZ[1_556]  | 1.81                     | 0.39              |
| 4:0:80:ASP:N    | 4:X:31:PHE:CD2[1_556]  | 1.81                     | 0.39              |
| 4:0:253:GLU:N   | 4:W:113:LYS:CA[1_556]  | 1.81                     | 0.39              |
| 4:1:125:GLU:CB  | 4:Y:21:PHE:CG[1_556]   | 1.81                     | 0.39              |
| 4:2:142:LEU:N   | 4:Z:310:ALA:C[1_556]   | 1.81                     | 0.39              |
| 4:1:362:TYR:CE2 | 4:Y:22:ALA:CB[1_556]   | 1.81                     | 0.39              |
| 4:0:233:SER:CB  | 4:W:367:PRO:CG[1_556]  | 1.81                     | 0.39              |
| 4:0:261:LEU:O   | 4:X:265:SER:OG[1_556]  | 1.81                     | 0.39              |
| 4:0:362:TYR:N   | 4:X:348:SER:OG[1_556]  | 1.81                     | 0.39              |
| 4:2:76:ILE:CD1  | 4:Z:18:LYS:CD[1_556]   | 1.81                     | 0.39              |
| 4:1:335:ARG:C   | 4:Y:219:VAL:N[1_556]   | 1.81                     | 0.39              |
| 4:0:203:THR:CB  | 4:X:205:GLU:OE2[1_556] | 1.81                     | 0.39              |
| 4:2:362:TYR:CD1 | 4:Z:344:SER:C[1_556]   | 1.81                     | 0.39              |
| 4:1:115:ASN:C   | 4:Y:11:ASP:CG[1_556]   | 1.81                     | 0.39              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:298:VAL:CB  | 4:Z:313:MET:N[1_556]   | 1.81                     | 0.39              |
| 4:2:203:THR:CB  | 4:Z:205:GLU:OE2[1_556] | 1.81                     | 0.39              |
| 4:1:195:GLU:OE2 | 4:X:109:PRO:O[1_556]   | 1.81                     | 0.39              |
| 4:2:143:TYR:CB  | 4:Z:329:ILE:O[1_556]   | 1.81                     | 0.39              |
| 4:1:66:THR:CG2  | 4:Y:62:ARG:N[1_556]    | 1.81                     | 0.39              |
| 4:2:266:PHE:O   | 4:Y:172:PRO:O[1_556]   | 1.81                     | 0.39              |
| 4:0:124:PHE:CA  | 4:X:24:ASP:N[1_556]    | 1.81                     | 0.39              |
| 4:0:134:VAL:CG1 | 4:X:338:SER:OG[1_556]  | 1.81                     | 0.39              |
| 4:0:300:SER:O   | 4:X:219:VAL:CG2[1_556] | 1.81                     | 0.39              |
| 4:1:305:MET:CB  | 4:Y:255:PHE:CA[1_556]  | 1.81                     | 0.39              |
| 4:2:178:LEU:CA  | 4:Z:180:LEU:CD2[1_556] | 1.81                     | 0.39              |
| 4:3:232:SER:CA  | 4:Z:366:GLY:O[1_556]   | 1.81                     | 0.39              |
| 4:4:40:HIS:CD2  | 4:Z:166:TYR:CD2[1_556] | 1.81                     | 0.39              |
| 4:2:80:ASP:N    | 4:Z:31:PHE:CD2[1_556]  | 1.81                     | 0.39              |
| 4:1:41:GLN:CG   | 4:W:167:GLU:OE1[1_556] | 1.81                     | 0.39              |
| 4:1:63:GLY:CA   | 4:W:287:ILE:C[1_556]   | 1.81                     | 0.39              |
| 4:2:240:TYR:OH  | 4:Z:198:TYR:OH[1_556]  | 1.81                     | 0.39              |
| 4:2:178:LEU:CD1 | 4:Z:269:MET:SD[1_556]  | 1.81                     | 0.39              |
| 4:2:118:LYS:CB  | 4:Z:10:CYS:C[1_556]    | 1.81                     | 0.39              |
| 4:0:167:GLU:CB  | 4:X:295:ALA:N[1_556]   | 1.81                     | 0.39              |
| 4:0:143:TYR:CB  | 4:X:329:ILE:O[1_556]   | 1.81                     | 0.39              |
| 4:0:311:ASP:N   | 4:X:224:GLU:CB[1_556]  | 1.81                     | 0.39              |
| 4:1:72:GLU:N    | 4:Y:157:ASP:OD1[1_556] | 1.81                     | 0.39              |
| 4:0:154:ASP:C   | 4:X:261:LEU:CD1[1_556] | 1.81                     | 0.39              |
| 4:1:180:LEU:CD2 | 4:Y:267:ILE:CA[1_556]  | 1.81                     | 0.39              |
| 4:2:336:LYS:CG  | 4:Z:218:TYR:CD2[1_556] | 1.81                     | 0.39              |
| 4:0:177:ARG:CA  | 4:X:178:LEU:CD2[1_556] | 1.81                     | 0.39              |
| 4:2:124:PHE:N   | 4:Z:24:ASP:CB[1_556]   | 1.81                     | 0.39              |
| 4:1:212:ILE:N   | 4:Y:196:ARG:CB[1_556]  | 1.81                     | 0.39              |
| 4:1:111:ASN:ND2 | 4:Y:339:VAL:CG2[1_556] | 1.81                     | 0.39              |
| 4:2:167:GLU:CB  | 4:Z:295:ALA:N[1_556]   | 1.81                     | 0.39              |
| 4:1:175:ILE:CA  | 4:Y:277:THR:CG2[1_556] | 1.81                     | 0.39              |
| 4:2:141:SER:O   | 4:Z:310:ALA:CB[1_556]  | 1.81                     | 0.39              |
| 4:0:148:THR:CB  | 4:X:328:LYS:CB[1_556]  | 1.81                     | 0.39              |
| 4:2:153:LEU:O   | 4:Z:262:PHE:CD2[1_556] | 1.81                     | 0.39              |
| 4:1:72:GLU:CB   | 4:Y:183:ARG:NH2[1_556] | 1.81                     | 0.39              |
| 4:1:124:PHE:CD2 | 4:Y:24:ASP:O[1_556]    | 1.81                     | 0.39              |
| 4:0:120:THR:CG2 | 4:X:344:SER:N[1_556]   | 1.81                     | 0.39              |
| 4:0:296:ASN:ND2 | 4:X:318:THR:C[1_556]   | 1.81                     | 0.39              |
| 4:2:122:ILE:CG2 | 4:Z:19:ALA:O[1_556]    | 1.81                     | 0.39              |
| 4:1:160:THR:CG2 | 4:Y:261:LEU:CA[1_556]  | 1.81                     | 0.39              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:267:ILE:N   | 4:X:173:HIS:ND1[1_556] | 1.81                     | 0.39              |
| 4:0:37:ARG:O    | 4:X:60:SER:O[1_556]    | 1.81                     | 0.39              |
| 4:2:166:TYR:O   | 4:Z:293:LEU:C[1_556]   | 1.81                     | 0.39              |
| 4:2:261:LEU:O   | 4:Z:266:PHE:N[1_556]   | 1.81                     | 0.39              |
| 4:0:372:ARG:CD  | 4:X:143:TYR:N[1_556]   | 1.81                     | 0.39              |
| 4:2:158:GLY:N   | 4:Z:182:GLY:O[1_556]   | 1.82                     | 0.38              |
| 4:2:170:ALA:N   | 4:Z:151:ILE:O[1_556]   | 1.82                     | 0.38              |
| 4:1:232:SER:N   | 4:X:369:ILE:CB[1_556]  | 1.82                     | 0.38              |
| 4:0:64:ILE:N    | 4:V:289:ILE:CA[1_556]  | 1.82                     | 0.38              |
| 4:0:183:ARG:CD  | 4:X:187:ASP:OD1[1_556] | 1.82                     | 0.38              |
| 4:2:167:GLU:OE1 | 4:Z:326:LYS:CG[1_556]  | 1.82                     | 0.38              |
| 4:2:11:ASP:CA   | 4:Z:305:MET:CE[1_556]  | 1.82                     | 0.38              |
| 4:2:210:ARG:CG  | 4:Z:193:LEU:CG[1_556]  | 1.82                     | 0.38              |
| 4:0:14:SER:C    | 4:X:213:LYS:NZ[1_556]  | 1.82                     | 0.38              |
| 4:2:370:VAL:CG1 | 4:Z:341:ILE:O[1_556]   | 1.82                     | 0.38              |
| 4:2:124:PHE:CD1 | 4:Z:24:ASP:C[1_556]    | 1.82                     | 0.38              |
| 4:2:211:ASP:OD1 | 4:Z:249:THR:C[1_556]   | 1.82                     | 0.38              |
| 4:1:362:TYR:CD1 | 4:Y:344:SER:C[1_556]   | 1.82                     | 0.38              |
| 4:1:183:ARG:CA  | 4:Y:186:THR:C[1_556]   | 1.82                     | 0.38              |
| 4:1:40:HIS:CD2  | 4:W:166:TYR:CD2[1_556] | 1.82                     | 0.38              |
| 4:2:183:ARG:CG  | 4:Z:187:ASP:CA[1_556]  | 1.82                     | 0.38              |
| 4:0:157:ASP:C   | 4:X:185:LEU:CA[1_556]  | 1.82                     | 0.38              |
| 4:0:286:ASP:N   | 4:X:283:MET:CG[1_556]  | 1.82                     | 0.38              |
| 4:1:162:ASN:CB  | 4:Y:274:ILE:N[1_556]   | 1.82                     | 0.38              |
| 4:2:144:ALA:O   | 4:Z:311:ASP:OD1[1_556] | 1.82                     | 0.38              |
| 4:1:158:GLY:CA  | 4:Y:182:GLY:C[1_556]   | 1.82                     | 0.38              |
| 4:2:142:LEU:N   | 4:Z:310:ALA:O[1_556]   | 1.82                     | 0.38              |
| 4:0:303:THR:CA  | 4:X:258:PRO:N[1_556]   | 1.82                     | 0.38              |
| 4:0:331:ALA:CB  | 4:X:222:ASP:CA[1_556]  | 1.82                     | 0.38              |
| 4:2:189:LEU:CB  | 4:Z:195:GLU:CG[1_556]  | 1.82                     | 0.38              |
| 4:1:141:SER:CB  | 4:Y:310:ALA:CA[1_556]  | 1.82                     | 0.38              |
| 4:0:232:SER:N   | 4:W:369:ILE:CB[1_556]  | 1.82                     | 0.38              |
| 4:2:117:GLU:C   | 4:Z:9:VAL:CG1[1_556]   | 1.82                     | 0.38              |
| 4:1:367:PRO:CA  | 4:Y:343:GLY:C[1_556]   | 1.82                     | 0.38              |
| 4:0:15:GLY:N    | 4:X:213:LYS:NZ[1_556]  | 1.82                     | 0.38              |
| 4:0:166:TYR:O   | 4:X:293:LEU:C[1_556]   | 1.82                     | 0.38              |
| 4:2:332:PRO:CD  | 4:Z:221:LEU:CD2[1_556] | 1.82                     | 0.38              |
| 4:1:271:SER:C   | 4:Y:270:GLU:CA[1_556]  | 1.82                     | 0.38              |
| 4:0:104:LEU:CD2 | 4:X:334:GLU:N[1_556]   | 1.82                     | 0.38              |
| 4:0:272:ALA:C   | 4:X:270:GLU:CA[1_556]  | 1.82                     | 0.38              |
| 4:2:367:PRO:N   | 4:Z:347:ALA:CA[1_556]  | 1.82                     | 0.38              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:266:PHE:O   | 4:W:172:PRO:O[1_556]   | 1.82                     | 0.38              |
| 4:2:296:ASN:ND2 | 4:Z:318:THR:C[1_556]   | 1.82                     | 0.38              |
| 4:4:39:ARG:NH1  | 4:Z:286:ASP:OD2[1_556] | 1.82                     | 0.38              |
| 4:0:304:THR:CA  | 4:X:223:PHE:CZ[1_556]  | 1.82                     | 0.38              |
| 4:0:62:ARG:CG   | 4:X:204:ALA:N[1_556]   | 1.82                     | 0.38              |
| 4:0:173:HIS:CB  | 4:X:174:ALA:CA[1_556]  | 1.82                     | 0.38              |
| 4:2:183:ARG:CD  | 4:Z:187:ASP:OD1[1_556] | 1.82                     | 0.38              |
| 4:2:272:ALA:C   | 4:Z:270:GLU:CA[1_556]  | 1.82                     | 0.38              |
| 4:0:139:VAL:CB  | 4:X:330:ILE:O[1_556]   | 1.82                     | 0.38              |
| 4:1:74:GLY:N    | 4:Y:157:ASP:N[1_556]   | 1.82                     | 0.38              |
| 4:0:169:TYR:CZ  | 4:X:150:GLY:O[1_556]   | 1.82                     | 0.38              |
| 4:2:305:MET:CB  | 4:Z:255:PHE:CD2[1_556] | 1.82                     | 0.38              |
| 4:0:124:PHE:C   | 4:X:24:ASP:CA[1_556]   | 1.82                     | 0.38              |
| 4:2:62:ARG:CG   | 4:Z:204:ALA:N[1_556]   | 1.82                     | 0.38              |
| 4:1:79:TRP:CD2  | 4:Y:17:VAL:CA[1_556]   | 1.82                     | 0.38              |
| 4:0:261:LEU:O   | 4:X:266:PHE:N[1_556]   | 1.82                     | 0.38              |
| 4:2:106:THR:CA  | 4:Z:336:LYS:N[1_556]   | 1.82                     | 0.38              |
| 4:0:179:ASP:OD1 | 4:X:179:ASP:C[1_556]   | 1.82                     | 0.38              |
| 4:1:293:LEU:C   | 4:Y:320:LEU:CB[1_556]  | 1.82                     | 0.38              |
| 4:0:169:TYR:CD2 | 4:X:293:LEU:CG[1_556]  | 1.82                     | 0.38              |
| 4:0:169:TYR:C   | 4:X:151:ILE:CG2[1_556] | 1.82                     | 0.38              |
| 4:1:162:ASN:CB  | 4:Y:274:ILE:CA[1_556]  | 1.82                     | 0.38              |
| 4:0:195:GLU:CD  | 4:W:110:LEU:CA[1_556]  | 1.82                     | 0.38              |
| 4:1:231:ALA:C   | 4:X:370:VAL:N[1_556]   | 1.82                     | 0.38              |
| 4:2:134:VAL:CG1 | 4:Z:338:SER:OG[1_556]  | 1.82                     | 0.38              |
| 4:1:109:PRO:O   | 4:Y:154:ASP:N[1_556]   | 1.82                     | 0.38              |
| 4:2:67:LEU:O    | 4:Z:62:ARG:CZ[1_556]   | 1.82                     | 0.38              |
| 4:0:197:GLY:O   | 4:W:76:ILE:N[1_556]    | 1.82                     | 0.38              |
| 4:2:164:PRO:N   | 4:Z:278:THR:CA[1_556]  | 1.82                     | 0.38              |
| 4:0:292:ASP:O   | 4:X:319:ALA:N[1_556]   | 1.82                     | 0.38              |
| 4:2:183:ARG:CA  | 4:Z:186:THR:C[1_556]   | 1.82                     | 0.38              |
| 4:1:309:ILE:CA  | 4:Y:259:GLU:OE2[1_556] | 1.82                     | 0.38              |
| 4:2:215:LYS:NZ  | 4:Z:249:THR:CG2[1_556] | 1.82                     | 0.38              |
| 4:2:262:PHE:CA  | 4:Z:265:SER:CB[1_556]  | 1.82                     | 0.38              |
| 4:0:164:PRO:N   | 4:X:278:THR:CA[1_556]  | 1.82                     | 0.38              |
| 4:2:64:ILE:N    | 4:X:289:ILE:CA[1_556]  | 1.82                     | 0.38              |
| 4:1:153:LEU:CD1 | 4:Y:262:PHE:CB[1_556]  | 1.82                     | 0.38              |
| 4:1:142:LEU:N   | 4:Y:310:ALA:O[1_556]   | 1.82                     | 0.38              |
| 4:0:185:LEU:CD2 | 4:X:188:TYR:CE1[1_556] | 1.82                     | 0.38              |
| 4:1:118:LYS:CB  | 4:Y:11:ASP:CA[1_556]   | 1.82                     | 0.38              |
| 4:1:126:THR:CB  | 4:Y:28:ARG:CD[1_556]   | 1.82                     | 0.38              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:40:HIS:O    | 4:Z:167:GLU:OE2[1_556] | 1.82                     | 0.38              |
| 4:0:286:ASP:OD1 | 4:X:290:ARG:NE[1_556]  | 1.82                     | 0.38              |
| 4:2:331:ALA:C   | 4:Z:221:LEU:CB[1_556]  | 1.82                     | 0.38              |
| 4:0:141:SER:OG  | 4:X:309:ILE:C[1_556]   | 1.82                     | 0.38              |
| 4:1:149:THR:OG1 | 4:Y:327:ILE:N[1_556]   | 1.82                     | 0.38              |
| 4:1:67:LEU:O    | 4:Y:62:ARG:CZ[1_556]   | 1.82                     | 0.38              |
| 4:0:118:LYS:CB  | 4:X:10:CYS:C[1_556]    | 1.82                     | 0.38              |
| 4:0:166:TYR:CA  | 4:X:294:TYR:CB[1_556]  | 1.82                     | 0.38              |
| 4:0:254:ARG:C   | 4:W:113:LYS:NZ[1_556]  | 1.82                     | 0.38              |
| 4:2:162:ASN:CB  | 4:Z:274:ILE:N[1_556]   | 1.82                     | 0.38              |
| 4:0:158:GLY:CA  | 4:X:182:GLY:C[1_556]   | 1.82                     | 0.38              |
| 4:1:108:ALA:CA  | 4:Y:300:SER:O[1_556]   | 1.82                     | 0.38              |
| 4:0:166:TYR:CD1 | 4:X:294:TYR:CB[1_556]  | 1.82                     | 0.38              |
| 4:2:153:LEU:CG  | 4:Z:262:PHE:N[1_556]   | 1.82                     | 0.38              |
| 4:0:213:LYS:CE  | 4:X:192:ILE:CG1[1_556] | 1.82                     | 0.38              |
| 4:1:339:VAL:CG2 | 4:Y:304:THR:O[1_556]   | 1.82                     | 0.38              |
| 4:2:167:GLU:C   | 4:Z:296:ASN:N[1_556]   | 1.82                     | 0.38              |
| 4:1:210:ARG:CG  | 4:Y:193:LEU:CG[1_556]  | 1.82                     | 0.38              |
| 4:1:113:LYS:O   | 4:Y:140:LEU:CD1[1_556] | 1.82                     | 0.38              |
| 4:0:240:TYR:OH  | 4:X:198:TYR:OH[1_556]  | 1.82                     | 0.38              |
| 4:0:63:GLY:O    | 4:V:289:ILE:CG2[1_556] | 1.82                     | 0.38              |
| 4:2:192:ILE:O   | 4:Y:112:PRO:N[1_556]   | 1.82                     | 0.38              |
| 4:4:64:ILE:N    | 4:Z:289:ILE:CA[1_556]  | 1.82                     | 0.38              |
| 4:1:254:ARG:C   | 4:X:113:LYS:NZ[1_556]  | 1.82                     | 0.38              |
| 4:4:63:GLY:CA   | 4:Z:287:ILE:C[1_556]   | 1.82                     | 0.38              |
| 4:2:162:ASN:ND2 | 4:Z:273:GLY:O[1_556]   | 1.82                     | 0.38              |
| 4:0:370:VAL:CG1 | 4:X:341:ILE:O[1_556]   | 1.82                     | 0.38              |
| 4:2:37:ARG:O    | 4:Z:60:SER:O[1_556]    | 1.82                     | 0.38              |
| 4:2:177:ARG:NH1 | 4:Z:159:VAL:O[1_556]   | 1.82                     | 0.38              |
| 4:2:67:LEU:CB   | 4:Z:207:GLU:CD[1_556]  | 1.82                     | 0.38              |
| 4:2:172:PRO:O   | 4:Z:162:ASN:O[1_556]   | 1.82                     | 0.38              |
| 4:0:162:ASN:CB  | 4:X:274:ILE:N[1_556]   | 1.82                     | 0.38              |
| 4:1:14:SER:C    | 4:Y:213:LYS:NZ[1_556]  | 1.82                     | 0.38              |
| 4:0:122:ILE:CG2 | 4:X:19:ALA:O[1_556]    | 1.82                     | 0.38              |
| 4:0:306:TYR:CG  | 4:X:256:ARG:CB[1_556]  | 1.82                     | 0.38              |
| 4:2:261:LEU:O   | 4:Z:265:SER:OG[1_556]  | 1.82                     | 0.38              |
| 4:2:253:GLU:N   | 4:Y:113:LYS:CA[1_556]  | 1.83                     | 0.37              |
| 4:0:214:GLU:O   | 4:X:252:ASN:CB[1_556]  | 1.83                     | 0.37              |
| 4:2:300:SER:OG  | 4:Z:309:ILE:CG1[1_556] | 1.83                     | 0.37              |
| 4:1:79:TRP:CZ3  | 4:Y:18:LYS:N[1_556]    | 1.83                     | 0.37              |
| 4:1:368:SER:OG  | 4:Y:346:LEU:CD2[1_556] | 1.83                     | 0.37              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:186:THR:CB  | 4:Y:191:LYS:N[1_556]   | 1.83                     | 0.37              |
| 4:1:68:LYS:CD   | 4:Y:59:GLN:CA[1_556]   | 1.83                     | 0.37              |
| 4:1:83:GLU:CB   | 4:Y:29:ALA:C[1_556]    | 1.83                     | 0.37              |
| 4:2:124:PHE:C   | 4:Z:24:ASP:CA[1_556]   | 1.83                     | 0.37              |
| 4:3:196:ARG:NH1 | 4:Z:115:ASN:C[1_556]   | 1.83                     | 0.37              |
| 4:2:165:ILE:CG1 | 4:Z:297:ASN:CB[1_556]  | 1.83                     | 0.37              |
| 4:1:148:THR:CB  | 4:Y:327:ILE:C[1_556]   | 1.83                     | 0.37              |
| 4:2:11:ASP:OD2  | 4:Z:305:MET:O[1_556]   | 1.83                     | 0.37              |
| 4:0:168:GLY:C   | 4:X:296:ASN:N[1_556]   | 1.83                     | 0.37              |
| 4:1:189:LEU:CD2 | 4:Y:195:GLU:CB[1_556]  | 1.83                     | 0.37              |
| 4:1:136:ILE:C   | 4:Y:299:MET:O[1_556]   | 1.83                     | 0.37              |
| 4:2:185:LEU:CD2 | 4:Z:188:TYR:CE1[1_556] | 1.83                     | 0.37              |
| 4:1:211:ASP:O   | 4:Y:196:ARG:CZ[1_556]  | 1.83                     | 0.37              |
| 4:0:167:GLU:CD  | 4:X:326:LYS:CB[1_556]  | 1.83                     | 0.37              |
| 4:0:123:MET:N   | 4:X:26:ALA:C[1_556]    | 1.83                     | 0.37              |
| 4:1:139:VAL:N   | 4:Y:299:MET:CE[1_556]  | 1.83                     | 0.37              |
| 4:2:124:PHE:CD2 | 4:Z:344:SER:OG[1_556]  | 1.83                     | 0.37              |
| 4:1:148:THR:CA  | 4:Y:327:ILE:O[1_556]   | 1.83                     | 0.37              |
| 4:0:298:VAL:CB  | 4:X:313:MET:N[1_556]   | 1.83                     | 0.37              |
| 4:1:178:LEU:CD1 | 4:Y:269:MET:CB[1_556]  | 1.83                     | 0.37              |
| 4:1:117:GLU:C   | 4:Y:9:VAL:CG1[1_556]   | 1.83                     | 0.37              |
| 4:2:264:PRO:CG  | 4:Z:269:MET:N[1_556]   | 1.83                     | 0.37              |
| 4:0:178:LEU:CD1 | 4:X:269:MET:SD[1_556]  | 1.83                     | 0.37              |
| 4:0:170:ALA:N   | 4:X:151:ILE:O[1_556]   | 1.83                     | 0.37              |
| 4:0:153:LEU:CG  | 4:X:262:PHE:N[1_556]   | 1.83                     | 0.37              |
| 4:0:106:THR:CA  | 4:X:336:LYS:N[1_556]   | 1.83                     | 0.37              |
| 4:0:208:ILE:CG1 | 4:X:198:TYR:CZ[1_556]  | 1.83                     | 0.37              |
| 4:2:298:VAL:C   | 4:Z:312:ARG:O[1_556]   | 1.83                     | 0.37              |
| 4:2:292:ASP:O   | 4:Z:319:ALA:N[1_556]   | 1.83                     | 0.37              |
| 4:0:206:ARG:N   | 4:X:199:SER:O[1_556]   | 1.83                     | 0.37              |
| 4:2:60:SER:CA   | 4:Z:243:PRO:CG[1_556]  | 1.83                     | 0.37              |
| 4:0:332:PRO:CD  | 4:X:221:LEU:CD2[1_556] | 1.83                     | 0.37              |
| 4:2:303:THR:CA  | 4:Z:257:CYS:CA[1_556]  | 1.83                     | 0.37              |
| 4:0:162:ASN:CA  | 4:X:274:ILE:N[1_556]   | 1.83                     | 0.37              |
| 4:0:60:SER:CB   | 4:X:243:PRO:CA[1_556]  | 1.83                     | 0.37              |
| 4:0:63:GLY:N    | 4:V:287:ILE:O[1_556]   | 1.83                     | 0.37              |
| 4:3:231:ALA:C   | 4:Z:370:VAL:N[1_556]   | 1.83                     | 0.37              |
| 4:1:68:LYS:N    | 4:Y:59:GLN:CG[1_556]   | 1.83                     | 0.37              |
| 4:2:169:TYR:C   | 4:Z:151:ILE:CG2[1_556] | 1.83                     | 0.37              |
| 4:0:76:ILE:CD1  | 4:X:18:LYS:CD[1_556]   | 1.83                     | 0.37              |
| 4:2:15:GLY:N    | 4:Z:213:LYS:NZ[1_556]  | 1.83                     | 0.37              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:124:PHE:CD2 | 4:X:344:SER:OG[1_556]  | 1.83                     | 0.37              |
| 4:1:331:ALA:C   | 4:Y:221:LEU:CB[1_556]  | 1.83                     | 0.37              |
| 4:0:59:GLN:OE1  | 4:X:208:ILE:CG2[1_556] | 1.83                     | 0.37              |
| 4:1:175:ILE:CA  | 4:Y:162:ASN:CG[1_556]  | 1.83                     | 0.37              |
| 4:0:67:LEU:CB   | 4:X:207:GLU:CD[1_556]  | 1.83                     | 0.37              |
| 4:0:177:ARG:NH1 | 4:X:159:VAL:O[1_556]   | 1.83                     | 0.37              |
| 4:2:179:ASP:OD1 | 4:Z:179:ASP:C[1_556]   | 1.83                     | 0.37              |
| 4:0:120:THR:CB  | 4:X:340:TRP:C[1_556]   | 1.83                     | 0.37              |
| 4:2:232:SER:N   | 4:Y:369:ILE:CB[1_556]  | 1.83                     | 0.37              |
| 4:0:281:SER:O   | 4:X:280:ASN:ND2[1_556] | 1.83                     | 0.37              |
| 4:2:177:ARG:CA  | 4:Z:178:LEU:CD2[1_556] | 1.83                     | 0.37              |
| 4:2:166:TYR:CA  | 4:Z:294:TYR:CB[1_556]  | 1.83                     | 0.37              |
| 4:2:208:ILE:CG1 | 4:Z:198:TYR:CZ[1_556]  | 1.83                     | 0.37              |
| 4:0:339:VAL:CG2 | 4:X:309:ILE:CG2[1_556] | 1.83                     | 0.37              |
| 4:0:68:LYS:CD   | 4:X:59:GLN:CA[1_556]   | 1.83                     | 0.37              |
| 4:0:136:ILE:C   | 4:X:299:MET:O[1_556]   | 1.83                     | 0.37              |
| 4:1:118:LYS:NZ  | 4:Y:19:ALA:CB[1_556]   | 1.83                     | 0.37              |
| 4:1:121:GLN:O   | 4:Y:21:PHE:N[1_556]    | 1.83                     | 0.37              |
| 4:1:185:LEU:O   | 4:Y:191:LYS:CD[1_556]  | 1.83                     | 0.37              |
| 4:2:162:ASN:CA  | 4:Z:274:ILE:O[1_556]   | 1.83                     | 0.37              |
| 4:0:367:PRO:N   | 4:X:347:ALA:CA[1_556]  | 1.83                     | 0.37              |
| 4:1:120:THR:CB  | 4:Y:340:TRP:C[1_556]   | 1.83                     | 0.37              |
| 4:1:288:ASP:O   | 4:Y:322:PRO:CB[1_556]  | 1.83                     | 0.37              |
| 4:1:217:CYS:CB  | 4:Y:256:ARG:NH2[1_556] | 1.83                     | 0.37              |
| 4:2:169:TYR:CD2 | 4:Z:293:LEU:CG[1_556]  | 1.83                     | 0.37              |
| 4:2:168:GLY:C   | 4:Z:296:ASN:N[1_556]   | 1.83                     | 0.37              |
| 4:2:140:LEU:C   | 4:Z:310:ALA:CB[1_556]  | 1.83                     | 0.37              |
| 4:2:157:ASP:C   | 4:Z:185:LEU:CA[1_556]  | 1.83                     | 0.37              |
| 4:0:267:ILE:N   | 4:W:173:HIS:ND1[1_556] | 1.83                     | 0.37              |
| 4:0:124:PHE:N   | 4:X:24:ASP:CB[1_556]   | 1.83                     | 0.37              |
| 4:1:123:MET:N   | 4:Y:26:ALA:O[1_556]    | 1.83                     | 0.37              |
| 4:1:135:ALA:N   | 4:Y:338:SER:OG[1_556]  | 1.83                     | 0.37              |
| 4:1:141:SER:OG  | 4:Y:309:ILE:C[1_556]   | 1.83                     | 0.37              |
| 4:0:211:ASP:OD1 | 4:X:249:THR:C[1_556]   | 1.83                     | 0.37              |
| 4:0:40:HIS:CD2  | 4:V:166:TYR:CG[1_556]  | 1.83                     | 0.37              |
| 4:0:122:ILE:N   | 4:X:340:TRP:CE2[1_556] | 1.83                     | 0.37              |
| 4:2:206:ARG:CA  | 4:Z:199:SER:O[1_556]   | 1.83                     | 0.37              |
| 4:0:158:GLY:N   | 4:X:182:GLY:O[1_556]   | 1.83                     | 0.37              |
| 4:1:131:ALA:O   | 4:Y:25:ASP:OD1[1_556]  | 1.83                     | 0.37              |
| 4:0:298:VAL:C   | 4:X:312:ARG:O[1_556]   | 1.83                     | 0.37              |
| 4:2:211:ASP:CG  | 4:Z:249:THR:CA[1_556]  | 1.83                     | 0.37              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:367:PRO:N   | 4:Y:347:ALA:CA[1_556]  | 1.83                     | 0.37              |
| 4:1:157:ASP:O   | 4:Y:185:LEU:O[1_556]   | 1.83                     | 0.37              |
| 4:1:151:ILE:CG1 | 4:Y:275:HIS:CA[1_556]  | 1.83                     | 0.37              |
| 4:0:141:SER:O   | 4:X:310:ALA:CB[1_556]  | 1.83                     | 0.37              |
| 4:2:108:ALA:N   | 4:Z:301:GLY:N[1_556]   | 1.83                     | 0.37              |
| 4:2:152:VAL:O   | 4:Z:274:ILE:CG2[1_556] | 1.83                     | 0.37              |
| 4:1:79:TRP:CZ2  | 4:Y:11:ASP:C[1_556]    | 1.83                     | 0.37              |
| 4:0:162:ASN:ND2 | 4:X:273:GLY:O[1_556]   | 1.83                     | 0.37              |
| 4:2:149:THR:CB  | 4:Z:327:ILE:CA[1_556]  | 1.83                     | 0.37              |
| 4:1:261:LEU:O   | 4:Y:265:SER:OG[1_556]  | 1.84                     | 0.36              |
| 4:1:113:LYS:CD  | 4:Y:136:ILE:CA[1_556]  | 1.84                     | 0.36              |
| 4:0:167:GLU:C   | 4:X:296:ASN:N[1_556]   | 1.84                     | 0.36              |
| 4:1:212:ILE:O   | 4:Y:196:ARG:CG[1_556]  | 1.84                     | 0.36              |
| 4:2:293:LEU:N   | 4:Z:317:ILE:O[1_556]   | 1.84                     | 0.36              |
| 4:2:217:CYS:SG  | 4:Z:256:ARG:NH2[1_556] | 1.84                     | 0.36              |
| 4:1:122:ILE:N   | 4:Y:340:TRP:CE2[1_556] | 1.84                     | 0.36              |
| 4:2:137:GLN:CA  | 4:Z:304:THR:OG1[1_556] | 1.84                     | 0.36              |
| 4:1:189:LEU:CB  | 4:Y:195:GLU:CG[1_556]  | 1.84                     | 0.36              |
| 4:0:83:GLU:N    | 4:X:30:VAL:O[1_556]    | 1.84                     | 0.36              |
| 4:1:80:ASP:CB   | 4:Y:31:PHE:CG[1_556]   | 1.84                     | 0.36              |
| 4:0:303:THR:CA  | 4:X:257:CYS:CA[1_556]  | 1.84                     | 0.36              |
| 4:0:124:PHE:CG  | 4:X:24:ASP:C[1_556]    | 1.84                     | 0.36              |
| 4:2:68:LYS:CD   | 4:Z:59:GLN:CA[1_556]   | 1.84                     | 0.36              |
| 4:2:14:SER:C    | 4:Z:213:LYS:NZ[1_556]  | 1.84                     | 0.36              |
| 4:1:309:ILE:CG1 | 4:Y:259:GLU:CG[1_556]  | 1.84                     | 0.36              |
| 4:1:183:ARG:NH2 | 4:Y:186:THR:OG1[1_556] | 1.84                     | 0.36              |
| 4:1:292:ASP:N   | 4:Y:321:ALA:CA[1_556]  | 1.84                     | 0.36              |
| 4:4:40:HIS:CD2  | 4:Z:166:TYR:O[1_556]   | 1.84                     | 0.36              |
| 4:3:229:THR:O   | 4:Z:369:ILE:N[1_556]   | 1.84                     | 0.36              |
| 4:1:155:SER:CB  | 4:Y:261:LEU:N[1_556]   | 1.84                     | 0.36              |
| 4:2:331:ALA:CB  | 4:Z:222:ASP:CA[1_556]  | 1.84                     | 0.36              |
| 4:0:262:PHE:CA  | 4:X:265:SER:CB[1_556]  | 1.84                     | 0.36              |
| 4:2:83:GLU:N    | 4:Z:30:VAL:O[1_556]    | 1.84                     | 0.36              |
| 4:1:264:PRO:C   | 4:Y:268:GLY:CA[1_556]  | 1.84                     | 0.36              |
| 4:1:294:TYR:N   | 4:Y:320:LEU:CB[1_556]  | 1.84                     | 0.36              |
| 4:2:40:HIS:O    | 4:X:167:GLU:OE2[1_556] | 1.84                     | 0.36              |
| 4:1:169:TYR:OH  | 4:Y:164:PRO:CA[1_556]  | 1.84                     | 0.36              |
| 4:1:217:CYS:SG  | 4:Y:256:ARG:NH2[1_556] | 1.84                     | 0.36              |
| 4:1:177:ARG:O   | 4:Y:178:LEU:CG[1_556]  | 1.84                     | 0.36              |
| 4:2:123:MET:N   | 4:Z:26:ALA:C[1_556]    | 1.84                     | 0.36              |
| 4:2:213:LYS:CE  | 4:Z:192:ILE:CG1[1_556] | 1.84                     | 0.36              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:162:ASN:CA  | 4:X:274:ILE:O[1_556]   | 1.84                     | 0.36              |
| 4:2:186:THR:CB  | 4:Z:189:LEU:C[1_556]   | 1.84                     | 0.36              |
| 4:1:67:LEU:CD2  | 4:Y:207:GLU:CD[1_556]  | 1.84                     | 0.36              |
| 4:1:167:GLU:C   | 4:Y:295:ALA:N[1_556]   | 1.84                     | 0.36              |
| 4:1:289:ILE:CD1 | 4:Y:294:TYR:CZ[1_556]  | 1.84                     | 0.36              |
| 4:0:175:ILE:CA  | 4:X:277:THR:CG2[1_556] | 1.84                     | 0.36              |
| 4:1:194:THR:OG1 | 4:X:177:ARG:CZ[1_556]  | 1.84                     | 0.36              |
| 4:0:331:ALA:C   | 4:X:221:LEU:CB[1_556]  | 1.84                     | 0.36              |
| 4:1:213:LYS:CB  | 4:Y:192:ILE:C[1_556]   | 1.84                     | 0.36              |
| 4:1:126:THR:OG1 | 4:Y:28:ARG:CG[1_556]   | 1.84                     | 0.36              |
| 4:4:64:ILE:CD1  | 4:Z:292:ASP:OD1[1_556] | 1.84                     | 0.36              |
| 4:2:286:ASP:N   | 4:Z:283:MET:CG[1_556]  | 1.84                     | 0.36              |
| 4:0:117:GLU:C   | 4:X:9:VAL:CG1[1_556]   | 1.84                     | 0.36              |
| 4:1:286:ASP:CG  | 4:Y:290:ARG:CZ[1_556]  | 1.84                     | 0.36              |
| 4:2:167:GLU:CD  | 4:Z:326:LYS:CB[1_556]  | 1.84                     | 0.36              |
| 4:1:113:LYS:CG  | 4:Y:136:ILE:O[1_556]   | 1.84                     | 0.36              |
| 4:1:140:LEU:N   | 4:Y:331:ALA:CB[1_556]  | 1.84                     | 0.36              |
| 4:2:59:GLN:OE1  | 4:Z:208:ILE:CG2[1_556] | 1.84                     | 0.36              |
| 4:1:185:LEU:O   | 4:Y:191:LYS:CG[1_556]  | 1.84                     | 0.36              |
| 4:2:104:LEU:C   | 4:Z:334:GLU:CG[1_556]  | 1.84                     | 0.36              |
| 4:1:370:VAL:CG1 | 4:Y:343:GLY:N[1_556]   | 1.84                     | 0.36              |
| 4:2:134:VAL:CB  | 4:Z:338:SER:C[1_556]   | 1.84                     | 0.36              |
| 4:1:206:ARG:N   | 4:Y:199:SER:O[1_556]   | 1.84                     | 0.36              |
| 4:1:179:ASP:CG  | 4:Y:179:ASP:O[1_556]   | 1.84                     | 0.36              |
| 4:1:272:ALA:CA  | 4:Y:270:GLU:CB[1_556]  | 1.84                     | 0.36              |
| 4:2:124:PHE:CG  | 4:Z:24:ASP:C[1_556]    | 1.84                     | 0.36              |
| 4:2:366:GLY:O   | 4:Z:347:ALA:CA[1_556]  | 1.84                     | 0.36              |
| 4:1:142:LEU:N   | 4:Y:310:ALA:C[1_556]   | 1.84                     | 0.36              |
| 4:1:41:GLN:N    | 4:W:167:GLU:OE1[1_556] | 1.84                     | 0.36              |
| 4:0:108:ALA:N   | 4:X:301:GLY:N[1_556]   | 1.84                     | 0.36              |
| 4:0:370:VAL:N   | 4:X:342:GLY:O[1_556]   | 1.84                     | 0.36              |
| 4:1:116:ARG:NE  | 4:Y:141:SER:OG[1_556]  | 1.84                     | 0.36              |
| 4:0:252:ASN:ND2 | 4:W:117:GLU:CD[1_556]  | 1.84                     | 0.36              |
| 4:3:39:ARG:C    | 4:Y:166:TYR:OH[1_556]  | 1.84                     | 0.36              |
| 4:2:133:TYR:CZ  | 4:Z:145:SER:CA[1_556]  | 1.84                     | 0.36              |
| 4:2:207:GLU:C   | 4:Z:200:PHE:CZ[1_556]  | 1.84                     | 0.36              |
| 4:0:41:GLN:CG   | 4:V:167:GLU:OE1[1_556] | 1.84                     | 0.36              |
| 4:0:137:GLN:CA  | 4:X:304:THR:OG1[1_556] | 1.84                     | 0.36              |
| 4:2:141:SER:OG  | 4:Z:309:ILE:C[1_556]   | 1.84                     | 0.36              |
| 4:1:121:GLN:NE2 | 4:Y:20:GLY:C[1_556]    | 1.84                     | 0.36              |
| 4:0:178:LEU:C   | 4:X:180:LEU:CD2[1_556] | 1.84                     | 0.36              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:306:TYR:CD2 | 4:Z:256:ARG:CB[1_556]  | 1.84                     | 0.36              |
| 4:0:165:ILE:CG1 | 4:X:297:ASN:CB[1_556]  | 1.84                     | 0.36              |
| 4:2:214:GLU:O   | 4:Z:252:ASN:CB[1_556]  | 1.84                     | 0.36              |
| 4:1:196:ARG:NH1 | 4:X:115:ASN:C[1_556]   | 1.84                     | 0.36              |
| 4:2:161:HIS:CD2 | 4:Z:160:THR:CB[1_556]  | 1.84                     | 0.36              |
| 4:1:151:ILE:N   | 4:Y:317:ILE:CB[1_556]  | 1.84                     | 0.36              |
| 4:2:126:THR:OG1 | 4:Z:28:ARG:CG[1_556]   | 1.84                     | 0.36              |
| 4:2:197:GLY:O   | 4:Y:76:ILE:N[1_556]    | 1.84                     | 0.36              |
| 4:0:183:ARG:CA  | 4:X:186:THR:C[1_556]   | 1.84                     | 0.36              |
| 4:2:162:ASN:CA  | 4:Z:274:ILE:N[1_556]   | 1.84                     | 0.36              |
| 4:0:211:ASP:CG  | 4:X:249:THR:CA[1_556]  | 1.84                     | 0.36              |
| 4:0:113:LYS:CD  | 4:X:136:ILE:CA[1_556]  | 1.84                     | 0.36              |
| 4:1:286:ASP:N   | 4:Y:283:MET:CG[1_556]  | 1.84                     | 0.36              |
| 4:0:189:LEU:CD2 | 4:X:195:GLU:C[1_556]   | 1.84                     | 0.36              |
| 4:1:171:LEU:CD1 | 4:Y:282:ILE:CB[1_556]  | 1.84                     | 0.36              |
| 4:1:303:THR:O   | 4:Y:256:ARG:O[1_556]   | 1.84                     | 0.36              |
| 4:0:178:LEU:CD1 | 4:X:269:MET:CB[1_556]  | 1.84                     | 0.36              |
| 4:1:172:PRO:O   | 4:Y:162:ASN:O[1_556]   | 1.84                     | 0.36              |
| 4:2:366:GLY:C   | 4:Z:347:ALA:C[1_556]   | 1.84                     | 0.36              |
| 4:1:116:ARG:CA  | 4:Y:339:VAL:CA[1_556]  | 1.84                     | 0.36              |
| 4:1:229:THR:O   | 4:X:369:ILE:N[1_556]   | 1.84                     | 0.36              |
| 4:2:295:ALA:C   | 4:Z:319:ALA:CA[1_556]  | 1.84                     | 0.36              |
| 4:2:339:VAL:CG2 | 4:Z:309:ILE:CG2[1_556] | 1.84                     | 0.36              |
| 4:2:254:ARG:C   | 4:Y:113:LYS:NZ[1_556]  | 1.84                     | 0.36              |
| 4:2:370:VAL:N   | 4:Z:342:GLY:O[1_556]   | 1.84                     | 0.36              |
| 4:0:32:PRO:CA   | 4:X:211:ASP:CB[1_556]  | 1.84                     | 0.36              |
| 4:0:295:ALA:C   | 4:X:319:ALA:CA[1_556]  | 1.84                     | 0.36              |
| 4:1:162:ASN:CA  | 4:Y:274:ILE:O[1_556]   | 1.85                     | 0.35              |
| 4:1:190:MET:CB  | 4:Y:194:THR:OG1[1_556] | 1.85                     | 0.35              |
| 4:1:371:HIS:ND1 | 4:Y:140:LEU:CA[1_556]  | 1.85                     | 0.35              |
| 4:2:121:GLN:O   | 4:Z:21:PHE:N[1_556]    | 1.85                     | 0.35              |
| 4:2:118:LYS:CE  | 4:Z:10:CYS:CB[1_556]   | 1.85                     | 0.35              |
| 4:0:300:SER:OG  | 4:X:309:ILE:CG1[1_556] | 1.85                     | 0.35              |
| 4:0:33:SER:CB   | 4:X:214:GLU:OE2[1_556] | 1.85                     | 0.35              |
| 4:2:131:ALA:O   | 4:Z:25:ASP:OD1[1_556]  | 1.85                     | 0.35              |
| 4:0:152:VAL:O   | 4:X:274:ILE:CG2[1_556] | 1.85                     | 0.35              |
| 4:2:267:ILE:N   | 4:Y:173:HIS:ND1[1_556] | 1.85                     | 0.35              |
| 4:1:211:ASP:OD2 | 4:Y:249:THR:O[1_556]   | 1.85                     | 0.35              |
| 4:2:125:GLU:CB  | 4:Z:21:PHE:CG[1_556]   | 1.85                     | 0.35              |
| 4:0:372:ARG:NH1 | 4:X:145:SER:CB[1_556]  | 1.85                     | 0.35              |
| 4:2:252:ASN:ND2 | 4:Y:117:GLU:CD[1_556]  | 1.85                     | 0.35              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:191:LYS:NZ  | 4:Y:110:LEU:CG[1_556]  | 1.85                     | 0.35              |
| 4:1:211:ASP:OD1 | 4:Y:249:THR:C[1_556]   | 1.85                     | 0.35              |
| 4:2:309:ILE:CA  | 4:Z:259:GLU:OE2[1_556] | 1.85                     | 0.35              |
| 4:1:133:TYR:CE1 | 4:Y:145:SER:CA[1_556]  | 1.85                     | 0.35              |
| 4:0:172:PRO:O   | 4:X:162:ASN:O[1_556]   | 1.85                     | 0.35              |
| 4:3:63:GLY:N    | 4:Y:287:ILE:O[1_556]   | 1.85                     | 0.35              |
| 4:1:140:LEU:C   | 4:Y:310:ALA:CB[1_556]  | 1.85                     | 0.35              |
| 4:2:185:LEU:O   | 4:Z:192:ILE:N[1_556]   | 1.85                     | 0.35              |
| 4:1:237:GLU:CD  | 4:X:114:ALA:O[1_556]   | 1.85                     | 0.35              |
| 4:3:40:HIS:ND1  | 4:Y:166:TYR:CB[1_556]  | 1.85                     | 0.35              |
| 4:0:134:VAL:CB  | 4:X:338:SER:C[1_556]   | 1.85                     | 0.35              |
| 4:0:293:LEU:N   | 4:X:317:ILE:O[1_556]   | 1.85                     | 0.35              |
| 4:2:151:ILE:N   | 4:Z:317:ILE:CB[1_556]  | 1.85                     | 0.35              |
| 4:1:177:ARG:CB  | 4:Y:178:LEU:C[1_556]   | 1.85                     | 0.35              |
| 4:0:149:THR:CG2 | 4:X:327:ILE:CG1[1_556] | 1.85                     | 0.35              |
| 4:2:162:ASN:N   | 4:Z:274:ILE:CG1[1_556] | 1.85                     | 0.35              |
| 4:0:264:PRO:CG  | 4:X:269:MET:N[1_556]   | 1.85                     | 0.35              |
| 4:2:64:ILE:CD1  | 4:X:292:ASP:OD1[1_556] | 1.85                     | 0.35              |
| 4:0:115:ASN:C   | 4:X:11:ASP:CG[1_556]   | 1.85                     | 0.35              |
| 4:0:207:GLU:C   | 4:X:200:PHE:CZ[1_556]  | 1.85                     | 0.35              |
| 4:1:167:GLU:OE2 | 4:Y:326:LYS:O[1_556]   | 1.85                     | 0.35              |
| 4:0:59:GLN:NE2  | 4:X:208:ILE:CA[1_556]  | 1.85                     | 0.35              |
| 4:0:40:HIS:O    | 4:V:167:GLU:OE2[1_556] | 1.85                     | 0.35              |
| 4:1:82:MET:N    | 4:Y:31:PHE:CA[1_556]   | 1.85                     | 0.35              |
| 4:0:116:ARG:NE  | 4:X:141:SER:OG[1_556]  | 1.85                     | 0.35              |
| 4:3:266:PHE:C   | 4:Z:172:PRO:C[1_556]   | 1.85                     | 0.35              |
| 4:1:266:PHE:C   | 4:X:172:PRO:C[1_556]   | 1.85                     | 0.35              |
| 4:1:120:THR:OG1 | 4:Y:341:ILE:CA[1_556]  | 1.85                     | 0.35              |
| 4:0:133:TYR:CZ  | 4:X:145:SER:CA[1_556]  | 1.85                     | 0.35              |
| 4:1:40:HIS:ND1  | 4:W:166:TYR:CB[1_556]  | 1.85                     | 0.35              |
| 4:1:172:PRO:CD  | 4:Y:164:PRO:CA[1_556]  | 1.85                     | 0.35              |
| 4:0:206:ARG:CA  | 4:X:199:SER:O[1_556]   | 1.85                     | 0.35              |
| 4:2:33:SER:CB   | 4:Z:214:GLU:OE2[1_556] | 1.85                     | 0.35              |
| 4:2:122:ILE:N   | 4:Z:340:TRP:CE2[1_556] | 1.85                     | 0.35              |
| 4:2:40:HIS:CD2  | 4:X:166:TYR:O[1_556]   | 1.85                     | 0.35              |
| 4:2:106:THR:CA  | 4:Z:335:ARG:O[1_556]   | 1.85                     | 0.35              |
| 4:0:118:LYS:CE  | 4:X:10:CYS:CB[1_556]   | 1.85                     | 0.35              |
| 4:1:56:ASP:OD2  | 4:Y:240:TYR:OH[1_556]  | 1.85                     | 0.35              |
| 4:0:182:GLY:C   | 4:X:188:TYR:C[1_556]   | 1.85                     | 0.35              |
| 4:1:107:GLU:N   | 4:Y:301:GLY:N[1_556]   | 1.85                     | 0.35              |
| 4:2:372:ARG:NH1 | 4:Z:145:SER:CB[1_556]  | 1.85                     | 0.35              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:120:THR:C   | 4:Y:340:TRP:CZ3[1_556] | 1.85                     | 0.35              |
| 4:1:133:TYR:CE1 | 4:Y:144:ALA:O[1_556]   | 1.85                     | 0.35              |
| 4:2:369:ILE:CA  | 4:Z:346:LEU:N[1_556]   | 1.85                     | 0.35              |
| 4:2:149:THR:CG2 | 4:Z:327:ILE:CG1[1_556] | 1.85                     | 0.35              |
| 4:2:40:HIS:CD2  | 4:X:166:TYR:CG[1_556]  | 1.85                     | 0.35              |
| 4:1:124:PHE:N   | 4:Y:24:ASP:CB[1_556]   | 1.85                     | 0.35              |
| 4:0:67:LEU:CD2  | 4:X:207:GLU:CD[1_556]  | 1.85                     | 0.35              |
| 4:2:63:GLY:N    | 4:X:287:ILE:O[1_556]   | 1.85                     | 0.35              |
| 4:1:166:TYR:CD1 | 4:Y:294:TYR:CB[1_556]  | 1.85                     | 0.35              |
| 4:1:111:ASN:O   | 4:Y:137:GLN:CB[1_556]  | 1.85                     | 0.35              |
| 4:1:369:ILE:CA  | 4:Y:346:LEU:N[1_556]   | 1.85                     | 0.35              |
| 4:2:281:SER:O   | 4:Z:280:ASN:ND2[1_556] | 1.85                     | 0.35              |
| 4:0:186:THR:CB  | 4:X:189:LEU:C[1_556]   | 1.85                     | 0.35              |
| 4:0:149:THR:CB  | 4:X:327:ILE:CA[1_556]  | 1.85                     | 0.35              |
| 4:2:60:SER:CB   | 4:Z:243:PRO:CA[1_556]  | 1.85                     | 0.35              |
| 4:1:79:TRP:CA   | 4:Y:17:VAL:CB[1_556]   | 1.85                     | 0.35              |
| 4:1:189:LEU:CD2 | 4:Y:195:GLU:C[1_556]   | 1.85                     | 0.35              |
| 4:0:173:HIS:N   | 4:X:174:ALA:O[1_556]   | 1.85                     | 0.35              |
| 4:2:113:LYS:CD  | 4:Z:136:ILE:CA[1_556]  | 1.85                     | 0.35              |
| 4:2:169:TYR:N   | 4:Z:296:ASN:O[1_556]   | 1.85                     | 0.35              |
| 4:0:161:HIS:C   | 4:X:274:ILE:CA[1_556]  | 1.85                     | 0.35              |
| 4:0:230:ALA:CA  | 4:W:368:SER:CA[1_556]  | 1.85                     | 0.35              |
| 4:2:115:ASN:C   | 4:Z:11:ASP:CG[1_556]   | 1.85                     | 0.35              |
| 4:0:151:ILE:N   | 4:X:317:ILE:CB[1_556]  | 1.85                     | 0.35              |
| 4:3:233:SER:CA  | 4:Z:367:PRO:CD[1_556]  | 1.85                     | 0.35              |
| 4:0:161:HIS:CD2 | 4:X:160:THR:CB[1_556]  | 1.85                     | 0.35              |
| 4:0:365:ALA:CA  | 4:X:349:LEU:CB[1_556]  | 1.85                     | 0.35              |
| 4:0:142:LEU:CD1 | 4:X:313:MET:C[1_556]   | 1.85                     | 0.35              |
| 4:2:67:LEU:CD2  | 4:Z:207:GLU:CD[1_556]  | 1.85                     | 0.35              |
| 4:2:172:PRO:CD  | 4:Z:164:PRO:CA[1_556]  | 1.85                     | 0.35              |
| 4:1:208:ILE:CG1 | 4:Y:198:TYR:CZ[1_556]  | 1.85                     | 0.35              |
| 4:2:120:THR:CB  | 4:Z:340:TRP:C[1_556]   | 1.85                     | 0.35              |
| 4:1:104:LEU:C   | 4:Y:334:GLU:CG[1_556]  | 1.85                     | 0.35              |
| 4:1:366:GLY:CA  | 4:Y:347:ALA:CB[1_556]  | 1.85                     | 0.35              |
| 4:2:189:LEU:CD2 | 4:Z:195:GLU:C[1_556]   | 1.85                     | 0.35              |
| 4:2:169:TYR:CE2 | 4:Z:293:LEU:CD1[1_556] | 1.85                     | 0.35              |
| 4:0:218:TYR:OH  | 4:X:231:ALA:CA[1_556]  | 1.85                     | 0.35              |
| 4:2:126:THR:CG2 | 4:Z:28:ARG:CG[1_556]   | 1.85                     | 0.35              |
| 4:2:296:ASN:C   | 4:Z:316:GLU:CA[1_556]  | 1.85                     | 0.35              |
| 4:0:371:HIS:O   | 4:X:139:VAL:C[1_556]   | 1.85                     | 0.35              |
| 4:2:368:SER:O   | 4:Z:346:LEU:CB[1_556]  | 1.85                     | 0.35              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:306:TYR:CD2 | 4:X:256:ARG:CB[1_556]  | 1.85                     | 0.35              |
| 4:0:197:GLY:CA  | 4:W:76:ILE:N[1_556]    | 1.85                     | 0.35              |
| 4:2:212:ILE:O   | 4:Z:196:ARG:CG[1_556]  | 1.85                     | 0.35              |
| 4:1:285:CYS:C   | 4:Y:283:MET:CG[1_556]  | 1.85                     | 0.35              |
| 4:1:183:ARG:CA  | 4:Y:188:TYR:N[1_556]   | 1.85                     | 0.35              |
| 4:0:363:ASP:N   | 4:X:348:SER:CB[1_556]  | 1.85                     | 0.35              |
| 4:1:170:ALA:CA  | 4:Y:151:ILE:CG2[1_556] | 1.85                     | 0.35              |
| 4:0:126:THR:CG2 | 4:X:28:ARG:CG[1_556]   | 1.85                     | 0.35              |
| 4:1:39:ARG:C    | 4:W:166:TYR:OH[1_556]  | 1.86                     | 0.34              |
| 4:0:371:HIS:CE1 | 4:X:136:ILE:O[1_556]   | 1.86                     | 0.34              |
| 4:0:217:CYS:SG  | 4:X:256:ARG:NH2[1_556] | 1.86                     | 0.34              |
| 4:1:300:SER:OG  | 4:Y:309:ILE:CA[1_556]  | 1.86                     | 0.34              |
| 4:1:166:TYR:CA  | 4:Y:294:TYR:CB[1_556]  | 1.86                     | 0.34              |
| 4:2:218:TYR:OH  | 4:Z:231:ALA:CA[1_556]  | 1.86                     | 0.34              |
| 4:2:121:GLN:N   | 4:Z:340:TRP:CZ2[1_556] | 1.86                     | 0.34              |
| 4:0:196:ARG:CZ  | 4:W:114:ALA:C[1_556]   | 1.86                     | 0.34              |
| 4:1:233:SER:CA  | 4:X:367:PRO:CD[1_556]  | 1.86                     | 0.34              |
| 4:1:72:GLU:O    | 4:Y:157:ASP:CB[1_556]  | 1.86                     | 0.34              |
| 4:2:296:ASN:ND2 | 4:Z:318:THR:OG1[1_556] | 1.86                     | 0.34              |
| 4:0:366:GLY:O   | 4:X:347:ALA:CA[1_556]  | 1.86                     | 0.34              |
| 4:1:59:GLN:OE1  | 4:Y:208:ILE:N[1_556]   | 1.86                     | 0.34              |
| 4:2:289:ILE:N   | 4:Z:283:MET:CE[1_556]  | 1.86                     | 0.34              |
| 4:2:309:ILE:CG1 | 4:Z:259:GLU:CG[1_556]  | 1.86                     | 0.34              |
| 4:1:121:GLN:CA  | 4:Y:340:TRP:CZ2[1_556] | 1.86                     | 0.34              |
| 4:0:104:LEU:C   | 4:X:334:GLU:CG[1_556]  | 1.86                     | 0.34              |
| 4:3:194:THR:OG1 | 4:Z:177:ARG:CZ[1_556]  | 1.86                     | 0.34              |
| 4:0:172:PRO:CG  | 4:X:164:PRO:CB[1_556]  | 1.86                     | 0.34              |
| 4:1:152:VAL:CB  | 4:Y:313:MET:CB[1_556]  | 1.86                     | 0.34              |
| 4:0:215:LYS:CD  | 4:X:196:ARG:NH2[1_556] | 1.86                     | 0.34              |
| 4:2:119:MET:C   | 4:Z:340:TRP:CE3[1_556] | 1.86                     | 0.34              |
| 4:3:267:ILE:CB  | 4:Z:173:HIS:CA[1_556]  | 1.86                     | 0.34              |
| 4:1:122:ILE:O   | 4:Y:28:ARG:N[1_556]    | 1.86                     | 0.34              |
| 4:0:289:ILE:N   | 4:X:283:MET:CE[1_556]  | 1.86                     | 0.34              |
| 4:0:79:TRP:CD2  | 4:X:17:VAL:CA[1_556]   | 1.86                     | 0.34              |
| 4:0:40:HIS:CD2  | 4:V:166:TYR:O[1_556]   | 1.86                     | 0.34              |
| 4:2:74:GLY:N    | 4:Z:157:ASP:N[1_556]   | 1.86                     | 0.34              |
| 4:1:166:TYR:CE1 | 4:Y:294:TYR:CD2[1_556] | 1.86                     | 0.34              |
| 4:0:169:TYR:CE2 | 4:X:293:LEU:CD1[1_556] | 1.86                     | 0.34              |
| 4:2:215:LYS:CD  | 4:Z:196:ARG:NH2[1_556] | 1.86                     | 0.34              |
| 4:2:161:HIS:C   | 4:Z:274:ILE:CA[1_556]  | 1.86                     | 0.34              |
| 4:0:106:THR:CA  | 4:X:335:ARG:O[1_556]   | 1.86                     | 0.34              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:297:ASN:C   | 4:Y:316:GLU:CG[1_556]  | 1.86                     | 0.34              |
| 4:2:280:ASN:O   | 4:Z:280:ASN:CG[1_556]  | 1.86                     | 0.34              |
| 4:0:185:LEU:O   | 4:X:192:ILE:N[1_556]   | 1.86                     | 0.34              |
| 4:2:175:ILE:CA  | 4:Z:277:THR:CG2[1_556] | 1.86                     | 0.34              |
| 4:2:178:LEU:C   | 4:Z:180:LEU:CD2[1_556] | 1.86                     | 0.34              |
| 4:1:68:LYS:CA   | 4:Y:59:GLN:CG[1_556]   | 1.86                     | 0.34              |
| 4:1:362:TYR:CG  | 4:Y:344:SER:O[1_556]   | 1.86                     | 0.34              |
| 4:2:307:PRO:CB  | 4:Z:227:MET:N[1_556]   | 1.86                     | 0.34              |
| 4:2:69:TYR:CE2  | 4:Z:210:ARG:CD[1_556]  | 1.86                     | 0.34              |
| 4:1:79:TRP:CD1  | 4:Y:17:VAL:CA[1_556]   | 1.86                     | 0.34              |
| 4:2:32:PRO:CA   | 4:Z:211:ASP:CB[1_556]  | 1.86                     | 0.34              |
| 4:1:231:ALA:N   | 4:X:371:HIS:N[1_556]   | 1.86                     | 0.34              |
| 4:0:124:PHE:CB  | 4:X:24:ASP:O[1_556]    | 1.86                     | 0.34              |
| 4:0:121:GLN:N   | 4:X:340:TRP:CZ2[1_556] | 1.86                     | 0.34              |
| 4:2:172:PRO:CG  | 4:Z:164:PRO:CB[1_556]  | 1.86                     | 0.34              |
| 4:3:41:GLN:N    | 4:Y:167:GLU:OE1[1_556] | 1.86                     | 0.34              |
| 4:0:296:ASN:C   | 4:X:316:GLU:CA[1_556]  | 1.86                     | 0.34              |
| 4:1:261:LEU:O   | 4:Y:265:SER:C[1_556]   | 1.86                     | 0.34              |
| 4:2:149:THR:CA  | 4:Z:327:ILE:CA[1_556]  | 1.86                     | 0.34              |
| 4:2:158:GLY:CA  | 4:Z:182:GLY:O[1_556]   | 1.86                     | 0.34              |
| 4:3:192:ILE:O   | 4:Z:112:PRO:N[1_556]   | 1.86                     | 0.34              |
| 4:1:115:ASN:O   | 4:Y:11:ASP:CB[1_556]   | 1.86                     | 0.34              |
| 4:1:292:ASP:CA  | 4:Y:321:ALA:C[1_556]   | 1.86                     | 0.34              |
| 4:2:304:THR:N   | 4:Z:259:GLU:N[1_556]   | 1.86                     | 0.34              |
| 4:0:369:ILE:CA  | 4:X:346:LEU:N[1_556]   | 1.86                     | 0.34              |
| 4:3:237:GLU:CD  | 4:Z:114:ALA:O[1_556]   | 1.86                     | 0.34              |
| 4:1:11:ASP:CB   | 4:Y:305:MET:SD[1_556]  | 1.86                     | 0.34              |
| 4:2:178:LEU:CD1 | 4:Z:269:MET:CB[1_556]  | 1.86                     | 0.34              |
| 4:2:151:ILE:CG1 | 4:Z:275:HIS:CA[1_556]  | 1.86                     | 0.34              |
| 4:1:60:SER:CB   | 4:Y:243:PRO:CA[1_556]  | 1.86                     | 0.34              |
| 4:0:303:THR:CG2 | 4:X:256:ARG:O[1_556]   | 1.86                     | 0.34              |
| 4:2:173:HIS:N   | 4:Z:174:ALA:O[1_556]   | 1.86                     | 0.34              |
| 4:2:362:TYR:CE2 | 4:Z:22:ALA:O[1_556]    | 1.86                     | 0.34              |
| 4:1:172:PRO:CD  | 4:Y:164:PRO:CG[1_556]  | 1.86                     | 0.34              |
| 4:2:134:VAL:CG1 | 4:Z:338:SER:N[1_556]   | 1.86                     | 0.34              |
| 4:1:173:HIS:CA  | 4:Y:174:ALA:C[1_556]   | 1.86                     | 0.34              |
| 4:0:64:ILE:CD1  | 4:V:292:ASP:OD1[1_556] | 1.86                     | 0.34              |
| 4:2:66:THR:CG2  | 4:Z:62:ARG:N[1_556]    | 1.86                     | 0.34              |
| 4:2:134:VAL:CG2 | 4:Z:338:SER:O[1_556]   | 1.86                     | 0.34              |
| 4:2:166:TYR:O   | 4:Z:293:LEU:O[1_556]   | 1.86                     | 0.34              |
| 4:2:330:ILE:CG1 | 4:Z:315:LYS:CG[1_556]  | 1.86                     | 0.34              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:185:LEU:C   | 4:Z:188:TYR:O[1_556]   | 1.86                     | 0.34              |
| 4:1:168:GLY:C   | 4:Y:296:ASN:N[1_556]   | 1.86                     | 0.34              |
| 4:3:231:ALA:CA  | 4:Z:370:VAL:CA[1_556]  | 1.86                     | 0.34              |
| 4:0:191:LYS:NZ  | 4:W:110:LEU:CG[1_556]  | 1.86                     | 0.34              |
| 4:0:173:HIS:CA  | 4:X:281:SER:OG[1_556]  | 1.86                     | 0.34              |
| 4:1:229:THR:C   | 4:X:368:SER:O[1_556]   | 1.86                     | 0.34              |
| 4:2:41:GLN:CG   | 4:X:167:GLU:OE1[1_556] | 1.86                     | 0.34              |
| 4:0:108:ALA:N   | 4:X:300:SER:O[1_556]   | 1.86                     | 0.34              |
| 4:0:304:THR:N   | 4:X:259:GLU:N[1_556]   | 1.86                     | 0.34              |
| 4:0:281:SER:C   | 4:X:280:ASN:OD1[1_556] | 1.86                     | 0.34              |
| 4:0:136:ILE:CG2 | 4:X:153:LEU:O[1_556]   | 1.86                     | 0.34              |
| 4:2:59:GLN:OE1  | 4:Z:208:ILE:N[1_556]   | 1.86                     | 0.34              |
| 4:2:194:THR:OG1 | 4:Y:177:ARG:CZ[1_556]  | 1.86                     | 0.34              |
| 4:1:231:ALA:CA  | 4:X:370:VAL:CA[1_556]  | 1.86                     | 0.34              |
| 4:1:169:TYR:CZ  | 4:Y:150:GLY:O[1_556]   | 1.86                     | 0.34              |
| 4:0:162:ASN:N   | 4:X:274:ILE:CG1[1_556] | 1.86                     | 0.34              |
| 4:2:154:ASP:O   | 4:Z:261:LEU:CD1[1_556] | 1.86                     | 0.34              |
| 4:0:170:ALA:CA  | 4:X:151:ILE:CG2[1_556] | 1.86                     | 0.34              |
| 4:0:180:LEU:O   | 4:X:260:THR:CG2[1_556] | 1.86                     | 0.34              |
| 4:1:161:HIS:C   | 4:Y:274:ILE:CA[1_556]  | 1.86                     | 0.34              |
| 4:2:173:HIS:CA  | 4:Z:281:SER:OG[1_556]  | 1.86                     | 0.34              |
| 4:0:151:ILE:N   | 4:X:317:ILE:CA[1_556]  | 1.86                     | 0.34              |
| 4:2:271:SER:OG  | 4:Z:269:MET:CB[1_556]  | 1.86                     | 0.34              |
| 4:2:371:HIS:CE1 | 4:Z:136:ILE:O[1_556]   | 1.86                     | 0.34              |
| 4:0:196:ARG:NH1 | 4:W:115:ASN:C[1_556]   | 1.86                     | 0.34              |
| 4:2:169:TYR:O   | 4:Z:293:LEU:O[1_556]   | 1.86                     | 0.34              |
| 4:1:224:GLU:OE2 | 4:Z:41:GLN:CG[1_556]   | 1.86                     | 0.34              |
| 4:0:169:TYR:O   | 4:X:293:LEU:O[1_556]   | 1.86                     | 0.34              |
| 4:1:115:ASN:N   | 4:Y:106:THR:CB[1_556]  | 1.86                     | 0.34              |
| 4:0:125:GLU:CB  | 4:X:21:PHE:CG[1_556]   | 1.86                     | 0.34              |
| 4:2:106:THR:CG2 | 4:Z:335:ARG:CB[1_556]  | 1.86                     | 0.34              |
| 4:2:59:GLN:NE2  | 4:Z:208:ILE:CA[1_556]  | 1.86                     | 0.34              |
| 4:2:124:PHE:CB  | 4:Z:23:GLY:C[1_556]    | 1.86                     | 0.34              |
| 4:0:267:ILE:C   | 4:W:173:HIS:CA[1_556]  | 1.86                     | 0.34              |
| 4:2:142:LEU:CD1 | 4:Z:313:MET:C[1_556]   | 1.86                     | 0.34              |
| 4:2:286:ASP:CG  | 4:Z:290:ARG:CD[1_556]  | 1.86                     | 0.34              |
| 4:1:159:VAL:CG1 | 4:Y:181:ALA:CB[1_556]  | 1.86                     | 0.34              |
| 4:1:186:THR:CB  | 4:Y:190:MET:CA[1_556]  | 1.86                     | 0.34              |
| 4:2:67:LEU:CG   | 4:Z:207:GLU:CD[1_556]  | 1.86                     | 0.34              |
| 4:2:164:PRO:CD  | 4:Z:278:THR:OG1[1_556] | 1.86                     | 0.34              |
| 4:2:182:GLY:C   | 4:Z:188:TYR:C[1_556]   | 1.86                     | 0.34              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:205:GLU:C   | 4:Z:199:SER:CA[1_556]  | 1.86                     | 0.34              |
| 4:0:126:THR:OG1 | 4:X:28:ARG:CG[1_556]   | 1.86                     | 0.34              |
| 4:2:116:ARG:NE  | 4:Z:141:SER:OG[1_556]  | 1.87                     | 0.33              |
| 4:0:296:ASN:ND2 | 4:X:318:THR:OG1[1_556] | 1.87                     | 0.33              |
| 4:2:281:SER:C   | 4:Z:280:ASN:OD1[1_556] | 1.87                     | 0.33              |
| 4:1:111:ASN:N   | 4:Y:154:ASP:CG[1_556]  | 1.87                     | 0.33              |
| 4:0:212:ILE:O   | 4:X:196:ARG:CG[1_556]  | 1.87                     | 0.33              |
| 4:0:366:GLY:C   | 4:X:347:ALA:C[1_556]   | 1.87                     | 0.33              |
| 4:1:104:LEU:CD1 | 4:Y:334:GLU:OE2[1_556] | 1.87                     | 0.33              |
| 4:0:166:TYR:O   | 4:X:293:LEU:O[1_556]   | 1.87                     | 0.33              |
| 4:0:114:ALA:CB  | 4:X:106:THR:O[1_556]   | 1.87                     | 0.33              |
| 4:1:32:PRO:CA   | 4:Y:211:ASP:CB[1_556]  | 1.87                     | 0.33              |
| 4:2:365:ALA:CA  | 4:Z:349:LEU:CB[1_556]  | 1.87                     | 0.33              |
| 4:2:79:TRP:CZ3  | 4:Z:18:LYS:N[1_556]    | 1.87                     | 0.33              |
| 4:0:134:VAL:CG2 | 4:X:338:SER:O[1_556]   | 1.87                     | 0.33              |
| 4:0:179:ASP:CG  | 4:X:179:ASP:O[1_556]   | 1.87                     | 0.33              |
| 4:2:196:ARG:CZ  | 4:Y:114:ALA:C[1_556]   | 1.87                     | 0.33              |
| 4:0:367:PRO:CB  | 4:X:343:GLY:O[1_556]   | 1.87                     | 0.33              |
| 4:1:150:GLY:CA  | 4:Y:317:ILE:CB[1_556]  | 1.87                     | 0.33              |
| 4:2:197:GLY:CA  | 4:Y:76:ILE:N[1_556]    | 1.87                     | 0.33              |
| 4:0:131:ALA:O   | 4:X:25:ASP:OD1[1_556]  | 1.87                     | 0.33              |
| 4:2:66:THR:CB   | 4:Z:59:GLN:O[1_556]    | 1.87                     | 0.33              |
| 4:0:309:ILE:CA  | 4:X:259:GLU:OE2[1_556] | 1.87                     | 0.33              |
| 4:3:191:LYS:CB  | 4:Z:110:LEU:CD1[1_556] | 1.87                     | 0.33              |
| 4:0:186:THR:C   | 4:X:191:LYS:CB[1_556]  | 1.87                     | 0.33              |
| 4:2:170:ALA:CA  | 4:Z:151:ILE:CG2[1_556] | 1.87                     | 0.33              |
| 4:0:169:TYR:N   | 4:X:296:ASN:O[1_556]   | 1.87                     | 0.33              |
| 4:0:271:SER:OG  | 4:X:269:MET:CB[1_556]  | 1.87                     | 0.33              |
| 4:0:121:GLN:O   | 4:X:21:PHE:N[1_556]    | 1.87                     | 0.33              |
| 4:0:151:ILE:CG1 | 4:X:275:HIS:CA[1_556]  | 1.87                     | 0.33              |
| 4:0:307:PRO:CB  | 4:X:227:MET:N[1_556]   | 1.87                     | 0.33              |
| 4:1:63:GLY:N    | 4:W:287:ILE:O[1_556]   | 1.87                     | 0.33              |
| 4:3:229:THR:C   | 4:Z:368:SER:O[1_556]   | 1.87                     | 0.33              |
| 4:1:274:ILE:CA  | 4:Y:264:PRO:CD[1_556]  | 1.87                     | 0.33              |
| 4:1:185:LEU:CB  | 4:Y:188:TYR:CE1[1_556] | 1.87                     | 0.33              |
| 4:2:74:GLY:N    | 4:Z:157:ASP:CA[1_556]  | 1.87                     | 0.33              |
| 4:2:367:PRO:CB  | 4:Z:343:GLY:O[1_556]   | 1.87                     | 0.33              |
| 4:2:230:ALA:CA  | 4:Y:368:SER:CA[1_556]  | 1.87                     | 0.33              |
| 4:2:79:TRP:CD2  | 4:Z:17:VAL:CA[1_556]   | 1.87                     | 0.33              |
| 4:0:123:MET:CA  | 4:X:26:ALA:CA[1_556]   | 1.87                     | 0.33              |
| 4:1:301:GLY:C   | 4:Y:258:PRO:CG[1_556]  | 1.87                     | 0.33              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:76:ILE:CG1  | 4:Z:18:LYS:NZ[1_556]   | 1.87                     | 0.33              |
| 4:0:118:LYS:CB  | 4:X:11:ASP:CA[1_556]   | 1.87                     | 0.33              |
| 4:2:136:ILE:CG2 | 4:Z:153:LEU:O[1_556]   | 1.87                     | 0.33              |
| 4:1:132:MET:CE  | 4:Y:341:ILE:CB[1_556]  | 1.87                     | 0.33              |
| 4:0:183:ARG:CG  | 4:X:186:THR:O[1_556]   | 1.87                     | 0.33              |
| 4:1:112:PRO:N   | 4:Y:137:GLN:CD[1_556]  | 1.87                     | 0.33              |
| 4:0:149:THR:CA  | 4:X:327:ILE:CA[1_556]  | 1.87                     | 0.33              |
| 4:2:371:HIS:O   | 4:Z:139:VAL:C[1_556]   | 1.87                     | 0.33              |
| 4:0:370:VAL:CG1 | 4:X:341:ILE:C[1_556]   | 1.87                     | 0.33              |
| 4:2:286:ASP:C   | 4:Z:283:MET:SD[1_556]  | 1.87                     | 0.33              |
| 4:0:205:GLU:C   | 4:X:199:SER:CA[1_556]  | 1.87                     | 0.33              |
| 4:2:363:ASP:N   | 4:Z:348:SER:CB[1_556]  | 1.87                     | 0.33              |
| 4:2:120:THR:C   | 4:Z:340:TRP:CH2[1_556] | 1.87                     | 0.33              |
| 4:2:121:GLN:CG  | 4:Z:20:GLY:O[1_556]    | 1.87                     | 0.33              |
| 4:4:63:GLY:N    | 4:Z:287:ILE:O[1_556]   | 1.87                     | 0.33              |
| 4:0:106:THR:CG2 | 4:X:335:ARG:CB[1_556]  | 1.87                     | 0.33              |
| 4:4:40:HIS:CD2  | 4:Z:166:TYR:CG[1_556]  | 1.87                     | 0.33              |
| 4:0:134:VAL:CG1 | 4:X:338:SER:N[1_556]   | 1.87                     | 0.33              |
| 4:1:305:MET:N   | 4:Y:255:PHE:C[1_556]   | 1.87                     | 0.33              |
| 4:1:339:VAL:CG2 | 4:Y:309:ILE:CG2[1_556] | 1.87                     | 0.33              |
| 4:2:16:LEU:N    | 4:Z:214:GLU:CB[1_556]  | 1.87                     | 0.33              |
| 4:1:331:ALA:CB  | 4:Y:222:ASP:CA[1_556]  | 1.87                     | 0.33              |
| 4:2:272:ALA:CA  | 4:Z:270:GLU:O[1_556]   | 1.87                     | 0.33              |
| 4:2:114:ALA:CB  | 4:Z:106:THR:O[1_556]   | 1.87                     | 0.33              |
| 4:1:308:GLY:N   | 4:Y:227:MET:CB[1_556]  | 1.87                     | 0.33              |
| 4:1:267:ILE:CB  | 4:X:173:HIS:CA[1_556]  | 1.87                     | 0.33              |
| 4:0:172:PRO:CD  | 4:X:164:PRO:CA[1_556]  | 1.87                     | 0.33              |
| 4:3:264:PRO:O   | 4:Z:173:HIS:CG[1_556]  | 1.87                     | 0.33              |
| 4:1:166:TYR:CA  | 4:Y:294:TYR:C[1_556]   | 1.87                     | 0.33              |
| 4:2:112:PRO:CA  | 4:Z:137:GLN:CB[1_556]  | 1.87                     | 0.33              |
| 4:0:66:THR:CG2  | 4:X:62:ARG:N[1_556]    | 1.87                     | 0.33              |
| 4:2:149:THR:C   | 4:Z:327:ILE:CB[1_556]  | 1.87                     | 0.33              |
| 4:0:212:ILE:N   | 4:X:196:ARG:CD[1_556]  | 1.87                     | 0.33              |
| 4:0:66:THR:CB   | 4:X:59:GLN:O[1_556]    | 1.87                     | 0.33              |
| 4:0:119:MET:C   | 4:X:340:TRP:CE3[1_556] | 1.87                     | 0.33              |
| 4:2:183:ARG:N   | 4:Z:185:LEU:O[1_556]   | 1.87                     | 0.33              |
| 4:2:111:ASN:O   | 4:Z:137:GLN:CB[1_556]  | 1.87                     | 0.33              |
| 4:0:59:GLN:OE1  | 4:X:208:ILE:N[1_556]   | 1.87                     | 0.33              |
| 4:0:266:PHE:C   | 4:W:172:PRO:C[1_556]   | 1.87                     | 0.33              |
| 4:1:296:ASN:ND2 | 4:Y:318:THR:OG1[1_556] | 1.87                     | 0.33              |
| 4:2:266:PHE:C   | 4:Y:172:PRO:C[1_556]   | 1.87                     | 0.33              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:298:VAL:C   | 4:Y:312:ARG:O[1_556]   | 1.87                     | 0.33              |
| 4:3:231:ALA:N   | 4:Z:371:HIS:N[1_556]   | 1.87                     | 0.33              |
| 4:0:164:PRO:CD  | 4:X:278:THR:OG1[1_556] | 1.87                     | 0.33              |
| 4:2:367:PRO:N   | 4:Z:347:ALA:N[1_556]   | 1.87                     | 0.33              |
| 4:0:113:LYS:N   | 4:X:137:GLN:CB[1_556]  | 1.87                     | 0.33              |
| 4:1:175:ILE:CB  | 4:Y:162:ASN:ND2[1_556] | 1.87                     | 0.33              |
| 4:1:366:GLY:C   | 4:Y:347:ALA:C[1_556]   | 1.87                     | 0.33              |
| 4:0:69:TYR:CE2  | 4:X:210:ARG:CD[1_556]  | 1.87                     | 0.33              |
| 4:0:367:PRO:N   | 4:X:347:ALA:N[1_556]   | 1.87                     | 0.33              |
| 4:0:83:GLU:CB   | 4:X:29:ALA:C[1_556]    | 1.87                     | 0.33              |
| 4:2:370:VAL:CG1 | 4:Z:341:ILE:C[1_556]   | 1.87                     | 0.33              |
| 4:1:266:PHE:N   | 4:X:173:HIS:CE1[1_556] | 1.87                     | 0.33              |
| 4:2:76:ILE:CG2  | 4:Z:16:LEU:C[1_556]    | 1.87                     | 0.33              |
| 4:0:104:LEU:CD1 | 4:X:333:PRO:CD[1_556]  | 1.87                     | 0.33              |
| 4:1:330:ILE:CG1 | 4:Y:315:LYS:CG[1_556]  | 1.87                     | 0.33              |
| 4:3:267:ILE:CG1 | 4:Z:173:HIS:CB[1_556]  | 1.87                     | 0.33              |
| 4:0:286:ASP:C   | 4:X:283:MET:SD[1_556]  | 1.87                     | 0.33              |
| 4:1:309:ILE:CD1 | 4:Y:259:GLU:OE1[1_556] | 1.87                     | 0.33              |
| 4:2:108:ALA:N   | 4:Z:300:SER:O[1_556]   | 1.87                     | 0.33              |
| 4:1:368:SER:O   | 4:Y:346:LEU:CB[1_556]  | 1.87                     | 0.33              |
| 4:1:292:ASP:O   | 4:Y:319:ALA:N[1_556]   | 1.87                     | 0.33              |
| 4:1:11:ASP:OD2  | 4:Y:305:MET:O[1_556]   | 1.87                     | 0.33              |
| 4:1:214:GLU:O   | 4:Y:252:ASN:N[1_556]   | 1.87                     | 0.33              |
| 4:0:79:TRP:CZ3  | 4:X:18:LYS:N[1_556]    | 1.87                     | 0.33              |
| 4:0:212:ILE:N   | 4:X:196:ARG:CB[1_556]  | 1.88                     | 0.32              |
| 4:1:369:ILE:N   | 4:Y:346:LEU:N[1_556]   | 1.88                     | 0.32              |
| 4:0:308:GLY:N   | 4:X:227:MET:CB[1_556]  | 1.88                     | 0.32              |
| 4:1:134:VAL:CG1 | 4:Y:338:SER:N[1_556]   | 1.88                     | 0.32              |
| 4:2:83:GLU:CB   | 4:Z:29:ALA:C[1_556]    | 1.88                     | 0.32              |
| 4:0:67:LEU:CB   | 4:X:62:ARG:NH2[1_556]  | 1.88                     | 0.32              |
| 4:2:151:ILE:N   | 4:Z:317:ILE:CA[1_556]  | 1.88                     | 0.32              |
| 4:2:159:VAL:CG1 | 4:Z:181:ALA:CB[1_556]  | 1.88                     | 0.32              |
| 4:1:371:HIS:O   | 4:Y:140:LEU:N[1_556]   | 1.88                     | 0.32              |
| 4:0:67:LEU:CG   | 4:X:207:GLU:CD[1_556]  | 1.88                     | 0.32              |
| 4:1:83:GLU:CB   | 4:Y:29:ALA:CA[1_556]   | 1.88                     | 0.32              |
| 4:1:81:ASP:CG   | 4:Y:32:PRO:CG[1_556]   | 1.88                     | 0.32              |
| 4:0:155:SER:C   | 4:X:258:PRO:CA[1_556]  | 1.88                     | 0.32              |
| 4:1:306:TYR:CD2 | 4:Y:256:ARG:CB[1_556]  | 1.88                     | 0.32              |
| 4:4:41:GLN:CG   | 4:Z:167:GLU:OE1[1_556] | 1.88                     | 0.32              |
| 4:1:124:PHE:CG  | 4:Y:24:ASP:C[1_556]    | 1.88                     | 0.32              |
| 4:0:272:ALA:CA  | 4:X:270:GLU:O[1_556]   | 1.88                     | 0.32              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:308:GLY:N   | 4:Z:227:MET:CB[1_556]  | 1.88                     | 0.32              |
| 4:0:132:MET:CE  | 4:X:341:ILE:CB[1_556]  | 1.88                     | 0.32              |
| 4:2:179:ASP:N   | 4:Z:180:LEU:CA[1_556]  | 1.88                     | 0.32              |
| 4:1:11:ASP:CA   | 4:Y:305:MET:CE[1_556]  | 1.88                     | 0.32              |
| 4:0:158:GLY:CA  | 4:X:182:GLY:O[1_556]   | 1.88                     | 0.32              |
| 4:2:180:LEU:O   | 4:Z:260:THR:CG2[1_556] | 1.88                     | 0.32              |
| 4:0:167:GLU:O   | 4:X:295:ALA:CB[1_556]  | 1.88                     | 0.32              |
| 4:2:267:ILE:C   | 4:Y:173:HIS:CA[1_556]  | 1.88                     | 0.32              |
| 4:0:186:THR:N   | 4:X:192:ILE:N[1_556]   | 1.88                     | 0.32              |
| 4:1:62:ARG:CB   | 4:W:288:ASP:OD1[1_556] | 1.88                     | 0.32              |
| 4:1:307:PRO:N   | 4:Y:227:MET:CG[1_556]  | 1.88                     | 0.32              |
| 4:2:186:THR:C   | 4:Z:191:LYS:CB[1_556]  | 1.88                     | 0.32              |
| 4:0:280:ASN:O   | 4:X:280:ASN:CG[1_556]  | 1.88                     | 0.32              |
| 4:0:76:ILE:CG2  | 4:X:16:LEU:C[1_556]    | 1.88                     | 0.32              |
| 4:2:173:HIS:C   | 4:Z:281:SER:OG[1_556]  | 1.88                     | 0.32              |
| 4:0:309:ILE:CG1 | 4:X:259:GLU:CG[1_556]  | 1.88                     | 0.32              |
| 4:2:183:ARG:CG  | 4:Z:186:THR:O[1_556]   | 1.88                     | 0.32              |
| 4:0:74:GLY:N    | 4:X:157:ASP:N[1_556]   | 1.88                     | 0.32              |
| 4:1:300:SER:O   | 4:Y:219:VAL:CG2[1_556] | 1.88                     | 0.32              |
| 4:0:368:SER:O   | 4:X:346:LEU:CB[1_556]  | 1.88                     | 0.32              |
| 4:1:264:PRO:O   | 4:X:173:HIS:CG[1_556]  | 1.88                     | 0.32              |
| 4:2:161:HIS:ND1 | 4:Z:155:SER:OG[1_556]  | 1.88                     | 0.32              |
| 4:0:154:ASP:O   | 4:X:261:LEU:CD1[1_556] | 1.88                     | 0.32              |
| 4:1:177:ARG:CA  | 4:Y:178:LEU:CD2[1_556] | 1.88                     | 0.32              |
| 4:3:40:HIS:CD2  | 4:Y:166:TYR:CG[1_556]  | 1.88                     | 0.32              |
| 4:1:179:ASP:O   | 4:Y:184:ASP:OD2[1_556] | 1.88                     | 0.32              |
| 4:0:112:PRO:CA  | 4:X:137:GLN:CB[1_556]  | 1.88                     | 0.32              |
| 4:0:194:THR:OG1 | 4:W:177:ARG:CZ[1_556]  | 1.88                     | 0.32              |
| 4:2:68:LYS:CA   | 4:Z:59:GLN:CG[1_556]   | 1.88                     | 0.32              |
| 4:1:214:GLU:O   | 4:Y:252:ASN:CB[1_556]  | 1.88                     | 0.32              |
| 4:2:124:PHE:CB  | 4:Z:24:ASP:O[1_556]    | 1.88                     | 0.32              |
| 4:0:76:ILE:CG1  | 4:X:18:LYS:NZ[1_556]   | 1.88                     | 0.32              |
| 4:1:192:ILE:O   | 4:X:112:PRO:N[1_556]   | 1.88                     | 0.32              |
| 4:1:167:GLU:OE1 | 4:Y:326:LYS:CG[1_556]  | 1.88                     | 0.32              |
| 4:0:330:ILE:CG1 | 4:X:315:LYS:CG[1_556]  | 1.88                     | 0.32              |
| 4:2:214:GLU:C   | 4:Z:253:GLU:CD[1_556]  | 1.88                     | 0.32              |
| 4:1:305:MET:CB  | 4:Y:255:PHE:CD2[1_556] | 1.88                     | 0.32              |
| 4:0:149:THR:C   | 4:X:327:ILE:CB[1_556]  | 1.88                     | 0.32              |
| 4:0:362:TYR:CE2 | 4:X:22:ALA:O[1_556]    | 1.88                     | 0.32              |
| 4:0:148:THR:CB  | 4:X:327:ILE:C[1_556]   | 1.88                     | 0.32              |
| 4:0:74:GLY:N    | 4:X:157:ASP:CA[1_556]  | 1.88                     | 0.32              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:191:LYS:CB  | 4:X:110:LEU:CD1[1_556] | 1.88                     | 0.32              |
| 4:0:124:PHE:CB  | 4:X:23:GLY:C[1_556]    | 1.88                     | 0.32              |
| 4:1:372:ARG:CG  | 4:Y:143:TYR:N[1_556]   | 1.88                     | 0.32              |
| 4:0:157:ASP:OD2 | 4:X:186:THR:CB[1_556]  | 1.88                     | 0.32              |
| 4:1:336:LYS:CG  | 4:Y:218:TYR:CD2[1_556] | 1.88                     | 0.32              |
| 4:2:303:THR:CG2 | 4:Z:256:ARG:O[1_556]   | 1.88                     | 0.32              |
| 4:2:339:VAL:CG2 | 4:Z:304:THR:O[1_556]   | 1.88                     | 0.32              |
| 4:1:64:ILE:CD1  | 4:W:292:ASP:OD1[1_556] | 1.88                     | 0.32              |
| 4:1:299:MET:O   | 4:Y:312:ARG:CB[1_556]  | 1.88                     | 0.32              |
| 4:2:292:ASP:N   | 4:Z:321:ALA:CA[1_556]  | 1.88                     | 0.32              |
| 4:0:304:THR:OG1 | 4:X:223:PHE:CE1[1_556] | 1.88                     | 0.32              |
| 4:0:185:LEU:C   | 4:X:188:TYR:O[1_556]   | 1.88                     | 0.32              |
| 4:0:16:LEU:N    | 4:X:214:GLU:CB[1_556]  | 1.88                     | 0.32              |
| 4:0:120:THR:C   | 4:X:340:TRP:CH2[1_556] | 1.88                     | 0.32              |
| 4:2:179:ASP:CG  | 4:Z:179:ASP:O[1_556]   | 1.88                     | 0.32              |
| 4:4:41:GLN:N    | 4:Z:167:GLU:OE1[1_556] | 1.88                     | 0.32              |
| 4:0:286:ASP:CG  | 4:X:290:ARG:CD[1_556]  | 1.88                     | 0.32              |
| 4:2:107:GLU:OE2 | 4:Z:141:SER:CB[1_556]  | 1.88                     | 0.32              |
| 4:2:149:THR:OG1 | 4:Z:326:LYS:O[1_556]   | 1.88                     | 0.32              |
| 4:2:196:ARG:NH1 | 4:Y:115:ASN:C[1_556]   | 1.88                     | 0.32              |
| 4:1:139:VAL:CB  | 4:Y:330:ILE:O[1_556]   | 1.88                     | 0.32              |
| 4:0:285:CYS:SG  | 4:X:279:TYR:CA[1_556]  | 1.88                     | 0.32              |
| 4:3:62:ARG:C    | 4:Y:288:ASP:N[1_556]   | 1.88                     | 0.32              |
| 4:1:59:GLN:NE2  | 4:Y:207:GLU:C[1_556]   | 1.88                     | 0.32              |
| 4:1:153:LEU:CD1 | 4:Y:262:PHE:O[1_556]   | 1.88                     | 0.32              |
| 4:0:40:HIS:CD2  | 4:V:166:TYR:CB[1_556]  | 1.88                     | 0.32              |
| 4:0:121:GLN:CG  | 4:X:20:GLY:O[1_556]    | 1.88                     | 0.32              |
| 4:1:335:ARG:C   | 4:Y:307:PRO:O[1_556]   | 1.88                     | 0.32              |
| 4:2:157:ASP:OD2 | 4:Z:186:THR:CB[1_556]  | 1.88                     | 0.32              |
| 4:1:122:ILE:CA  | 4:Y:19:ALA:O[1_556]    | 1.88                     | 0.32              |
| 4:2:179:ASP:O   | 4:Z:184:ASP:OD2[1_556] | 1.88                     | 0.32              |
| 4:2:296:ASN:C   | 4:Z:316:GLU:C[1_556]   | 1.88                     | 0.32              |
| 4:3:267:ILE:C   | 4:Z:173:HIS:CB[1_556]  | 1.88                     | 0.32              |
| 4:0:372:ARG:CG  | 4:X:143:TYR:N[1_556]   | 1.88                     | 0.32              |
| 4:0:214:GLU:C   | 4:X:253:GLU:CD[1_556]  | 1.88                     | 0.32              |
| 4:1:178:LEU:CA  | 4:Y:180:LEU:CD2[1_556] | 1.88                     | 0.32              |
| 4:2:40:HIS:ND1  | 4:X:166:TYR:CE1[1_556] | 1.88                     | 0.32              |
| 4:1:304:THR:CA  | 4:Y:223:PHE:CZ[1_556]  | 1.88                     | 0.32              |
| 4:1:362:TYR:CB  | 4:Y:348:SER:OG[1_556]  | 1.88                     | 0.32              |
| 4:1:293:LEU:N   | 4:Y:317:ILE:O[1_556]   | 1.88                     | 0.32              |
| 4:3:266:PHE:N   | 4:Z:173:HIS:CE1[1_556] | 1.88                     | 0.32              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:40:HIS:ND1  | 4:V:166:TYR:CE1[1_556] | 1.88                     | 0.32              |
| 4:2:68:LYS:N    | 4:Z:59:GLN:CG[1_556]   | 1.88                     | 0.32              |
| 4:3:196:ARG:NE  | 4:Z:115:ASN:CA[1_556]  | 1.88                     | 0.32              |
| 4:1:186:THR:CB  | 4:Y:189:LEU:C[1_556]   | 1.88                     | 0.32              |
| 4:3:63:GLY:N    | 4:Y:287:ILE:C[1_556]   | 1.88                     | 0.32              |
| 4:2:132:MET:CE  | 4:Z:341:ILE:CB[1_556]  | 1.88                     | 0.32              |
| 4:1:289:ILE:CA  | 4:Y:322:PRO:CD[1_556]  | 1.89                     | 0.31              |
| 4:1:372:ARG:NH2 | 4:Y:145:SER:CA[1_556]  | 1.89                     | 0.31              |
| 4:2:135:ALA:CB  | 4:Z:332:PRO:CG[1_556]  | 1.89                     | 0.31              |
| 4:2:124:PHE:C   | 4:Z:24:ASP:OD1[1_556]  | 1.89                     | 0.31              |
| 4:2:123:MET:CA  | 4:Z:26:ALA:CA[1_556]   | 1.89                     | 0.31              |
| 4:2:372:ARG:CG  | 4:Z:143:TYR:N[1_556]   | 1.89                     | 0.31              |
| 4:0:32:PRO:CB   | 4:X:211:ASP:CA[1_556]  | 1.89                     | 0.31              |
| 4:1:286:ASP:CG  | 4:Y:290:ARG:CD[1_556]  | 1.89                     | 0.31              |
| 4:0:284:LYS:N   | 4:X:280:ASN:ND2[1_556] | 1.89                     | 0.31              |
| 4:1:104:LEU:CA  | 4:Y:334:GLU:CB[1_556]  | 1.89                     | 0.31              |
| 4:1:370:VAL:CG1 | 4:Y:341:ILE:O[1_556]   | 1.89                     | 0.31              |
| 4:2:118:LYS:CB  | 4:Z:11:ASP:CA[1_556]   | 1.89                     | 0.31              |
| 4:1:213:LYS:N   | 4:Y:196:ARG:CB[1_556]  | 1.89                     | 0.31              |
| 4:2:113:LYS:N   | 4:Z:137:GLN:CB[1_556]  | 1.89                     | 0.31              |
| 4:1:121:GLN:N   | 4:Y:340:TRP:CZ2[1_556] | 1.89                     | 0.31              |
| 4:0:213:LYS:N   | 4:X:196:ARG:CB[1_556]  | 1.89                     | 0.31              |
| 4:2:104:LEU:CD1 | 4:Z:333:PRO:CD[1_556]  | 1.89                     | 0.31              |
| 4:1:72:GLU:CA   | 4:Y:157:ASP:OD1[1_556] | 1.89                     | 0.31              |
| 4:1:306:TYR:CE1 | 4:Y:256:ARG:CG[1_556]  | 1.89                     | 0.31              |
| 4:2:260:THR:O   | 4:Z:265:SER:C[1_556]   | 1.89                     | 0.31              |
| 4:1:267:ILE:CG1 | 4:X:173:HIS:CB[1_556]  | 1.89                     | 0.31              |
| 4:0:40:HIS:CD2  | 4:V:166:TYR:CA[1_556]  | 1.89                     | 0.31              |
| 4:1:195:GLU:CD  | 4:X:110:LEU:CA[1_556]  | 1.89                     | 0.31              |
| 4:1:206:ARG:CA  | 4:Y:199:SER:O[1_556]   | 1.89                     | 0.31              |
| 4:2:83:GLU:CD   | 4:Z:28:ARG:O[1_556]    | 1.89                     | 0.31              |
| 4:0:203:THR:OG1 | 4:X:205:GLU:OE2[1_556] | 1.89                     | 0.31              |
| 4:1:37:ARG:CZ   | 4:Y:56:ASP:CA[1_556]   | 1.89                     | 0.31              |
| 4:2:285:CYS:SG  | 4:Z:279:TYR:CA[1_556]  | 1.89                     | 0.31              |
| 4:0:167:GLU:C   | 4:X:295:ALA:N[1_556]   | 1.89                     | 0.31              |
| 4:1:116:ARG:NH1 | 4:Y:142:LEU:N[1_556]   | 1.89                     | 0.31              |
| 4:0:183:ARG:N   | 4:X:185:LEU:O[1_556]   | 1.89                     | 0.31              |
| 4:2:291:LYS:CE  | 4:Z:322:PRO:C[1_556]   | 1.89                     | 0.31              |
| 4:1:307:PRO:CB  | 4:Y:227:MET:N[1_556]   | 1.89                     | 0.31              |
| 4:2:330:ILE:CD1 | 4:Z:315:LYS:CG[1_556]  | 1.89                     | 0.31              |
| 4:0:211:ASP:OD2 | 4:X:249:THR:O[1_556]   | 1.89                     | 0.31              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:213:LYS:N   | 4:Z:196:ARG:CB[1_556]  | 1.89                     | 0.31              |
| 4:0:9:VAL:CG2   | 4:X:333:PRO:CB[1_556]  | 1.89                     | 0.31              |
| 4:2:284:LYS:N   | 4:Z:280:ASN:ND2[1_556] | 1.89                     | 0.31              |
| 4:1:182:GLY:O   | 4:Y:188:TYR:O[1_556]   | 1.89                     | 0.31              |
| 4:2:212:ILE:N   | 4:Z:196:ARG:CD[1_556]  | 1.89                     | 0.31              |
| 4:1:120:THR:CA  | 4:Y:340:TRP:CD2[1_556] | 1.89                     | 0.31              |
| 4:1:281:SER:CA  | 4:Y:276:GLU:O[1_556]   | 1.89                     | 0.31              |
| 4:2:67:LEU:CB   | 4:Z:62:ARG:NH2[1_556]  | 1.89                     | 0.31              |
| 4:0:83:GLU:CD   | 4:X:28:ARG:O[1_556]    | 1.89                     | 0.31              |
| 4:0:260:THR:O   | 4:X:265:SER:C[1_556]   | 1.89                     | 0.31              |
| 4:2:79:TRP:CZ2  | 4:Z:11:ASP:C[1_556]    | 1.89                     | 0.31              |
| 4:2:157:ASP:CB  | 4:Z:213:LYS:CG[1_556]  | 1.89                     | 0.31              |
| 4:2:338:SER:OG  | 4:Z:308:GLY:N[1_556]   | 1.89                     | 0.31              |
| 4:4:40:HIS:ND1  | 4:Z:166:TYR:CE1[1_556] | 1.89                     | 0.31              |
| 4:1:332:PRO:CA  | 4:Y:221:LEU:CD2[1_556] | 1.89                     | 0.31              |
| 4:1:272:ALA:CA  | 4:Y:270:GLU:O[1_556]   | 1.89                     | 0.31              |
| 4:1:338:SER:OG  | 4:Y:308:GLY:N[1_556]   | 1.89                     | 0.31              |
| 4:0:372:ARG:CG  | 4:X:147:ARG:O[1_556]   | 1.89                     | 0.31              |
| 4:2:212:ILE:N   | 4:Z:196:ARG:CB[1_556]  | 1.89                     | 0.31              |
| 4:2:305:MET:CB  | 4:Z:255:PHE:CA[1_556]  | 1.89                     | 0.31              |
| 4:1:214:GLU:N   | 4:Y:253:GLU:OE2[1_556] | 1.89                     | 0.31              |
| 4:2:72:GLU:OE1  | 4:Z:183:ARG:NH2[1_556] | 1.89                     | 0.31              |
| 4:0:157:ASP:CB  | 4:X:213:LYS:CG[1_556]  | 1.89                     | 0.31              |
| 4:1:151:ILE:N   | 4:Y:317:ILE:CA[1_556]  | 1.89                     | 0.31              |
| 4:1:165:ILE:CG1 | 4:Y:297:ASN:CB[1_556]  | 1.89                     | 0.31              |
| 4:2:372:ARG:CG  | 4:Z:143:TYR:CA[1_556]  | 1.89                     | 0.31              |
| 4:1:311:ASP:N   | 4:Y:224:GLU:CB[1_556]  | 1.89                     | 0.31              |
| 4:3:62:ARG:CB   | 4:Y:288:ASP:OD1[1_556] | 1.89                     | 0.31              |
| 4:2:232:SER:CB  | 4:Y:366:GLY:O[1_556]   | 1.89                     | 0.31              |
| 4:0:296:ASN:C   | 4:X:316:GLU:C[1_556]   | 1.89                     | 0.31              |
| 4:0:362:TYR:CG  | 4:X:344:SER:O[1_556]   | 1.89                     | 0.31              |
| 4:2:167:GLU:O   | 4:Z:295:ALA:CB[1_556]  | 1.89                     | 0.31              |
| 4:1:172:PRO:CG  | 4:Y:164:PRO:CB[1_556]  | 1.89                     | 0.31              |
| 4:3:64:ILE:CD1  | 4:Y:292:ASP:OD1[1_556] | 1.89                     | 0.31              |
| 4:1:362:TYR:CE2 | 4:Y:22:ALA:O[1_556]    | 1.89                     | 0.31              |
| 4:3:40:HIS:CD2  | 4:Y:166:TYR:CB[1_556]  | 1.89                     | 0.31              |
| 4:2:9:VAL:CG2   | 4:Z:333:PRO:CB[1_556]  | 1.89                     | 0.31              |
| 4:2:155:SER:C   | 4:Z:258:PRO:CA[1_556]  | 1.89                     | 0.31              |
| 4:2:231:ALA:C   | 4:Y:370:VAL:N[1_556]   | 1.89                     | 0.31              |
| 4:0:111:ASN:O   | 4:X:137:GLN:CB[1_556]  | 1.89                     | 0.31              |
| 4:2:186:THR:N   | 4:Z:192:ILE:N[1_556]   | 1.89                     | 0.31              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:185:LEU:CB  | 4:X:188:TYR:CE1[1_556] | 1.89                     | 0.31              |
| 4:1:169:TYR:CE2 | 4:Y:293:LEU:CD1[1_556] | 1.89                     | 0.31              |
| 4:2:118:LYS:O   | 4:Z:340:TRP:CE2[1_556] | 1.89                     | 0.31              |
| 4:2:110:LEU:N   | 4:Z:154:ASP:CB[1_556]  | 1.89                     | 0.31              |
| 4:1:161:HIS:ND1 | 4:Y:155:SER:OG[1_556]  | 1.89                     | 0.31              |
| 4:0:171:LEU:CG  | 4:X:282:ILE:CD1[1_556] | 1.89                     | 0.31              |
| 4:2:40:HIS:CD2  | 4:X:166:TYR:CA[1_556]  | 1.89                     | 0.31              |
| 4:1:253:GLU:OE2 | 4:X:112:PRO:C[1_556]   | 1.89                     | 0.31              |
| 4:1:33:SER:CB   | 4:Y:214:GLU:OE2[1_556] | 1.89                     | 0.31              |
| 4:2:104:LEU:CD1 | 4:Z:334:GLU:OE2[1_556] | 1.89                     | 0.31              |
| 4:0:68:LYS:CA   | 4:X:59:GLN:CG[1_556]   | 1.89                     | 0.31              |
| 4:0:149:THR:OG1 | 4:X:326:LYS:O[1_556]   | 1.89                     | 0.31              |
| 4:0:173:HIS:C   | 4:X:281:SER:OG[1_556]  | 1.89                     | 0.31              |
| 4:2:362:TYR:CE2 | 4:Z:22:ALA:CB[1_556]   | 1.89                     | 0.31              |
| 4:0:135:ALA:CB  | 4:X:332:PRO:CG[1_556]  | 1.89                     | 0.31              |
| 4:1:66:THR:CB   | 4:Y:59:GLN:O[1_556]    | 1.89                     | 0.31              |
| 4:2:203:THR:OG1 | 4:Z:205:GLU:OE2[1_556] | 1.89                     | 0.31              |
| 4:2:372:ARG:CG  | 4:Z:147:ARG:O[1_556]   | 1.89                     | 0.31              |
| 4:2:79:TRP:NE1  | 4:Z:11:ASP:O[1_556]    | 1.89                     | 0.31              |
| 4:0:291:LYS:CE  | 4:X:322:PRO:C[1_556]   | 1.89                     | 0.31              |
| 4:1:332:PRO:N   | 4:Y:221:LEU:N[1_556]   | 1.89                     | 0.31              |
| 4:2:217:CYS:CB  | 4:Z:256:ARG:NH2[1_556] | 1.90                     | 0.30              |
| 4:0:79:TRP:NE1  | 4:X:11:ASP:O[1_556]    | 1.90                     | 0.30              |
| 4:0:60:SER:C    | 4:X:243:PRO:CB[1_556]  | 1.90                     | 0.30              |
| 4:1:368:SER:C   | 4:Y:346:LEU:CD2[1_556] | 1.90                     | 0.30              |
| 4:1:267:ILE:C   | 4:X:173:HIS:CB[1_556]  | 1.90                     | 0.30              |
| 4:1:115:ASN:O   | 4:Y:11:ASP:CG[1_556]   | 1.90                     | 0.30              |
| 4:0:169:TYR:OH  | 4:X:164:PRO:CA[1_556]  | 1.90                     | 0.30              |
| 4:0:159:VAL:CG1 | 4:X:181:ALA:CB[1_556]  | 1.90                     | 0.30              |
| 4:2:304:THR:OG1 | 4:Z:223:PHE:CE1[1_556] | 1.90                     | 0.30              |
| 4:3:195:GLU:CD  | 4:Z:110:LEU:CA[1_556]  | 1.90                     | 0.30              |
| 4:1:62:ARG:C    | 4:W:288:ASP:N[1_556]   | 1.90                     | 0.30              |
| 4:1:335:ARG:CD  | 4:Y:220:ALA:O[1_556]   | 1.90                     | 0.30              |
| 4:0:339:VAL:CG2 | 4:X:304:THR:O[1_556]   | 1.90                     | 0.30              |
| 4:0:179:ASP:N   | 4:X:180:LEU:CA[1_556]  | 1.90                     | 0.30              |
| 4:0:207:GLU:CD  | 4:X:242:LEU:CD2[1_556] | 1.90                     | 0.30              |
| 4:0:231:ALA:C   | 4:W:370:VAL:N[1_556]   | 1.90                     | 0.30              |
| 4:1:40:HIS:CD2  | 4:W:166:TYR:CG[1_556]  | 1.90                     | 0.30              |
| 4:2:303:THR:CG2 | 4:Z:257:CYS:C[1_556]   | 1.90                     | 0.30              |
| 4:1:68:LYS:CA   | 4:Y:59:GLN:OE1[1_556]  | 1.90                     | 0.30              |
| 4:1:185:LEU:C   | 4:Y:188:TYR:O[1_556]   | 1.90                     | 0.30              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:362:TYR:CE2 | 4:X:22:ALA:CB[1_556]   | 1.90                     | 0.30              |
| 4:2:335:ARG:C   | 4:Z:307:PRO:O[1_556]   | 1.90                     | 0.30              |
| 4:2:148:THR:CB  | 4:Z:327:ILE:C[1_556]   | 1.90                     | 0.30              |
| 4:2:83:GLU:CB   | 4:Z:29:ALA:CA[1_556]   | 1.90                     | 0.30              |
| 4:1:332:PRO:CD  | 4:Y:221:LEU:CD2[1_556] | 1.90                     | 0.30              |
| 4:1:170:ALA:N   | 4:Y:151:ILE:CG2[1_556] | 1.90                     | 0.30              |
| 4:0:107:GLU:OE2 | 4:X:141:SER:CB[1_556]  | 1.90                     | 0.30              |
| 4:1:124:PHE:C   | 4:Y:24:ASP:CA[1_556]   | 1.90                     | 0.30              |
| 4:0:292:ASP:N   | 4:X:321:ALA:CA[1_556]  | 1.90                     | 0.30              |
| 4:2:297:ASN:N   | 4:Z:315:LYS:C[1_556]   | 1.90                     | 0.30              |
| 4:0:161:HIS:ND1 | 4:X:155:SER:OG[1_556]  | 1.90                     | 0.30              |
| 4:1:162:ASN:N   | 4:Y:274:ILE:CG1[1_556] | 1.90                     | 0.30              |
| 4:2:207:GLU:CD  | 4:Z:242:LEU:CD2[1_556] | 1.90                     | 0.30              |
| 4:0:366:GLY:CA  | 4:X:347:ALA:CB[1_556]  | 1.90                     | 0.30              |
| 4:0:118:LYS:O   | 4:X:340:TRP:CE2[1_556] | 1.90                     | 0.30              |
| 4:0:121:GLN:N   | 4:X:340:TRP:CE2[1_556] | 1.90                     | 0.30              |
| 4:2:332:PRO:CA  | 4:Z:221:LEU:CD2[1_556] | 1.90                     | 0.30              |
| 4:2:140:LEU:CG  | 4:Z:331:ALA:O[1_556]   | 1.90                     | 0.30              |
| 4:0:301:GLY:C   | 4:X:258:PRO:CB[1_556]  | 1.90                     | 0.30              |
| 4:2:169:TYR:OH  | 4:Z:164:PRO:CA[1_556]  | 1.90                     | 0.30              |
| 4:2:186:THR:CB  | 4:Z:190:MET:CA[1_556]  | 1.90                     | 0.30              |
| 4:0:367:PRO:O   | 4:X:342:GLY:O[1_556]   | 1.90                     | 0.30              |
| 4:3:253:GLU:OE2 | 4:Z:112:PRO:C[1_556]   | 1.90                     | 0.30              |
| 4:2:362:TYR:CD2 | 4:Z:23:GLY:CA[1_556]   | 1.90                     | 0.30              |
| 4:1:14:SER:OG   | 4:Y:182:GLY:CA[1_556]  | 1.90                     | 0.30              |
| 4:0:335:ARG:C   | 4:X:219:VAL:N[1_556]   | 1.90                     | 0.30              |
| 4:0:171:LEU:CD2 | 4:X:282:ILE:CG1[1_556] | 1.90                     | 0.30              |
| 4:4:64:ILE:CB   | 4:Z:292:ASP:OD2[1_556] | 1.90                     | 0.30              |
| 4:1:337:TYR:CA  | 4:Y:307:PRO:CD[1_556]  | 1.90                     | 0.30              |
| 4:1:84:LYS:CE   | 4:Y:56:ASP:OD1[1_556]  | 1.90                     | 0.30              |
| 4:0:305:MET:CB  | 4:X:255:PHE:CA[1_556]  | 1.90                     | 0.30              |
| 4:2:177:ARG:NH2 | 4:Z:159:VAL:CA[1_556]  | 1.90                     | 0.30              |
| 4:1:233:SER:CB  | 4:X:367:PRO:CG[1_556]  | 1.90                     | 0.30              |
| 4:2:167:GLU:C   | 4:Z:295:ALA:N[1_556]   | 1.90                     | 0.30              |
| 4:0:68:LYS:N    | 4:X:59:GLN:CG[1_556]   | 1.90                     | 0.30              |
| 4:2:301:GLY:C   | 4:Z:258:PRO:CB[1_556]  | 1.90                     | 0.30              |
| 4:2:362:TYR:C   | 4:Z:348:SER:CA[1_556]  | 1.90                     | 0.30              |
| 4:1:167:GLU:CD  | 4:Y:326:LYS:CB[1_556]  | 1.90                     | 0.30              |
| 4:0:124:PHE:C   | 4:X:24:ASP:OD1[1_556]  | 1.90                     | 0.30              |
| 4:0:79:TRP:CZ2  | 4:X:11:ASP:C[1_556]    | 1.90                     | 0.30              |
| 4:2:112:PRO:N   | 4:Z:137:GLN:CD[1_556]  | 1.90                     | 0.30              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:362:TYR:C   | 4:X:348:SER:CA[1_556]  | 1.90                     | 0.30              |
| 4:2:214:GLU:CB  | 4:Z:250:ILE:CG2[1_556] | 1.90                     | 0.30              |
| 4:0:168:GLY:N   | 4:X:295:ALA:CA[1_556]  | 1.90                     | 0.30              |
| 4:1:215:LYS:NZ  | 4:Y:249:THR:CA[1_556]  | 1.90                     | 0.30              |
| 4:1:191:LYS:NZ  | 4:X:110:LEU:CG[1_556]  | 1.90                     | 0.30              |
| 4:2:32:PRO:CB   | 4:Z:211:ASP:CA[1_556]  | 1.90                     | 0.30              |
| 4:3:233:SER:CB  | 4:Z:367:PRO:CG[1_556]  | 1.90                     | 0.30              |
| 4:2:41:GLN:N    | 4:X:167:GLU:OE1[1_556] | 1.90                     | 0.30              |
| 4:0:171:LEU:CD1 | 4:X:282:ILE:CB[1_556]  | 1.90                     | 0.30              |
| 4:1:196:ARG:NE  | 4:X:115:ASN:CA[1_556]  | 1.90                     | 0.30              |
| 4:2:40:HIS:CD2  | 4:X:166:TYR:CB[1_556]  | 1.90                     | 0.30              |
| 4:1:63:GLY:N    | 4:W:287:ILE:C[1_556]   | 1.90                     | 0.30              |
| 4:1:150:GLY:N   | 4:Y:317:ILE:CD1[1_556] | 1.90                     | 0.30              |
| 4:1:134:VAL:CG1 | 4:Y:338:SER:OG[1_556]  | 1.90                     | 0.30              |
| 4:2:31:PHE:CA   | 4:Z:215:LYS:NZ[1_556]  | 1.90                     | 0.30              |
| 4:1:251:GLY:CA  | 4:X:114:ALA:CA[1_556]  | 1.90                     | 0.30              |
| 4:4:40:HIS:CD2  | 4:Z:166:TYR:CA[1_556]  | 1.90                     | 0.30              |
| 4:0:14:SER:OG   | 4:X:182:GLY:CA[1_556]  | 1.90                     | 0.30              |
| 4:2:168:GLY:N   | 4:Z:295:ALA:CA[1_556]  | 1.90                     | 0.30              |
| 4:1:203:THR:CB  | 4:Y:205:GLU:OE2[1_556] | 1.90                     | 0.30              |
| 4:0:205:GLU:C   | 4:X:199:SER:CB[1_556]  | 1.90                     | 0.30              |
| 4:0:37:ARG:CZ   | 4:X:56:ASP:CA[1_556]   | 1.90                     | 0.30              |
| 4:2:157:ASP:N   | 4:Z:306:TYR:OH[1_556]  | 1.90                     | 0.30              |
| 4:1:209:VAL:CG1 | 4:Y:194:THR:CB[1_556]  | 1.90                     | 0.30              |
| 4:0:33:SER:C    | 4:X:210:ARG:NH1[1_556] | 1.90                     | 0.30              |
| 4:1:158:GLY:CA  | 4:Y:182:GLY:O[1_556]   | 1.90                     | 0.30              |
| 4:1:206:ARG:CD  | 4:Y:200:PHE:O[1_556]   | 1.90                     | 0.30              |
| 4:1:158:GLY:CA  | 4:Y:185:LEU:N[1_556]   | 1.91                     | 0.29              |
| 4:1:149:THR:OG1 | 4:Y:326:LYS:O[1_556]   | 1.91                     | 0.29              |
| 4:0:179:ASP:O   | 4:X:184:ASP:OD2[1_556] | 1.91                     | 0.29              |
| 4:0:133:TYR:CE1 | 4:X:145:SER:CA[1_556]  | 1.91                     | 0.29              |
| 4:0:72:GLU:OE1  | 4:X:183:ARG:NH2[1_556] | 1.91                     | 0.29              |
| 4:0:372:ARG:CG  | 4:X:143:TYR:CA[1_556]  | 1.91                     | 0.29              |
| 4:2:205:GLU:C   | 4:Z:199:SER:CB[1_556]  | 1.91                     | 0.29              |
| 4:2:335:ARG:C   | 4:Z:219:VAL:N[1_556]   | 1.91                     | 0.29              |
| 4:0:362:TYR:CD2 | 4:X:23:GLY:CA[1_556]   | 1.91                     | 0.29              |
| 4:3:196:ARG:CB  | 4:Z:111:ASN:OD1[1_556] | 1.91                     | 0.29              |
| 4:1:120:THR:C   | 4:Y:340:TRP:CH2[1_556] | 1.91                     | 0.29              |
| 4:0:330:ILE:CD1 | 4:X:315:LYS:CG[1_556]  | 1.91                     | 0.29              |
| 4:2:211:ASP:OD2 | 4:Z:249:THR:O[1_556]   | 1.91                     | 0.29              |
| 4:2:185:LEU:CB  | 4:Z:188:TYR:CE1[1_556] | 1.91                     | 0.29              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:362:TYR:CG  | 4:Z:344:SER:O[1_556]   | 1.91                     | 0.29              |
| 4:0:232:SER:CB  | 4:W:366:GLY:O[1_556]   | 1.91                     | 0.29              |
| 4:1:67:LEU:CG   | 4:Y:207:GLU:CD[1_556]  | 1.91                     | 0.29              |
| 4:1:277:THR:CG2 | 4:Y:272:ALA:CA[1_556]  | 1.91                     | 0.29              |
| 4:1:202:THR:C   | 4:Y:201:VAL:CG2[1_556] | 1.91                     | 0.29              |
| 4:0:40:HIS:ND1  | 4:V:166:TYR:CB[1_556]  | 1.91                     | 0.29              |
| 4:0:191:LYS:CB  | 4:W:110:LEU:CD1[1_556] | 1.91                     | 0.29              |
| 4:0:31:PHE:CA   | 4:X:215:LYS:NZ[1_556]  | 1.91                     | 0.29              |
| 4:0:338:SER:OG  | 4:X:308:GLY:N[1_556]   | 1.91                     | 0.29              |
| 4:1:154:ASP:O   | 4:Y:261:LEU:CD1[1_556] | 1.91                     | 0.29              |
| 4:0:122:ILE:O   | 4:X:28:ARG:N[1_556]    | 1.91                     | 0.29              |
| 4:2:367:PRO:O   | 4:Z:343:GLY:C[1_556]   | 1.91                     | 0.29              |
| 4:0:110:LEU:N   | 4:X:154:ASP:CB[1_556]  | 1.91                     | 0.29              |
| 4:3:250:ILE:CA  | 4:Z:114:ALA:CB[1_556]  | 1.91                     | 0.29              |
| 4:3:197:GLY:CA  | 4:Z:76:ILE:N[1_556]    | 1.91                     | 0.29              |
| 4:0:232:SER:OG  | 4:W:365:ALA:CB[1_556]  | 1.91                     | 0.29              |
| 4:1:121:GLN:N   | 4:Y:340:TRP:CE2[1_556] | 1.91                     | 0.29              |
| 4:0:56:ASP:OD2  | 4:X:240:TYR:OH[1_556]  | 1.91                     | 0.29              |
| 4:3:251:GLY:CA  | 4:Z:114:ALA:CA[1_556]  | 1.91                     | 0.29              |
| 4:0:196:ARG:NE  | 4:W:115:ASN:CA[1_556]  | 1.91                     | 0.29              |
| 4:1:307:PRO:CB  | 4:Y:227:MET:CB[1_556]  | 1.91                     | 0.29              |
| 4:2:120:THR:N   | 4:Z:340:TRP:CE3[1_556] | 1.91                     | 0.29              |
| 4:1:33:SER:C    | 4:Y:210:ARG:NH1[1_556] | 1.91                     | 0.29              |
| 4:3:196:ARG:CZ  | 4:Z:114:ALA:C[1_556]   | 1.91                     | 0.29              |
| 4:0:107:GLU:N   | 4:X:301:GLY:N[1_556]   | 1.91                     | 0.29              |
| 4:0:140:LEU:CG  | 4:X:331:ALA:O[1_556]   | 1.91                     | 0.29              |
| 4:3:40:HIS:CD2  | 4:Y:166:TYR:CA[1_556]  | 1.91                     | 0.29              |
| 4:2:112:PRO:C   | 4:Z:137:GLN:CA[1_556]  | 1.91                     | 0.29              |
| 4:4:40:HIS:ND1  | 4:Z:166:TYR:CB[1_556]  | 1.91                     | 0.29              |
| 4:2:260:THR:C   | 4:Z:266:PHE:CA[1_556]  | 1.91                     | 0.29              |
| 4:0:112:PRO:C   | 4:X:137:GLN:CA[1_556]  | 1.91                     | 0.29              |
| 4:1:339:VAL:CG1 | 4:Y:335:ARG:NE[1_556]  | 1.91                     | 0.29              |
| 4:2:121:GLN:N   | 4:Z:340:TRP:CE2[1_556] | 1.91                     | 0.29              |
| 4:2:40:HIS:ND1  | 4:X:166:TYR:CB[1_556]  | 1.91                     | 0.29              |
| 4:0:264:PRO:O   | 4:W:173:HIS:CG[1_556]  | 1.91                     | 0.29              |
| 4:0:177:ARG:NH2 | 4:X:159:VAL:CA[1_556]  | 1.91                     | 0.29              |
| 4:0:307:PRO:N   | 4:X:227:MET:CG[1_556]  | 1.91                     | 0.29              |
| 4:2:232:SER:N   | 4:Y:369:ILE:N[1_556]   | 1.91                     | 0.29              |
| 4:1:104:LEU:CA  | 4:Y:334:GLU:CD[1_556]  | 1.91                     | 0.29              |
| 4:0:281:SER:CB  | 4:X:276:GLU:CA[1_556]  | 1.91                     | 0.29              |
| 4:1:271:SER:C   | 4:Y:270:GLU:CB[1_556]  | 1.91                     | 0.29              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:72:GLU:CB   | 4:Z:183:ARG:NH2[1_556] | 1.91                     | 0.29              |
| 4:1:149:THR:CB  | 4:Y:327:ILE:CA[1_556]  | 1.91                     | 0.29              |
| 4:2:171:LEU:CG  | 4:Z:282:ILE:CD1[1_556] | 1.91                     | 0.29              |
| 4:2:171:LEU:CD1 | 4:Z:282:ILE:CB[1_556]  | 1.91                     | 0.29              |
| 4:0:217:CYS:CB  | 4:X:256:ARG:NH2[1_556] | 1.91                     | 0.29              |
| 4:2:366:GLY:CA  | 4:Z:347:ALA:CB[1_556]  | 1.91                     | 0.29              |
| 4:3:230:ALA:CA  | 4:Z:368:SER:CA[1_556]  | 1.91                     | 0.29              |
| 4:2:367:PRO:O   | 4:Z:342:GLY:O[1_556]   | 1.91                     | 0.29              |
| 4:3:267:ILE:CA  | 4:Z:173:HIS:N[1_556]   | 1.91                     | 0.29              |
| 4:0:183:ARG:CA  | 4:X:188:TYR:N[1_556]   | 1.91                     | 0.29              |
| 4:2:133:TYR:CE1 | 4:Z:144:ALA:O[1_556]   | 1.91                     | 0.29              |
| 4:1:231:ALA:CB  | 4:X:370:VAL:C[1_556]   | 1.91                     | 0.29              |
| 4:3:191:LYS:NZ  | 4:Z:110:LEU:CG[1_556]  | 1.91                     | 0.29              |
| 4:2:116:ARG:CA  | 4:Z:339:VAL:O[1_556]   | 1.91                     | 0.29              |
| 4:2:64:ILE:CB   | 4:X:292:ASP:OD2[1_556] | 1.91                     | 0.29              |
| 4:0:83:GLU:CB   | 4:X:29:ALA:CA[1_556]   | 1.91                     | 0.29              |
| 4:2:60:SER:C    | 4:Z:243:PRO:CB[1_556]  | 1.91                     | 0.29              |
| 4:1:40:HIS:CD2  | 4:W:166:TYR:CB[1_556]  | 1.91                     | 0.29              |
| 4:2:187:ASP:OD1 | 4:Z:190:MET:CB[1_556]  | 1.91                     | 0.29              |
| 4:2:366:GLY:CA  | 4:Z:348:SER:N[1_556]   | 1.91                     | 0.29              |
| 4:2:183:ARG:CB  | 4:Z:186:THR:CA[1_556]  | 1.91                     | 0.29              |
| 4:1:123:MET:N   | 4:Y:26:ALA:C[1_556]    | 1.91                     | 0.29              |
| 4:1:286:ASP:N   | 4:Y:283:MET:N[1_556]   | 1.91                     | 0.29              |
| 4:0:293:LEU:C   | 4:X:320:LEU:CB[1_556]  | 1.91                     | 0.29              |
| 4:1:185:LEU:O   | 4:Y:192:ILE:N[1_556]   | 1.91                     | 0.29              |
| 4:0:72:GLU:CB   | 4:X:183:ARG:NH2[1_556] | 1.91                     | 0.29              |
| 4:1:365:ALA:CA  | 4:Y:349:LEU:O[1_556]   | 1.91                     | 0.29              |
| 4:0:292:ASP:CA  | 4:X:321:ALA:C[1_556]   | 1.91                     | 0.29              |
| 4:0:179:ASP:OD1 | 4:X:180:LEU:CA[1_556]  | 1.91                     | 0.29              |
| 4:0:229:THR:O   | 4:W:369:ILE:N[1_556]   | 1.91                     | 0.29              |
| 4:0:104:LEU:CD1 | 4:X:334:GLU:OE2[1_556] | 1.91                     | 0.29              |
| 4:2:33:SER:C    | 4:Z:210:ARG:NH1[1_556] | 1.91                     | 0.29              |
| 4:2:122:ILE:O   | 4:Z:28:ARG:N[1_556]    | 1.91                     | 0.29              |
| 4:2:292:ASP:CA  | 4:Z:321:ALA:C[1_556]   | 1.91                     | 0.29              |
| 4:0:271:SER:C   | 4:X:270:GLU:CB[1_556]  | 1.91                     | 0.29              |
| 4:0:158:GLY:CA  | 4:X:185:LEU:N[1_556]   | 1.91                     | 0.29              |
| 4:2:274:ILE:CA  | 4:Z:264:PRO:CD[1_556]  | 1.91                     | 0.29              |
| 4:0:297:ASN:N   | 4:X:315:LYS:C[1_556]   | 1.91                     | 0.29              |
| 4:2:9:VAL:CG1   | 4:Z:333:PRO:CB[1_556]  | 1.92                     | 0.28              |
| 4:0:303:THR:CG2 | 4:X:257:CYS:C[1_556]   | 1.92                     | 0.28              |
| 4:2:11:ASP:CB   | 4:Z:305:MET:SD[1_556]  | 1.92                     | 0.28              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:121:GLN:CB  | 4:Y:9:VAL:CA[1_556]    | 1.92                     | 0.28              |
| 4:0:299:MET:O   | 4:X:312:ARG:CB[1_556]  | 1.92                     | 0.28              |
| 4:1:253:GLU:N   | 4:X:113:LYS:N[1_556]   | 1.92                     | 0.28              |
| 4:0:150:GLY:C   | 4:X:317:ILE:CA[1_556]  | 1.92                     | 0.28              |
| 4:1:260:THR:O   | 4:Y:265:SER:C[1_556]   | 1.92                     | 0.28              |
| 4:1:183:ARG:N   | 4:Y:185:LEU:O[1_556]   | 1.92                     | 0.28              |
| 4:1:178:LEU:C   | 4:Y:180:LEU:CD2[1_556] | 1.92                     | 0.28              |
| 4:2:133:TYR:CE1 | 4:Z:145:SER:CA[1_556]  | 1.92                     | 0.28              |
| 4:0:185:LEU:O   | 4:X:191:LYS:CD[1_556]  | 1.92                     | 0.28              |
| 4:1:365:ALA:CA  | 4:Y:349:LEU:CB[1_556]  | 1.92                     | 0.28              |
| 4:1:209:VAL:O   | 4:Y:193:LEU:CA[1_556]  | 1.92                     | 0.28              |
| 4:1:59:GLN:NE2  | 4:Y:208:ILE:CA[1_556]  | 1.92                     | 0.28              |
| 4:2:135:ALA:N   | 4:Z:338:SER:OG[1_556]  | 1.92                     | 0.28              |
| 4:0:366:GLY:CA  | 4:X:348:SER:N[1_556]   | 1.92                     | 0.28              |
| 4:0:335:ARG:C   | 4:X:307:PRO:O[1_556]   | 1.92                     | 0.28              |
| 4:2:293:LEU:C   | 4:Z:320:LEU:CB[1_556]  | 1.92                     | 0.28              |
| 4:2:232:SER:OG  | 4:Y:365:ALA:CB[1_556]  | 1.92                     | 0.28              |
| 4:0:267:ILE:CA  | 4:W:173:HIS:N[1_556]   | 1.92                     | 0.28              |
| 4:1:69:TYR:CE2  | 4:Y:210:ARG:CD[1_556]  | 1.92                     | 0.28              |
| 4:0:116:ARG:NH1 | 4:X:142:LEU:N[1_556]   | 1.92                     | 0.28              |
| 4:1:372:ARG:NE  | 4:Y:143:TYR:N[1_556]   | 1.92                     | 0.28              |
| 4:1:162:ASN:C   | 4:Y:274:ILE:CA[1_556]  | 1.92                     | 0.28              |
| 4:0:107:GLU:OE2 | 4:X:300:SER:OG[1_556]  | 1.92                     | 0.28              |
| 4:0:155:SER:CB  | 4:X:261:LEU:N[1_556]   | 1.92                     | 0.28              |
| 4:2:173:HIS:CA  | 4:Z:174:ALA:C[1_556]   | 1.92                     | 0.28              |
| 4:0:186:THR:CB  | 4:X:191:LYS:N[1_556]   | 1.92                     | 0.28              |
| 4:1:148:THR:CB  | 4:Y:328:LYS:N[1_556]   | 1.92                     | 0.28              |
| 4:2:299:MET:O   | 4:Z:312:ARG:CB[1_556]  | 1.92                     | 0.28              |
| 4:3:253:GLU:N   | 4:Z:113:LYS:N[1_556]   | 1.92                     | 0.28              |
| 4:0:112:PRO:N   | 4:X:137:GLN:CD[1_556]  | 1.92                     | 0.28              |
| 4:1:35:VAL:CG1  | 4:Y:56:ASP:OD2[1_556]  | 1.92                     | 0.28              |
| 4:2:264:PRO:O   | 4:Y:173:HIS:CG[1_556]  | 1.92                     | 0.28              |
| 4:2:335:ARG:NE  | 4:Z:220:ALA:CA[1_556]  | 1.92                     | 0.28              |
| 4:1:196:ARG:CB  | 4:X:111:ASN:OD1[1_556] | 1.92                     | 0.28              |
| 4:2:294:TYR:N   | 4:Z:320:LEU:CB[1_556]  | 1.92                     | 0.28              |
| 4:0:367:PRO:O   | 4:X:343:GLY:C[1_556]   | 1.92                     | 0.28              |
| 4:0:77:THR:N    | 4:X:15:GLY:C[1_556]    | 1.92                     | 0.28              |
| 4:1:40:HIS:CD2  | 4:W:166:TYR:CA[1_556]  | 1.92                     | 0.28              |
| 4:0:157:ASP:N   | 4:X:306:TYR:OH[1_556]  | 1.92                     | 0.28              |
| 4:2:37:ARG:CZ   | 4:Z:56:ASP:CA[1_556]   | 1.92                     | 0.28              |
| 4:0:41:GLN:N    | 4:V:167:GLU:OE1[1_556] | 1.92                     | 0.28              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:362:TYR:CB  | 4:Z:348:SER:OG[1_556]  | 1.92                     | 0.28              |
| 4:0:120:THR:C   | 4:X:340:TRP:CE3[1_556] | 1.92                     | 0.28              |
| 4:3:192:ILE:CA  | 4:Z:110:LEU:C[1_556]   | 1.92                     | 0.28              |
| 4:2:115:ASN:N   | 4:Z:106:THR:CB[1_556]  | 1.92                     | 0.28              |
| 4:0:208:ILE:C   | 4:X:198:TYR:CD1[1_556] | 1.92                     | 0.28              |
| 4:0:293:LEU:CB  | 4:X:320:LEU:CB[1_556]  | 1.92                     | 0.28              |
| 4:2:208:ILE:C   | 4:Z:198:TYR:CD1[1_556] | 1.92                     | 0.28              |
| 4:2:281:SER:CB  | 4:Z:276:GLU:CA[1_556]  | 1.92                     | 0.28              |
| 4:1:372:ARG:CG  | 4:Y:143:TYR:CA[1_556]  | 1.92                     | 0.28              |
| 4:0:120:THR:N   | 4:X:340:TRP:CE3[1_556] | 1.92                     | 0.28              |
| 4:0:332:PRO:CA  | 4:X:221:LEU:CD2[1_556] | 1.92                     | 0.28              |
| 4:1:67:LEU:CB   | 4:Y:207:GLU:CD[1_556]  | 1.92                     | 0.28              |
| 4:1:186:THR:CB  | 4:Y:190:MET:O[1_556]   | 1.92                     | 0.28              |
| 4:1:68:LYS:CD   | 4:Y:59:GLN:N[1_556]    | 1.92                     | 0.28              |
| 4:0:306:TYR:O   | 4:X:227:MET:CG[1_556]  | 1.92                     | 0.28              |
| 4:1:124:PHE:CB  | 4:Y:23:GLY:C[1_556]    | 1.92                     | 0.28              |
| 4:0:186:THR:CB  | 4:X:190:MET:CA[1_556]  | 1.92                     | 0.28              |
| 4:0:211:ASP:OD1 | 4:X:249:THR:CG2[1_556] | 1.92                     | 0.28              |
| 4:2:171:LEU:CD2 | 4:Z:282:ILE:CG1[1_556] | 1.92                     | 0.28              |
| 4:1:207:GLU:CD  | 4:Y:242:LEU:CD2[1_556] | 1.92                     | 0.28              |
| 4:0:189:LEU:CD2 | 4:X:195:GLU:CB[1_556]  | 1.92                     | 0.28              |
| 4:1:171:LEU:CD2 | 4:Y:282:ILE:CG1[1_556] | 1.92                     | 0.28              |
| 4:1:196:ARG:CZ  | 4:X:114:ALA:C[1_556]   | 1.92                     | 0.28              |
| 4:1:108:ALA:N   | 4:Y:300:SER:O[1_556]   | 1.92                     | 0.28              |
| 4:1:120:THR:CA  | 4:Y:340:TRP:O[1_556]   | 1.92                     | 0.28              |
| 4:2:305:MET:N   | 4:Z:255:PHE:C[1_556]   | 1.92                     | 0.28              |
| 4:1:296:ASN:N   | 4:Y:319:ALA:CA[1_556]  | 1.92                     | 0.28              |
| 4:0:267:ILE:CB  | 4:W:173:HIS:CA[1_556]  | 1.92                     | 0.28              |
| 4:2:119:MET:CE  | 4:Z:337:TYR:C[1_556]   | 1.92                     | 0.28              |
| 4:1:286:ASP:C   | 4:Y:283:MET:SD[1_556]  | 1.92                     | 0.28              |
| 4:1:206:ARG:CB  | 4:Y:200:PHE:C[1_556]   | 1.92                     | 0.28              |
| 4:1:303:THR:CG2 | 4:Y:256:ARG:O[1_556]   | 1.92                     | 0.28              |
| 4:1:177:ARG:NH1 | 4:Y:159:VAL:O[1_556]   | 1.92                     | 0.28              |
| 4:2:86:TRP:CZ3  | 4:Z:27:PRO:CG[1_556]   | 1.92                     | 0.28              |
| 4:1:80:ASP:C    | 4:Y:31:PHE:CG[1_556]   | 1.92                     | 0.28              |
| 4:1:280:ASN:O   | 4:Y:280:ASN:CG[1_556]  | 1.92                     | 0.28              |
| 4:1:171:LEU:O   | 4:Y:281:SER:CB[1_556]  | 1.92                     | 0.28              |
| 4:0:214:GLU:CB  | 4:X:250:ILE:CG2[1_556] | 1.92                     | 0.28              |
| 4:2:155:SER:CB  | 4:Z:261:LEU:N[1_556]   | 1.92                     | 0.28              |
| 4:1:121:GLN:CG  | 4:Y:20:GLY:O[1_556]    | 1.92                     | 0.28              |
| 4:1:304:THR:OG1 | 4:Y:223:PHE:CE1[1_556] | 1.92                     | 0.28              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:367:PRO:N   | 4:Y:347:ALA:N[1_556]   | 1.92                     | 0.28              |
| 4:4:40:HIS:CD2  | 4:Z:166:TYR:CB[1_556]  | 1.92                     | 0.28              |
| 4:1:264:PRO:CB  | 4:Y:268:GLY:O[1_556]   | 1.92                     | 0.28              |
| 4:1:293:LEU:CB  | 4:Y:320:LEU:CB[1_556]  | 1.92                     | 0.28              |
| 4:2:79:TRP:CA   | 4:Z:17:VAL:CB[1_556]   | 1.92                     | 0.28              |
| 4:0:261:LEU:O   | 4:X:265:SER:C[1_556]   | 1.92                     | 0.28              |
| 4:0:232:SER:N   | 4:W:369:ILE:N[1_556]   | 1.92                     | 0.28              |
| 4:1:124:PHE:CB  | 4:Y:24:ASP:O[1_556]    | 1.92                     | 0.28              |
| 4:0:73:HIS:NE2  | 4:X:184:ASP:OD1[1_556] | 1.92                     | 0.28              |
| 4:1:167:GLU:O   | 4:Y:295:ALA:CB[1_556]  | 1.92                     | 0.28              |
| 4:0:120:THR:CA  | 4:X:340:TRP:CD2[1_556] | 1.92                     | 0.28              |
| 4:2:191:LYS:CB  | 4:Y:110:LEU:CD1[1_556] | 1.92                     | 0.28              |
| 4:3:40:HIS:N    | 4:Y:166:TYR:CE2[1_556] | 1.92                     | 0.28              |
| 4:1:150:GLY:C   | 4:Y:317:ILE:CA[1_556]  | 1.92                     | 0.28              |
| 4:0:138:ALA:N   | 4:X:299:MET:SD[1_556]  | 1.92                     | 0.28              |
| 4:1:210:ARG:NE  | 4:Y:193:LEU:CD2[1_556] | 1.92                     | 0.28              |
| 4:1:151:ILE:CD1 | 4:Y:276:GLU:CA[1_556]  | 1.92                     | 0.28              |
| 4:1:197:GLY:CA  | 4:X:76:ILE:N[1_556]    | 1.92                     | 0.28              |
| 4:2:186:THR:CB  | 4:Z:191:LYS:N[1_556]   | 1.92                     | 0.28              |
| 4:0:79:TRP:CH2  | 4:X:18:LYS:CE[1_556]   | 1.92                     | 0.28              |
| 4:0:187:ASP:OD1 | 4:X:190:MET:CB[1_556]  | 1.92                     | 0.28              |
| 4:1:179:ASP:N   | 4:Y:180:LEU:CA[1_556]  | 1.92                     | 0.28              |
| 4:2:265:SER:O   | 4:Y:173:HIS:ND1[1_556] | 1.92                     | 0.28              |
| 4:0:119:MET:CE  | 4:X:337:TYR:C[1_556]   | 1.92                     | 0.28              |
| 4:2:185:LEU:O   | 4:Z:191:LYS:CD[1_556]  | 1.92                     | 0.28              |
| 4:2:56:ASP:OD2  | 4:Z:240:TYR:OH[1_556]  | 1.92                     | 0.28              |
| 4:0:362:TYR:O   | 4:X:348:SER:OG[1_556]  | 1.92                     | 0.28              |
| 4:0:206:ARG:N   | 4:X:199:SER:N[1_556]   | 1.92                     | 0.28              |
| 4:2:107:GLU:N   | 4:Z:301:GLY:N[1_556]   | 1.92                     | 0.28              |
| 4:0:11:ASP:CB   | 4:X:305:MET:SD[1_556]  | 1.92                     | 0.28              |
| 4:1:82:MET:O    | 4:Y:30:VAL:CB[1_556]   | 1.92                     | 0.28              |
| 4:0:196:ARG:NH1 | 4:W:114:ALA:C[1_556]   | 1.92                     | 0.28              |
| 4:2:73:HIS:CB   | 4:Z:157:ASP:C[1_556]   | 1.92                     | 0.28              |
| 4:1:32:PRO:CB   | 4:Y:211:ASP:CA[1_556]  | 1.93                     | 0.27              |
| 4:0:153:LEU:CD1 | 4:X:262:PHE:O[1_556]   | 1.93                     | 0.27              |
| 4:1:175:ILE:CG1 | 4:Y:162:ASN:OD1[1_556] | 1.93                     | 0.27              |
| 4:0:135:ALA:N   | 4:X:338:SER:OG[1_556]  | 1.93                     | 0.27              |
| 4:0:79:TRP:CA   | 4:X:17:VAL:CB[1_556]   | 1.93                     | 0.27              |
| 4:1:370:VAL:CG1 | 4:Y:341:ILE:C[1_556]   | 1.93                     | 0.27              |
| 4:3:267:ILE:C   | 4:Z:173:HIS:CA[1_556]  | 1.93                     | 0.27              |
| 4:2:307:PRO:N   | 4:Z:227:MET:CG[1_556]  | 1.93                     | 0.27              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:77:THR:N    | 4:Z:15:GLY:C[1_556]    | 1.93                     | 0.27              |
| 4:0:121:GLN:C   | 4:X:340:TRP:CH2[1_556] | 1.93                     | 0.27              |
| 4:2:183:ARG:CA  | 4:Z:188:TYR:N[1_556]   | 1.93                     | 0.27              |
| 4:2:14:SER:OG   | 4:Z:182:GLY:CA[1_556]  | 1.93                     | 0.27              |
| 4:2:189:LEU:CD2 | 4:Z:195:GLU:CB[1_556]  | 1.93                     | 0.27              |
| 4:0:362:TYR:CB  | 4:X:348:SER:OG[1_556]  | 1.93                     | 0.27              |
| 4:1:149:THR:CG2 | 4:Y:327:ILE:CG1[1_556] | 1.93                     | 0.27              |
| 4:0:177:ARG:N   | 4:X:178:LEU:CD2[1_556] | 1.93                     | 0.27              |
| 4:2:136:ILE:CG2 | 4:Z:299:MET:CA[1_556]  | 1.93                     | 0.27              |
| 4:2:281:SER:OG  | 4:Z:277:THR:C[1_556]   | 1.93                     | 0.27              |
| 4:1:134:VAL:CG1 | 4:Y:338:SER:C[1_556]   | 1.93                     | 0.27              |
| 4:2:120:THR:CA  | 4:Z:340:TRP:CD2[1_556] | 1.93                     | 0.27              |
| 4:2:196:ARG:NH1 | 4:Y:114:ALA:C[1_556]   | 1.93                     | 0.27              |
| 4:1:37:ARG:CZ   | 4:Y:57:GLU:N[1_556]    | 1.93                     | 0.27              |
| 4:0:133:TYR:CE1 | 4:X:144:ALA:O[1_556]   | 1.93                     | 0.27              |
| 4:1:59:GLN:OE1  | 4:Y:208:ILE:CG2[1_556] | 1.93                     | 0.27              |
| 4:0:260:THR:C   | 4:X:266:PHE:CA[1_556]  | 1.93                     | 0.27              |
| 4:2:261:LEU:O   | 4:Z:265:SER:C[1_556]   | 1.93                     | 0.27              |
| 4:0:9:VAL:CG1   | 4:X:333:PRO:CB[1_556]  | 1.93                     | 0.27              |
| 4:2:167:GLU:OE2 | 4:Z:326:LYS:CG[1_556]  | 1.93                     | 0.27              |
| 4:0:63:GLY:N    | 4:V:287:ILE:C[1_556]   | 1.93                     | 0.27              |
| 4:0:116:ARG:CA  | 4:X:339:VAL:O[1_556]   | 1.93                     | 0.27              |
| 4:1:77:THR:N    | 4:Y:15:GLY:C[1_556]    | 1.93                     | 0.27              |
| 4:2:211:ASP:OD1 | 4:Z:249:THR:CG2[1_556] | 1.93                     | 0.27              |
| 4:1:252:ASN:N   | 4:X:114:ALA:N[1_556]   | 1.93                     | 0.27              |
| 4:2:229:THR:O   | 4:Y:369:ILE:N[1_556]   | 1.93                     | 0.27              |
| 4:2:213:LYS:C   | 4:Z:253:GLU:CG[1_556]  | 1.93                     | 0.27              |
| 4:1:250:ILE:CA  | 4:X:114:ALA:CB[1_556]  | 1.93                     | 0.27              |
| 4:0:335:ARG:CD  | 4:X:220:ALA:O[1_556]   | 1.93                     | 0.27              |
| 4:1:305:MET:O   | 4:Y:255:PHE:CG[1_556]  | 1.93                     | 0.27              |
| 4:2:170:ALA:O   | 4:Z:151:ILE:C[1_556]   | 1.93                     | 0.27              |
| 4:0:183:ARG:NE  | 4:X:186:THR:CG2[1_556] | 1.93                     | 0.27              |
| 4:2:183:ARG:NE  | 4:Z:186:THR:CG2[1_556] | 1.93                     | 0.27              |
| 4:0:303:THR:O   | 4:X:256:ARG:O[1_556]   | 1.93                     | 0.27              |
| 4:1:83:GLU:CG   | 4:Y:29:ALA:CA[1_556]   | 1.93                     | 0.27              |
| 4:2:303:THR:O   | 4:Z:256:ARG:O[1_556]   | 1.93                     | 0.27              |
| 4:2:286:ASP:CG  | 4:Z:290:ARG:CZ[1_556]  | 1.93                     | 0.27              |
| 4:2:138:ALA:N   | 4:Z:299:MET:SD[1_556]  | 1.93                     | 0.27              |
| 4:2:196:ARG:NE  | 4:Y:115:ASN:CA[1_556]  | 1.93                     | 0.27              |
| 4:2:211:ASP:CG  | 4:Z:249:THR:N[1_556]   | 1.93                     | 0.27              |
| 4:0:122:ILE:O   | 4:X:26:ALA:O[1_556]    | 1.93                     | 0.27              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:175:ILE:CD1 | 4:Y:162:ASN:CB[1_556]  | 1.93                     | 0.27              |
| 4:1:230:ALA:CA  | 4:X:368:SER:CA[1_556]  | 1.93                     | 0.27              |
| 4:1:149:THR:CA  | 4:Y:327:ILE:CA[1_556]  | 1.93                     | 0.27              |
| 4:2:339:VAL:CG1 | 4:Z:335:ARG:NE[1_556]  | 1.93                     | 0.27              |
| 4:0:294:TYR:N   | 4:X:320:LEU:CB[1_556]  | 1.93                     | 0.27              |
| 4:0:173:HIS:CA  | 4:X:174:ALA:C[1_556]   | 1.93                     | 0.27              |
| 4:1:211:ASP:CG  | 4:Y:249:THR:CA[1_556]  | 1.93                     | 0.27              |
| 4:2:185:LEU:O   | 4:Z:191:LYS:CG[1_556]  | 1.93                     | 0.27              |
| 4:2:179:ASP:OD1 | 4:Z:180:LEU:CA[1_556]  | 1.93                     | 0.27              |
| 4:0:81:ASP:CG   | 4:X:32:PRO:CG[1_556]   | 1.93                     | 0.27              |
| 4:0:305:MET:N   | 4:X:255:PHE:C[1_556]   | 1.93                     | 0.27              |
| 4:0:64:ILE:CB   | 4:V:292:ASP:OD2[1_556] | 1.93                     | 0.27              |
| 4:2:116:ARG:NH1 | 4:Z:142:LEU:N[1_556]   | 1.93                     | 0.27              |
| 4:0:183:ARG:CB  | 4:X:186:THR:CA[1_556]  | 1.93                     | 0.27              |
| 4:2:207:GLU:CD  | 4:Z:242:LEU:CG[1_556]  | 1.93                     | 0.27              |
| 4:1:104:LEU:N   | 4:Y:334:GLU:CG[1_556]  | 1.93                     | 0.27              |
| 4:1:232:SER:CB  | 4:X:366:GLY:O[1_556]   | 1.93                     | 0.27              |
| 4:2:106:THR:N   | 4:Z:334:GLU:O[1_556]   | 1.93                     | 0.27              |
| 4:0:162:ASN:C   | 4:X:274:ILE:CA[1_556]  | 1.93                     | 0.27              |
| 4:0:115:ASN:N   | 4:X:106:THR:CB[1_556]  | 1.93                     | 0.27              |
| 4:0:136:ILE:CG2 | 4:X:299:MET:CA[1_556]  | 1.93                     | 0.27              |
| 4:1:104:LEU:CD1 | 4:Y:333:PRO:CD[1_556]  | 1.93                     | 0.27              |
| 4:2:271:SER:C   | 4:Z:270:GLU:CB[1_556]  | 1.93                     | 0.27              |
| 4:2:115:ASN:O   | 4:Z:11:ASP:CB[1_556]   | 1.93                     | 0.27              |
| 4:2:365:ALA:CA  | 4:Z:349:LEU:O[1_556]   | 1.93                     | 0.27              |
| 4:3:231:ALA:CB  | 4:Z:370:VAL:C[1_556]   | 1.93                     | 0.27              |
| 4:1:72:GLU:OE1  | 4:Y:183:ARG:NH2[1_556] | 1.93                     | 0.27              |
| 4:4:62:ARG:CB   | 4:Z:288:ASP:OD1[1_556] | 1.93                     | 0.27              |
| 4:2:106:THR:C   | 4:Z:336:LYS:N[1_556]   | 1.93                     | 0.27              |
| 4:2:237:GLU:CD  | 4:Y:114:ALA:O[1_556]   | 1.93                     | 0.27              |
| 4:0:274:ILE:CA  | 4:X:264:PRO:CD[1_556]  | 1.93                     | 0.27              |
| 4:3:252:ASN:ND2 | 4:Z:117:GLU:CD[1_556]  | 1.93                     | 0.27              |
| 4:2:252:ASN:CB  | 4:Y:113:LYS:C[1_556]   | 1.93                     | 0.27              |
| 4:1:295:ALA:C   | 4:Y:319:ALA:N[1_556]   | 1.93                     | 0.27              |
| 4:2:213:LYS:CB  | 4:Z:192:ILE:C[1_556]   | 1.93                     | 0.27              |
| 4:1:163:VAL:N   | 4:Y:274:ILE:C[1_556]   | 1.93                     | 0.27              |
| 4:1:164:PRO:CD  | 4:Y:278:THR:OG1[1_556] | 1.93                     | 0.27              |
| 4:2:202:THR:C   | 4:Z:201:VAL:CG2[1_556] | 1.93                     | 0.27              |
| 4:1:80:ASP:N    | 4:Y:31:PHE:CE1[1_556]  | 1.93                     | 0.27              |
| 4:0:180:LEU:N   | 4:X:267:ILE:CD1[1_556] | 1.93                     | 0.27              |
| 4:0:183:ARG:C   | 4:X:188:TYR:CA[1_556]  | 1.93                     | 0.27              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:267:ILE:CA  | 4:X:173:HIS:N[1_556]   | 1.93                     | 0.27              |
| 4:1:108:ALA:N   | 4:Y:301:GLY:N[1_556]   | 1.93                     | 0.27              |
| 4:2:107:GLU:OE2 | 4:Z:300:SER:OG[1_556]  | 1.93                     | 0.27              |
| 4:2:76:ILE:C    | 4:Z:16:LEU:O[1_556]    | 1.93                     | 0.27              |
| 4:1:140:LEU:CB  | 4:Y:331:ALA:CA[1_556]  | 1.93                     | 0.27              |
| 4:2:300:SER:OG  | 4:Z:309:ILE:CB[1_556]  | 1.93                     | 0.27              |
| 4:1:369:ILE:CB  | 4:Y:346:LEU:CA[1_556]  | 1.93                     | 0.27              |
| 4:0:86:TRP:CZ3  | 4:X:27:PRO:CG[1_556]   | 1.93                     | 0.27              |
| 4:0:207:GLU:OE1 | 4:X:242:LEU:CD1[1_556] | 1.93                     | 0.27              |
| 4:3:192:ILE:CB  | 4:Z:110:LEU:O[1_556]   | 1.93                     | 0.27              |
| 4:0:250:ILE:CA  | 4:W:114:ALA:CB[1_556]  | 1.93                     | 0.27              |
| 4:1:339:VAL:O   | 4:Y:335:ARG:NH2[1_556] | 1.93                     | 0.27              |
| 4:2:335:ARG:CD  | 4:Z:220:ALA:O[1_556]   | 1.93                     | 0.27              |
| 4:0:81:ASP:OD1  | 4:X:56:ASP:OD2[1_556]  | 1.93                     | 0.27              |
| 4:2:120:THR:C   | 4:Z:340:TRP:CE3[1_556] | 1.93                     | 0.27              |
| 4:2:82:MET:N    | 4:Z:31:PHE:CA[1_556]   | 1.93                     | 0.27              |
| 4:0:104:LEU:CD2 | 4:X:333:PRO:CA[1_556]  | 1.94                     | 0.26              |
| 4:0:272:ALA:CA  | 4:X:270:GLU:CB[1_556]  | 1.94                     | 0.26              |
| 4:1:367:PRO:O   | 4:Y:343:GLY:C[1_556]   | 1.94                     | 0.26              |
| 4:1:168:GLY:N   | 4:Y:295:ALA:CA[1_556]  | 1.94                     | 0.26              |
| 4:1:124:PHE:C   | 4:Y:24:ASP:OD1[1_556]  | 1.94                     | 0.26              |
| 4:1:40:HIS:N    | 4:W:166:TYR:CE2[1_556] | 1.94                     | 0.26              |
| 4:1:119:MET:C   | 4:Y:340:TRP:CE3[1_556] | 1.94                     | 0.26              |
| 4:1:292:ASP:CB  | 4:Y:321:ALA:CA[1_556]  | 1.94                     | 0.26              |
| 4:1:169:TYR:O   | 4:Y:293:LEU:O[1_556]   | 1.94                     | 0.26              |
| 4:2:121:GLN:C   | 4:Z:340:TRP:CH2[1_556] | 1.94                     | 0.26              |
| 4:0:213:LYS:CB  | 4:X:192:ILE:C[1_556]   | 1.94                     | 0.26              |
| 4:1:168:GLY:O   | 4:Y:296:ASN:O[1_556]   | 1.94                     | 0.26              |
| 4:1:79:TRP:O    | 4:Y:31:PHE:CD1[1_556]  | 1.94                     | 0.26              |
| 4:1:192:ILE:CA  | 4:X:110:LEU:C[1_556]   | 1.94                     | 0.26              |
| 4:1:162:ASN:ND2 | 4:Y:273:GLY:CA[1_556]  | 1.94                     | 0.26              |
| 4:2:305:MET:O   | 4:Z:255:PHE:CG[1_556]  | 1.94                     | 0.26              |
| 4:0:168:GLY:CA  | 4:X:295:ALA:C[1_556]   | 1.94                     | 0.26              |
| 4:2:267:ILE:CA  | 4:Y:173:HIS:N[1_556]   | 1.94                     | 0.26              |
| 4:1:120:THR:N   | 4:Y:340:TRP:CB[1_556]  | 1.94                     | 0.26              |
| 4:1:31:PHE:CA   | 4:Y:215:LYS:NZ[1_556]  | 1.94                     | 0.26              |
| 4:2:150:GLY:C   | 4:Z:317:ILE:CA[1_556]  | 1.94                     | 0.26              |
| 4:1:107:GLU:OE2 | 4:Y:141:SER:CB[1_556]  | 1.94                     | 0.26              |
| 4:0:286:ASP:CG  | 4:X:290:ARG:CZ[1_556]  | 1.94                     | 0.26              |
| 4:0:335:ARG:NE  | 4:X:220:ALA:CA[1_556]  | 1.94                     | 0.26              |
| 4:0:207:GLU:CD  | 4:X:242:LEU:CG[1_556]  | 1.94                     | 0.26              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:172:PRO:CD  | 4:X:164:PRO:CG[1_556]  | 1.94                     | 0.26              |
| 4:1:126:THR:CG2 | 4:Y:28:ARG:CG[1_556]   | 1.94                     | 0.26              |
| 4:1:282:ILE:C   | 4:Y:280:ASN:ND2[1_556] | 1.94                     | 0.26              |
| 4:2:233:SER:CA  | 4:Y:367:PRO:CG[1_556]  | 1.94                     | 0.26              |
| 4:2:168:GLY:CA  | 4:Z:295:ALA:C[1_556]   | 1.94                     | 0.26              |
| 4:2:72:GLU:CG   | 4:Z:157:ASP:OD2[1_556] | 1.94                     | 0.26              |
| 4:1:180:LEU:CD2 | 4:Y:267:ILE:O[1_556]   | 1.94                     | 0.26              |
| 4:3:252:ASN:N   | 4:Z:114:ALA:N[1_556]   | 1.94                     | 0.26              |
| 4:2:73:HIS:NE2  | 4:Z:184:ASP:OD1[1_556] | 1.94                     | 0.26              |
| 4:2:81:ASP:OD1  | 4:Z:56:ASP:OD2[1_556]  | 1.94                     | 0.26              |
| 4:0:167:GLU:OE2 | 4:X:326:LYS:CG[1_556]  | 1.94                     | 0.26              |
| 4:0:115:ASN:O   | 4:X:11:ASP:CB[1_556]   | 1.94                     | 0.26              |
| 4:0:182:GLY:O   | 4:X:188:TYR:O[1_556]   | 1.94                     | 0.26              |
| 4:2:267:ILE:CB  | 4:Y:173:HIS:CA[1_556]  | 1.94                     | 0.26              |
| 4:2:158:GLY:CA  | 4:Z:185:LEU:N[1_556]   | 1.94                     | 0.26              |
| 4:2:286:ASP:N   | 4:Z:283:MET:N[1_556]   | 1.94                     | 0.26              |
| 4:0:167:GLU:OE2 | 4:X:326:LYS:O[1_556]   | 1.94                     | 0.26              |
| 4:1:192:ILE:CB  | 4:X:110:LEU:O[1_556]   | 1.94                     | 0.26              |
| 4:2:206:ARG:N   | 4:Z:199:SER:N[1_556]   | 1.94                     | 0.26              |
| 4:0:107:GLU:CD  | 4:X:300:SER:OG[1_556]  | 1.94                     | 0.26              |
| 4:2:370:VAL:CG1 | 4:Z:343:GLY:N[1_556]   | 1.94                     | 0.26              |
| 4:3:252:ASN:O   | 4:Z:113:LYS:CB[1_556]  | 1.94                     | 0.26              |
| 4:0:59:GLN:NE2  | 4:X:207:GLU:C[1_556]   | 1.94                     | 0.26              |
| 4:0:265:SER:O   | 4:W:173:HIS:ND1[1_556] | 1.94                     | 0.26              |
| 4:2:86:TRP:NE1  | 4:Z:337:TYR:CE2[1_556] | 1.94                     | 0.26              |
| 4:1:372:ARG:NH1 | 4:Y:145:SER:CB[1_556]  | 1.94                     | 0.26              |
| 4:1:149:THR:C   | 4:Y:327:ILE:CB[1_556]  | 1.94                     | 0.26              |
| 4:0:72:GLU:CG   | 4:X:157:ASP:OD2[1_556] | 1.94                     | 0.26              |
| 4:0:370:VAL:CG1 | 4:X:343:GLY:N[1_556]   | 1.94                     | 0.26              |
| 4:1:176:MET:O   | 4:Y:178:LEU:CD2[1_556] | 1.94                     | 0.26              |
| 4:2:79:TRP:CH2  | 4:Z:18:LYS:CE[1_556]   | 1.94                     | 0.26              |
| 4:2:165:ILE:CB  | 4:Z:297:ASN:CB[1_556]  | 1.94                     | 0.26              |
| 4:1:113:LYS:N   | 4:Y:137:GLN:CB[1_556]  | 1.94                     | 0.26              |
| 4:1:293:LEU:CD2 | 4:Y:279:TYR:CG[1_556]  | 1.94                     | 0.26              |
| 4:0:106:THR:C   | 4:X:336:LYS:N[1_556]   | 1.94                     | 0.26              |
| 4:0:37:ARG:CG   | 4:X:60:SER:CB[1_556]   | 1.94                     | 0.26              |
| 4:0:185:LEU:O   | 4:X:191:LYS:CG[1_556]  | 1.94                     | 0.26              |
| 4:3:266:PHE:CB  | 4:Z:172:PRO:CG[1_556]  | 1.94                     | 0.26              |
| 4:2:209:VAL:O   | 4:Z:193:LEU:CA[1_556]  | 1.94                     | 0.26              |
| 4:1:209:VAL:CG1 | 4:Y:194:THR:CG2[1_556] | 1.94                     | 0.26              |
| 4:1:212:ILE:N   | 4:Y:196:ARG:CD[1_556]  | 1.94                     | 0.26              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:296:ASN:N   | 4:X:319:ALA:CA[1_556]  | 1.94                     | 0.26              |
| 4:2:272:ALA:CA  | 4:Z:270:GLU:CB[1_556]  | 1.94                     | 0.26              |
| 4:2:122:ILE:O   | 4:Z:26:ALA:O[1_556]    | 1.94                     | 0.26              |
| 4:1:109:PRO:O   | 4:Y:154:ASP:CB[1_556]  | 1.94                     | 0.26              |
| 4:2:79:TRP:CE3  | 4:Z:18:LYS:CB[1_556]   | 1.94                     | 0.26              |
| 4:2:177:ARG:N   | 4:Z:178:LEU:CD2[1_556] | 1.94                     | 0.26              |
| 4:1:252:ASN:ND2 | 4:X:117:GLU:CD[1_556]  | 1.94                     | 0.26              |
| 4:2:293:LEU:CB  | 4:Z:320:LEU:CB[1_556]  | 1.94                     | 0.26              |
| 4:2:306:TYR:O   | 4:Z:227:MET:CG[1_556]  | 1.94                     | 0.26              |
| 4:0:136:ILE:CB  | 4:X:299:MET:N[1_556]   | 1.94                     | 0.26              |
| 4:2:207:GLU:OE1 | 4:Z:242:LEU:CD1[1_556] | 1.94                     | 0.26              |
| 4:0:290:ARG:CA  | 4:X:320:LEU:O[1_556]   | 1.94                     | 0.26              |
| 4:2:109:PRO:O   | 4:Z:154:ASP:CB[1_556]  | 1.94                     | 0.26              |
| 4:0:237:GLU:CD  | 4:W:114:ALA:O[1_556]   | 1.94                     | 0.26              |
| 4:0:79:TRP:N    | 4:X:17:VAL:N[1_556]    | 1.94                     | 0.26              |
| 4:1:233:SER:O   | 4:X:367:PRO:N[1_556]   | 1.94                     | 0.26              |
| 4:1:285:CYS:SG  | 4:Y:279:TYR:CA[1_556]  | 1.94                     | 0.26              |
| 4:2:369:ILE:CB  | 4:Z:345:ILE:O[1_556]   | 1.94                     | 0.26              |
| 4:1:186:THR:N   | 4:Y:192:ILE:N[1_556]   | 1.94                     | 0.26              |
| 4:2:167:GLU:OE2 | 4:Z:326:LYS:O[1_556]   | 1.94                     | 0.26              |
| 4:0:79:TRP:CE3  | 4:X:18:LYS:CB[1_556]   | 1.94                     | 0.26              |
| 4:1:267:ILE:C   | 4:X:173:HIS:CA[1_556]  | 1.94                     | 0.26              |
| 4:4:63:GLY:O    | 4:Z:289:ILE:CB[1_556]  | 1.94                     | 0.26              |
| 4:2:162:ASN:C   | 4:Z:274:ILE:CA[1_556]  | 1.94                     | 0.26              |
| 4:0:82:MET:N    | 4:X:31:PHE:CA[1_556]   | 1.94                     | 0.26              |
| 4:2:166:TYR:CE1 | 4:Z:294:TYR:CD2[1_556] | 1.94                     | 0.26              |
| 4:2:181:ALA:CB  | 4:Z:185:LEU:CG[1_556]  | 1.94                     | 0.26              |
| 4:0:267:ILE:CG1 | 4:W:173:HIS:CB[1_556]  | 1.94                     | 0.26              |
| 4:1:232:SER:N   | 4:X:369:ILE:N[1_556]   | 1.94                     | 0.26              |
| 4:0:120:THR:N   | 4:X:340:TRP:CB[1_556]  | 1.94                     | 0.26              |
| 4:0:339:VAL:CG1 | 4:X:335:ARG:NE[1_556]  | 1.94                     | 0.26              |
| 4:0:170:ALA:O   | 4:X:151:ILE:C[1_556]   | 1.94                     | 0.26              |
| 4:2:172:PRO:CD  | 4:Z:164:PRO:CG[1_556]  | 1.94                     | 0.26              |
| 4:2:362:TYR:O   | 4:Z:348:SER:OG[1_556]  | 1.94                     | 0.26              |
| 4:1:172:PRO:C   | 4:Y:162:ASN:O[1_556]   | 1.94                     | 0.26              |
| 4:1:126:THR:CA  | 4:Y:28:ARG:CG[1_556]   | 1.94                     | 0.26              |
| 4:0:233:SER:CA  | 4:W:367:PRO:CG[1_556]  | 1.94                     | 0.26              |
| 4:0:211:ASP:CG  | 4:X:249:THR:N[1_556]   | 1.94                     | 0.26              |
| 4:2:80:ASP:N    | 4:Z:31:PHE:CE1[1_556]  | 1.94                     | 0.26              |
| 4:3:232:SER:CB  | 4:Z:366:GLY:O[1_556]   | 1.94                     | 0.26              |
| 4:2:82:MET:N    | 4:Z:30:VAL:O[1_556]    | 1.94                     | 0.26              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:281:SER:OG  | 4:Y:277:THR:C[1_556]   | 1.94                     | 0.26              |
| 4:0:202:THR:C   | 4:X:201:VAL:CG2[1_556] | 1.94                     | 0.26              |
| 4:1:214:GLU:CB  | 4:Y:250:ILE:CG2[1_556] | 1.94                     | 0.26              |
| 4:1:155:SER:N   | 4:Y:261:LEU:CD1[1_556] | 1.94                     | 0.26              |
| 4:1:155:SER:C   | 4:Y:258:PRO:CA[1_556]  | 1.94                     | 0.26              |
| 4:1:123:MET:CA  | 4:Y:26:ALA:CA[1_556]   | 1.94                     | 0.26              |
| 4:1:59:GLN:CG   | 4:Y:208:ILE:CG2[1_556] | 1.94                     | 0.26              |
| 4:2:158:GLY:C   | 4:Z:181:ALA:C[1_556]   | 1.94                     | 0.26              |
| 4:0:166:TYR:CE1 | 4:X:294:TYR:CD2[1_556] | 1.94                     | 0.26              |
| 4:0:62:ARG:C    | 4:V:288:ASP:N[1_556]   | 1.94                     | 0.26              |
| 4:1:180:LEU:O   | 4:Y:260:THR:CG2[1_556] | 1.94                     | 0.26              |
| 4:0:40:HIS:CG   | 4:V:166:TYR:CD1[1_556] | 1.94                     | 0.26              |
| 4:1:158:GLY:C   | 4:Y:181:ALA:C[1_556]   | 1.95                     | 0.25              |
| 4:0:252:ASN:CB  | 4:W:113:LYS:C[1_556]   | 1.95                     | 0.25              |
| 4:0:110:LEU:N   | 4:X:154:ASP:O[1_556]   | 1.95                     | 0.25              |
| 4:1:252:ASN:CB  | 4:X:113:LYS:C[1_556]   | 1.95                     | 0.25              |
| 4:2:59:GLN:NE2  | 4:Z:207:GLU:C[1_556]   | 1.95                     | 0.25              |
| 4:1:252:ASN:O   | 4:X:113:LYS:CB[1_556]  | 1.95                     | 0.25              |
| 4:2:305:MET:O   | 4:Z:255:PHE:CD2[1_556] | 1.95                     | 0.25              |
| 4:1:116:ARG:CZ  | 4:Y:141:SER:N[1_556]   | 1.95                     | 0.25              |
| 4:2:197:GLY:N   | 4:Y:75:ILE:CB[1_556]   | 1.95                     | 0.25              |
| 4:2:104:LEU:CD2 | 4:Z:333:PRO:CA[1_556]  | 1.95                     | 0.25              |
| 4:0:186:THR:CB  | 4:X:190:MET:O[1_556]   | 1.95                     | 0.25              |
| 4:2:81:ASP:CG   | 4:Z:32:PRO:CG[1_556]   | 1.95                     | 0.25              |
| 4:1:215:LYS:CA  | 4:Y:196:ARG:NH1[1_556] | 1.95                     | 0.25              |
| 4:1:9:VAL:CG1   | 4:Y:333:PRO:CB[1_556]  | 1.95                     | 0.25              |
| 4:1:137:GLN:CB  | 4:Y:304:THR:CG2[1_556] | 1.95                     | 0.25              |
| 4:1:166:TYR:CE2 | 4:Y:291:LYS:CA[1_556]  | 1.95                     | 0.25              |
| 4:2:290:ARG:CA  | 4:Z:320:LEU:O[1_556]   | 1.95                     | 0.25              |
| 4:0:162:ASN:CA  | 4:X:275:HIS:N[1_556]   | 1.95                     | 0.25              |
| 4:2:213:LYS:NZ  | 4:Z:189:LEU:CD1[1_556] | 1.95                     | 0.25              |
| 4:1:123:MET:CE  | 4:Y:27:PRO:CD[1_556]   | 1.95                     | 0.25              |
| 4:2:153:LEU:CD1 | 4:Z:262:PHE:O[1_556]   | 1.95                     | 0.25              |
| 4:1:171:LEU:O   | 4:Y:281:SER:OG[1_556]  | 1.95                     | 0.25              |
| 4:0:209:VAL:N   | 4:X:198:TYR:CD2[1_556] | 1.95                     | 0.25              |
| 4:1:180:LEU:N   | 4:Y:267:ILE:CD1[1_556] | 1.95                     | 0.25              |
| 4:0:177:ARG:CB  | 4:X:178:LEU:C[1_556]   | 1.95                     | 0.25              |
| 4:0:170:ALA:N   | 4:X:151:ILE:CG2[1_556] | 1.95                     | 0.25              |
| 4:1:76:ILE:CG2  | 4:Y:16:LEU:O[1_556]    | 1.95                     | 0.25              |
| 4:1:183:ARG:CB  | 4:Y:187:ASP:CA[1_556]  | 1.95                     | 0.25              |
| 4:1:160:THR:CA  | 4:Y:180:LEU:CD1[1_556] | 1.95                     | 0.25              |

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| Atom-1         | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|------------------------|--------------------------|-------------------|
| 4:0:73:HIS:CB  | 4:X:157:ASP:C[1_556]   | 1.95                     | 0.25              |
| 4:1:291:LYS:CE | 4:Y:322:PRO:C[1_556]   | 1.95                     | 0.25              |
| 4:2:136:ILE:CB | 4:Z:299:MET:N[1_556]   | 1.95                     | 0.25              |
| 4:1:73:HIS:C   | 4:Y:157:ASP:CA[1_556]  | 1.95                     | 0.25              |
| 4:2:186:THR:CB | 4:Z:190:MET:O[1_556]   | 1.95                     | 0.25              |
| 4:1:233:SER:CA | 4:X:367:PRO:C[1_556]   | 1.95                     | 0.25              |
| 4:1:81:ASP:CB  | 4:Y:32:PRO:N[1_556]    | 1.95                     | 0.25              |
| 4:1:166:TYR:C  | 4:Y:294:TYR:N[1_556]   | 1.95                     | 0.25              |
| 4:2:177:ARG:CB | 4:Z:178:LEU:C[1_556]   | 1.95                     | 0.25              |
| 4:0:86:TRP:NE1 | 4:X:337:TYR:CE2[1_556] | 1.95                     | 0.25              |
| 4:2:301:GLY:C  | 4:Z:258:PRO:CG[1_556]  | 1.95                     | 0.25              |
| 4:0:281:SER:OG | 4:X:277:THR:C[1_556]   | 1.95                     | 0.25              |
| 4:2:209:VAL:N  | 4:Z:198:TYR:CD2[1_556] | 1.95                     | 0.25              |
| 4:1:71:ILE:O   | 4:Y:157:ASP:CG[1_556]  | 1.95                     | 0.25              |
| 4:0:365:ALA:CB | 4:X:349:LEU:CG[1_556]  | 1.95                     | 0.25              |
| 4:1:372:ARG:CG | 4:Y:147:ARG:O[1_556]   | 1.95                     | 0.25              |
| 4:2:231:ALA:N  | 4:Y:371:HIS:N[1_556]   | 1.95                     | 0.25              |
| 4:1:207:GLU:CA | 4:Y:200:PHE:CD1[1_556] | 1.95                     | 0.25              |
| 4:1:362:TYR:O  | 4:Y:348:SER:N[1_556]   | 1.95                     | 0.25              |
| 4:2:183:ARG:C  | 4:Z:188:TYR:CA[1_556]  | 1.95                     | 0.25              |
| 4:2:63:GLY:N   | 4:X:287:ILE:C[1_556]   | 1.95                     | 0.25              |
| 4:1:123:MET:O  | 4:Y:26:ALA:O[1_556]    | 1.95                     | 0.25              |
| 4:1:63:GLY:O   | 4:W:289:ILE:CB[1_556]  | 1.95                     | 0.25              |
| 4:1:284:LYS:N  | 4:Y:280:ASN:ND2[1_556] | 1.95                     | 0.25              |
| 4:0:122:ILE:CA | 4:X:19:ALA:O[1_556]    | 1.95                     | 0.25              |
| 4:1:209:VAL:CB | 4:Y:194:THR:C[1_556]   | 1.95                     | 0.25              |
| 4:2:62:ARG:CB  | 4:X:288:ASP:OD1[1_556] | 1.95                     | 0.25              |
| 4:0:182:GLY:C  | 4:X:189:LEU:CA[1_556]  | 1.95                     | 0.25              |
| 4:0:365:ALA:CA | 4:X:349:LEU:O[1_556]   | 1.95                     | 0.25              |
| 4:2:297:ASN:C  | 4:Z:316:GLU:CG[1_556]  | 1.95                     | 0.25              |
| 4:1:272:ALA:O  | 4:Y:270:GLU:N[1_556]   | 1.95                     | 0.25              |
| 4:1:30:VAL:CG1 | 4:Y:215:LYS:CB[1_556]  | 1.95                     | 0.25              |
| 4:0:296:ASN:O  | 4:X:315:LYS:C[1_556]   | 1.95                     | 0.25              |
| 4:0:104:LEU:CA | 4:X:334:GLU:CD[1_556]  | 1.95                     | 0.25              |
| 4:1:367:PRO:CB | 4:Y:343:GLY:O[1_556]   | 1.95                     | 0.25              |
| 4:2:104:LEU:CA | 4:Z:334:GLU:CD[1_556]  | 1.95                     | 0.25              |
| 4:0:213:LYS:C  | 4:X:253:GLU:CG[1_556]  | 1.95                     | 0.25              |
| 4:2:296:ASN:N  | 4:Z:319:ALA:CA[1_556]  | 1.95                     | 0.25              |
| 4:0:286:ASP:N  | 4:X:283:MET:N[1_556]   | 1.95                     | 0.25              |
| 4:0:69:TYR:CE2 | 4:X:210:ARG:CB[1_556]  | 1.95                     | 0.25              |
| 4:0:109:PRO:O  | 4:X:154:ASP:CB[1_556]  | 1.95                     | 0.25              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:112:PRO:C   | 4:Y:137:GLN:CD[1_556]  | 1.95                     | 0.25              |
| 4:2:140:LEU:CB  | 4:Z:331:ALA:CA[1_556]  | 1.95                     | 0.25              |
| 4:3:233:SER:O   | 4:Z:367:PRO:N[1_556]   | 1.95                     | 0.25              |
| 4:0:371:HIS:O   | 4:X:140:LEU:N[1_556]   | 1.95                     | 0.25              |
| 4:0:224:GLU:OE2 | 4:Y:41:GLN:CG[1_556]   | 1.95                     | 0.25              |
| 4:2:122:ILE:CA  | 4:Z:19:ALA:O[1_556]    | 1.95                     | 0.25              |
| 4:0:59:GLN:CG   | 4:X:208:ILE:CG2[1_556] | 1.95                     | 0.25              |
| 4:1:161:HIS:NE2 | 4:Y:160:THR:CA[1_556]  | 1.95                     | 0.25              |
| 4:2:206:ARG:CB  | 4:Z:199:SER:O[1_556]   | 1.95                     | 0.25              |
| 4:0:277:THR:CG2 | 4:X:272:ALA:CA[1_556]  | 1.95                     | 0.25              |
| 4:2:63:GLY:O    | 4:X:289:ILE:CB[1_556]  | 1.95                     | 0.25              |
| 4:0:206:ARG:CB  | 4:X:199:SER:O[1_556]   | 1.95                     | 0.25              |
| 4:2:172:PRO:C   | 4:Z:162:ASN:O[1_556]   | 1.95                     | 0.25              |
| 4:1:173:HIS:CG  | 4:Y:174:ALA:O[1_556]   | 1.95                     | 0.25              |
| 4:1:218:TYR:OH  | 4:Y:231:ALA:CA[1_556]  | 1.95                     | 0.25              |
| 4:1:330:ILE:CD1 | 4:Y:315:LYS:CG[1_556]  | 1.95                     | 0.25              |
| 4:3:232:SER:N   | 4:Z:369:ILE:N[1_556]   | 1.95                     | 0.25              |
| 4:0:301:GLY:C   | 4:X:258:PRO:CG[1_556]  | 1.95                     | 0.25              |
| 4:1:372:ARG:NE  | 4:Y:143:TYR:CA[1_556]  | 1.95                     | 0.25              |
| 4:0:106:THR:N   | 4:X:334:GLU:O[1_556]   | 1.95                     | 0.25              |
| 4:1:126:THR:OG1 | 4:Y:28:ARG:N[1_556]    | 1.95                     | 0.25              |
| 4:1:266:PHE:CB  | 4:X:172:PRO:CG[1_556]  | 1.95                     | 0.25              |
| 4:0:176:MET:CB  | 4:X:277:THR:OG1[1_556] | 1.95                     | 0.25              |
| 4:2:79:TRP:CZ3  | 4:Z:18:LYS:CA[1_556]   | 1.95                     | 0.25              |
| 4:1:115:ASN:O   | 4:Y:11:ASP:OD2[1_556]  | 1.95                     | 0.25              |
| 4:2:182:GLY:C   | 4:Z:189:LEU:CA[1_556]  | 1.95                     | 0.25              |
| 4:1:81:ASP:C    | 4:Y:31:PHE:CA[1_556]   | 1.95                     | 0.25              |
| 4:1:83:GLU:CD   | 4:Y:29:ALA:CB[1_556]   | 1.95                     | 0.25              |
| 4:2:180:LEU:N   | 4:Z:267:ILE:CD1[1_556] | 1.95                     | 0.25              |
| 4:2:250:ILE:CA  | 4:Y:114:ALA:CB[1_556]  | 1.95                     | 0.25              |
| 4:0:336:LYS:CA  | 4:X:218:TYR:CB[1_556]  | 1.95                     | 0.25              |
| 4:2:182:GLY:O   | 4:Z:188:TYR:O[1_556]   | 1.95                     | 0.25              |
| 4:1:82:MET:C    | 4:Y:30:VAL:CG1[1_556]  | 1.95                     | 0.25              |
| 4:0:297:ASN:C   | 4:X:316:GLU:CG[1_556]  | 1.96                     | 0.24              |
| 4:2:79:TRP:N    | 4:Z:17:VAL:N[1_556]    | 1.96                     | 0.24              |
| 4:0:120:THR:CA  | 4:X:340:TRP:O[1_556]   | 1.96                     | 0.24              |
| 4:2:35:VAL:CG1  | 4:Z:56:ASP:OD2[1_556]  | 1.96                     | 0.24              |
| 4:0:300:SER:OG  | 4:X:309:ILE:CB[1_556]  | 1.96                     | 0.24              |
| 4:0:231:ALA:CA  | 4:W:370:VAL:CA[1_556]  | 1.96                     | 0.24              |
| 4:0:209:VAL:O   | 4:X:193:LEU:CA[1_556]  | 1.96                     | 0.24              |
| 4:3:252:ASN:CB  | 4:Z:113:LYS:C[1_556]   | 1.96                     | 0.24              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:369:ILE:CB  | 4:Y:345:ILE:O[1_556]   | 1.96                     | 0.24              |
| 4:1:117:GLU:CB  | 4:Y:104:LEU:CD2[1_556] | 1.96                     | 0.24              |
| 4:2:365:ALA:CB  | 4:Z:349:LEU:CG[1_556]  | 1.96                     | 0.24              |
| 4:2:231:ALA:CB  | 4:Y:370:VAL:C[1_556]   | 1.96                     | 0.24              |
| 4:3:270:GLU:CG  | 4:Z:286:ASP:N[1_556]   | 1.96                     | 0.24              |
| 4:1:298:VAL:N   | 4:Y:316:GLU:CB[1_556]  | 1.96                     | 0.24              |
| 4:0:231:ALA:N   | 4:W:371:HIS:N[1_556]   | 1.96                     | 0.24              |
| 4:1:206:ARG:CD  | 4:Y:200:PHE:C[1_556]   | 1.96                     | 0.24              |
| 4:0:76:ILE:C    | 4:X:16:LEU:O[1_556]    | 1.96                     | 0.24              |
| 4:1:157:ASP:N   | 4:Y:306:TYR:OH[1_556]  | 1.96                     | 0.24              |
| 4:1:64:ILE:CB   | 4:W:292:ASP:OD2[1_556] | 1.96                     | 0.24              |
| 4:0:116:ARG:CD  | 4:X:141:SER:CA[1_556]  | 1.96                     | 0.24              |
| 4:1:210:ARG:N   | 4:Y:193:LEU:CA[1_556]  | 1.96                     | 0.24              |
| 4:2:37:ARG:CG   | 4:Z:60:SER:CB[1_556]   | 1.96                     | 0.24              |
| 4:1:72:GLU:CG   | 4:Y:183:ARG:NE[1_556]  | 1.96                     | 0.24              |
| 4:2:168:GLY:O   | 4:Z:296:ASN:CA[1_556]  | 1.96                     | 0.24              |
| 4:2:267:ILE:CG1 | 4:Y:173:HIS:CB[1_556]  | 1.96                     | 0.24              |
| 4:1:309:ILE:CG2 | 4:Y:259:GLU:OE2[1_556] | 1.96                     | 0.24              |
| 4:0:126:THR:OG1 | 4:X:28:ARG:N[1_556]    | 1.96                     | 0.24              |
| 4:2:229:THR:C   | 4:Y:368:SER:O[1_556]   | 1.96                     | 0.24              |
| 4:2:189:LEU:CD2 | 4:Z:196:ARG:N[1_556]   | 1.96                     | 0.24              |
| 4:2:176:MET:CB  | 4:Z:277:THR:OG1[1_556] | 1.96                     | 0.24              |
| 4:0:231:ALA:C   | 4:W:369:ILE:CG2[1_556] | 1.96                     | 0.24              |
| 4:0:84:LYS:CE   | 4:X:56:ASP:OD1[1_556]  | 1.96                     | 0.24              |
| 4:2:68:LYS:CD   | 4:Z:59:GLN:N[1_556]    | 1.96                     | 0.24              |
| 4:0:307:PRO:CB  | 4:X:227:MET:O[1_556]   | 1.96                     | 0.24              |
| 4:0:305:MET:O   | 4:X:255:PHE:CG[1_556]  | 1.96                     | 0.24              |
| 4:1:277:THR:O   | 4:Y:272:ALA:CB[1_556]  | 1.96                     | 0.24              |
| 4:1:79:TRP:NE1  | 4:Y:11:ASP:O[1_556]    | 1.96                     | 0.24              |
| 4:1:73:HIS:C    | 4:Y:157:ASP:C[1_556]   | 1.96                     | 0.24              |
| 4:1:306:TYR:O   | 4:Y:227:MET:CG[1_556]  | 1.96                     | 0.24              |
| 4:0:181:ALA:CB  | 4:X:185:LEU:CG[1_556]  | 1.96                     | 0.24              |
| 4:2:110:LEU:N   | 4:Z:154:ASP:O[1_556]   | 1.96                     | 0.24              |
| 4:2:371:HIS:O   | 4:Z:140:LEU:N[1_556]   | 1.96                     | 0.24              |
| 4:1:107:GLU:OE2 | 4:Y:300:SER:OG[1_556]  | 1.96                     | 0.24              |
| 4:1:167:GLU:CA  | 4:Y:294:TYR:C[1_556]   | 1.96                     | 0.24              |
| 4:0:189:LEU:CD2 | 4:X:196:ARG:N[1_556]   | 1.96                     | 0.24              |
| 4:0:168:GLY:O   | 4:X:296:ASN:CA[1_556]  | 1.96                     | 0.24              |
| 4:1:60:SER:CB   | 4:Y:243:PRO:CB[1_556]  | 1.96                     | 0.24              |
| 4:1:183:ARG:C   | 4:Y:188:TYR:CA[1_556]  | 1.96                     | 0.24              |
| 4:2:170:ALA:N   | 4:Z:151:ILE:CG2[1_556] | 1.96                     | 0.24              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:107:GLU:CD  | 4:Z:300:SER:OG[1_556]  | 1.96                     | 0.24              |
| 4:0:16:LEU:CD1  | 4:X:215:LYS:N[1_556]   | 1.96                     | 0.24              |
| 4:1:177:ARG:NH2 | 4:Y:159:VAL:CA[1_556]  | 1.96                     | 0.24              |
| 4:1:37:ARG:CG   | 4:Y:60:SER:CB[1_556]   | 1.96                     | 0.24              |
| 4:1:311:ASP:OD1 | 4:Y:224:GLU:OE2[1_556] | 1.96                     | 0.24              |
| 4:1:183:ARG:CG  | 4:Y:186:THR:O[1_556]   | 1.96                     | 0.24              |
| 4:3:63:GLY:O    | 4:Y:289:ILE:CB[1_556]  | 1.96                     | 0.24              |
| 4:2:296:ASN:O   | 4:Z:315:LYS:C[1_556]   | 1.96                     | 0.24              |
| 4:2:62:ARG:C    | 4:X:288:ASP:N[1_556]   | 1.96                     | 0.24              |
| 4:0:229:THR:C   | 4:W:368:SER:O[1_556]   | 1.96                     | 0.24              |
| 4:0:158:GLY:C   | 4:X:181:ALA:C[1_556]   | 1.96                     | 0.24              |
| 4:2:16:LEU:CD1  | 4:Z:215:LYS:N[1_556]   | 1.96                     | 0.24              |
| 4:1:76:ILE:C    | 4:Y:16:LEU:O[1_556]    | 1.96                     | 0.24              |
| 4:2:73:HIS:C    | 4:Z:157:ASP:CA[1_556]  | 1.96                     | 0.24              |
| 4:2:306:TYR:CE2 | 4:Z:256:ARG:CA[1_556]  | 1.96                     | 0.24              |
| 4:0:369:ILE:CB  | 4:X:345:ILE:O[1_556]   | 1.96                     | 0.24              |
| 4:3:233:SER:CA  | 4:Z:367:PRO:C[1_556]   | 1.96                     | 0.24              |
| 4:1:281:SER:C   | 4:Y:280:ASN:ND2[1_556] | 1.96                     | 0.24              |
| 4:1:173:HIS:C   | 4:Y:281:SER:OG[1_556]  | 1.96                     | 0.24              |
| 4:1:168:GLY:CA  | 4:Y:295:ALA:C[1_556]   | 1.96                     | 0.24              |
| 4:2:231:ALA:CA  | 4:Y:370:VAL:CA[1_556]  | 1.96                     | 0.24              |
| 4:1:118:LYS:CE  | 4:Y:10:CYS:SG[1_556]   | 1.96                     | 0.24              |
| 4:0:62:ARG:CB   | 4:V:288:ASP:OD1[1_556] | 1.96                     | 0.24              |
| 4:3:40:HIS:ND1  | 4:Y:166:TYR:CE1[1_556] | 1.96                     | 0.24              |
| 4:2:285:CYS:C   | 4:Z:283:MET:N[1_556]   | 1.96                     | 0.24              |
| 4:2:162:ASN:CA  | 4:Z:275:HIS:N[1_556]   | 1.96                     | 0.24              |
| 4:2:69:TYR:CE2  | 4:Z:210:ARG:CB[1_556]  | 1.96                     | 0.24              |
| 4:1:173:HIS:CA  | 4:Y:281:SER:OG[1_556]  | 1.96                     | 0.24              |
| 4:1:303:THR:CG2 | 4:Y:257:CYS:C[1_556]   | 1.96                     | 0.24              |
| 4:1:194:THR:CB  | 4:X:177:ARG:CZ[1_556]  | 1.96                     | 0.24              |
| 4:1:265:SER:O   | 4:X:173:HIS:NE2[1_556] | 1.96                     | 0.24              |
| 4:2:279:TYR:O   | 4:Z:276:GLU:OE1[1_556] | 1.96                     | 0.24              |
| 4:0:115:ASN:O   | 4:X:11:ASP:CG[1_556]   | 1.96                     | 0.24              |
| 4:0:115:ASN:O   | 4:X:11:ASP:OD2[1_556]  | 1.96                     | 0.24              |
| 4:2:258:PRO:CG  | 4:Z:256:ARG:NH1[1_556] | 1.96                     | 0.24              |
| 4:1:302:GLY:CA  | 4:Y:258:PRO:CD[1_556]  | 1.96                     | 0.24              |
| 4:1:135:ALA:CB  | 4:Y:332:PRO:CG[1_556]  | 1.96                     | 0.24              |
| 4:0:165:ILE:CB  | 4:X:297:ASN:CB[1_556]  | 1.96                     | 0.24              |
| 4:1:165:ILE:CB  | 4:Y:297:ASN:CB[1_556]  | 1.96                     | 0.24              |
| 4:1:40:HIS:ND1  | 4:W:166:TYR:CE1[1_556] | 1.96                     | 0.24              |
| 4:2:299:MET:N   | 4:Z:312:ARG:CA[1_556]  | 1.96                     | 0.24              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:292:ASP:OD2 | 4:X:322:PRO:O[1_556]   | 1.96                     | 0.24              |
| 4:0:82:MET:N    | 4:X:30:VAL:O[1_556]    | 1.96                     | 0.24              |
| 4:0:189:LEU:CG  | 4:X:195:GLU:C[1_556]   | 1.96                     | 0.24              |
| 4:2:266:PHE:N   | 4:Y:173:HIS:CE1[1_556] | 1.96                     | 0.24              |
| 4:0:174:ALA:CA  | 4:X:277:THR:O[1_556]   | 1.96                     | 0.24              |
| 4:1:213:LYS:C   | 4:Y:253:GLU:CG[1_556]  | 1.96                     | 0.24              |
| 4:2:215:LYS:NZ  | 4:Z:249:THR:CA[1_556]  | 1.96                     | 0.24              |
| 4:2:109:PRO:CB  | 4:Z:154:ASP:N[1_556]   | 1.96                     | 0.24              |
| 4:2:134:VAL:CG1 | 4:Z:338:SER:C[1_556]   | 1.96                     | 0.24              |
| 4:0:108:ALA:N   | 4:X:300:SER:C[1_556]   | 1.96                     | 0.24              |
| 4:2:120:THR:CA  | 4:Z:340:TRP:O[1_556]   | 1.96                     | 0.24              |
| 4:0:213:LYS:NZ  | 4:X:189:LEU:CD1[1_556] | 1.96                     | 0.24              |
| 4:2:120:THR:N   | 4:Z:340:TRP:CB[1_556]  | 1.96                     | 0.24              |
| 4:0:68:LYS:CA   | 4:X:59:GLN:OE1[1_556]  | 1.96                     | 0.24              |
| 4:0:150:GLY:CA  | 4:X:317:ILE:CB[1_556]  | 1.96                     | 0.24              |
| 4:1:60:SER:C    | 4:Y:243:PRO:CB[1_556]  | 1.96                     | 0.24              |
| 4:1:118:LYS:CG  | 4:Y:10:CYS:C[1_556]    | 1.96                     | 0.24              |
| 4:0:163:VAL:N   | 4:X:274:ILE:C[1_556]   | 1.96                     | 0.24              |
| 4:1:271:SER:OG  | 4:Y:269:MET:CB[1_556]  | 1.96                     | 0.24              |
| 4:0:63:GLY:O    | 4:V:289:ILE:CB[1_556]  | 1.96                     | 0.24              |
| 4:2:336:LYS:CD  | 4:Z:218:TYR:CE1[1_556] | 1.96                     | 0.24              |
| 4:4:63:GLY:N    | 4:Z:287:ILE:C[1_556]   | 1.96                     | 0.24              |
| 4:2:40:HIS:CG   | 4:X:166:TYR:CD1[1_556] | 1.96                     | 0.24              |
| 4:0:279:TYR:O   | 4:X:276:GLU:OE1[1_556] | 1.96                     | 0.24              |
| 4:0:305:MET:O   | 4:X:255:PHE:CD2[1_556] | 1.96                     | 0.24              |
| 4:1:112:PRO:CA  | 4:Y:137:GLN:CB[1_556]  | 1.96                     | 0.24              |
| 4:0:183:ARG:CZ  | 4:X:186:THR:CB[1_556]  | 1.96                     | 0.24              |
| 4:2:189:LEU:CG  | 4:Z:195:GLU:C[1_556]   | 1.96                     | 0.24              |
| 4:1:16:LEU:N    | 4:Y:214:GLU:CB[1_556]  | 1.96                     | 0.24              |
| 4:1:336:LYS:N   | 4:Y:218:TYR:CB[1_556]  | 1.97                     | 0.23              |
| 4:2:108:ALA:N   | 4:Z:300:SER:C[1_556]   | 1.97                     | 0.23              |
| 4:2:277:THR:CG2 | 4:Z:272:ALA:CA[1_556]  | 1.97                     | 0.23              |
| 4:0:140:LEU:CB  | 4:X:331:ALA:CA[1_556]  | 1.97                     | 0.23              |
| 4:1:171:LEU:CG  | 4:Y:282:ILE:CD1[1_556] | 1.97                     | 0.23              |
| 4:0:80:ASP:N    | 4:X:31:PHE:CE1[1_556]  | 1.97                     | 0.23              |
| 4:1:208:ILE:C   | 4:Y:198:TYR:CD1[1_556] | 1.97                     | 0.23              |
| 4:1:37:ARG:C    | 4:Y:60:SER:CB[1_556]   | 1.97                     | 0.23              |
| 4:1:73:HIS:CB   | 4:Y:157:ASP:C[1_556]   | 1.97                     | 0.23              |
| 4:2:279:TYR:N   | 4:Z:276:GLU:CG[1_556]  | 1.97                     | 0.23              |
| 4:1:298:VAL:N   | 4:Y:316:GLU:CG[1_556]  | 1.97                     | 0.23              |
| 4:2:150:GLY:CA  | 4:Z:317:ILE:CB[1_556]  | 1.97                     | 0.23              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:210:ARG:NE  | 4:X:193:LEU:CD2[1_556] | 1.97                     | 0.23              |
| 4:0:35:VAL:CG1  | 4:X:56:ASP:OD2[1_556]  | 1.97                     | 0.23              |
| 4:2:40:HIS:CE1  | 4:X:166:TYR:CD1[1_556] | 1.97                     | 0.23              |
| 4:1:40:HIS:C    | 4:W:167:GLU:CG[1_556]  | 1.97                     | 0.23              |
| 4:0:192:ILE:CB  | 4:W:110:LEU:O[1_556]   | 1.97                     | 0.23              |
| 4:0:309:ILE:CD1 | 4:X:259:GLU:OE2[1_556] | 1.97                     | 0.23              |
| 4:2:298:VAL:N   | 4:Z:316:GLU:N[1_556]   | 1.97                     | 0.23              |
| 4:4:62:ARG:C    | 4:Z:288:ASP:N[1_556]   | 1.97                     | 0.23              |
| 4:1:337:TYR:C   | 4:Y:307:PRO:C[1_556]   | 1.97                     | 0.23              |
| 4:0:172:PRO:C   | 4:X:162:ASN:O[1_556]   | 1.97                     | 0.23              |
| 4:1:293:LEU:N   | 4:Y:320:LEU:C[1_556]   | 1.97                     | 0.23              |
| 4:2:12:ASN:CG   | 4:Z:336:LYS:CG[1_556]  | 1.97                     | 0.23              |
| 4:0:171:LEU:O   | 4:X:281:SER:CB[1_556]  | 1.97                     | 0.23              |
| 4:1:270:GLU:CG  | 4:X:286:ASP:N[1_556]   | 1.97                     | 0.23              |
| 4:0:298:VAL:N   | 4:X:316:GLU:N[1_556]   | 1.97                     | 0.23              |
| 4:1:299:MET:CG  | 4:Y:312:ARG:NH2[1_556] | 1.97                     | 0.23              |
| 4:0:231:ALA:N   | 4:W:368:SER:C[1_556]   | 1.97                     | 0.23              |
| 4:1:116:ARG:CB  | 4:Y:339:VAL:CG1[1_556] | 1.97                     | 0.23              |
| 4:0:294:TYR:N   | 4:X:319:ALA:O[1_556]   | 1.97                     | 0.23              |
| 4:1:197:GLY:N   | 4:X:75:ILE:CB[1_556]   | 1.97                     | 0.23              |
| 4:0:197:GLY:N   | 4:W:75:ILE:CB[1_556]   | 1.97                     | 0.23              |
| 4:0:266:PHE:N   | 4:W:173:HIS:CE1[1_556] | 1.97                     | 0.23              |
| 4:0:258:PRO:CG  | 4:X:256:ARG:NH1[1_556] | 1.97                     | 0.23              |
| 4:0:33:SER:CB   | 4:X:214:GLU:OE1[1_556] | 1.97                     | 0.23              |
| 4:0:68:LYS:CD   | 4:X:59:GLN:N[1_556]    | 1.97                     | 0.23              |
| 4:1:279:TYR:O   | 4:Y:276:GLU:OE1[1_556] | 1.97                     | 0.23              |
| 4:2:231:ALA:N   | 4:Y:368:SER:C[1_556]   | 1.97                     | 0.23              |
| 4:1:172:PRO:CA  | 4:Y:162:ASN:C[1_556]   | 1.97                     | 0.23              |
| 4:0:59:GLN:CG   | 4:X:208:ILE:CD1[1_556] | 1.97                     | 0.23              |
| 4:1:106:THR:N   | 4:Y:334:GLU:O[1_556]   | 1.97                     | 0.23              |
| 4:1:134:VAL:CG2 | 4:Y:337:TYR:O[1_556]   | 1.97                     | 0.23              |
| 4:0:40:HIS:CE1  | 4:V:166:TYR:CD1[1_556] | 1.97                     | 0.23              |
| 4:0:306:TYR:CB  | 4:X:227:MET:CE[1_556]  | 1.97                     | 0.23              |
| 4:2:59:GLN:CG   | 4:Z:208:ILE:CD1[1_556] | 1.97                     | 0.23              |
| 4:2:84:LYS:CE   | 4:Z:56:ASP:OD1[1_556]  | 1.97                     | 0.23              |
| 4:1:41:GLN:O    | 4:W:148:THR:OG1[1_556] | 1.97                     | 0.23              |
| 4:1:260:THR:C   | 4:Y:266:PHE:CA[1_556]  | 1.97                     | 0.23              |
| 4:1:30:VAL:O    | 4:Y:215:LYS:CG[1_556]  | 1.97                     | 0.23              |
| 4:1:110:LEU:N   | 4:Y:154:ASP:CB[1_556]  | 1.97                     | 0.23              |
| 4:0:209:VAL:CB  | 4:X:194:THR:C[1_556]   | 1.97                     | 0.23              |
| 4:0:79:TRP:CZ3  | 4:X:18:LYS:CA[1_556]   | 1.97                     | 0.23              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:274:ILE:CG1 | 4:Y:263:GLN:O[1_556]   | 1.97                     | 0.23              |
| 4:0:12:ASN:CG   | 4:X:336:LYS:CG[1_556]  | 1.97                     | 0.23              |
| 4:1:67:LEU:C    | 4:Y:59:GLN:OE1[1_556]  | 1.97                     | 0.23              |
| 4:2:169:TYR:CG  | 4:Z:150:GLY:CA[1_556]  | 1.97                     | 0.23              |
| 4:2:190:MET:CA  | 4:Z:194:THR:OG1[1_556] | 1.97                     | 0.23              |
| 4:2:164:PRO:CG  | 4:Z:278:THR:CB[1_556]  | 1.97                     | 0.23              |
| 4:1:236:LEU:CG  | 4:X:117:GLU:OE1[1_556] | 1.97                     | 0.23              |
| 4:1:332:PRO:CG  | 4:Y:221:LEU:CB[1_556]  | 1.97                     | 0.23              |
| 4:0:83:GLU:OE1  | 4:X:29:ALA:N[1_556]    | 1.97                     | 0.23              |
| 4:0:253:GLU:N   | 4:W:113:LYS:N[1_556]   | 1.97                     | 0.23              |
| 4:0:148:THR:O   | 4:X:327:ILE:C[1_556]   | 1.97                     | 0.23              |
| 4:1:194:THR:CG2 | 4:X:177:ARG:NH2[1_556] | 1.97                     | 0.23              |
| 4:1:332:PRO:CD  | 4:Y:221:LEU:CA[1_556]  | 1.97                     | 0.23              |
| 4:2:253:GLU:N   | 4:Y:113:LYS:N[1_556]   | 1.97                     | 0.23              |
| 4:3:198:TYR:O   | 4:Z:72:GLU:O[1_556]    | 1.97                     | 0.23              |
| 4:2:192:ILE:CB  | 4:Y:110:LEU:O[1_556]   | 1.97                     | 0.23              |
| 4:0:82:MET:C    | 4:X:30:VAL:CG1[1_556]  | 1.97                     | 0.23              |
| 4:2:206:ARG:CD  | 4:Z:200:PHE:C[1_556]   | 1.97                     | 0.23              |
| 4:1:138:ALA:N   | 4:Y:299:MET:SD[1_556]  | 1.97                     | 0.23              |
| 4:0:160:THR:CG2 | 4:X:261:LEU:C[1_556]   | 1.97                     | 0.23              |
| 4:3:64:ILE:CB   | 4:Y:292:ASP:OD2[1_556] | 1.97                     | 0.23              |
| 4:2:106:THR:N   | 4:Z:334:GLU:C[1_556]   | 1.97                     | 0.23              |
| 4:2:292:ASP:OD2 | 4:Z:325:MET:CB[1_556]  | 1.97                     | 0.23              |
| 4:1:107:GLU:CD  | 4:Y:300:SER:OG[1_556]  | 1.97                     | 0.23              |
| 4:1:79:TRP:N    | 4:Y:17:VAL:CB[1_556]   | 1.97                     | 0.23              |
| 4:2:336:LYS:CA  | 4:Z:218:TYR:CB[1_556]  | 1.97                     | 0.23              |
| 4:2:116:ARG:NH2 | 4:Z:141:SER:O[1_556]   | 1.97                     | 0.23              |
| 4:2:72:GLU:CA   | 4:Z:157:ASP:CB[1_556]  | 1.97                     | 0.23              |
| 4:0:148:THR:N   | 4:X:314:GLN:NE2[1_556] | 1.97                     | 0.23              |
| 4:2:166:TYR:CE2 | 4:Z:291:LYS:CA[1_556]  | 1.97                     | 0.23              |
| 4:3:40:HIS:C    | 4:Y:167:GLU:CG[1_556]  | 1.97                     | 0.23              |
| 4:4:40:HIS:CE1  | 4:Z:166:TYR:CD1[1_556] | 1.97                     | 0.23              |
| 4:3:254:ARG:CA  | 4:Z:113:LYS:NZ[1_556]  | 1.97                     | 0.23              |
| 4:1:79:TRP:CH2  | 4:Y:11:ASP:O[1_556]    | 1.97                     | 0.23              |
| 4:1:252:ASN:N   | 4:X:113:LYS:C[1_556]   | 1.97                     | 0.23              |
| 4:2:83:GLU:CG   | 4:Z:28:ARG:O[1_556]    | 1.97                     | 0.23              |
| 4:2:307:PRO:CB  | 4:Z:227:MET:O[1_556]   | 1.97                     | 0.23              |
| 4:2:68:LYS:CA   | 4:Z:59:GLN:OE1[1_556]  | 1.97                     | 0.23              |
| 4:2:174:ALA:CA  | 4:Z:277:THR:O[1_556]   | 1.97                     | 0.23              |
| 4:3:227:MET:CG  | 4:Z:372:ARG:C[1_556]   | 1.97                     | 0.23              |
| 4:2:33:SER:CB   | 4:Z:214:GLU:OE1[1_556] | 1.97                     | 0.23              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:186:THR:CB  | 4:Y:190:MET:N[1_556]   | 1.97                     | 0.23              |
| 4:2:115:ASN:O   | 4:Z:11:ASP:CG[1_556]   | 1.97                     | 0.23              |
| 4:1:120:THR:C   | 4:Y:340:TRP:CE3[1_556] | 1.97                     | 0.23              |
| 4:0:336:LYS:N   | 4:X:218:TYR:CB[1_556]  | 1.97                     | 0.23              |
| 4:1:296:ASN:CG  | 4:Y:318:THR:CA[1_556]  | 1.97                     | 0.23              |
| 4:2:116:ARG:CD  | 4:Z:141:SER:CA[1_556]  | 1.97                     | 0.23              |
| 4:0:192:ILE:CA  | 4:W:110:LEU:C[1_556]   | 1.97                     | 0.23              |
| 4:0:306:TYR:CE2 | 4:X:256:ARG:CA[1_556]  | 1.97                     | 0.23              |
| 4:0:210:ARG:N   | 4:X:193:LEU:CA[1_556]  | 1.97                     | 0.23              |
| 4:2:295:ALA:C   | 4:Z:319:ALA:N[1_556]   | 1.97                     | 0.23              |
| 4:2:59:GLN:CG   | 4:Z:208:ILE:CG2[1_556] | 1.97                     | 0.23              |
| 4:0:231:ALA:CB  | 4:W:370:VAL:C[1_556]   | 1.97                     | 0.23              |
| 4:2:160:THR:CG2 | 4:Z:261:LEU:C[1_556]   | 1.98                     | 0.22              |
| 4:2:252:ASN:N   | 4:Y:114:ALA:N[1_556]   | 1.98                     | 0.22              |
| 4:1:141:SER:C   | 4:Y:310:ALA:N[1_556]   | 1.98                     | 0.22              |
| 4:0:113:LYS:CB  | 4:X:137:GLN:N[1_556]   | 1.98                     | 0.22              |
| 4:1:206:ARG:N   | 4:Y:199:SER:N[1_556]   | 1.98                     | 0.22              |
| 4:1:129:VAL:CG2 | 4:Y:25:ASP:N[1_556]    | 1.98                     | 0.22              |
| 4:2:126:THR:OG1 | 4:Z:28:ARG:N[1_556]    | 1.98                     | 0.22              |
| 4:1:278:THR:CA  | 4:Y:276:GLU:CG[1_556]  | 1.98                     | 0.22              |
| 4:3:252:ASN:N   | 4:Z:113:LYS:C[1_556]   | 1.98                     | 0.22              |
| 4:1:79:TRP:CH2  | 4:Y:18:LYS:CE[1_556]   | 1.98                     | 0.22              |
| 4:1:112:PRO:C   | 4:Y:137:GLN:CA[1_556]  | 1.98                     | 0.22              |
| 4:1:86:TRP:CZ3  | 4:Y:27:PRO:CG[1_556]   | 1.98                     | 0.22              |
| 4:0:307:PRO:CB  | 4:X:227:MET:CB[1_556]  | 1.98                     | 0.22              |
| 4:1:170:ALA:O   | 4:Y:151:ILE:C[1_556]   | 1.98                     | 0.22              |
| 4:0:30:VAL:CG1  | 4:X:215:LYS:CB[1_556]  | 1.98                     | 0.22              |
| 4:0:155:SER:CB  | 4:X:258:PRO:C[1_556]   | 1.98                     | 0.22              |
| 4:2:278:THR:CA  | 4:Z:276:GLU:CG[1_556]  | 1.98                     | 0.22              |
| 4:2:206:ARG:CD  | 4:Z:200:PHE:O[1_556]   | 1.98                     | 0.22              |
| 4:1:331:ALA:C   | 4:Y:221:LEU:N[1_556]   | 1.98                     | 0.22              |
| 4:2:149:THR:OG1 | 4:Z:326:LYS:C[1_556]   | 1.98                     | 0.22              |
| 4:2:116:ARG:O   | 4:Z:340:TRP:C[1_556]   | 1.98                     | 0.22              |
| 4:1:68:LYS:CB   | 4:Y:59:GLN:NE2[1_556]  | 1.98                     | 0.22              |
| 4:2:165:ILE:N   | 4:Z:297:ASN:OD1[1_556] | 1.98                     | 0.22              |
| 4:2:231:ALA:C   | 4:Y:369:ILE:CG2[1_556] | 1.98                     | 0.22              |
| 4:0:108:ALA:CB  | 4:X:155:SER:O[1_556]   | 1.98                     | 0.22              |
| 4:0:299:MET:N   | 4:X:312:ARG:CA[1_556]  | 1.98                     | 0.22              |
| 4:2:289:ILE:CG2 | 4:Z:294:TYR:CE2[1_556] | 1.98                     | 0.22              |
| 4:2:292:ASP:OD2 | 4:Z:322:PRO:O[1_556]   | 1.98                     | 0.22              |
| 4:2:148:THR:N   | 4:Z:314:GLN:NE2[1_556] | 1.98                     | 0.22              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:186:THR:CB  | 4:Z:190:MET:N[1_556]   | 1.98                     | 0.22              |
| 4:0:75:ILE:N    | 4:X:156:GLY:CA[1_556]  | 1.98                     | 0.22              |
| 4:1:285:CYS:C   | 4:Y:283:MET:N[1_556]   | 1.98                     | 0.22              |
| 4:2:150:GLY:N   | 4:Z:317:ILE:CD1[1_556] | 1.98                     | 0.22              |
| 4:2:265:SER:O   | 4:Y:173:HIS:NE2[1_556] | 1.98                     | 0.22              |
| 4:0:206:ARG:CD  | 4:X:200:PHE:C[1_556]   | 1.98                     | 0.22              |
| 4:2:332:PRO:N   | 4:Z:221:LEU:N[1_556]   | 1.98                     | 0.22              |
| 4:3:233:SER:C   | 4:Z:366:GLY:C[1_556]   | 1.98                     | 0.22              |
| 4:1:300:SER:OG  | 4:Y:309:ILE:CB[1_556]  | 1.98                     | 0.22              |
| 4:0:278:THR:CA  | 4:X:276:GLU:CG[1_556]  | 1.98                     | 0.22              |
| 4:3:236:LEU:CG  | 4:Z:117:GLU:OE1[1_556] | 1.98                     | 0.22              |
| 4:0:215:LYS:NZ  | 4:X:249:THR:CA[1_556]  | 1.98                     | 0.22              |
| 4:1:203:THR:OG1 | 4:Y:205:GLU:OE2[1_556] | 1.98                     | 0.22              |
| 4:0:308:GLY:N   | 4:X:224:GLU:O[1_556]   | 1.98                     | 0.22              |
| 4:2:82:MET:O    | 4:Z:30:VAL:CB[1_556]   | 1.98                     | 0.22              |
| 4:1:132:MET:SD  | 4:Y:341:ILE:CG1[1_556] | 1.98                     | 0.22              |
| 4:2:73:HIS:N    | 4:Z:157:ASP:CA[1_556]  | 1.98                     | 0.22              |
| 4:2:183:ARG:CZ  | 4:Z:186:THR:CB[1_556]  | 1.98                     | 0.22              |
| 4:0:196:ARG:CB  | 4:W:111:ASN:OD1[1_556] | 1.98                     | 0.22              |
| 4:1:73:HIS:NE2  | 4:Y:184:ASP:OD1[1_556] | 1.98                     | 0.22              |
| 4:3:194:THR:CG2 | 4:Z:177:ARG:NH2[1_556] | 1.98                     | 0.22              |
| 4:1:121:GLN:O   | 4:Y:20:GLY:C[1_556]    | 1.98                     | 0.22              |
| 4:0:11:ASP:OD1  | 4:X:305:MET:CA[1_556]  | 1.98                     | 0.22              |
| 4:2:370:VAL:C   | 4:Z:342:GLY:CA[1_556]  | 1.98                     | 0.22              |
| 4:2:83:GLU:OE1  | 4:Z:29:ALA:N[1_556]    | 1.98                     | 0.22              |
| 4:0:206:ARG:CD  | 4:X:200:PHE:O[1_556]   | 1.98                     | 0.22              |
| 4:0:332:PRO:N   | 4:X:221:LEU:N[1_556]   | 1.98                     | 0.22              |
| 4:3:194:THR:CB  | 4:Z:177:ARG:CZ[1_556]  | 1.98                     | 0.22              |
| 4:2:148:THR:O   | 4:Z:327:ILE:C[1_556]   | 1.98                     | 0.22              |
| 4:0:73:HIS:C    | 4:X:157:ASP:CA[1_556]  | 1.98                     | 0.22              |
| 4:1:180:LEU:CD1 | 4:Y:267:ILE:N[1_556]   | 1.98                     | 0.22              |
| 4:1:297:ASN:N   | 4:Y:315:LYS:C[1_556]   | 1.98                     | 0.22              |
| 4:2:104:LEU:CA  | 4:Z:334:GLU:CB[1_556]  | 1.98                     | 0.22              |
| 4:0:104:LEU:CA  | 4:X:334:GLU:CB[1_556]  | 1.98                     | 0.22              |
| 4:1:110:LEU:N   | 4:Y:154:ASP:O[1_556]   | 1.98                     | 0.22              |
| 4:1:86:TRP:NE1  | 4:Y:337:TYR:CE2[1_556] | 1.98                     | 0.22              |
| 4:0:72:GLU:CA   | 4:X:157:ASP:CB[1_556]  | 1.98                     | 0.22              |
| 4:1:116:ARG:CA  | 4:Y:339:VAL:O[1_556]   | 1.98                     | 0.22              |
| 4:0:109:PRO:CB  | 4:X:154:ASP:N[1_556]   | 1.98                     | 0.22              |
| 4:1:162:ASN:N   | 4:Y:274:ILE:CD1[1_556] | 1.98                     | 0.22              |
| 4:2:162:ASN:CA  | 4:Z:274:ILE:CB[1_556]  | 1.98                     | 0.22              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:168:GLY:O   | 4:Y:296:ASN:CA[1_556]  | 1.98                     | 0.22              |
| 4:1:198:TYR:O   | 4:X:72:GLU:O[1_556]    | 1.98                     | 0.22              |
| 4:3:41:GLN:CA   | 4:Y:167:GLU:CD[1_556]  | 1.98                     | 0.22              |
| 4:0:227:MET:CG  | 4:W:372:ARG:C[1_556]   | 1.98                     | 0.22              |
| 4:0:112:PRO:C   | 4:X:137:GLN:CD[1_556]  | 1.98                     | 0.22              |
| 4:2:336:LYS:N   | 4:Z:218:TYR:CB[1_556]  | 1.98                     | 0.22              |
| 4:1:370:VAL:C   | 4:Y:342:GLY:CA[1_556]  | 1.98                     | 0.22              |
| 4:0:149:THR:OG1 | 4:X:326:LYS:C[1_556]   | 1.98                     | 0.22              |
| 4:3:232:SER:OG  | 4:Z:365:ALA:CB[1_556]  | 1.98                     | 0.22              |
| 4:0:370:VAL:C   | 4:X:342:GLY:CA[1_556]  | 1.98                     | 0.22              |
| 4:0:134:VAL:CG1 | 4:X:338:SER:C[1_556]   | 1.98                     | 0.22              |
| 4:3:231:ALA:C   | 4:Z:369:ILE:CG2[1_556] | 1.98                     | 0.22              |
| 4:2:163:VAL:N   | 4:Z:274:ILE:C[1_556]   | 1.98                     | 0.22              |
| 4:2:149:THR:O   | 4:Z:327:ILE:CB[1_556]  | 1.98                     | 0.22              |
| 4:0:176:MET:O   | 4:X:178:LEU:CD2[1_556] | 1.98                     | 0.22              |
| 4:1:79:TRP:N    | 4:Y:17:VAL:N[1_556]    | 1.98                     | 0.22              |
| 4:0:174:ALA:CA  | 4:X:281:SER:N[1_556]   | 1.98                     | 0.22              |
| 4:0:285:CYS:C   | 4:X:283:MET:N[1_556]   | 1.98                     | 0.22              |
| 4:2:206:ARG:CB  | 4:Z:200:PHE:C[1_556]   | 1.98                     | 0.22              |
| 4:2:79:TRP:N    | 4:Z:17:VAL:CB[1_556]   | 1.98                     | 0.22              |
| 4:2:337:TYR:CA  | 4:Z:307:PRO:CD[1_556]  | 1.98                     | 0.22              |
| 4:2:210:ARG:N   | 4:Z:193:LEU:CA[1_556]  | 1.98                     | 0.22              |
| 4:0:252:ASN:N   | 4:W:114:ALA:N[1_556]   | 1.98                     | 0.22              |
| 4:3:265:SER:O   | 4:Z:173:HIS:NE2[1_556] | 1.98                     | 0.22              |
| 4:2:115:ASN:O   | 4:Z:11:ASP:OD2[1_556]  | 1.98                     | 0.22              |
| 4:1:211:ASP:CG  | 4:Y:249:THR:N[1_556]   | 1.98                     | 0.22              |
| 4:1:119:MET:CE  | 4:Y:337:TYR:C[1_556]   | 1.98                     | 0.22              |
| 4:1:367:PRO:O   | 4:Y:342:GLY:O[1_556]   | 1.98                     | 0.22              |
| 4:1:305:MET:CG  | 4:Y:255:PHE:CA[1_556]  | 1.98                     | 0.22              |
| 4:2:171:LEU:O   | 4:Z:281:SER:CB[1_556]  | 1.98                     | 0.22              |
| 4:2:30:VAL:CG1  | 4:Z:215:LYS:CB[1_556]  | 1.98                     | 0.22              |
| 4:0:114:ALA:CA  | 4:X:106:THR:OG1[1_556] | 1.98                     | 0.22              |
| 4:2:308:GLY:N   | 4:Z:224:GLU:O[1_556]   | 1.98                     | 0.22              |
| 4:1:183:ARG:CB  | 4:Y:186:THR:CA[1_556]  | 1.98                     | 0.22              |
| 4:2:309:ILE:CD1 | 4:Z:259:GLU:OE2[1_556] | 1.98                     | 0.22              |
| 4:0:209:VAL:CG1 | 4:X:194:THR:CB[1_556]  | 1.98                     | 0.22              |
| 4:0:288:ASP:OD2 | 4:Z:205:GLU:OE1[1_556] | 1.98                     | 0.22              |
| 4:2:172:PRO:CA  | 4:Z:162:ASN:C[1_556]   | 1.98                     | 0.22              |
| 4:2:82:MET:C    | 4:Z:30:VAL:CG1[1_556]  | 1.98                     | 0.22              |
| 4:1:83:GLU:CD   | 4:Y:28:ARG:O[1_556]    | 1.98                     | 0.22              |
| 4:1:73:HIS:O    | 4:Y:181:ALA:CB[1_556]  | 1.98                     | 0.22              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:307:PRO:CB  | 4:Z:227:MET:CB[1_556]  | 1.98                     | 0.22              |
| 4:0:336:LYS:CD  | 4:X:218:TYR:CE1[1_556] | 1.98                     | 0.22              |
| 4:0:73:HIS:O    | 4:X:181:ALA:CB[1_556]  | 1.98                     | 0.22              |
| 4:0:164:PRO:CG  | 4:X:278:THR:CB[1_556]  | 1.98                     | 0.22              |
| 4:2:155:SER:CB  | 4:Z:258:PRO:C[1_556]   | 1.98                     | 0.22              |
| 4:2:210:ARG:NE  | 4:Z:193:LEU:CD2[1_556] | 1.98                     | 0.22              |
| 4:1:157:ASP:CB  | 4:Y:213:LYS:CG[1_556]  | 1.98                     | 0.22              |
| 4:1:335:ARG:NE  | 4:Y:220:ALA:CA[1_556]  | 1.98                     | 0.22              |
| 4:1:164:PRO:CD  | 4:Y:278:THR:C[1_556]   | 1.98                     | 0.22              |
| 4:0:166:TYR:CE2 | 4:X:291:LYS:CA[1_556]  | 1.98                     | 0.22              |
| 4:2:125:GLU:CD  | 4:Z:21:PHE:CB[1_556]   | 1.99                     | 0.21              |
| 4:1:154:ASP:C   | 4:Y:261:LEU:CG[1_556]  | 1.99                     | 0.21              |
| 4:2:108:ALA:CB  | 4:Z:155:SER:O[1_556]   | 1.99                     | 0.21              |
| 4:1:292:ASP:CA  | 4:Y:321:ALA:CA[1_556]  | 1.99                     | 0.21              |
| 4:0:279:TYR:N   | 4:X:276:GLU:CG[1_556]  | 1.99                     | 0.21              |
| 4:4:40:HIS:CG   | 4:Z:166:TYR:CD1[1_556] | 1.99                     | 0.21              |
| 4:1:79:TRP:CZ3  | 4:Y:18:LYS:CA[1_556]   | 1.99                     | 0.21              |
| 4:3:197:GLY:N   | 4:Z:75:ILE:CB[1_556]   | 1.99                     | 0.21              |
| 4:2:178:LEU:CA  | 4:Z:180:LEU:CG[1_556]  | 1.99                     | 0.21              |
| 4:0:125:GLU:CD  | 4:X:21:PHE:CB[1_556]   | 1.99                     | 0.21              |
| 4:1:362:TYR:CD2 | 4:Y:23:GLY:CA[1_556]   | 1.99                     | 0.21              |
| 4:1:41:GLN:CA   | 4:W:167:GLU:CD[1_556]  | 1.99                     | 0.21              |
| 4:1:11:ASP:CG   | 4:Y:305:MET:CA[1_556]  | 1.99                     | 0.21              |
| 4:0:126:THR:CA  | 4:X:28:ARG:CG[1_556]   | 1.99                     | 0.21              |
| 4:2:75:ILE:N    | 4:Z:156:GLY:CA[1_556]  | 1.99                     | 0.21              |
| 4:2:155:SER:N   | 4:Z:261:LEU:CD1[1_556] | 1.99                     | 0.21              |
| 4:0:82:MET:O    | 4:X:30:VAL:CB[1_556]   | 1.99                     | 0.21              |
| 4:3:40:HIS:CG   | 4:Y:166:TYR:CD1[1_556] | 1.99                     | 0.21              |
| 4:1:169:TYR:CD2 | 4:Y:293:LEU:CD1[1_556] | 1.99                     | 0.21              |
| 4:2:112:PRO:C   | 4:Z:137:GLN:CD[1_556]  | 1.99                     | 0.21              |
| 4:1:114:ALA:CA  | 4:Y:106:THR:OG1[1_556] | 1.99                     | 0.21              |
| 4:0:106:THR:N   | 4:X:334:GLU:C[1_556]   | 1.99                     | 0.21              |
| 4:0:83:GLU:CG   | 4:X:29:ALA:CA[1_556]   | 1.99                     | 0.21              |
| 4:0:110:LEU:CD2 | 4:X:161:HIS:C[1_556]   | 1.99                     | 0.21              |
| 4:2:179:ASP:CA  | 4:Z:180:LEU:CA[1_556]  | 1.99                     | 0.21              |
| 4:0:125:GLU:OE1 | 4:X:21:PHE:CA[1_556]   | 1.99                     | 0.21              |
| 4:1:254:ARG:CA  | 4:X:113:LYS:NZ[1_556]  | 1.99                     | 0.21              |
| 4:0:190:MET:CA  | 4:X:194:THR:OG1[1_556] | 1.99                     | 0.21              |
| 4:1:118:LYS:O   | 4:Y:340:TRP:CE2[1_556] | 1.99                     | 0.21              |
| 4:2:174:ALA:CA  | 4:Z:281:SER:N[1_556]   | 1.99                     | 0.21              |
| 4:0:162:ASN:CA  | 4:X:274:ILE:CB[1_556]  | 1.99                     | 0.21              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:207:GLU:N   | 4:Y:199:SER:O[1_556]   | 1.99                     | 0.21              |
| 4:0:116:ARG:O   | 4:X:340:TRP:C[1_556]   | 1.99                     | 0.21              |
| 4:1:299:MET:O   | 4:Y:312:ARG:CG[1_556]  | 1.99                     | 0.21              |
| 4:0:116:ARG:NH2 | 4:X:141:SER:O[1_556]   | 1.99                     | 0.21              |
| 4:1:285:CYS:CA  | 4:Y:283:MET:CB[1_556]  | 1.99                     | 0.21              |
| 4:2:62:ARG:CZ   | 4:Z:204:ALA:O[1_556]   | 1.99                     | 0.21              |
| 4:0:195:GLU:N   | 4:W:75:ILE:CD1[1_556]  | 1.99                     | 0.21              |
| 4:2:251:GLY:CA  | 4:Y:114:ALA:CA[1_556]  | 1.99                     | 0.21              |
| 4:0:337:TYR:CA  | 4:X:307:PRO:CD[1_556]  | 1.99                     | 0.21              |
| 4:0:289:ILE:CG2 | 4:X:294:TYR:CE2[1_556] | 1.99                     | 0.21              |
| 4:0:194:THR:C   | 4:W:75:ILE:CD1[1_556]  | 1.99                     | 0.21              |
| 4:2:294:TYR:N   | 4:Z:319:ALA:O[1_556]   | 1.99                     | 0.21              |
| 4:2:83:GLU:CG   | 4:Z:29:ALA:CA[1_556]   | 1.99                     | 0.21              |
| 4:0:295:ALA:C   | 4:X:319:ALA:N[1_556]   | 1.99                     | 0.21              |
| 4:1:233:SER:C   | 4:X:366:GLY:C[1_556]   | 1.99                     | 0.21              |
| 4:0:167:GLU:C   | 4:X:295:ALA:CB[1_556]  | 1.99                     | 0.21              |
| 4:1:298:VAL:N   | 4:Y:316:GLU:N[1_556]   | 1.99                     | 0.21              |
| 4:3:198:TYR:N   | 4:Z:75:ILE:CA[1_556]   | 1.99                     | 0.21              |
| 4:0:172:PRO:CA  | 4:X:162:ASN:C[1_556]   | 1.99                     | 0.21              |
| 4:2:209:VAL:CB  | 4:Z:194:THR:C[1_556]   | 1.99                     | 0.21              |
| 4:2:253:GLU:OE2 | 4:Y:112:PRO:C[1_556]   | 1.99                     | 0.21              |
| 4:0:251:GLY:CA  | 4:W:114:ALA:CA[1_556]  | 1.99                     | 0.21              |
| 4:1:82:MET:N    | 4:Y:30:VAL:O[1_556]    | 1.99                     | 0.21              |
| 4:0:112:PRO:CB  | 4:X:137:GLN:OE1[1_556] | 1.99                     | 0.21              |
| 4:2:114:ALA:CA  | 4:Z:106:THR:OG1[1_556] | 1.99                     | 0.21              |
| 4:3:41:GLN:O    | 4:Y:148:THR:OG1[1_556] | 1.99                     | 0.21              |
| 4:0:180:LEU:CD1 | 4:X:267:ILE:N[1_556]   | 1.99                     | 0.21              |
| 4:0:285:CYS:CA  | 4:X:283:MET:CB[1_556]  | 1.99                     | 0.21              |
| 4:0:368:SER:C   | 4:X:346:LEU:CD2[1_556] | 1.99                     | 0.21              |
| 4:1:177:ARG:CG  | 4:Y:178:LEU:C[1_556]   | 1.99                     | 0.21              |
| 4:0:115:ASN:C   | 4:X:339:VAL:CG1[1_556] | 1.99                     | 0.21              |
| 4:0:83:GLU:CG   | 4:X:28:ARG:O[1_556]    | 1.99                     | 0.21              |
| 4:1:227:MET:CG  | 4:X:372:ARG:C[1_556]   | 1.99                     | 0.21              |
| 4:0:150:GLY:N   | 4:X:317:ILE:CD1[1_556] | 1.99                     | 0.21              |
| 4:1:106:THR:C   | 4:Y:336:LYS:N[1_556]   | 1.99                     | 0.21              |
| 4:1:306:TYR:CB  | 4:Y:227:MET:CE[1_556]  | 1.99                     | 0.21              |
| 4:0:175:ILE:CD1 | 4:X:162:ASN:CB[1_556]  | 1.99                     | 0.21              |
| 4:2:167:GLU:C   | 4:Z:295:ALA:CB[1_556]  | 1.99                     | 0.21              |
| 4:1:206:ARG:C   | 4:Y:200:PHE:N[1_556]   | 1.99                     | 0.21              |
| 4:0:253:GLU:OE2 | 4:W:112:PRO:C[1_556]   | 1.99                     | 0.21              |
| 4:0:367:PRO:N   | 4:X:343:GLY:O[1_556]   | 1.99                     | 0.21              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:111:ASN:CB  | 4:X:154:ASP:CG[1_556]  | 1.99                     | 0.21              |
| 4:1:187:ASP:OD1 | 4:Y:190:MET:CB[1_556]  | 1.99                     | 0.21              |
| 4:2:306:TYR:CB  | 4:Z:227:MET:CE[1_556]  | 1.99                     | 0.21              |
| 4:1:179:ASP:OD1 | 4:Y:180:LEU:CA[1_556]  | 1.99                     | 0.21              |
| 4:1:336:LYS:CA  | 4:Y:218:TYR:CB[1_556]  | 1.99                     | 0.21              |
| 4:0:123:MET:N   | 4:X:27:PRO:N[1_556]    | 1.99                     | 0.21              |
| 4:0:164:PRO:CD  | 4:X:278:THR:C[1_556]   | 1.99                     | 0.21              |
| 4:0:292:ASP:OD2 | 4:X:325:MET:CB[1_556]  | 1.99                     | 0.21              |
| 4:2:176:MET:O   | 4:Z:178:LEU:CD2[1_556] | 1.99                     | 0.21              |
| 4:1:109:PRO:CB  | 4:Y:154:ASP:N[1_556]   | 1.99                     | 0.21              |
| 4:0:169:TYR:CG  | 4:X:150:GLY:CA[1_556]  | 1.99                     | 0.21              |
| 4:1:76:ILE:CD1  | 4:Y:18:LYS:CE[1_556]   | 1.99                     | 0.21              |
| 4:0:73:HIS:CE1  | 4:X:184:ASP:N[1_556]   | 1.99                     | 0.21              |
| 4:2:277:THR:CB  | 4:Z:273:GLY:N[1_556]   | 1.99                     | 0.21              |
| 4:0:72:GLU:CG   | 4:X:183:ARG:NE[1_556]  | 1.99                     | 0.21              |
| 4:2:139:VAL:O   | 4:Z:329:ILE:O[1_556]   | 1.99                     | 0.21              |
| 4:1:305:MET:O   | 4:Y:255:PHE:CD2[1_556] | 1.99                     | 0.21              |
| 4:2:78:ASN:CA   | 4:Z:31:PHE:O[1_556]    | 1.99                     | 0.21              |
| 4:0:194:THR:O   | 4:W:75:ILE:CD1[1_556]  | 1.99                     | 0.21              |
| 4:2:192:ILE:CA  | 4:Y:110:LEU:C[1_556]   | 1.99                     | 0.21              |
| 4:1:339:VAL:CG1 | 4:Y:304:THR:O[1_556]   | 1.99                     | 0.21              |
| 4:0:178:LEU:CA  | 4:X:180:LEU:CG[1_556]  | 1.99                     | 0.21              |
| 4:2:368:SER:C   | 4:Z:346:LEU:CD2[1_556] | 1.99                     | 0.21              |
| 4:0:254:ARG:CA  | 4:W:113:LYS:NZ[1_556]  | 1.99                     | 0.21              |
| 4:1:181:ALA:C   | 4:Y:188:TYR:CB[1_556]  | 1.99                     | 0.21              |
| 4:2:126:THR:CA  | 4:Z:28:ARG:CG[1_556]   | 1.99                     | 0.21              |
| 4:0:252:ASN:O   | 4:W:113:LYS:CB[1_556]  | 1.99                     | 0.21              |
| 4:1:232:SER:OG  | 4:X:365:ALA:CB[1_556]  | 1.99                     | 0.21              |
| 4:2:121:GLN:OE1 | 4:Z:20:GLY:N[1_556]    | 1.99                     | 0.21              |
| 4:2:76:ILE:O    | 4:Z:16:LEU:O[1_556]    | 1.99                     | 0.21              |
| 4:1:292:ASP:N   | 4:Y:321:ALA:N[1_556]   | 1.99                     | 0.21              |
| 4:0:121:GLN:OE1 | 4:X:20:GLY:N[1_556]    | 1.99                     | 0.21              |
| 4:1:120:THR:N   | 4:Y:340:TRP:CE3[1_556] | 1.99                     | 0.21              |
| 4:1:177:ARG:N   | 4:Y:178:LEU:CD2[1_556] | 1.99                     | 0.21              |
| 4:2:113:LYS:CB  | 4:Z:137:GLN:N[1_556]   | 1.99                     | 0.21              |
| 4:0:265:SER:O   | 4:W:173:HIS:NE2[1_556] | 1.99                     | 0.21              |
| 4:2:294:TYR:C   | 4:Z:319:ALA:CA[1_556]  | 1.99                     | 0.21              |
| 4:0:79:TRP:N    | 4:X:17:VAL:CB[1_556]   | 2.00                     | 0.20              |
| 4:2:282:ILE:O   | 4:Z:279:TYR:CD2[1_556] | 2.00                     | 0.20              |
| 4:1:291:LYS:NZ  | 4:Y:322:PRO:N[1_556]   | 2.00                     | 0.20              |
| 4:4:41:GLN:O    | 4:Z:148:THR:OG1[1_556] | 2.00                     | 0.20              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:189:LEU:CD2 | 4:Y:195:GLU:CA[1_556]  | 2.00                     | 0.20              |
| 4:1:149:THR:O   | 4:Y:327:ILE:CB[1_556]  | 2.00                     | 0.20              |
| 4:0:149:THR:O   | 4:X:327:ILE:CB[1_556]  | 2.00                     | 0.20              |
| 4:0:155:SER:O   | 4:X:258:PRO:N[1_556]   | 2.00                     | 0.20              |
| 4:2:209:VAL:CG1 | 4:Z:194:THR:CB[1_556]  | 2.00                     | 0.20              |
| 4:2:196:ARG:CB  | 4:Y:111:ASN:OD1[1_556] | 2.00                     | 0.20              |
| 4:0:118:LYS:CE  | 4:X:10:CYS:CA[1_556]   | 2.00                     | 0.20              |
| 4:1:258:PRO:CG  | 4:Y:256:ARG:NH1[1_556] | 2.00                     | 0.20              |
| 4:0:335:ARG:CB  | 4:X:220:ALA:CA[1_556]  | 2.00                     | 0.20              |
| 4:2:372:ARG:N   | 4:Z:143:TYR:CG[1_556]  | 2.00                     | 0.20              |
| 4:1:297:ASN:CA  | 4:Y:316:GLU:CB[1_556]  | 2.00                     | 0.20              |
| 4:2:305:MET:N   | 4:Z:255:PHE:CB[1_556]  | 2.00                     | 0.20              |
| 4:0:32:PRO:CA   | 4:X:211:ASP:CA[1_556]  | 2.00                     | 0.20              |
| 4:0:104:LEU:CD2 | 4:X:333:PRO:C[1_556]   | 2.00                     | 0.20              |
| 4:2:125:GLU:OE1 | 4:Z:21:PHE:CA[1_556]   | 2.00                     | 0.20              |
| 4:0:139:VAL:O   | 4:X:329:ILE:O[1_556]   | 2.00                     | 0.20              |
| 4:1:140:LEU:CG  | 4:Y:331:ALA:O[1_556]   | 2.00                     | 0.20              |
| 4:1:160:THR:CB  | 4:Y:180:LEU:CD1[1_556] | 2.00                     | 0.20              |
| 4:0:73:HIS:N    | 4:X:157:ASP:CA[1_556]  | 2.00                     | 0.20              |
| 4:0:132:MET:SD  | 4:X:341:ILE:CG1[1_556] | 2.00                     | 0.20              |
| 4:1:62:ARG:CB   | 4:Y:204:ALA:N[1_556]   | 2.00                     | 0.20              |
| 4:2:310:ALA:N   | 4:Z:224:GLU:N[1_556]   | 2.00                     | 0.20              |
| 4:2:104:LEU:CD2 | 4:Z:333:PRO:C[1_556]   | 2.00                     | 0.20              |
| 4:0:186:THR:CB  | 4:X:190:MET:N[1_556]   | 2.00                     | 0.20              |
| 4:0:79:TRP:CA   | 4:X:17:VAL:O[1_556]    | 2.00                     | 0.20              |
| 4:2:112:PRO:CB  | 4:Z:137:GLN:OE1[1_556] | 2.00                     | 0.20              |
| 4:2:159:VAL:O   | 4:Z:185:LEU:CD2[1_556] | 2.00                     | 0.20              |
| 4:2:184:ASP:CA  | 4:Z:188:TYR:N[1_556]   | 2.00                     | 0.20              |
| 4:1:233:SER:CA  | 4:X:367:PRO:CG[1_556]  | 2.00                     | 0.20              |
| 4:0:125:GLU:O   | 4:X:28:ARG:CZ[1_556]   | 2.00                     | 0.20              |
| 4:1:72:GLU:C    | 4:Y:157:ASP:OD2[1_556] | 2.00                     | 0.20              |
| 4:0:206:ARG:CB  | 4:X:200:PHE:C[1_556]   | 2.00                     | 0.20              |
| 4:0:299:MET:CG  | 4:X:312:ARG:NH2[1_556] | 2.00                     | 0.20              |
| 4:1:104:LEU:CD2 | 4:Y:333:PRO:C[1_556]   | 2.00                     | 0.20              |
| 4:2:164:PRO:CD  | 4:Z:278:THR:C[1_556]   | 2.00                     | 0.20              |
| 4:1:183:ARG:NE  | 4:Y:186:THR:CG2[1_556] | 2.00                     | 0.20              |
| 4:2:73:HIS:CE1  | 4:Z:184:ASP:N[1_556]   | 2.00                     | 0.20              |
| 4:2:118:LYS:CE  | 4:Z:10:CYS:CA[1_556]   | 2.00                     | 0.20              |
| 4:2:285:CYS:CA  | 4:Z:283:MET:CB[1_556]  | 2.00                     | 0.20              |
| 4:2:108:ALA:C   | 4:Z:300:SER:O[1_556]   | 2.00                     | 0.20              |
| 4:0:310:ALA:N   | 4:X:224:GLU:N[1_556]   | 2.00                     | 0.20              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:298:VAL:CG1 | 4:X:311:ASP:O[1_556]   | 2.00                     | 0.20              |
| 4:1:362:TYR:O   | 4:Y:348:SER:OG[1_556]  | 2.00                     | 0.20              |
| 4:0:123:MET:O   | 4:X:26:ALA:O[1_556]    | 2.00                     | 0.20              |
| 4:2:110:LEU:CD2 | 4:Z:161:HIS:C[1_556]   | 2.00                     | 0.20              |
| 4:1:104:LEU:CD2 | 4:Y:333:PRO:CA[1_556]  | 2.00                     | 0.20              |
| 4:2:362:TYR:CG  | 4:Z:23:GLY:N[1_556]    | 2.00                     | 0.20              |
| 4:1:16:LEU:CD2  | 4:Y:213:LYS:CA[1_556]  | 2.00                     | 0.20              |
| 4:1:182:GLY:C   | 4:Y:189:LEU:CA[1_556]  | 2.00                     | 0.20              |
| 4:0:215:LYS:CA  | 4:X:196:ARG:NH1[1_556] | 2.00                     | 0.20              |
| 4:0:165:ILE:N   | 4:X:297:ASN:OD1[1_556] | 2.00                     | 0.20              |
| 4:1:123:MET:CG  | 4:Y:26:ALA:C[1_556]    | 2.00                     | 0.20              |
| 4:3:233:SER:CA  | 4:Z:367:PRO:CG[1_556]  | 2.00                     | 0.20              |
| 4:1:270:GLU:OE2 | 4:X:286:ASP:N[1_556]   | 2.00                     | 0.20              |
| 4:1:369:ILE:CD1 | 4:Y:143:TYR:OH[1_556]  | 2.00                     | 0.20              |
| 4:1:291:LYS:CD  | 4:Y:322:PRO:CB[1_556]  | 2.00                     | 0.20              |
| 4:0:124:PHE:CB  | 4:X:24:ASP:C[1_556]    | 2.00                     | 0.20              |
| 4:0:40:HIS:N    | 4:V:166:TYR:CE2[1_556] | 2.00                     | 0.20              |
| 4:1:139:VAL:CG2 | 4:Y:298:VAL:C[1_556]   | 2.00                     | 0.20              |
| 4:2:175:ILE:CD1 | 4:Z:162:ASN:CB[1_556]  | 2.00                     | 0.20              |
| 4:1:176:MET:CB  | 4:Y:277:THR:OG1[1_556] | 2.00                     | 0.20              |
| 4:1:113:LYS:CB  | 4:Y:137:GLN:N[1_556]   | 2.00                     | 0.20              |
| 4:1:147:ARG:NH1 | 4:Y:315:LYS:CG[1_556]  | 2.00                     | 0.20              |
| 4:2:252:ASN:O   | 4:Y:113:LYS:CB[1_556]  | 2.00                     | 0.20              |
| 4:0:139:VAL:CG1 | 4:X:330:ILE:N[1_556]   | 2.00                     | 0.20              |
| 4:0:179:ASP:CA  | 4:X:180:LEU:CA[1_556]  | 2.00                     | 0.20              |
| 4:3:194:THR:C   | 4:Z:75:ILE:CD1[1_556]  | 2.00                     | 0.20              |
| 4:0:166:TYR:CD2 | 4:X:294:TYR:CB[1_556]  | 2.00                     | 0.20              |
| 4:2:11:ASP:OD1  | 4:Z:305:MET:CA[1_556]  | 2.00                     | 0.20              |
| 4:2:227:MET:CG  | 4:Y:372:ARG:C[1_556]   | 2.00                     | 0.20              |
| 4:1:159:VAL:CA  | 4:Y:181:ALA:O[1_556]   | 2.00                     | 0.20              |
| 4:2:311:ASP:OD1 | 4:Z:224:GLU:OE2[1_556] | 2.00                     | 0.20              |
| 4:1:231:ALA:C   | 4:X:369:ILE:CG2[1_556] | 2.00                     | 0.20              |
| 4:1:362:TYR:CE1 | 4:Y:22:ALA:CB[1_556]   | 2.00                     | 0.20              |
| 4:0:11:ASP:CG   | 4:X:305:MET:CA[1_556]  | 2.00                     | 0.20              |
| 4:1:253:GLU:CG  | 4:X:112:PRO:CB[1_556]  | 2.00                     | 0.20              |
| 4:3:41:GLN:CB   | 4:Y:167:GLU:OE1[1_556] | 2.00                     | 0.20              |
| 4:0:122:ILE:C   | 4:X:27:PRO:CA[1_556]   | 2.00                     | 0.20              |
| 4:0:196:ARG:CG  | 4:W:115:ASN:CB[1_556]  | 2.00                     | 0.20              |
| 4:0:281:SER:C   | 4:X:280:ASN:ND2[1_556] | 2.00                     | 0.20              |
| 4:0:159:VAL:O   | 4:X:185:LEU:CD2[1_556] | 2.00                     | 0.20              |
| 4:1:232:SER:N   | 4:X:369:ILE:CA[1_556]  | 2.00                     | 0.20              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:233:SER:O   | 4:Y:367:PRO:N[1_556]   | 2.00                     | 0.20              |
| 4:1:169:TYR:OH  | 4:Y:164:PRO:C[1_556]   | 2.00                     | 0.20              |
| 4:0:108:ALA:C   | 4:X:300:SER:O[1_556]   | 2.00                     | 0.20              |
| 4:2:125:GLU:O   | 4:Z:28:ARG:CZ[1_556]   | 2.00                     | 0.20              |
| 4:2:282:ILE:C   | 4:Z:280:ASN:ND2[1_556] | 2.00                     | 0.20              |
| 4:2:115:ASN:C   | 4:Z:339:VAL:CG1[1_556] | 2.00                     | 0.20              |
| 4:1:303:THR:CG2 | 4:Y:260:THR:OG1[1_556] | 2.00                     | 0.20              |
| 4:1:297:ASN:CB  | 4:Y:316:GLU:CD[1_556]  | 2.00                     | 0.20              |
| 4:1:72:GLU:CG   | 4:Y:157:ASP:OD2[1_556] | 2.00                     | 0.20              |
| 4:2:79:TRP:CA   | 4:Z:17:VAL:O[1_556]    | 2.00                     | 0.20              |
| 4:2:80:ASP:C    | 4:Z:31:PHE:CG[1_556]   | 2.00                     | 0.20              |
| 4:0:80:ASP:C    | 4:X:31:PHE:CG[1_556]   | 2.00                     | 0.20              |
| 4:0:104:LEU:N   | 4:X:334:GLU:CG[1_556]  | 2.00                     | 0.20              |
| 4:1:147:ARG:C   | 4:Y:314:GLN:CD[1_556]  | 2.00                     | 0.20              |
| 4:0:119:MET:N   | 4:X:340:TRP:CB[1_556]  | 2.00                     | 0.20              |
| 4:1:281:SER:CB  | 4:Y:276:GLU:CA[1_556]  | 2.00                     | 0.20              |
| 4:2:294:TYR:O   | 4:Z:319:ALA:CB[1_556]  | 2.00                     | 0.20              |
| 4:2:121:GLN:CB  | 4:Z:9:VAL:CA[1_556]    | 2.00                     | 0.20              |
| 4:2:306:TYR:C   | 4:Z:255:PHE:CE1[1_556] | 2.00                     | 0.20              |
| 4:0:78:ASN:CA   | 4:X:31:PHE:O[1_556]    | 2.00                     | 0.20              |
| 4:2:173:HIS:CG  | 4:Z:174:ALA:O[1_556]   | 2.00                     | 0.20              |
| 4:0:121:GLN:CB  | 4:X:9:VAL:CA[1_556]    | 2.00                     | 0.20              |
| 4:0:106:THR:OG1 | 4:X:305:MET:SD[1_556]  | 2.00                     | 0.20              |
| 4:0:69:TYR:CE2  | 4:X:210:ARG:CG[1_556]  | 2.00                     | 0.20              |
| 4:1:335:ARG:CB  | 4:Y:220:ALA:CA[1_556]  | 2.00                     | 0.20              |
| 4:2:298:VAL:CG1 | 4:Z:311:ASP:O[1_556]   | 2.00                     | 0.20              |
| 4:0:175:ILE:CG1 | 4:X:162:ASN:OD1[1_556] | 2.00                     | 0.20              |
| 4:1:369:ILE:N   | 4:Y:346:LEU:CG[1_556]  | 2.00                     | 0.20              |
| 4:2:184:ASP:C   | 4:Z:188:TYR:CA[1_556]  | 2.00                     | 0.20              |
| 4:1:165:ILE:N   | 4:Y:297:ASN:OD1[1_556] | 2.00                     | 0.20              |
| 4:2:69:TYR:CE2  | 4:Z:210:ARG:CG[1_556]  | 2.01                     | 0.19              |
| 4:1:125:GLU:CD  | 4:Y:7:ALA:O[1_556]     | 2.01                     | 0.19              |
| 4:2:264:PRO:CB  | 4:Z:268:GLY:O[1_556]   | 2.01                     | 0.19              |
| 4:2:134:VAL:CG2 | 4:Z:337:TYR:O[1_556]   | 2.01                     | 0.19              |
| 4:2:294:TYR:C   | 4:Z:319:ALA:CB[1_556]  | 2.01                     | 0.19              |
| 4:1:292:ASP:OD2 | 4:Y:322:PRO:O[1_556]   | 2.01                     | 0.19              |
| 4:2:215:LYS:CA  | 4:Z:196:ARG:NH1[1_556] | 2.01                     | 0.19              |
| 4:2:167:GLU:N   | 4:Z:295:ALA:CA[1_556]  | 2.01                     | 0.19              |
| 4:0:155:SER:N   | 4:X:261:LEU:CD1[1_556] | 2.01                     | 0.19              |
| 4:2:195:GLU:N   | 4:Y:75:ILE:CD1[1_556]  | 2.01                     | 0.19              |
| 4:1:66:THR:CB   | 4:Y:62:ARG:N[1_556]    | 2.01                     | 0.19              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:372:ARG:N   | 4:X:143:TYR:CG[1_556]  | 2.01                     | 0.19              |
| 4:2:79:TRP:O    | 4:Z:31:PHE:CD1[1_556]  | 2.01                     | 0.19              |
| 4:0:214:GLU:CB  | 4:X:253:GLU:OE2[1_556] | 2.01                     | 0.19              |
| 4:0:173:HIS:CG  | 4:X:174:ALA:O[1_556]   | 2.01                     | 0.19              |
| 4:0:282:ILE:O   | 4:X:279:TYR:CD2[1_556] | 2.01                     | 0.19              |
| 4:1:213:LYS:CA  | 4:Y:192:ILE:O[1_556]   | 2.01                     | 0.19              |
| 4:1:198:TYR:N   | 4:X:75:ILE:CA[1_556]   | 2.01                     | 0.19              |
| 4:3:232:SER:N   | 4:Z:369:ILE:CA[1_556]  | 2.01                     | 0.19              |
| 4:2:162:ASN:N   | 4:Z:274:ILE:CD1[1_556] | 2.01                     | 0.19              |
| 4:0:305:MET:N   | 4:X:255:PHE:CB[1_556]  | 2.01                     | 0.19              |
| 4:0:153:LEU:C   | 4:X:262:PHE:CE2[1_556] | 2.01                     | 0.19              |
| 4:1:307:PRO:CG  | 4:Y:227:MET:CA[1_556]  | 2.01                     | 0.19              |
| 4:1:301:GLY:CA  | 4:Y:258:PRO:CB[1_556]  | 2.01                     | 0.19              |
| 4:3:253:GLU:CG  | 4:Z:112:PRO:CB[1_556]  | 2.01                     | 0.19              |
| 4:0:362:TYR:CG  | 4:X:23:GLY:N[1_556]    | 2.01                     | 0.19              |
| 4:1:33:SER:OG   | 4:Y:210:ARG:NH1[1_556] | 2.01                     | 0.19              |
| 4:2:291:LYS:CD  | 4:Z:322:PRO:CB[1_556]  | 2.01                     | 0.19              |
| 4:2:73:HIS:O    | 4:Z:181:ALA:CB[1_556]  | 2.01                     | 0.19              |
| 4:1:129:VAL:CG2 | 4:Y:25:ASP:C[1_556]    | 2.01                     | 0.19              |
| 4:0:277:THR:CB  | 4:X:273:GLY:N[1_556]   | 2.01                     | 0.19              |
| 4:0:148:THR:CB  | 4:X:328:LYS:N[1_556]   | 2.01                     | 0.19              |
| 4:1:40:HIS:CG   | 4:W:166:TYR:CD1[1_556] | 2.01                     | 0.19              |
| 4:0:231:ALA:CB  | 4:W:369:ILE:O[1_556]   | 2.01                     | 0.19              |
| 4:2:37:ARG:C    | 4:Z:60:SER:CB[1_556]   | 2.01                     | 0.19              |
| 4:0:147:ARG:C   | 4:X:314:GLN:CD[1_556]  | 2.01                     | 0.19              |
| 4:2:207:GLU:CA  | 4:Z:200:PHE:CD1[1_556] | 2.01                     | 0.19              |
| 4:2:106:THR:OG1 | 4:Z:305:MET:SD[1_556]  | 2.01                     | 0.19              |
| 4:2:274:ILE:N   | 4:Z:264:PRO:CD[1_556]  | 2.01                     | 0.19              |
| 4:2:139:VAL:CG1 | 4:Z:330:ILE:N[1_556]   | 2.01                     | 0.19              |
| 4:1:265:SER:O   | 4:X:173:HIS:ND1[1_556] | 2.01                     | 0.19              |
| 4:2:371:HIS:N   | 4:Z:342:GLY:O[1_556]   | 2.01                     | 0.19              |
| 4:1:125:GLU:N   | 4:Y:21:PHE:O[1_556]    | 2.01                     | 0.19              |
| 4:2:117:GLU:CB  | 4:Z:104:LEU:CD2[1_556] | 2.01                     | 0.19              |
| 4:0:113:LYS:N   | 4:X:137:GLN:CG[1_556]  | 2.01                     | 0.19              |
| 4:1:32:PRO:CA   | 4:Y:211:ASP:CA[1_556]  | 2.01                     | 0.19              |
| 4:0:270:GLU:CG  | 4:W:286:ASP:N[1_556]   | 2.01                     | 0.19              |
| 4:0:60:SER:CB   | 4:X:243:PRO:CB[1_556]  | 2.01                     | 0.19              |
| 4:2:274:ILE:CG1 | 4:Z:263:GLN:O[1_556]   | 2.01                     | 0.19              |
| 4:1:336:LYS:CD  | 4:Y:218:TYR:CE1[1_556] | 2.01                     | 0.19              |
| 4:2:296:ASN:CA  | 4:Z:315:LYS:C[1_556]   | 2.01                     | 0.19              |
| 4:2:104:LEU:N   | 4:Z:334:GLU:CG[1_556]  | 2.01                     | 0.19              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:211:ASP:C   | 4:X:196:ARG:NE[1_556]  | 2.01                     | 0.19              |
| 4:1:172:PRO:CA  | 4:Y:162:ASN:O[1_556]   | 2.01                     | 0.19              |
| 4:0:76:ILE:O    | 4:X:16:LEU:O[1_556]    | 2.01                     | 0.19              |
| 4:1:70:PRO:O    | 4:Y:15:GLY:O[1_556]    | 2.01                     | 0.19              |
| 4:1:189:LEU:CD2 | 4:Y:196:ARG:N[1_556]   | 2.01                     | 0.19              |
| 4:1:41:GLN:CB   | 4:W:167:GLU:OE1[1_556] | 2.01                     | 0.19              |
| 4:2:194:THR:O   | 4:Y:75:ILE:CD1[1_556]  | 2.01                     | 0.19              |
| 4:1:208:ILE:CD1 | 4:Y:198:TYR:CE1[1_556] | 2.01                     | 0.19              |
| 4:0:266:PHE:CB  | 4:W:172:PRO:CG[1_556]  | 2.01                     | 0.19              |
| 4:0:311:ASP:OD1 | 4:X:224:GLU:OE2[1_556] | 2.01                     | 0.19              |
| 4:0:62:ARG:CZ   | 4:X:204:ALA:O[1_556]   | 2.01                     | 0.19              |
| 4:2:367:PRO:N   | 4:Z:343:GLY:O[1_556]   | 2.01                     | 0.19              |
| 4:0:294:TYR:C   | 4:X:319:ALA:CA[1_556]  | 2.01                     | 0.19              |
| 4:1:107:GLU:CA  | 4:Y:301:GLY:CA[1_556]  | 2.01                     | 0.19              |
| 4:1:122:ILE:C   | 4:Y:27:PRO:CA[1_556]   | 2.01                     | 0.19              |
| 4:2:119:MET:N   | 4:Z:340:TRP:CB[1_556]  | 2.01                     | 0.19              |
| 4:0:134:VAL:CG2 | 4:X:337:TYR:O[1_556]   | 2.01                     | 0.19              |
| 4:2:111:ASN:CB  | 4:Z:154:ASP:CG[1_556]  | 2.01                     | 0.19              |
| 4:0:274:ILE:CG1 | 4:X:263:GLN:O[1_556]   | 2.01                     | 0.19              |
| 4:2:194:THR:C   | 4:Y:75:ILE:CD1[1_556]  | 2.01                     | 0.19              |
| 4:1:74:GLY:CA   | 4:Y:157:ASP:N[1_556]   | 2.01                     | 0.19              |
| 4:1:292:ASP:OD2 | 4:Y:325:MET:CB[1_556]  | 2.01                     | 0.19              |
| 4:0:233:SER:O   | 4:W:367:PRO:N[1_556]   | 2.01                     | 0.19              |
| 4:0:281:SER:OG  | 4:X:276:GLU:O[1_556]   | 2.01                     | 0.19              |
| 4:2:138:ALA:O   | 4:Z:299:MET:CE[1_556]  | 2.01                     | 0.19              |
| 4:1:166:TYR:CD2 | 4:Y:290:ARG:O[1_556]   | 2.01                     | 0.19              |
| 4:1:122:ILE:O   | 4:Y:26:ALA:O[1_556]    | 2.01                     | 0.19              |
| 4:3:231:ALA:CB  | 4:Z:369:ILE:O[1_556]   | 2.01                     | 0.19              |
| 4:1:211:ASP:OD1 | 4:Y:249:THR:CG2[1_556] | 2.01                     | 0.19              |
| 4:0:122:ILE:CG2 | 4:X:27:PRO:CA[1_556]   | 2.01                     | 0.19              |
| 4:1:169:TYR:CG  | 4:Y:150:GLY:CA[1_556]  | 2.01                     | 0.19              |
| 4:1:72:GLU:OE1  | 4:Y:183:ARG:NH1[1_556] | 2.01                     | 0.19              |
| 4:1:118:LYS:CE  | 4:Y:10:CYS:CA[1_556]   | 2.01                     | 0.19              |
| 4:1:265:SER:C   | 4:X:173:HIS:NE2[1_556] | 2.01                     | 0.19              |
| 4:0:337:TYR:C   | 4:X:307:PRO:C[1_556]   | 2.01                     | 0.19              |
| 4:2:123:MET:N   | 4:Z:27:PRO:N[1_556]    | 2.01                     | 0.19              |
| 4:2:155:SER:O   | 4:Z:258:PRO:N[1_556]   | 2.01                     | 0.19              |
| 4:1:114:ALA:CB  | 4:Y:107:GLU:N[1_556]   | 2.01                     | 0.19              |
| 4:1:148:THR:N   | 4:Y:314:GLN:NE2[1_556] | 2.01                     | 0.19              |
| 4:2:166:TYR:CD2 | 4:Z:294:TYR:CB[1_556]  | 2.01                     | 0.19              |
| 4:1:181:ALA:CB  | 4:Y:185:LEU:CG[1_556]  | 2.01                     | 0.19              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:37:ARG:C    | 4:X:60:SER:CB[1_556]   | 2.01                     | 0.19              |
| 4:2:281:SER:C   | 4:Z:280:ASN:ND2[1_556] | 2.01                     | 0.19              |
| 4:1:304:THR:CG2 | 4:Y:259:GLU:N[1_556]   | 2.01                     | 0.19              |
| 4:1:366:GLY:CA  | 4:Y:348:SER:N[1_556]   | 2.01                     | 0.19              |
| 4:2:113:LYS:N   | 4:Z:137:GLN:CG[1_556]  | 2.01                     | 0.19              |
| 4:0:184:ASP:CA  | 4:X:188:TYR:N[1_556]   | 2.01                     | 0.19              |
| 4:1:86:TRP:CG   | 4:Y:337:TYR:OH[1_556]  | 2.01                     | 0.19              |
| 4:2:72:GLU:CG   | 4:Z:183:ARG:NE[1_556]  | 2.01                     | 0.19              |
| 4:0:292:ASP:CA  | 4:X:318:THR:O[1_556]   | 2.01                     | 0.19              |
| 4:2:73:HIS:C    | 4:Z:156:GLY:C[1_556]   | 2.01                     | 0.19              |
| 4:2:124:PHE:CB  | 4:Z:24:ASP:C[1_556]    | 2.01                     | 0.19              |
| 4:0:294:TYR:C   | 4:X:319:ALA:CB[1_556]  | 2.01                     | 0.19              |
| 4:1:174:ALA:CB  | 4:Y:281:SER:CA[1_556]  | 2.01                     | 0.19              |
| 4:1:207:GLU:CD  | 4:Y:242:LEU:CG[1_556]  | 2.01                     | 0.19              |
| 4:2:254:ARG:CA  | 4:Y:113:LYS:NZ[1_556]  | 2.01                     | 0.19              |
| 4:2:180:LEU:CD1 | 4:Z:267:ILE:N[1_556]   | 2.01                     | 0.19              |
| 4:0:332:PRO:CD  | 4:X:221:LEU:CA[1_556]  | 2.01                     | 0.19              |
| 4:0:338:SER:CA  | 4:X:308:GLY:CA[1_556]  | 2.01                     | 0.19              |
| 4:1:115:ASN:OD1 | 4:Y:12:ASN:O[1_556]    | 2.01                     | 0.19              |
| 4:2:175:ILE:CG1 | 4:Z:162:ASN:OD1[1_556] | 2.01                     | 0.19              |
| 4:1:155:SER:O   | 4:Y:258:PRO:N[1_556]   | 2.01                     | 0.19              |
| 4:1:174:ALA:CA  | 4:Y:281:SER:N[1_556]   | 2.01                     | 0.19              |
| 4:2:231:ALA:CB  | 4:Y:369:ILE:O[1_556]   | 2.01                     | 0.19              |
| 4:1:213:LYS:NZ  | 4:Y:189:LEU:CD1[1_556] | 2.01                     | 0.19              |
| 4:1:366:GLY:N   | 4:Y:347:ALA:CA[1_556]  | 2.01                     | 0.19              |
| 4:2:303:THR:O   | 4:Z:255:PHE:O[1_556]   | 2.01                     | 0.19              |
| 4:0:79:TRP:O    | 4:X:31:PHE:CD1[1_556]  | 2.01                     | 0.19              |
| 4:0:362:TYR:O   | 4:X:348:SER:N[1_556]   | 2.01                     | 0.19              |
| 4:2:177:ARG:CZ  | 4:Z:159:VAL:C[1_556]   | 2.01                     | 0.19              |
| 4:2:137:GLN:CD  | 4:Z:304:THR:OG1[1_556] | 2.01                     | 0.19              |
| 4:2:132:MET:SD  | 4:Z:341:ILE:CG1[1_556] | 2.01                     | 0.19              |
| 4:2:272:ALA:N   | 4:Z:271:SER:N[1_556]   | 2.01                     | 0.19              |
| 4:2:279:TYR:CA  | 4:Z:276:GLU:OE2[1_556] | 2.01                     | 0.19              |
| 4:2:233:SER:CA  | 4:Y:367:PRO:C[1_556]   | 2.01                     | 0.19              |
| 4:0:166:TYR:CZ  | 4:X:325:MET:CG[1_556]  | 2.02                     | 0.18              |
| 4:3:270:GLU:OE2 | 4:Z:286:ASP:N[1_556]   | 2.02                     | 0.18              |
| 4:0:208:ILE:CA  | 4:X:198:TYR:CD2[1_556] | 2.02                     | 0.18              |
| 4:0:183:ARG:CD  | 4:X:187:ASP:N[1_556]   | 2.02                     | 0.18              |
| 4:2:41:GLN:O    | 4:X:148:THR:OG1[1_556] | 2.02                     | 0.18              |
| 4:0:282:ILE:C   | 4:X:280:ASN:ND2[1_556] | 2.02                     | 0.18              |
| 4:1:231:ALA:CB  | 4:X:369:ILE:O[1_556]   | 2.02                     | 0.18              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:153:LEU:C   | 4:Z:262:PHE:CE2[1_556] | 2.02                     | 0.18              |
| 4:0:264:PRO:CB  | 4:X:268:GLY:O[1_556]   | 2.02                     | 0.18              |
| 4:2:123:MET:CG  | 4:Z:26:ALA:C[1_556]    | 2.02                     | 0.18              |
| 4:0:293:LEU:N   | 4:X:320:LEU:C[1_556]   | 2.02                     | 0.18              |
| 4:1:362:TYR:CG  | 4:Y:23:GLY:N[1_556]    | 2.02                     | 0.18              |
| 4:0:137:GLN:CD  | 4:X:304:THR:OG1[1_556] | 2.02                     | 0.18              |
| 4:2:148:THR:CB  | 4:Z:328:LYS:N[1_556]   | 2.02                     | 0.18              |
| 4:1:206:ARG:O   | 4:Y:200:PHE:CD2[1_556] | 2.02                     | 0.18              |
| 4:1:364:GLU:C   | 4:Y:349:LEU:O[1_556]   | 2.02                     | 0.18              |
| 4:1:197:GLY:CA  | 4:X:75:ILE:N[1_556]    | 2.02                     | 0.18              |
| 4:2:40:HIS:N    | 4:X:166:TYR:CE2[1_556] | 2.02                     | 0.18              |
| 4:0:198:TYR:O   | 4:W:72:GLU:O[1_556]    | 2.02                     | 0.18              |
| 4:1:120:THR:CG2 | 4:Y:344:SER:CA[1_556]  | 2.02                     | 0.18              |
| 4:1:114:ALA:O   | 4:Y:106:THR:OG1[1_556] | 2.02                     | 0.18              |
| 4:0:151:ILE:CD1 | 4:X:276:GLU:CA[1_556]  | 2.02                     | 0.18              |
| 4:1:62:ARG:CZ   | 4:Y:204:ALA:O[1_556]   | 2.02                     | 0.18              |
| 4:2:292:ASP:CA  | 4:Z:318:THR:O[1_556]   | 2.02                     | 0.18              |
| 4:0:162:ASN:N   | 4:X:274:ILE:CD1[1_556] | 2.02                     | 0.18              |
| 4:2:72:GLU:C    | 4:Z:157:ASP:OD2[1_556] | 2.02                     | 0.18              |
| 4:0:141:SER:C   | 4:X:310:ALA:N[1_556]   | 2.02                     | 0.18              |
| 4:0:211:ASP:CA  | 4:X:249:THR:O[1_556]   | 2.02                     | 0.18              |
| 4:0:307:PRO:CG  | 4:X:227:MET:CA[1_556]  | 2.02                     | 0.18              |
| 4:3:196:ARG:NH1 | 4:Z:114:ALA:C[1_556]   | 2.02                     | 0.18              |
| 4:1:183:ARG:C   | 4:Y:187:ASP:CA[1_556]  | 2.02                     | 0.18              |
| 4:1:214:GLU:O   | 4:Y:253:GLU:N[1_556]   | 2.02                     | 0.18              |
| 4:2:169:TYR:CD2 | 4:Z:293:LEU:CD1[1_556] | 2.02                     | 0.18              |
| 4:0:233:SER:C   | 4:W:366:GLY:C[1_556]   | 2.02                     | 0.18              |
| 4:2:185:LEU:CA  | 4:Z:188:TYR:O[1_556]   | 2.02                     | 0.18              |
| 4:2:372:ARG:NE  | 4:Z:143:TYR:N[1_556]   | 2.02                     | 0.18              |
| 4:3:265:SER:O   | 4:Z:173:HIS:ND1[1_556] | 2.02                     | 0.18              |
| 4:1:214:GLU:CB  | 4:Y:253:GLU:OE2[1_556] | 2.02                     | 0.18              |
| 4:2:122:ILE:CG2 | 4:Z:27:PRO:CA[1_556]   | 2.02                     | 0.18              |
| 4:1:118:LYS:CD  | 4:Y:10:CYS:C[1_556]    | 2.02                     | 0.18              |
| 4:0:296:ASN:CA  | 4:X:315:LYS:C[1_556]   | 2.02                     | 0.18              |
| 4:2:299:MET:CG  | 4:Z:312:ARG:NH2[1_556] | 2.02                     | 0.18              |
| 4:1:290:ARG:CA  | 4:Y:320:LEU:O[1_556]   | 2.02                     | 0.18              |
| 4:0:299:MET:O   | 4:X:312:ARG:CG[1_556]  | 2.02                     | 0.18              |
| 4:1:278:THR:C   | 4:Y:276:GLU:CB[1_556]  | 2.02                     | 0.18              |
| 4:2:123:MET:CE  | 4:Z:27:PRO:CD[1_556]   | 2.02                     | 0.18              |
| 4:2:123:MET:O   | 4:Z:26:ALA:O[1_556]    | 2.02                     | 0.18              |
| 4:2:32:PRO:CA   | 4:Z:211:ASP:CA[1_556]  | 2.02                     | 0.18              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:112:PRO:O   | 4:Y:137:GLN:CD[1_556]  | 2.02                     | 0.18              |
| 4:2:211:ASP:CA  | 4:Z:249:THR:O[1_556]   | 2.02                     | 0.18              |
| 4:1:157:ASP:C   | 4:Y:186:THR:N[1_556]   | 2.02                     | 0.18              |
| 4:0:81:ASP:CB   | 4:X:32:PRO:N[1_556]    | 2.02                     | 0.18              |
| 4:0:294:TYR:O   | 4:X:319:ALA:CB[1_556]  | 2.02                     | 0.18              |
| 4:0:180:LEU:CD2 | 4:X:267:ILE:O[1_556]   | 2.02                     | 0.18              |
| 4:1:138:ALA:O   | 4:Y:299:MET:CE[1_556]  | 2.02                     | 0.18              |
| 4:2:372:ARG:NE  | 4:Z:143:TYR:CA[1_556]  | 2.02                     | 0.18              |
| 4:2:262:PHE:C   | 4:Z:265:SER:CB[1_556]  | 2.02                     | 0.18              |
| 4:0:184:ASP:C   | 4:X:188:TYR:CA[1_556]  | 2.02                     | 0.18              |
| 4:0:372:ARG:NE  | 4:X:143:TYR:N[1_556]   | 2.02                     | 0.18              |
| 4:1:296:ASN:CA  | 4:Y:315:LYS:C[1_556]   | 2.02                     | 0.18              |
| 4:3:195:GLU:N   | 4:Z:75:ILE:CD1[1_556]  | 2.02                     | 0.18              |
| 4:1:121:GLN:C   | 4:Y:340:TRP:CH2[1_556] | 2.02                     | 0.18              |
| 4:2:148:THR:O   | 4:Z:328:LYS:CA[1_556]  | 2.02                     | 0.18              |
| 4:1:173:HIS:ND1 | 4:Y:174:ALA:CB[1_556]  | 2.02                     | 0.18              |
| 4:1:116:ARG:CD  | 4:Y:141:SER:CA[1_556]  | 2.02                     | 0.18              |
| 4:2:335:ARG:CB  | 4:Z:220:ALA:CA[1_556]  | 2.02                     | 0.18              |
| 4:1:338:SER:CA  | 4:Y:308:GLY:CA[1_556]  | 2.02                     | 0.18              |
| 4:0:86:TRP:CG   | 4:X:337:TYR:OH[1_556]  | 2.02                     | 0.18              |
| 4:2:168:GLY:O   | 4:Z:296:ASN:O[1_556]   | 2.02                     | 0.18              |
| 4:0:12:ASN:ND2  | 4:X:336:LYS:CD[1_556]  | 2.02                     | 0.18              |
| 4:1:272:ALA:CA  | 4:Y:270:GLU:N[1_556]   | 2.02                     | 0.18              |
| 4:1:73:HIS:N    | 4:Y:157:ASP:CA[1_556]  | 2.02                     | 0.18              |
| 4:2:155:SER:O   | 4:Z:258:PRO:CG[1_556]  | 2.02                     | 0.18              |
| 4:2:11:ASP:CG   | 4:Z:305:MET:CA[1_556]  | 2.02                     | 0.18              |
| 4:1:370:VAL:CG2 | 4:Y:342:GLY:N[1_556]   | 2.02                     | 0.18              |
| 4:1:279:TYR:N   | 4:Y:276:GLU:CG[1_556]  | 2.02                     | 0.18              |
| 4:2:270:GLU:CG  | 4:Y:286:ASP:N[1_556]   | 2.02                     | 0.18              |
| 4:2:105:LEU:CA  | 4:Z:334:GLU:CB[1_556]  | 2.02                     | 0.18              |
| 4:1:162:ASN:CA  | 4:Y:274:ILE:CB[1_556]  | 2.02                     | 0.18              |
| 4:1:292:ASP:OD1 | 4:Y:322:PRO:O[1_556]   | 2.02                     | 0.18              |
| 4:2:185:LEU:CG  | 4:Z:188:TYR:CE2[1_556] | 2.02                     | 0.18              |
| 4:1:136:ILE:CD1 | 4:Y:152:VAL:CG1[1_556] | 2.02                     | 0.18              |
| 4:1:292:ASP:CB  | 4:Y:321:ALA:C[1_556]   | 2.02                     | 0.18              |
| 4:1:180:LEU:CD1 | 4:Y:267:ILE:CA[1_556]  | 2.02                     | 0.18              |
| 4:2:12:ASN:ND2  | 4:Z:336:LYS:CD[1_556]  | 2.02                     | 0.18              |
| 4:2:122:ILE:C   | 4:Z:27:PRO:CA[1_556]   | 2.02                     | 0.18              |
| 4:0:12:ASN:CG   | 4:X:336:LYS:CB[1_556]  | 2.02                     | 0.18              |
| 4:0:16:LEU:CD2  | 4:X:212:ILE:O[1_556]   | 2.02                     | 0.18              |
| 4:2:236:LEU:CG  | 4:Y:117:GLU:OE1[1_556] | 2.02                     | 0.18              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:163:VAL:O   | 4:Y:278:THR:OG1[1_556] | 2.02                     | 0.18              |
| 4:1:289:ILE:CG2 | 4:Y:294:TYR:CE2[1_556] | 2.02                     | 0.18              |
| 4:0:279:TYR:CA  | 4:X:276:GLU:OE2[1_556] | 2.02                     | 0.18              |
| 4:1:283:MET:N   | 4:Y:280:ASN:ND2[1_556] | 2.02                     | 0.18              |
| 4:1:207:GLU:OE1 | 4:Y:242:LEU:CD1[1_556] | 2.02                     | 0.18              |
| 4:0:207:GLU:CA  | 4:X:200:PHE:CD1[1_556] | 2.02                     | 0.18              |
| 4:2:151:ILE:CD1 | 4:Z:276:GLU:CA[1_556]  | 2.02                     | 0.18              |
| 4:0:233:SER:CA  | 4:W:367:PRO:C[1_556]   | 2.02                     | 0.18              |
| 4:1:213:LYS:CG  | 4:Y:192:ILE:CG1[1_556] | 2.02                     | 0.18              |
| 4:1:147:ARG:N   | 4:Y:314:GLN:NE2[1_556] | 2.02                     | 0.18              |
| 4:1:137:GLN:CB  | 4:Y:304:THR:CA[1_556]  | 2.02                     | 0.18              |
| 4:1:365:ALA:CB  | 4:Y:349:LEU:CG[1_556]  | 2.02                     | 0.18              |
| 4:1:153:LEU:CD2 | 4:Y:262:PHE:CA[1_556]  | 2.02                     | 0.18              |
| 4:0:169:TYR:CD2 | 4:X:293:LEU:CD1[1_556] | 2.02                     | 0.18              |
| 4:4:40:HIS:N    | 4:Z:166:TYR:CE2[1_556] | 2.02                     | 0.18              |
| 4:1:81:ASP:OD1  | 4:Y:56:ASP:OD2[1_556]  | 2.02                     | 0.18              |
| 4:2:289:ILE:CB  | 4:Z:294:TYR:CZ[1_556]  | 2.02                     | 0.18              |
| 4:2:180:LEU:CD2 | 4:Z:267:ILE:O[1_556]   | 2.02                     | 0.18              |
| 4:0:370:VAL:O   | 4:X:144:ALA:N[1_556]   | 2.02                     | 0.18              |
| 4:1:148:THR:CG2 | 4:Y:328:LYS:CA[1_556]  | 2.02                     | 0.18              |
| 4:1:167:GLU:OE2 | 4:Y:326:LYS:CG[1_556]  | 2.02                     | 0.18              |
| 4:0:123:MET:CE  | 4:X:27:PRO:CD[1_556]   | 2.02                     | 0.18              |
| 4:1:196:ARG:NH1 | 4:X:115:ASN:CB[1_556]  | 2.02                     | 0.18              |
| 4:2:81:ASP:CB   | 4:Z:32:PRO:N[1_556]    | 2.02                     | 0.18              |
| 4:0:306:TYR:C   | 4:X:255:PHE:CE1[1_556] | 2.02                     | 0.18              |
| 4:2:262:PHE:CA  | 4:Z:265:SER:OG[1_556]  | 2.02                     | 0.18              |
| 4:0:292:ASP:CB  | 4:X:321:ALA:CA[1_556]  | 2.02                     | 0.18              |
| 4:2:281:SER:OG  | 4:Z:276:GLU:O[1_556]   | 2.02                     | 0.18              |
| 4:1:11:ASP:OD1  | 4:Y:305:MET:CA[1_556]  | 2.02                     | 0.18              |
| 4:2:141:SER:C   | 4:Z:310:ALA:N[1_556]   | 2.02                     | 0.18              |
| 4:1:370:VAL:CG1 | 4:Y:342:GLY:O[1_556]   | 2.02                     | 0.18              |
| 4:1:194:THR:C   | 4:X:75:ILE:CD1[1_556]  | 2.02                     | 0.18              |
| 4:2:147:ARG:C   | 4:Z:314:GLN:CD[1_556]  | 2.02                     | 0.18              |
| 4:0:168:GLY:O   | 4:X:296:ASN:O[1_556]   | 2.02                     | 0.18              |
| 4:2:196:ARG:CG  | 4:Y:115:ASN:CB[1_556]  | 2.02                     | 0.18              |
| 4:0:183:ARG:CB  | 4:X:187:ASP:CA[1_556]  | 2.02                     | 0.18              |
| 4:1:196:ARG:NH1 | 4:X:114:ALA:C[1_556]   | 2.02                     | 0.18              |
| 4:2:278:THR:C   | 4:Z:276:GLU:CB[1_556]  | 2.02                     | 0.18              |
| 4:0:303:THR:O   | 4:X:255:PHE:O[1_556]   | 2.02                     | 0.18              |
| 4:1:202:THR:O   | 4:Y:201:VAL:CG2[1_556] | 2.02                     | 0.18              |
| 4:2:307:PRO:C   | 4:Z:227:MET:CA[1_556]  | 2.02                     | 0.18              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:185:LEU:CB  | 4:Y:188:TYR:CG[1_556]  | 2.02                     | 0.18              |
| 4:1:82:MET:C    | 4:Y:30:VAL:CA[1_556]   | 2.02                     | 0.18              |
| 4:1:176:MET:C   | 4:Y:178:LEU:CB[1_556]  | 2.02                     | 0.18              |
| 4:2:37:ARG:CZ   | 4:Z:57:GLU:N[1_556]    | 2.02                     | 0.18              |
| 4:1:261:LEU:O   | 4:Y:265:SER:CB[1_556]  | 2.02                     | 0.18              |
| 4:2:232:SER:O   | 4:Y:366:GLY:C[1_556]   | 2.02                     | 0.18              |
| 4:0:177:ARG:CZ  | 4:X:159:VAL:C[1_556]   | 2.02                     | 0.18              |
| 4:0:37:ARG:CZ   | 4:X:57:GLU:N[1_556]    | 2.02                     | 0.18              |
| 4:2:73:HIS:O    | 4:Z:156:GLY:O[1_556]   | 2.03                     | 0.17              |
| 4:0:261:LEU:CG  | 4:X:266:PHE:CD1[1_556] | 2.03                     | 0.17              |
| 4:3:194:THR:O   | 4:Z:75:ILE:CD1[1_556]  | 2.03                     | 0.17              |
| 4:2:211:ASP:C   | 4:Z:196:ARG:NE[1_556]  | 2.03                     | 0.17              |
| 4:1:113:LYS:N   | 4:Y:137:GLN:CG[1_556]  | 2.03                     | 0.17              |
| 4:0:80:ASP:N    | 4:X:31:PHE:CB[1_556]   | 2.03                     | 0.17              |
| 4:0:167:GLU:N   | 4:X:295:ALA:CA[1_556]  | 2.03                     | 0.17              |
| 4:2:266:PHE:CB  | 4:Y:172:PRO:CG[1_556]  | 2.03                     | 0.17              |
| 4:0:117:GLU:CB  | 4:X:104:LEU:CD2[1_556] | 2.03                     | 0.17              |
| 4:1:108:ALA:CB  | 4:Y:155:SER:O[1_556]   | 2.03                     | 0.17              |
| 4:1:162:ASN:CA  | 4:Y:275:HIS:N[1_556]   | 2.03                     | 0.17              |
| 4:1:175:ILE:CD1 | 4:Y:162:ASN:CG[1_556]  | 2.03                     | 0.17              |
| 4:3:41:GLN:N    | 4:Y:167:GLU:CG[1_556]  | 2.03                     | 0.17              |
| 4:2:139:VAL:CG2 | 4:Z:298:VAL:C[1_556]   | 2.03                     | 0.17              |
| 4:2:60:SER:CB   | 4:Z:243:PRO:CB[1_556]  | 2.03                     | 0.17              |
| 4:0:339:VAL:O   | 4:X:335:ARG:NH2[1_556] | 2.03                     | 0.17              |
| 4:0:155:SER:O   | 4:X:258:PRO:CG[1_556]  | 2.03                     | 0.17              |
| 4:0:310:ALA:CB  | 4:X:224:GLU:N[1_556]   | 2.03                     | 0.17              |
| 4:2:297:ASN:N   | 4:Z:316:GLU:N[1_556]   | 2.03                     | 0.17              |
| 4:3:228:ALA:O   | 4:Z:369:ILE:C[1_556]   | 2.03                     | 0.17              |
| 4:2:162:ASN:ND2 | 4:Z:273:GLY:CA[1_556]  | 2.03                     | 0.17              |
| 4:1:307:PRO:CB  | 4:Y:227:MET:O[1_556]   | 2.03                     | 0.17              |
| 4:1:208:ILE:CA  | 4:Y:198:TYR:CD2[1_556] | 2.03                     | 0.17              |
| 4:0:14:SER:CB   | 4:X:213:LYS:NZ[1_556]  | 2.03                     | 0.17              |
| 4:1:136:ILE:CG2 | 4:Y:299:MET:CA[1_556]  | 2.03                     | 0.17              |
| 4:0:162:ASN:ND2 | 4:X:273:GLY:CA[1_556]  | 2.03                     | 0.17              |
| 4:0:369:ILE:CD1 | 4:X:143:TYR:OH[1_556]  | 2.03                     | 0.17              |
| 4:1:179:ASP:CA  | 4:Y:180:LEU:CA[1_556]  | 2.03                     | 0.17              |
| 4:2:71:ILE:O    | 4:Z:157:ASP:CG[1_556]  | 2.03                     | 0.17              |
| 4:0:307:PRO:C   | 4:X:227:MET:CA[1_556]  | 2.03                     | 0.17              |
| 4:1:279:TYR:CA  | 4:Y:276:GLU:OE2[1_556] | 2.03                     | 0.17              |
| 4:1:125:GLU:O   | 4:Y:21:PHE:CD1[1_556]  | 2.03                     | 0.17              |
| 4:2:298:VAL:C   | 4:Z:312:ARG:CA[1_556]  | 2.03                     | 0.17              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:118:LYS:CG  | 4:Z:10:CYS:C[1_556]    | 2.03                     | 0.17              |
| 4:1:123:MET:N   | 4:Y:27:PRO:N[1_556]    | 2.03                     | 0.17              |
| 4:0:179:ASP:CA  | 4:X:180:LEU:CB[1_556]  | 2.03                     | 0.17              |
| 4:0:332:PRO:CG  | 4:X:221:LEU:CB[1_556]  | 2.03                     | 0.17              |
| 4:0:195:GLU:OE1 | 4:W:111:ASN:N[1_556]   | 2.03                     | 0.17              |
| 4:3:196:ARG:CG  | 4:Z:115:ASN:CB[1_556]  | 2.03                     | 0.17              |
| 4:1:251:GLY:CA  | 4:X:114:ALA:CB[1_556]  | 2.03                     | 0.17              |
| 4:0:195:GLU:CA  | 4:W:75:ILE:CD1[1_556]  | 2.03                     | 0.17              |
| 4:1:357:ILE:CG2 | 4:Y:345:ILE:CD1[1_556] | 2.03                     | 0.17              |
| 4:2:232:SER:N   | 4:Y:369:ILE:CA[1_556]  | 2.03                     | 0.17              |
| 4:1:274:ILE:N   | 4:Y:264:PRO:CD[1_556]  | 2.03                     | 0.17              |
| 4:1:136:ILE:CB  | 4:Y:300:SER:N[1_556]   | 2.03                     | 0.17              |
| 4:0:371:HIS:N   | 4:X:342:GLY:O[1_556]   | 2.03                     | 0.17              |
| 4:2:362:TYR:CE1 | 4:Z:22:ALA:CB[1_556]   | 2.03                     | 0.17              |
| 4:2:257:CYS:SG  | 4:Z:192:ILE:CG2[1_556] | 2.03                     | 0.17              |
| 4:0:172:PRO:C   | 4:X:281:SER:OG[1_556]  | 2.03                     | 0.17              |
| 4:2:198:TYR:O   | 4:Y:72:GLU:O[1_556]    | 2.03                     | 0.17              |
| 4:0:71:ILE:O    | 4:X:157:ASP:CG[1_556]  | 2.03                     | 0.17              |
| 4:2:12:ASN:CG   | 4:Z:336:LYS:CB[1_556]  | 2.03                     | 0.17              |
| 4:2:331:ALA:C   | 4:Z:221:LEU:N[1_556]   | 2.03                     | 0.17              |
| 4:2:310:ALA:CB  | 4:Z:224:GLU:N[1_556]   | 2.03                     | 0.17              |
| 4:2:214:GLU:CB  | 4:Z:253:GLU:OE2[1_556] | 2.03                     | 0.17              |
| 4:2:337:TYR:C   | 4:Z:307:PRO:C[1_556]   | 2.03                     | 0.17              |
| 4:1:310:ALA:CB  | 4:Y:224:GLU:N[1_556]   | 2.03                     | 0.17              |
| 4:0:162:ASN:OD1 | 4:X:273:GLY:O[1_556]   | 2.03                     | 0.17              |
| 4:2:362:TYR:O   | 4:Z:348:SER:N[1_556]   | 2.03                     | 0.17              |
| 4:2:253:GLU:CG  | 4:Y:112:PRO:CB[1_556]  | 2.03                     | 0.17              |
| 4:0:236:LEU:CG  | 4:W:117:GLU:OE1[1_556] | 2.03                     | 0.17              |
| 4:2:283:MET:N   | 4:Z:280:ASN:ND2[1_556] | 2.03                     | 0.17              |
| 4:2:161:HIS:NE2 | 4:Z:160:THR:CA[1_556]  | 2.03                     | 0.17              |
| 4:1:111:ASN:CB  | 4:Y:154:ASP:CG[1_556]  | 2.03                     | 0.17              |
| 4:0:274:ILE:N   | 4:X:264:PRO:CD[1_556]  | 2.03                     | 0.17              |
| 4:0:138:ALA:O   | 4:X:299:MET:CE[1_556]  | 2.03                     | 0.17              |
| 4:2:233:SER:C   | 4:Y:366:GLY:C[1_556]   | 2.03                     | 0.17              |
| 4:1:228:ALA:O   | 4:X:369:ILE:C[1_556]   | 2.03                     | 0.17              |
| 4:0:232:SER:N   | 4:W:369:ILE:CA[1_556]  | 2.03                     | 0.17              |
| 4:0:357:ILE:CG2 | 4:X:345:ILE:CD1[1_556] | 2.03                     | 0.17              |
| 4:3:265:SER:C   | 4:Z:173:HIS:NE2[1_556] | 2.03                     | 0.17              |
| 4:2:297:ASN:CA  | 4:Z:316:GLU:CB[1_556]  | 2.03                     | 0.17              |
| 4:0:293:LEU:CD2 | 4:X:279:TYR:CG[1_556]  | 2.03                     | 0.17              |
| 4:0:125:GLU:CA  | 4:X:24:ASP:CG[1_556]   | 2.03                     | 0.17              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:291:LYS:CD  | 4:X:322:PRO:CB[1_556]  | 2.03                     | 0.17              |
| 4:1:119:MET:O   | 4:Y:340:TRP:CG[1_556]  | 2.03                     | 0.17              |
| 4:2:62:ARG:NE   | 4:Z:204:ALA:O[1_556]   | 2.03                     | 0.17              |
| 4:2:195:GLU:OE1 | 4:Y:111:ASN:N[1_556]   | 2.03                     | 0.17              |
| 4:0:72:GLU:C    | 4:X:157:ASP:OD2[1_556] | 2.03                     | 0.17              |
| 4:2:372:ARG:CA  | 4:Z:143:TYR:CG[1_556]  | 2.03                     | 0.17              |
| 4:2:307:PRO:CG  | 4:Z:227:MET:CA[1_556]  | 2.03                     | 0.17              |
| 4:0:118:LYS:CG  | 4:X:10:CYS:C[1_556]    | 2.03                     | 0.17              |
| 4:0:147:ARG:NH1 | 4:X:315:LYS:CG[1_556]  | 2.03                     | 0.17              |
| 4:2:166:TYR:C   | 4:Z:294:TYR:N[1_556]   | 2.03                     | 0.17              |
| 4:0:148:THR:O   | 4:X:328:LYS:CA[1_556]  | 2.03                     | 0.17              |
| 4:0:109:PRO:CG  | 4:X:153:LEU:CG[1_556]  | 2.03                     | 0.17              |
| 4:2:208:ILE:CA  | 4:Z:198:TYR:CD2[1_556] | 2.03                     | 0.17              |
| 4:0:116:ARG:CB  | 4:X:339:VAL:CG1[1_556] | 2.03                     | 0.17              |
| 4:0:137:GLN:CB  | 4:X:304:THR:CA[1_556]  | 2.03                     | 0.17              |
| 4:2:195:GLU:CA  | 4:Y:75:ILE:CD1[1_556]  | 2.03                     | 0.17              |
| 4:2:175:ILE:C   | 4:Z:162:ASN:OD1[1_556] | 2.03                     | 0.17              |
| 4:2:179:ASP:CA  | 4:Z:180:LEU:CB[1_556]  | 2.03                     | 0.17              |
| 4:0:73:HIS:C    | 4:X:156:GLY:C[1_556]   | 2.03                     | 0.17              |
| 4:2:116:ARG:CZ  | 4:Z:141:SER:N[1_556]   | 2.03                     | 0.17              |
| 4:1:210:ARG:N   | 4:Y:193:LEU:CB[1_556]  | 2.03                     | 0.17              |
| 4:1:79:TRP:N    | 4:Y:17:VAL:CG2[1_556]  | 2.03                     | 0.17              |
| 4:0:41:GLN:O    | 4:V:148:THR:OG1[1_556] | 2.03                     | 0.17              |
| 4:2:16:LEU:CD2  | 4:Z:212:ILE:O[1_556]   | 2.03                     | 0.17              |
| 4:0:166:TYR:CE1 | 4:X:325:MET:SD[1_556]  | 2.03                     | 0.17              |
| 4:0:206:ARG:CA  | 4:X:199:SER:N[1_556]   | 2.03                     | 0.17              |
| 4:3:196:ARG:NH1 | 4:Z:115:ASN:CB[1_556]  | 2.03                     | 0.17              |
| 4:0:272:ALA:N   | 4:X:271:SER:N[1_556]   | 2.03                     | 0.17              |
| 4:1:371:HIS:N   | 4:Y:342:GLY:O[1_556]   | 2.03                     | 0.17              |
| 4:1:116:ARG:NH2 | 4:Y:141:SER:O[1_556]   | 2.03                     | 0.17              |
| 4:4:63:GLY:C    | 4:Z:288:ASP:O[1_556]   | 2.03                     | 0.17              |
| 4:2:212:ILE:CB  | 4:Z:196:ARG:CG[1_556]  | 2.03                     | 0.17              |
| 4:2:332:PRO:CD  | 4:Z:221:LEU:CA[1_556]  | 2.03                     | 0.17              |
| 4:2:166:TYR:CE1 | 4:Z:325:MET:SD[1_556]  | 2.03                     | 0.17              |
| 4:0:372:ARG:NH1 | 4:X:145:SER:OG[1_556]  | 2.03                     | 0.17              |
| 4:0:73:HIS:O    | 4:X:156:GLY:O[1_556]   | 2.03                     | 0.17              |
| 4:0:176:MET:C   | 4:X:178:LEU:CD2[1_556] | 2.03                     | 0.17              |
| 4:0:59:GLN:CD   | 4:X:208:ILE:CG2[1_556] | 2.03                     | 0.17              |
| 4:3:197:GLY:CA  | 4:Z:75:ILE:N[1_556]    | 2.03                     | 0.17              |
| 4:2:369:ILE:CB  | 4:Z:346:LEU:CA[1_556]  | 2.03                     | 0.17              |
| 4:1:83:GLU:CG   | 4:Y:28:ARG:O[1_556]    | 2.03                     | 0.17              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:32:PRO:N    | 4:Y:211:ASP:CB[1_556]  | 2.03                     | 0.17              |
| 4:2:116:ARG:CB  | 4:Z:339:VAL:CG1[1_556] | 2.03                     | 0.17              |
| 4:2:293:LEU:N   | 4:Z:320:LEU:C[1_556]   | 2.03                     | 0.17              |
| 4:2:63:GLY:C    | 4:X:288:ASP:O[1_556]   | 2.03                     | 0.17              |
| 4:0:303:THR:O   | 4:X:256:ARG:CA[1_556]  | 2.03                     | 0.17              |
| 4:2:339:VAL:O   | 4:Z:335:ARG:NH2[1_556] | 2.03                     | 0.17              |
| 4:0:306:TYR:CE1 | 4:X:256:ARG:CD[1_556]  | 2.03                     | 0.17              |
| 4:2:120:THR:CG2 | 4:Z:344:SER:CA[1_556]  | 2.03                     | 0.17              |
| 4:1:41:GLN:N    | 4:W:167:GLU:CG[1_556]  | 2.03                     | 0.17              |
| 4:0:123:MET:CG  | 4:X:26:ALA:C[1_556]    | 2.03                     | 0.17              |
| 4:0:185:LEU:CG  | 4:X:188:TYR:CE2[1_556] | 2.03                     | 0.17              |
| 4:2:162:ASN:OD1 | 4:Z:273:GLY:O[1_556]   | 2.03                     | 0.17              |
| 4:0:253:GLU:CG  | 4:W:112:PRO:CB[1_556]  | 2.03                     | 0.17              |
| 4:2:306:TYR:CD2 | 4:Z:256:ARG:CA[1_556]  | 2.03                     | 0.17              |
| 4:1:131:ALA:N   | 4:Y:25:ASP:CG[1_556]   | 2.03                     | 0.17              |
| 4:0:369:ILE:CB  | 4:X:346:LEU:CA[1_556]  | 2.03                     | 0.17              |
| 4:1:158:GLY:O   | 4:Y:184:ASP:CB[1_556]  | 2.03                     | 0.17              |
| 4:2:159:VAL:CA  | 4:Z:181:ALA:O[1_556]   | 2.03                     | 0.17              |
| 4:2:183:ARG:CB  | 4:Z:187:ASP:CA[1_556]  | 2.03                     | 0.17              |
| 4:1:299:MET:N   | 4:Y:312:ARG:CA[1_556]  | 2.03                     | 0.17              |
| 4:2:292:ASP:CB  | 4:Z:321:ALA:CA[1_556]  | 2.03                     | 0.17              |
| 4:0:185:LEU:CA  | 4:X:188:TYR:O[1_556]   | 2.03                     | 0.17              |
| 4:2:370:VAL:O   | 4:Z:144:ALA:N[1_556]   | 2.03                     | 0.17              |
| 4:1:72:GLU:CA   | 4:Y:157:ASP:CB[1_556]  | 2.03                     | 0.17              |
| 4:1:183:ARG:CA  | 4:Y:187:ASP:C[1_556]   | 2.03                     | 0.17              |
| 4:2:166:TYR:CZ  | 4:Z:325:MET:CG[1_556]  | 2.03                     | 0.17              |
| 4:0:83:GLU:CD   | 4:X:29:ALA:CB[1_556]   | 2.03                     | 0.17              |
| 4:1:79:TRP:CE3  | 4:Y:18:LYS:CB[1_556]   | 2.03                     | 0.17              |
| 4:0:166:TYR:C   | 4:X:294:TYR:N[1_556]   | 2.03                     | 0.17              |
| 4:0:372:ARG:NE  | 4:X:143:TYR:CA[1_556]  | 2.03                     | 0.17              |
| 4:1:118:LYS:CD  | 4:Y:10:CYS:CB[1_556]   | 2.03                     | 0.17              |
| 4:1:16:LEU:CD1  | 4:Y:215:LYS:N[1_556]   | 2.03                     | 0.17              |
| 4:2:209:VAL:CG1 | 4:Z:194:THR:CG2[1_556] | 2.03                     | 0.17              |
| 4:1:136:ILE:CB  | 4:Y:299:MET:N[1_556]   | 2.03                     | 0.17              |
| 4:1:294:TYR:N   | 4:Y:319:ALA:O[1_556]   | 2.03                     | 0.17              |
| 4:2:194:THR:CB  | 4:Y:177:ARG:CZ[1_556]  | 2.03                     | 0.17              |
| 4:2:210:ARG:CZ  | 4:Z:212:ILE:CG2[1_556] | 2.03                     | 0.17              |
| 4:1:372:ARG:NE  | 4:Y:143:TYR:C[1_556]   | 2.03                     | 0.17              |
| 4:1:304:THR:CG2 | 4:Y:259:GLU:CA[1_556]  | 2.03                     | 0.17              |
| 4:2:80:ASP:N    | 4:Z:31:PHE:CB[1_556]   | 2.03                     | 0.17              |
| 4:1:196:ARG:CZ  | 4:X:115:ASN:CB[1_556]  | 2.04                     | 0.16              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:289:ILE:CB  | 4:X:294:TYR:CZ[1_556]  | 2.04                     | 0.16              |
| 4:1:166:TYR:CD2 | 4:Y:294:TYR:CB[1_556]  | 2.04                     | 0.16              |
| 4:2:81:ASP:C    | 4:Z:31:PHE:CA[1_556]   | 2.04                     | 0.16              |
| 4:1:189:LEU:CG  | 4:Y:195:GLU:C[1_556]   | 2.04                     | 0.16              |
| 4:0:107:GLU:CA  | 4:X:301:GLY:CA[1_556]  | 2.04                     | 0.16              |
| 4:2:197:GLY:CA  | 4:Y:75:ILE:CB[1_556]   | 2.04                     | 0.16              |
| 4:2:299:MET:O   | 4:Z:312:ARG:CG[1_556]  | 2.04                     | 0.16              |
| 4:2:59:GLN:OE1  | 4:Z:208:ILE:CB[1_556]  | 2.04                     | 0.16              |
| 4:2:147:ARG:NH1 | 4:Z:315:LYS:CG[1_556]  | 2.04                     | 0.16              |
| 4:0:301:GLY:N   | 4:X:219:VAL:CA[1_556]  | 2.04                     | 0.16              |
| 4:2:338:SER:CA  | 4:Z:308:GLY:CA[1_556]  | 2.04                     | 0.16              |
| 4:0:298:VAL:C   | 4:X:312:ARG:CA[1_556]  | 2.04                     | 0.16              |
| 4:2:129:VAL:CG2 | 4:Z:25:ASP:N[1_556]    | 2.04                     | 0.16              |
| 4:0:121:GLN:OE1 | 4:X:9:VAL:O[1_556]     | 2.04                     | 0.16              |
| 4:1:309:ILE:CD1 | 4:Y:259:GLU:OE2[1_556] | 2.04                     | 0.16              |
| 4:0:105:LEU:CA  | 4:X:334:GLU:CB[1_556]  | 2.04                     | 0.16              |
| 4:1:195:GLU:N   | 4:X:75:ILE:CD1[1_556]  | 2.04                     | 0.16              |
| 4:2:14:SER:CB   | 4:Z:213:LYS:NZ[1_556]  | 2.04                     | 0.16              |
| 4:2:272:ALA:CA  | 4:Z:270:GLU:N[1_556]   | 2.04                     | 0.16              |
| 4:2:83:GLU:CD   | 4:Z:29:ALA:CB[1_556]   | 2.04                     | 0.16              |
| 4:2:73:HIS:C    | 4:Z:157:ASP:C[1_556]   | 2.04                     | 0.16              |
| 4:1:167:GLU:C   | 4:Y:295:ALA:CB[1_556]  | 2.04                     | 0.16              |
| 4:1:294:TYR:O   | 4:Y:319:ALA:O[1_556]   | 2.04                     | 0.16              |
| 4:2:206:ARG:O   | 4:Z:200:PHE:CD2[1_556] | 2.04                     | 0.16              |
| 4:2:293:LEU:CD2 | 4:Z:279:TYR:CG[1_556]  | 2.04                     | 0.16              |
| 4:1:177:ARG:C   | 4:Y:178:LEU:CD1[1_556] | 2.04                     | 0.16              |
| 4:0:174:ALA:CB  | 4:X:277:THR:O[1_556]   | 2.04                     | 0.16              |
| 4:0:125:GLU:N   | 4:X:24:ASP:CB[1_556]   | 2.04                     | 0.16              |
| 4:2:125:GLU:CA  | 4:Z:24:ASP:CG[1_556]   | 2.04                     | 0.16              |
| 4:0:104:LEU:O   | 4:X:333:PRO:C[1_556]   | 2.04                     | 0.16              |
| 4:3:196:ARG:CZ  | 4:Z:115:ASN:CB[1_556]  | 2.04                     | 0.16              |
| 4:1:296:ASN:O   | 4:Y:315:LYS:C[1_556]   | 2.04                     | 0.16              |
| 4:0:160:THR:CA  | 4:X:180:LEU:CD1[1_556] | 2.04                     | 0.16              |
| 4:0:191:LYS:CD  | 4:W:110:LEU:CD2[1_556] | 2.04                     | 0.16              |
| 4:2:183:ARG:CD  | 4:Z:187:ASP:N[1_556]   | 2.04                     | 0.16              |
| 4:2:15:GLY:C    | 4:Z:214:GLU:CG[1_556]  | 2.04                     | 0.16              |
| 4:2:197:GLY:N   | 4:Y:75:ILE:CG2[1_556]  | 2.04                     | 0.16              |
| 4:1:336:LYS:N   | 4:Y:218:TYR:CA[1_556]  | 2.04                     | 0.16              |
| 4:0:171:LEU:O   | 4:X:281:SER:OG[1_556]  | 2.04                     | 0.16              |
| 4:1:292:ASP:CA  | 4:Y:321:ALA:N[1_556]   | 2.04                     | 0.16              |
| 4:2:86:TRP:CG   | 4:Z:337:TYR:OH[1_556]  | 2.04                     | 0.16              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:262:PHE:C   | 4:X:265:SER:CB[1_556]  | 2.04                     | 0.16              |
| 4:0:30:VAL:O    | 4:X:215:LYS:CG[1_556]  | 2.04                     | 0.16              |
| 4:1:115:ASN:C   | 4:Y:339:VAL:CG1[1_556] | 2.04                     | 0.16              |
| 4:0:72:GLU:OE1  | 4:X:183:ARG:NH1[1_556] | 2.04                     | 0.16              |
| 4:2:303:THR:O   | 4:Z:256:ARG:CA[1_556]  | 2.04                     | 0.16              |
| 4:0:212:ILE:CB  | 4:X:196:ARG:CG[1_556]  | 2.04                     | 0.16              |
| 4:1:183:ARG:CZ  | 4:Y:186:THR:CB[1_556]  | 2.04                     | 0.16              |
| 4:0:80:ASP:O    | 4:X:30:VAL:O[1_556]    | 2.04                     | 0.16              |
| 4:3:267:ILE:O   | 4:Z:173:HIS:C[1_556]   | 2.04                     | 0.16              |
| 4:1:371:HIS:CA  | 4:Y:140:LEU:CA[1_556]  | 2.04                     | 0.16              |
| 4:0:267:ILE:O   | 4:W:173:HIS:C[1_556]   | 2.04                     | 0.16              |
| 4:0:137:GLN:CB  | 4:X:304:THR:CG2[1_556] | 2.04                     | 0.16              |
| 4:0:63:GLY:C    | 4:V:288:ASP:O[1_556]   | 2.04                     | 0.16              |
| 4:2:210:ARG:N   | 4:Z:193:LEU:CB[1_556]  | 2.04                     | 0.16              |
| 4:2:160:THR:CA  | 4:Z:180:LEU:CD1[1_556] | 2.04                     | 0.16              |
| 4:1:190:MET:CA  | 4:Y:194:THR:OG1[1_556] | 2.04                     | 0.16              |
| 4:0:116:ARG:CZ  | 4:X:141:SER:N[1_556]   | 2.04                     | 0.16              |
| 4:1:185:LEU:CD2 | 4:Y:188:TYR:CD2[1_556] | 2.04                     | 0.16              |
| 4:3:231:ALA:N   | 4:Z:368:SER:C[1_556]   | 2.04                     | 0.16              |
| 4:1:173:HIS:C   | 4:Y:174:ALA:O[1_556]   | 2.04                     | 0.16              |
| 4:0:209:VAL:CG1 | 4:X:194:THR:CG2[1_556] | 2.04                     | 0.16              |
| 4:0:159:VAL:CA  | 4:X:181:ALA:O[1_556]   | 2.04                     | 0.16              |
| 4:0:262:PHE:CA  | 4:X:265:SER:OG[1_556]  | 2.04                     | 0.16              |
| 4:0:86:TRP:CH2  | 4:X:337:TYR:CE1[1_556] | 2.04                     | 0.16              |
| 4:2:137:GLN:CB  | 4:Z:304:THR:CA[1_556]  | 2.04                     | 0.16              |
| 4:0:116:ARG:CB  | 4:X:339:VAL:CB[1_556]  | 2.04                     | 0.16              |
| 4:2:372:ARG:NE  | 4:Z:143:TYR:C[1_556]   | 2.04                     | 0.16              |
| 4:2:176:MET:C   | 4:Z:178:LEU:CD2[1_556] | 2.04                     | 0.16              |
| 4:1:265:SER:CA  | 4:X:173:HIS:NE2[1_556] | 2.04                     | 0.16              |
| 4:1:159:VAL:O   | 4:Y:185:LEU:CD2[1_556] | 2.04                     | 0.16              |
| 4:1:165:ILE:N   | 4:Y:278:THR:CG2[1_556] | 2.04                     | 0.16              |
| 4:0:30:VAL:CG1  | 4:X:215:LYS:C[1_556]   | 2.04                     | 0.16              |
| 4:1:177:ARG:CB  | 4:Y:178:LEU:CA[1_556]  | 2.04                     | 0.16              |
| 4:1:173:HIS:CG  | 4:Y:174:ALA:CB[1_556]  | 2.04                     | 0.16              |
| 4:1:194:THR:O   | 4:X:75:ILE:CD1[1_556]  | 2.04                     | 0.16              |
| 4:1:296:ASN:OD1 | 4:Y:318:THR:CG2[1_556] | 2.04                     | 0.16              |
| 4:0:167:GLU:CA  | 4:X:294:TYR:C[1_556]   | 2.04                     | 0.16              |
| 4:1:12:ASN:CG   | 4:Y:336:LYS:CB[1_556]  | 2.04                     | 0.16              |
| 4:0:305:MET:C   | 4:X:255:PHE:CZ[1_556]  | 2.04                     | 0.16              |
| 4:0:161:HIS:NE2 | 4:X:160:THR:CA[1_556]  | 2.04                     | 0.16              |
| 4:1:122:ILE:CB  | 4:Y:19:ALA:C[1_556]    | 2.04                     | 0.16              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:12:ASN:CG   | 4:Y:336:LYS:CG[1_556]  | 2.04                     | 0.16              |
| 4:2:231:ALA:N   | 4:Y:367:PRO:O[1_556]   | 2.04                     | 0.16              |
| 4:2:171:LEU:O   | 4:Z:281:SER:OG[1_556]  | 2.04                     | 0.16              |
| 4:2:105:LEU:N   | 4:Z:334:GLU:CG[1_556]  | 2.04                     | 0.16              |
| 4:0:331:ALA:C   | 4:X:221:LEU:N[1_556]   | 2.04                     | 0.16              |
| 4:1:206:ARG:CB  | 4:Y:199:SER:O[1_556]   | 2.04                     | 0.16              |
| 4:0:232:SER:O   | 4:W:366:GLY:C[1_556]   | 2.04                     | 0.16              |
| 4:2:174:ALA:CB  | 4:Z:277:THR:O[1_556]   | 2.04                     | 0.16              |
| 4:0:362:TYR:CE1 | 4:X:344:SER:O[1_556]   | 2.04                     | 0.16              |
| 4:3:251:GLY:CA  | 4:Z:114:ALA:CB[1_556]  | 2.04                     | 0.16              |
| 4:0:181:ALA:C   | 4:X:188:TYR:CB[1_556]  | 2.04                     | 0.16              |
| 4:0:59:GLN:OE1  | 4:X:208:ILE:CB[1_556]  | 2.04                     | 0.16              |
| 4:0:67:LEU:C    | 4:X:59:GLN:OE1[1_556]  | 2.04                     | 0.16              |
| 4:0:81:ASP:C    | 4:X:31:PHE:CA[1_556]   | 2.04                     | 0.16              |
| 4:1:281:SER:OG  | 4:Y:276:GLU:O[1_556]   | 2.04                     | 0.16              |
| 4:2:292:ASP:N   | 4:Z:321:ALA:N[1_556]   | 2.04                     | 0.16              |
| 4:1:174:ALA:CA  | 4:Y:277:THR:O[1_556]   | 2.04                     | 0.16              |
| 4:0:184:ASP:CA  | 4:X:188:TYR:CA[1_556]  | 2.04                     | 0.16              |
| 4:1:164:PRO:CG  | 4:Y:278:THR:CB[1_556]  | 2.04                     | 0.16              |
| 4:2:372:ARG:NH1 | 4:Z:145:SER:OG[1_556]  | 2.04                     | 0.16              |
| 4:2:184:ASP:CA  | 4:Z:188:TYR:CA[1_556]  | 2.04                     | 0.16              |
| 4:0:83:GLU:OE2  | 4:X:28:ARG:O[1_556]    | 2.04                     | 0.16              |
| 4:2:261:LEU:CG  | 4:Z:266:PHE:CD1[1_556] | 2.04                     | 0.16              |
| 4:0:73:HIS:C    | 4:X:157:ASP:C[1_556]   | 2.04                     | 0.16              |
| 4:0:298:VAL:N   | 4:X:316:GLU:CB[1_556]  | 2.04                     | 0.16              |
| 4:2:153:LEU:CD1 | 4:Z:262:PHE:N[1_556]   | 2.04                     | 0.16              |
| 4:2:296:ASN:CG  | 4:Z:318:THR:CA[1_556]  | 2.04                     | 0.16              |
| 4:0:367:PRO:C   | 4:X:343:GLY:C[1_556]   | 2.04                     | 0.16              |
| 4:2:332:PRO:CG  | 4:Z:221:LEU:CB[1_556]  | 2.04                     | 0.16              |
| 4:2:67:LEU:C    | 4:Z:59:GLN:OE1[1_556]  | 2.04                     | 0.16              |
| 4:2:298:VAL:N   | 4:Z:316:GLU:CB[1_556]  | 2.04                     | 0.16              |
| 4:2:109:PRO:CG  | 4:Z:153:LEU:CG[1_556]  | 2.04                     | 0.16              |
| 4:0:231:ALA:N   | 4:W:367:PRO:O[1_556]   | 2.04                     | 0.16              |
| 4:2:136:ILE:CB  | 4:Z:300:SER:N[1_556]   | 2.04                     | 0.16              |
| 4:2:172:PRO:C   | 4:Z:281:SER:OG[1_556]  | 2.04                     | 0.16              |
| 4:1:136:ILE:C   | 4:Y:300:SER:N[1_556]   | 2.04                     | 0.16              |
| 4:0:62:ARG:NE   | 4:X:204:ALA:O[1_556]   | 2.05                     | 0.15              |
| 4:2:76:ILE:CG2  | 4:Z:16:LEU:O[1_556]    | 2.05                     | 0.15              |
| 4:2:148:THR:C   | 4:Z:328:LYS:CA[1_556]  | 2.05                     | 0.15              |
| 4:3:195:GLU:CD  | 4:Z:109:PRO:CA[1_556]  | 2.05                     | 0.15              |
| 4:2:369:ILE:CD1 | 4:Z:143:TYR:OH[1_556]  | 2.05                     | 0.15              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:195:GLU:CD  | 4:X:109:PRO:CA[1_556]  | 2.05                     | 0.15              |
| 4:0:76:ILE:CG2  | 4:X:16:LEU:O[1_556]    | 2.05                     | 0.15              |
| 4:2:268:GLY:N   | 4:Y:173:HIS:C[1_556]   | 2.05                     | 0.15              |
| 4:2:305:MET:N   | 4:Z:223:PHE:CE1[1_556] | 2.05                     | 0.15              |
| 4:0:372:ARG:CA  | 4:X:143:TYR:CG[1_556]  | 2.05                     | 0.15              |
| 4:2:207:GLU:N   | 4:Z:199:SER:O[1_556]   | 2.05                     | 0.15              |
| 4:0:278:THR:C   | 4:X:276:GLU:CB[1_556]  | 2.05                     | 0.15              |
| 4:1:367:PRO:N   | 4:Y:343:GLY:O[1_556]   | 2.05                     | 0.15              |
| 4:1:138:ALA:O   | 4:Y:299:MET:SD[1_556]  | 2.05                     | 0.15              |
| 4:2:279:TYR:C   | 4:Z:276:GLU:CD[1_556]  | 2.05                     | 0.15              |
| 4:2:306:TYR:CA  | 4:Z:255:PHE:CE1[1_556] | 2.05                     | 0.15              |
| 4:2:72:GLU:OE1  | 4:Z:183:ARG:NH1[1_556] | 2.05                     | 0.15              |
| 4:3:61:LYS:O    | 4:Y:288:ASP:O[1_556]   | 2.05                     | 0.15              |
| 4:1:209:VAL:N   | 4:Y:198:TYR:CD2[1_556] | 2.05                     | 0.15              |
| 4:1:176:MET:C   | 4:Y:178:LEU:CD2[1_556] | 2.05                     | 0.15              |
| 4:0:210:ARG:CZ  | 4:X:212:ILE:CG2[1_556] | 2.05                     | 0.15              |
| 4:2:137:GLN:CB  | 4:Z:304:THR:CG2[1_556] | 2.05                     | 0.15              |
| 4:2:289:ILE:CB  | 4:Z:294:TYR:CE2[1_556] | 2.05                     | 0.15              |
| 4:2:306:TYR:CE1 | 4:Z:256:ARG:CD[1_556]  | 2.05                     | 0.15              |
| 4:1:125:GLU:O   | 4:Y:28:ARG:CZ[1_556]   | 2.05                     | 0.15              |
| 4:0:139:VAL:CG2 | 4:X:298:VAL:C[1_556]   | 2.05                     | 0.15              |
| 4:2:367:PRO:C   | 4:Z:343:GLY:C[1_556]   | 2.05                     | 0.15              |
| 4:0:272:ALA:O   | 4:X:270:GLU:N[1_556]   | 2.05                     | 0.15              |
| 4:0:207:GLU:N   | 4:X:199:SER:O[1_556]   | 2.05                     | 0.15              |
| 4:1:208:ILE:CB  | 4:Y:198:TYR:CG[1_556]  | 2.05                     | 0.15              |
| 4:2:124:PHE:CG  | 4:Z:23:GLY:O[1_556]    | 2.05                     | 0.15              |
| 4:2:125:GLU:N   | 4:Z:24:ASP:CB[1_556]   | 2.05                     | 0.15              |
| 4:2:169:TYR:C   | 4:Z:296:ASN:O[1_556]   | 2.05                     | 0.15              |
| 4:1:196:ARG:CG  | 4:X:115:ASN:CB[1_556]  | 2.05                     | 0.15              |
| 4:0:272:ALA:CA  | 4:X:270:GLU:N[1_556]   | 2.05                     | 0.15              |
| 4:0:362:TYR:CE1 | 4:X:22:ALA:CB[1_556]   | 2.05                     | 0.15              |
| 4:2:139:VAL:O   | 4:Z:329:ILE:C[1_556]   | 2.05                     | 0.15              |
| 4:1:114:ALA:O   | 4:Y:106:THR:CB[1_556]  | 2.05                     | 0.15              |
| 4:0:194:THR:CB  | 4:W:177:ARG:CZ[1_556]  | 2.05                     | 0.15              |
| 4:1:210:ARG:CZ  | 4:Y:212:ILE:CG2[1_556] | 2.05                     | 0.15              |
| 4:2:362:TYR:CE1 | 4:Z:344:SER:O[1_556]   | 2.05                     | 0.15              |
| 4:1:61:LYS:O    | 4:W:288:ASP:O[1_556]   | 2.05                     | 0.15              |
| 4:1:337:TYR:CA  | 4:Y:307:PRO:N[1_556]   | 2.05                     | 0.15              |
| 4:1:289:ILE:CB  | 4:Y:294:TYR:CZ[1_556]  | 2.05                     | 0.15              |
| 4:1:231:ALA:N   | 4:X:368:SER:C[1_556]   | 2.05                     | 0.15              |
| 4:2:106:THR:O   | 4:Z:336:LYS:C[1_556]   | 2.05                     | 0.15              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:185:LEU:CD2 | 4:Z:188:TYR:CD2[1_556] | 2.05                     | 0.15              |
| 4:1:116:ARG:CB  | 4:Y:339:VAL:CB[1_556]  | 2.05                     | 0.15              |
| 4:0:297:ASN:N   | 4:X:316:GLU:N[1_556]   | 2.05                     | 0.15              |
| 4:0:72:GLU:CD   | 4:X:183:ARG:CD[1_556]  | 2.05                     | 0.15              |
| 4:0:210:ARG:N   | 4:X:193:LEU:CB[1_556]  | 2.05                     | 0.15              |
| 4:2:194:THR:CG2 | 4:Y:177:ARG:NH2[1_556] | 2.05                     | 0.15              |
| 4:3:230:ALA:CA  | 4:Z:368:SER:O[1_556]   | 2.05                     | 0.15              |
| 4:0:291:LYS:NZ  | 4:X:322:PRO:N[1_556]   | 2.05                     | 0.15              |
| 4:2:118:LYS:CD  | 4:Z:10:CYS:N[1_556]    | 2.05                     | 0.15              |
| 4:1:83:GLU:OE1  | 4:Y:29:ALA:N[1_556]    | 2.05                     | 0.15              |
| 4:0:305:MET:N   | 4:X:223:PHE:CE1[1_556] | 2.05                     | 0.15              |
| 4:0:136:ILE:CB  | 4:X:300:SER:N[1_556]   | 2.05                     | 0.15              |
| 4:1:149:THR:OG1 | 4:Y:326:LYS:C[1_556]   | 2.05                     | 0.15              |
| 4:2:157:ASP:O   | 4:Z:185:LEU:CB[1_556]  | 2.05                     | 0.15              |
| 4:1:308:GLY:N   | 4:Y:224:GLU:O[1_556]   | 2.05                     | 0.15              |
| 4:1:30:VAL:CG1  | 4:Y:215:LYS:C[1_556]   | 2.05                     | 0.15              |
| 4:0:302:GLY:CA  | 4:X:258:PRO:CD[1_556]  | 2.05                     | 0.15              |
| 4:1:69:TYR:CE2  | 4:Y:210:ARG:CB[1_556]  | 2.05                     | 0.15              |
| 4:0:297:ASN:CA  | 4:X:316:GLU:CB[1_556]  | 2.05                     | 0.15              |
| 4:0:175:ILE:O   | 4:X:277:THR:CG2[1_556] | 2.05                     | 0.15              |
| 4:2:294:TYR:CA  | 4:Z:320:LEU:N[1_556]   | 2.05                     | 0.15              |
| 4:1:106:THR:O   | 4:Y:336:LYS:C[1_556]   | 2.05                     | 0.15              |
| 4:2:121:GLN:OE1 | 4:Z:9:VAL:O[1_556]     | 2.05                     | 0.15              |
| 4:1:336:LYS:CG  | 4:Y:218:TYR:CB[1_556]  | 2.05                     | 0.15              |
| 4:1:76:ILE:O    | 4:Y:16:LEU:O[1_556]    | 2.05                     | 0.15              |
| 4:1:121:GLN:OE1 | 4:Y:9:VAL:O[1_556]     | 2.05                     | 0.15              |
| 4:0:33:SER:N    | 4:X:214:GLU:OE1[1_556] | 2.05                     | 0.15              |
| 4:2:191:LYS:CD  | 4:Y:110:LEU:CD2[1_556] | 2.05                     | 0.15              |
| 4:1:370:VAL:O   | 4:Y:140:LEU:O[1_556]   | 2.05                     | 0.15              |
| 4:2:272:ALA:O   | 4:Z:270:GLU:N[1_556]   | 2.05                     | 0.15              |
| 4:0:198:TYR:N   | 4:W:75:ILE:CA[1_556]   | 2.05                     | 0.15              |
| 4:2:172:PRO:CG  | 4:Z:163:VAL:C[1_556]   | 2.05                     | 0.15              |
| 4:0:257:CYS:SG  | 4:X:192:ILE:CG2[1_556] | 2.05                     | 0.15              |
| 4:0:283:MET:N   | 4:X:280:ASN:ND2[1_556] | 2.05                     | 0.15              |
| 4:2:206:ARG:CA  | 4:Z:199:SER:N[1_556]   | 2.05                     | 0.15              |
| 4:0:296:ASN:CG  | 4:X:318:THR:CA[1_556]  | 2.05                     | 0.15              |
| 4:2:59:GLN:CD   | 4:Z:208:ILE:CG2[1_556] | 2.05                     | 0.15              |
| 4:1:169:TYR:CG  | 4:Y:151:ILE:N[1_556]   | 2.05                     | 0.15              |
| 4:0:233:SER:OG  | 4:W:367:PRO:CA[1_556]  | 2.05                     | 0.15              |
| 4:1:108:ALA:N   | 4:Y:300:SER:C[1_556]   | 2.05                     | 0.15              |
| 4:0:279:TYR:C   | 4:X:276:GLU:CD[1_556]  | 2.05                     | 0.15              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:296:ASN:OD1 | 4:Z:318:THR:CG2[1_556] | 2.05                     | 0.15              |
| 4:2:33:SER:N    | 4:Z:214:GLU:OE1[1_556] | 2.05                     | 0.15              |
| 4:0:157:ASP:O   | 4:X:185:LEU:CB[1_556]  | 2.05                     | 0.15              |
| 4:2:185:LEU:CB  | 4:Z:188:TYR:CG[1_556]  | 2.05                     | 0.15              |
| 4:1:118:LYS:CD  | 4:Y:10:CYS:N[1_556]    | 2.05                     | 0.15              |
| 4:3:234:SER:CA  | 4:Z:367:PRO:CD[1_556]  | 2.05                     | 0.15              |
| 4:2:181:ALA:C   | 4:Z:188:TYR:CB[1_556]  | 2.05                     | 0.15              |
| 4:0:274:ILE:CG1 | 4:X:263:GLN:CB[1_556]  | 2.05                     | 0.15              |
| 4:1:130:PRO:CA  | 4:Y:25:ASP:OD2[1_556]  | 2.05                     | 0.15              |
| 4:0:118:LYS:CE  | 4:X:10:CYS:SG[1_556]   | 2.05                     | 0.15              |
| 4:0:298:VAL:N   | 4:X:316:GLU:CG[1_556]  | 2.05                     | 0.15              |
| 4:0:268:GLY:N   | 4:W:173:HIS:C[1_556]   | 2.05                     | 0.15              |
| 4:2:121:GLN:O   | 4:Z:20:GLY:C[1_556]    | 2.05                     | 0.15              |
| 4:2:167:GLU:CA  | 4:Z:294:TYR:C[1_556]   | 2.05                     | 0.15              |
| 4:2:195:GLU:OE1 | 4:Y:110:LEU:C[1_556]   | 2.05                     | 0.15              |
| 4:0:194:THR:O   | 4:W:75:ILE:CB[1_556]   | 2.05                     | 0.15              |
| 4:2:357:ILE:CG2 | 4:Z:345:ILE:CD1[1_556] | 2.05                     | 0.15              |
| 4:1:371:HIS:CB  | 4:Y:140:LEU:CG[1_556]  | 2.05                     | 0.15              |
| 4:2:116:ARG:CB  | 4:Z:339:VAL:CB[1_556]  | 2.05                     | 0.15              |
| 4:0:120:THR:CG2 | 4:X:344:SER:CA[1_556]  | 2.05                     | 0.15              |
| 4:0:175:ILE:C   | 4:X:162:ASN:OD1[1_556] | 2.05                     | 0.15              |
| 4:1:234:SER:CA  | 4:X:367:PRO:CD[1_556]  | 2.05                     | 0.15              |
| 4:1:306:TYR:CE2 | 4:Y:256:ARG:CA[1_556]  | 2.05                     | 0.15              |
| 4:0:129:VAL:CG2 | 4:X:25:ASP:N[1_556]    | 2.05                     | 0.15              |
| 4:0:206:ARG:O   | 4:X:200:PHE:CD2[1_556] | 2.05                     | 0.15              |
| 4:2:112:PRO:CG  | 4:Z:137:GLN:OE1[1_556] | 2.05                     | 0.15              |
| 4:0:292:ASP:N   | 4:X:321:ALA:N[1_556]   | 2.05                     | 0.15              |
| 4:0:139:VAL:O   | 4:X:329:ILE:C[1_556]   | 2.05                     | 0.15              |
| 4:2:301:GLY:N   | 4:Z:219:VAL:CA[1_556]  | 2.05                     | 0.15              |
| 4:2:291:LYS:NZ  | 4:Z:322:PRO:N[1_556]   | 2.05                     | 0.15              |
| 4:0:309:ILE:CG2 | 4:X:259:GLU:OE2[1_556] | 2.05                     | 0.15              |
| 4:2:30:VAL:O    | 4:Z:215:LYS:CG[1_556]  | 2.05                     | 0.15              |
| 4:1:260:THR:C   | 4:Y:265:SER:O[1_556]   | 2.05                     | 0.15              |
| 4:0:110:LEU:CD1 | 4:X:161:HIS:N[1_556]   | 2.05                     | 0.15              |
| 4:0:15:GLY:C    | 4:X:214:GLU:CG[1_556]  | 2.05                     | 0.15              |
| 4:0:113:LYS:CA  | 4:X:136:ILE:O[1_556]   | 2.05                     | 0.15              |
| 4:0:112:PRO:CA  | 4:X:137:GLN:OE1[1_556] | 2.05                     | 0.15              |
| 4:1:183:ARG:CD  | 4:Y:187:ASP:N[1_556]   | 2.05                     | 0.15              |
| 4:0:33:SER:OG   | 4:X:210:ARG:NH1[1_556] | 2.05                     | 0.15              |
| 4:1:164:PRO:CB  | 4:Y:278:THR:CA[1_556]  | 2.05                     | 0.15              |
| 4:2:80:ASP:O    | 4:Z:30:VAL:O[1_556]    | 2.05                     | 0.15              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:62:ARG:CB   | 4:X:204:ALA:N[1_556]   | 2.05                     | 0.15              |
| 4:2:113:LYS:CA  | 4:Z:136:ILE:O[1_556]   | 2.05                     | 0.15              |
| 4:1:167:GLU:O   | 4:Y:296:ASN:N[1_556]   | 2.05                     | 0.15              |
| 4:2:107:GLU:CA  | 4:Z:301:GLY:CA[1_556]  | 2.05                     | 0.15              |
| 4:0:309:ILE:CG2 | 4:X:223:PHE:C[1_556]   | 2.05                     | 0.15              |
| 4:1:75:ILE:N    | 4:Y:156:GLY:CA[1_556]  | 2.05                     | 0.15              |
| 4:0:197:GLY:N   | 4:W:75:ILE:CG2[1_556]  | 2.05                     | 0.15              |
| 4:0:118:LYS:CD  | 4:X:10:CYS:C[1_556]    | 2.05                     | 0.15              |
| 4:1:262:PHE:CA  | 4:Y:265:SER:OG[1_556]  | 2.05                     | 0.15              |
| 4:2:174:ALA:CB  | 4:Z:281:SER:CA[1_556]  | 2.05                     | 0.15              |
| 4:0:306:TYR:CD2 | 4:X:256:ARG:CA[1_556]  | 2.05                     | 0.15              |
| 4:2:208:ILE:CD1 | 4:Z:198:TYR:CE1[1_556] | 2.05                     | 0.15              |
| 4:2:110:LEU:CD1 | 4:Z:161:HIS:N[1_556]   | 2.05                     | 0.15              |
| 4:2:83:GLU:OE2  | 4:Z:28:ARG:O[1_556]    | 2.05                     | 0.15              |
| 4:0:194:THR:CG2 | 4:W:177:ARG:NH2[1_556] | 2.05                     | 0.15              |
| 4:2:203:THR:C   | 4:Z:205:GLU:OE2[1_556] | 2.05                     | 0.15              |
| 4:3:265:SER:CA  | 4:Z:173:HIS:NE2[1_556] | 2.05                     | 0.15              |
| 4:1:127:PHE:N   | 4:Y:28:ARG:NE[1_556]   | 2.05                     | 0.15              |
| 4:2:277:THR:O   | 4:Z:272:ALA:CB[1_556]  | 2.05                     | 0.15              |
| 4:0:302:GLY:N   | 4:X:218:TYR:O[1_556]   | 2.05                     | 0.15              |
| 4:2:302:GLY:CA  | 4:Z:258:PRO:CD[1_556]  | 2.05                     | 0.15              |
| 4:2:142:LEU:N   | 4:Z:310:ALA:CB[1_556]  | 2.05                     | 0.15              |
| 4:2:170:ALA:CA  | 4:Z:151:ILE:O[1_556]   | 2.05                     | 0.15              |
| 4:1:274:ILE:CD1 | 4:Y:264:PRO:CA[1_556]  | 2.06                     | 0.14              |
| 4:1:106:THR:N   | 4:Y:334:GLU:C[1_556]   | 2.06                     | 0.14              |
| 4:0:306:TYR:CA  | 4:X:255:PHE:CE1[1_556] | 2.06                     | 0.14              |
| 4:0:306:TYR:C   | 4:X:227:MET:CG[1_556]  | 2.06                     | 0.14              |
| 4:0:208:ILE:CD1 | 4:X:198:TYR:CE1[1_556] | 2.06                     | 0.14              |
| 4:3:191:LYS:CD  | 4:Z:110:LEU:CD2[1_556] | 2.06                     | 0.14              |
| 4:0:125:GLU:N   | 4:X:21:PHE:O[1_556]    | 2.06                     | 0.14              |
| 4:2:305:MET:C   | 4:Z:255:PHE:CZ[1_556]  | 2.06                     | 0.14              |
| 4:2:202:THR:O   | 4:Z:201:VAL:CG2[1_556] | 2.06                     | 0.14              |
| 4:1:297:ASN:N   | 4:Y:316:GLU:N[1_556]   | 2.06                     | 0.14              |
| 4:1:153:LEU:CD1 | 4:Y:262:PHE:N[1_556]   | 2.06                     | 0.14              |
| 4:1:110:LEU:CD2 | 4:Y:161:HIS:C[1_556]   | 2.06                     | 0.14              |
| 4:1:125:GLU:CD  | 4:Y:21:PHE:CB[1_556]   | 2.06                     | 0.14              |
| 4:0:153:LEU:CD1 | 4:X:262:PHE:N[1_556]   | 2.06                     | 0.14              |
| 4:0:277:THR:O   | 4:X:272:ALA:CB[1_556]  | 2.06                     | 0.14              |
| 4:2:304:THR:C   | 4:Z:223:PHE:CZ[1_556]  | 2.06                     | 0.14              |
| 4:2:86:TRP:CH2  | 4:Z:337:TYR:CE1[1_556] | 2.06                     | 0.14              |
| 4:2:309:ILE:CG2 | 4:Z:259:GLU:OE2[1_556] | 2.06                     | 0.14              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:262:PHE:C   | 4:Y:265:SER:CB[1_556]  | 2.06                     | 0.14              |
| 4:0:302:GLY:O   | 4:X:255:PHE:N[1_556]   | 2.06                     | 0.14              |
| 4:1:306:TYR:C   | 4:Y:255:PHE:CE1[1_556] | 2.06                     | 0.14              |
| 4:2:267:ILE:O   | 4:Y:173:HIS:C[1_556]   | 2.06                     | 0.14              |
| 4:1:210:ARG:NH2 | 4:Y:212:ILE:CD1[1_556] | 2.06                     | 0.14              |
| 4:2:171:LEU:C   | 4:Z:151:ILE:CG1[1_556] | 2.06                     | 0.14              |
| 4:1:261:LEU:CG  | 4:Y:266:PHE:CD1[1_556] | 2.06                     | 0.14              |
| 4:2:125:GLU:N   | 4:Z:21:PHE:O[1_556]    | 2.06                     | 0.14              |
| 4:0:170:ALA:O   | 4:X:151:ILE:CG2[1_556] | 2.06                     | 0.14              |
| 4:0:105:LEU:N   | 4:X:334:GLU:CG[1_556]  | 2.06                     | 0.14              |
| 4:1:183:ARG:CA  | 4:Y:187:ASP:N[1_556]   | 2.06                     | 0.14              |
| 4:2:298:VAL:C   | 4:Z:312:ARG:CB[1_556]  | 2.06                     | 0.14              |
| 4:1:203:THR:O   | 4:Y:199:SER:O[1_556]   | 2.06                     | 0.14              |
| 4:0:110:LEU:CG  | 4:X:162:ASN:N[1_556]   | 2.06                     | 0.14              |
| 4:2:112:PRO:CA  | 4:Z:137:GLN:OE1[1_556] | 2.06                     | 0.14              |
| 4:0:197:GLY:CA  | 4:W:75:ILE:CB[1_556]   | 2.06                     | 0.14              |
| 4:0:135:ALA:CB  | 4:X:332:PRO:N[1_556]   | 2.06                     | 0.14              |
| 4:4:40:HIS:C    | 4:Z:167:GLU:CG[1_556]  | 2.06                     | 0.14              |
| 4:1:174:ALA:CB  | 4:Y:277:THR:O[1_556]   | 2.06                     | 0.14              |
| 4:3:196:ARG:NH1 | 4:Z:116:ARG:N[1_556]   | 2.06                     | 0.14              |
| 4:0:73:HIS:CE1  | 4:X:184:ASP:CG[1_556]  | 2.06                     | 0.14              |
| 4:0:169:TYR:N   | 4:X:297:ASN:N[1_556]   | 2.06                     | 0.14              |
| 4:0:114:ALA:CB  | 4:X:107:GLU:N[1_556]   | 2.06                     | 0.14              |
| 4:1:148:THR:O   | 4:Y:327:ILE:C[1_556]   | 2.06                     | 0.14              |
| 4:2:194:THR:O   | 4:Y:75:ILE:CB[1_556]   | 2.06                     | 0.14              |
| 4:2:297:ASN:CB  | 4:Z:316:GLU:CD[1_556]  | 2.06                     | 0.14              |
| 4:1:336:LYS:O   | 4:Y:217:CYS:O[1_556]   | 2.06                     | 0.14              |
| 4:0:177:ARG:C   | 4:X:178:LEU:CD1[1_556] | 2.06                     | 0.14              |
| 4:1:155:SER:OG  | 4:Y:260:THR:C[1_556]   | 2.06                     | 0.14              |
| 4:0:187:ASP:CA  | 4:X:191:LYS:CB[1_556]  | 2.06                     | 0.14              |
| 4:0:331:ALA:CB  | 4:X:222:ASP:C[1_556]   | 2.06                     | 0.14              |
| 4:1:167:GLU:N   | 4:Y:295:ALA:CA[1_556]  | 2.06                     | 0.14              |
| 4:2:118:LYS:CE  | 4:Z:10:CYS:SG[1_556]   | 2.06                     | 0.14              |
| 4:1:267:ILE:O   | 4:X:173:HIS:C[1_556]   | 2.06                     | 0.14              |
| 4:2:367:PRO:O   | 4:Z:343:GLY:O[1_556]   | 2.06                     | 0.14              |
| 4:0:112:PRO:CG  | 4:X:137:GLN:OE1[1_556] | 2.06                     | 0.14              |
| 4:0:118:LYS:CD  | 4:X:10:CYS:N[1_556]    | 2.06                     | 0.14              |
| 4:1:172:PRO:C   | 4:Y:281:SER:OG[1_556]  | 2.06                     | 0.14              |
| 4:2:298:VAL:N   | 4:Z:316:GLU:CG[1_556]  | 2.06                     | 0.14              |
| 4:2:104:LEU:O   | 4:Z:333:PRO:C[1_556]   | 2.06                     | 0.14              |
| 4:1:261:LEU:CB  | 4:Y:266:PHE:CA[1_556]  | 2.06                     | 0.14              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:371:HIS:CA  | 4:X:140:LEU:CA[1_556]  | 2.06                     | 0.14              |
| 4:0:304:THR:CG2 | 4:X:259:GLU:N[1_556]   | 2.06                     | 0.14              |
| 4:0:175:ILE:CD1 | 4:X:162:ASN:CG[1_556]  | 2.06                     | 0.14              |
| 4:1:104:LEU:O   | 4:Y:333:PRO:C[1_556]   | 2.06                     | 0.14              |
| 4:0:292:ASP:OD1 | 4:X:322:PRO:O[1_556]   | 2.06                     | 0.14              |
| 4:1:186:THR:CA  | 4:Y:190:MET:C[1_556]   | 2.06                     | 0.14              |
| 4:1:72:GLU:CD   | 4:Y:183:ARG:CD[1_556]  | 2.06                     | 0.14              |
| 4:1:197:GLY:N   | 4:X:75:ILE:CD1[1_556]  | 2.06                     | 0.14              |
| 4:0:292:ASP:CB  | 4:X:321:ALA:C[1_556]   | 2.06                     | 0.14              |
| 4:2:116:ARG:CD  | 4:Z:140:LEU:O[1_556]   | 2.06                     | 0.14              |
| 4:1:73:HIS:CE1  | 4:Y:184:ASP:CG[1_556]  | 2.06                     | 0.14              |
| 4:1:172:PRO:CD  | 4:Y:164:PRO:CB[1_556]  | 2.06                     | 0.14              |
| 4:2:251:GLY:CA  | 4:Y:114:ALA:CB[1_556]  | 2.06                     | 0.14              |
| 4:2:292:ASP:OD1 | 4:Z:322:PRO:O[1_556]   | 2.06                     | 0.14              |
| 4:0:114:ALA:O   | 4:X:106:THR:OG1[1_556] | 2.06                     | 0.14              |
| 4:3:227:MET:SD  | 4:Z:372:ARG:O[1_556]   | 2.06                     | 0.14              |
| 4:1:113:LYS:CB  | 4:Y:135:ALA:C[1_556]   | 2.06                     | 0.14              |
| 4:0:78:ASN:N    | 4:X:15:GLY:O[1_556]    | 2.06                     | 0.14              |
| 4:0:62:ARG:CA   | 4:X:204:ALA:CB[1_556]  | 2.06                     | 0.14              |
| 4:0:372:ARG:NE  | 4:X:143:TYR:C[1_556]   | 2.06                     | 0.14              |
| 4:2:169:TYR:N   | 4:Z:297:ASN:N[1_556]   | 2.06                     | 0.14              |
| 4:2:233:SER:OG  | 4:Y:367:PRO:CA[1_556]  | 2.06                     | 0.14              |
| 4:0:195:GLU:OE1 | 4:W:110:LEU:C[1_556]   | 2.06                     | 0.14              |
| 4:0:153:LEU:CA  | 4:X:262:PHE:CG[1_556]  | 2.06                     | 0.14              |
| 4:0:193:LEU:CA  | 4:W:112:PRO:CG[1_556]  | 2.06                     | 0.14              |
| 4:1:230:ALA:CA  | 4:X:368:SER:O[1_556]   | 2.06                     | 0.14              |
| 4:0:121:GLN:O   | 4:X:20:GLY:C[1_556]    | 2.06                     | 0.14              |
| 4:0:252:ASN:N   | 4:W:113:LYS:C[1_556]   | 2.06                     | 0.14              |
| 4:1:304:THR:CA  | 4:Y:259:GLU:CB[1_556]  | 2.06                     | 0.14              |
| 4:2:33:SER:OG   | 4:Z:210:ARG:NH1[1_556] | 2.06                     | 0.14              |
| 4:2:304:THR:CG2 | 4:Z:259:GLU:N[1_556]   | 2.06                     | 0.14              |
| 4:2:304:THR:CA  | 4:Z:255:PHE:O[1_556]   | 2.06                     | 0.14              |
| 4:1:141:SER:CB  | 4:Y:309:ILE:O[1_556]   | 2.06                     | 0.14              |
| 4:0:189:LEU:CD2 | 4:X:195:GLU:CA[1_556]  | 2.06                     | 0.14              |
| 4:1:62:ARG:CZ   | 4:Y:204:ALA:C[1_556]   | 2.06                     | 0.14              |
| 4:2:76:ILE:CD1  | 4:Z:18:LYS:CE[1_556]   | 2.06                     | 0.14              |
| 4:0:269:MET:CB  | 4:X:268:GLY:O[1_556]   | 2.06                     | 0.14              |
| 4:2:154:ASP:C   | 4:Z:261:LEU:CG[1_556]  | 2.06                     | 0.14              |
| 4:0:79:TRP:N    | 4:X:31:PHE:O[1_556]    | 2.06                     | 0.14              |
| 4:1:209:VAL:CB  | 4:Y:194:THR:N[1_556]   | 2.06                     | 0.14              |
| 4:2:252:ASN:N   | 4:Y:113:LYS:C[1_556]   | 2.06                     | 0.14              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:175:ILE:O   | 4:Z:277:THR:CG2[1_556] | 2.06                     | 0.14              |
| 4:2:30:VAL:CG1  | 4:Z:215:LYS:C[1_556]   | 2.06                     | 0.14              |
| 4:2:216:LEU:N   | 4:Z:252:ASN:OD1[1_556] | 2.06                     | 0.14              |
| 4:1:272:ALA:CB  | 4:Y:270:GLU:CA[1_556]  | 2.06                     | 0.14              |
| 4:2:191:LYS:CE  | 4:Y:110:LEU:CD1[1_556] | 2.06                     | 0.14              |
| 4:1:110:LEU:CD1 | 4:Y:161:HIS:CG[1_556]  | 2.06                     | 0.14              |
| 4:1:303:THR:N   | 4:Y:257:CYS:C[1_556]   | 2.06                     | 0.14              |
| 4:2:309:ILE:CG2 | 4:Z:223:PHE:C[1_556]   | 2.06                     | 0.14              |
| 4:0:185:LEU:C   | 4:X:192:ILE:N[1_556]   | 2.06                     | 0.14              |
| 4:0:172:PRO:CG  | 4:X:163:VAL:C[1_556]   | 2.06                     | 0.14              |
| 4:1:62:ARG:NH2  | 4:Y:205:GLU:C[1_556]   | 2.06                     | 0.14              |
| 4:1:304:THR:C   | 4:Y:223:PHE:CZ[1_556]  | 2.06                     | 0.14              |
| 4:0:185:LEU:CB  | 4:X:188:TYR:CG[1_556]  | 2.06                     | 0.14              |
| 4:1:303:THR:O   | 4:Y:256:ARG:CA[1_556]  | 2.06                     | 0.14              |
| 4:1:160:THR:CG2 | 4:Y:261:LEU:C[1_556]   | 2.06                     | 0.14              |
| 4:2:260:THR:C   | 4:Z:266:PHE:C[1_556]   | 2.06                     | 0.14              |
| 4:2:160:THR:CB  | 4:Z:180:LEU:CD1[1_556] | 2.06                     | 0.14              |
| 4:0:296:ASN:OD1 | 4:X:318:THR:CG2[1_556] | 2.06                     | 0.14              |
| 4:2:171:LEU:N   | 4:Z:151:ILE:CB[1_556]  | 2.06                     | 0.14              |
| 4:2:186:THR:C   | 4:Z:190:MET:C[1_556]   | 2.06                     | 0.14              |
| 4:3:40:HIS:CE1  | 4:Y:166:TYR:CD1[1_556] | 2.06                     | 0.14              |
| 4:0:148:THR:C   | 4:X:328:LYS:CA[1_556]  | 2.07                     | 0.13              |
| 4:1:116:ARG:O   | 4:Y:340:TRP:C[1_556]   | 2.07                     | 0.13              |
| 4:0:124:PHE:CG  | 4:X:23:GLY:O[1_556]    | 2.07                     | 0.13              |
| 4:0:216:LEU:N   | 4:X:252:ASN:OD1[1_556] | 2.07                     | 0.13              |
| 4:1:40:HIS:CE1  | 4:W:166:TYR:CD1[1_556] | 2.07                     | 0.13              |
| 4:0:268:GLY:N   | 4:W:173:HIS:CG[1_556]  | 2.07                     | 0.13              |
| 4:0:68:LYS:CB   | 4:X:59:GLN:NE2[1_556]  | 2.07                     | 0.13              |
| 4:1:73:HIS:CB   | 4:Y:158:GLY:CA[1_556]  | 2.07                     | 0.13              |
| 4:2:189:LEU:CD2 | 4:Z:195:GLU:CA[1_556]  | 2.07                     | 0.13              |
| 4:0:106:THR:O   | 4:X:336:LYS:C[1_556]   | 2.07                     | 0.13              |
| 4:1:161:HIS:CE1 | 4:Y:160:THR:CB[1_556]  | 2.07                     | 0.13              |
| 4:0:142:LEU:N   | 4:X:310:ALA:CB[1_556]  | 2.07                     | 0.13              |
| 4:0:169:TYR:C   | 4:X:296:ASN:O[1_556]   | 2.07                     | 0.13              |
| 4:2:185:LEU:C   | 4:Z:192:ILE:N[1_556]   | 2.07                     | 0.13              |
| 4:1:271:SER:O   | 4:Y:270:GLU:CG[1_556]  | 2.07                     | 0.13              |
| 4:1:161:HIS:C   | 4:Y:274:ILE:N[1_556]   | 2.07                     | 0.13              |
| 4:2:304:THR:CA  | 4:Z:223:PHE:CE1[1_556] | 2.07                     | 0.13              |
| 4:1:197:GLY:CA  | 4:X:75:ILE:CB[1_556]   | 2.07                     | 0.13              |
| 4:0:198:TYR:N   | 4:W:75:ILE:CG2[1_556]  | 2.07                     | 0.13              |
| 4:2:79:TRP:CH2  | 4:Z:11:ASP:O[1_556]    | 2.07                     | 0.13              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:304:THR:CA  | 4:X:223:PHE:CE1[1_556] | 2.07                     | 0.13              |
| 4:2:210:ARG:N   | 4:Z:193:LEU:CG[1_556]  | 2.07                     | 0.13              |
| 4:2:164:PRO:CB  | 4:Z:278:THR:CB[1_556]  | 2.07                     | 0.13              |
| 4:1:305:MET:N   | 4:Y:223:PHE:CE1[1_556] | 2.07                     | 0.13              |
| 4:0:174:ALA:CB  | 4:X:281:SER:CA[1_556]  | 2.07                     | 0.13              |
| 4:1:37:ARG:NH1  | 4:Y:56:ASP:O[1_556]    | 2.07                     | 0.13              |
| 4:0:304:THR:CA  | 4:X:255:PHE:O[1_556]   | 2.07                     | 0.13              |
| 4:1:191:LYS:CD  | 4:X:110:LEU:CD2[1_556] | 2.07                     | 0.13              |
| 4:0:366:GLY:N   | 4:X:347:ALA:CA[1_556]  | 2.07                     | 0.13              |
| 4:0:298:VAL:C   | 4:X:312:ARG:CB[1_556]  | 2.07                     | 0.13              |
| 4:2:294:TYR:O   | 4:Z:319:ALA:O[1_556]   | 2.07                     | 0.13              |
| 4:2:118:LYS:CD  | 4:Z:10:CYS:C[1_556]    | 2.07                     | 0.13              |
| 4:1:78:ASN:CA   | 4:Y:33:SER:N[1_556]    | 2.07                     | 0.13              |
| 4:0:40:HIS:C    | 4:V:167:GLU:CG[1_556]  | 2.07                     | 0.13              |
| 4:2:302:GLY:O   | 4:Z:255:PHE:N[1_556]   | 2.07                     | 0.13              |
| 4:1:133:TYR:OH  | 4:Y:145:SER:OG[1_556]  | 2.07                     | 0.13              |
| 4:2:125:GLU:CD  | 4:Z:7:ALA:O[1_556]     | 2.07                     | 0.13              |
| 4:0:330:ILE:CD1 | 4:X:315:LYS:CE[1_556]  | 2.07                     | 0.13              |
| 4:0:154:ASP:C   | 4:X:261:LEU:CG[1_556]  | 2.07                     | 0.13              |
| 4:0:41:GLN:CA   | 4:V:167:GLU:CD[1_556]  | 2.07                     | 0.13              |
| 4:1:232:SER:CB  | 4:X:369:ILE:CB[1_556]  | 2.07                     | 0.13              |
| 4:0:261:LEU:O   | 4:X:265:SER:CB[1_556]  | 2.07                     | 0.13              |
| 4:0:177:ARG:NH1 | 4:X:160:THR:N[1_556]   | 2.07                     | 0.13              |
| 4:2:198:TYR:N   | 4:Y:75:ILE:CA[1_556]   | 2.07                     | 0.13              |
| 4:1:59:GLN:CG   | 4:Y:208:ILE:CD1[1_556] | 2.07                     | 0.13              |
| 4:1:80:ASP:N    | 4:Y:31:PHE:CB[1_556]   | 2.07                     | 0.13              |
| 4:1:16:LEU:CD2  | 4:Y:212:ILE:O[1_556]   | 2.07                     | 0.13              |
| 4:0:297:ASN:CB  | 4:X:316:GLU:CD[1_556]  | 2.07                     | 0.13              |
| 4:2:169:TYR:CG  | 4:Z:151:ILE:N[1_556]   | 2.07                     | 0.13              |
| 4:0:160:THR:CG2 | 4:X:260:THR:O[1_556]   | 2.07                     | 0.13              |
| 4:0:289:ILE:CB  | 4:X:294:TYR:CE2[1_556] | 2.07                     | 0.13              |
| 4:2:302:GLY:N   | 4:Z:218:TYR:O[1_556]   | 2.07                     | 0.13              |
| 4:0:185:LEU:CD2 | 4:X:188:TYR:CD2[1_556] | 2.07                     | 0.13              |
| 4:0:339:VAL:CG1 | 4:X:304:THR:O[1_556]   | 2.07                     | 0.13              |
| 4:2:169:TYR:OH  | 4:Z:164:PRO:C[1_556]   | 2.07                     | 0.13              |
| 4:2:135:ALA:CB  | 4:Z:332:PRO:N[1_556]   | 2.07                     | 0.13              |
| 4:1:338:SER:OG  | 4:Y:308:GLY:O[1_556]   | 2.07                     | 0.13              |
| 4:0:174:ALA:C   | 4:X:277:THR:C[1_556]   | 2.07                     | 0.13              |
| 4:0:177:ARG:CG  | 4:X:178:LEU:C[1_556]   | 2.07                     | 0.13              |
| 4:0:157:ASP:C   | 4:X:186:THR:N[1_556]   | 2.07                     | 0.13              |
| 4:0:303:THR:CB  | 4:X:257:CYS:N[1_556]   | 2.07                     | 0.13              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:162:ASN:OD1 | 4:Y:273:GLY:O[1_556]   | 2.07                     | 0.13              |
| 4:2:82:MET:CA   | 4:Z:30:VAL:CB[1_556]   | 2.07                     | 0.13              |
| 4:1:155:SER:CB  | 4:Y:258:PRO:C[1_556]   | 2.07                     | 0.13              |
| 4:2:40:HIS:C    | 4:X:167:GLU:CG[1_556]  | 2.07                     | 0.13              |
| 4:2:365:ALA:CB  | 4:Z:349:LEU:N[1_556]   | 2.07                     | 0.13              |
| 4:1:178:LEU:CA  | 4:Y:180:LEU:CG[1_556]  | 2.07                     | 0.13              |
| 4:2:72:GLU:CD   | 4:Z:183:ARG:CD[1_556]  | 2.07                     | 0.13              |
| 4:2:177:ARG:C   | 4:Z:178:LEU:CD1[1_556] | 2.07                     | 0.13              |
| 4:0:294:TYR:CA  | 4:X:320:LEU:N[1_556]   | 2.07                     | 0.13              |
| 4:2:187:ASP:CA  | 4:Z:191:LYS:CB[1_556]  | 2.07                     | 0.13              |
| 4:1:367:PRO:O   | 4:Y:343:GLY:O[1_556]   | 2.07                     | 0.13              |
| 4:1:166:TYR:CE1 | 4:Y:325:MET:SD[1_556]  | 2.07                     | 0.13              |
| 4:1:105:LEU:CD2 | 4:Y:337:TYR:CD2[1_556] | 2.07                     | 0.13              |
| 4:2:206:ARG:CZ  | 4:Z:190:MET:SD[1_556]  | 2.07                     | 0.13              |
| 4:2:370:VAL:CG1 | 4:Z:342:GLY:O[1_556]   | 2.07                     | 0.13              |
| 4:1:278:THR:CA  | 4:Y:276:GLU:OE2[1_556] | 2.07                     | 0.13              |
| 4:2:110:LEU:CG  | 4:Z:162:ASN:N[1_556]   | 2.07                     | 0.13              |
| 4:2:209:VAL:CB  | 4:Z:194:THR:N[1_556]   | 2.07                     | 0.13              |
| 4:1:73:HIS:CE1  | 4:Y:184:ASP:N[1_556]   | 2.07                     | 0.13              |
| 4:1:257:CYS:SG  | 4:Y:192:ILE:CG2[1_556] | 2.07                     | 0.13              |
| 4:0:116:ARG:CD  | 4:X:140:LEU:O[1_556]   | 2.07                     | 0.13              |
| 4:1:147:ARG:CB  | 4:Y:314:GLN:NE2[1_556] | 2.07                     | 0.13              |
| 4:0:171:LEU:C   | 4:X:151:ILE:CG1[1_556] | 2.07                     | 0.13              |
| 4:1:33:SER:CB   | 4:Y:210:ARG:CZ[1_556]  | 2.07                     | 0.13              |
| 4:2:170:ALA:O   | 4:Z:151:ILE:CG2[1_556] | 2.07                     | 0.13              |
| 4:2:39:ARG:NH1  | 4:X:289:ILE:CG2[1_556] | 2.07                     | 0.13              |
| 4:1:277:THR:CB  | 4:Y:273:GLY:N[1_556]   | 2.07                     | 0.13              |
| 4:1:33:SER:N    | 4:Y:210:ARG:NH2[1_556] | 2.07                     | 0.13              |
| 4:1:33:SER:CB   | 4:Y:214:GLU:OE1[1_556] | 2.07                     | 0.13              |
| 4:2:173:HIS:C   | 4:Z:174:ALA:O[1_556]   | 2.07                     | 0.13              |
| 4:1:184:ASP:N   | 4:Y:187:ASP:O[1_556]   | 2.07                     | 0.13              |
| 4:1:185:LEU:CA  | 4:Y:188:TYR:O[1_556]   | 2.07                     | 0.13              |
| 4:2:274:ILE:CG1 | 4:Z:263:GLN:CB[1_556]  | 2.07                     | 0.13              |
| 4:2:183:ARG:C   | 4:Z:187:ASP:CA[1_556]  | 2.07                     | 0.13              |
| 4:1:304:THR:CA  | 4:Y:255:PHE:O[1_556]   | 2.07                     | 0.13              |
| 4:2:62:ARG:CB   | 4:Z:204:ALA:N[1_556]   | 2.07                     | 0.13              |
| 4:1:62:ARG:CD   | 4:Y:204:ALA:N[1_556]   | 2.07                     | 0.13              |
| 4:2:114:ALA:CB  | 4:Z:107:GLU:N[1_556]   | 2.07                     | 0.13              |
| 4:0:213:LYS:CA  | 4:X:253:GLU:OE1[1_556] | 2.07                     | 0.13              |
| 4:1:79:TRP:C    | 4:Y:31:PHE:CG[1_556]   | 2.07                     | 0.13              |
| 4:2:264:PRO:CB  | 4:Z:268:GLY:N[1_556]   | 2.07                     | 0.13              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:125:GLU:CD  | 4:X:7:ALA:O[1_556]     | 2.07                     | 0.13              |
| 4:2:289:ILE:C   | 4:Z:322:PRO:CD[1_556]  | 2.07                     | 0.13              |
| 4:2:68:LYS:CB   | 4:Z:59:GLN:NE2[1_556]  | 2.07                     | 0.13              |
| 4:0:169:TYR:CG  | 4:X:151:ILE:N[1_556]   | 2.07                     | 0.13              |
| 4:2:330:ILE:CD1 | 4:Z:315:LYS:CE[1_556]  | 2.07                     | 0.13              |
| 4:1:357:ILE:CG2 | 4:Y:345:ILE:CB[1_556]  | 2.07                     | 0.13              |
| 4:2:214:GLU:O   | 4:Z:253:GLU:N[1_556]   | 2.07                     | 0.13              |
| 4:2:268:GLY:N   | 4:Y:173:HIS:CG[1_556]  | 2.07                     | 0.13              |
| 4:1:196:ARG:NH1 | 4:X:116:ARG:N[1_556]   | 2.07                     | 0.13              |
| 4:0:79:TRP:CH2  | 4:X:11:ASP:O[1_556]    | 2.07                     | 0.13              |
| 4:1:305:MET:N   | 4:Y:255:PHE:CB[1_556]  | 2.07                     | 0.13              |
| 4:1:139:VAL:O   | 4:Y:329:ILE:O[1_556]   | 2.07                     | 0.13              |
| 4:2:274:ILE:CA  | 4:Z:263:GLN:CA[1_556]  | 2.07                     | 0.13              |
| 4:4:39:ARG:NH1  | 4:Z:289:ILE:CG2[1_556] | 2.07                     | 0.13              |
| 4:0:304:THR:C   | 4:X:223:PHE:CZ[1_556]  | 2.07                     | 0.13              |
| 4:1:186:THR:OG1 | 4:Y:190:MET:N[1_556]   | 2.07                     | 0.13              |
| 4:1:170:ALA:CA  | 4:Y:151:ILE:O[1_556]   | 2.07                     | 0.13              |
| 4:0:293:LEU:O   | 4:X:320:LEU:N[1_556]   | 2.07                     | 0.13              |
| 4:2:157:ASP:C   | 4:Z:186:THR:N[1_556]   | 2.07                     | 0.13              |
| 4:2:213:LYS:CG  | 4:Z:192:ILE:CG1[1_556] | 2.07                     | 0.13              |
| 4:1:68:LYS:CG   | 4:Y:59:GLN:CA[1_556]   | 2.07                     | 0.13              |
| 4:0:305:MET:CG  | 4:X:255:PHE:CA[1_556]  | 2.07                     | 0.13              |
| 4:0:289:ILE:C   | 4:X:322:PRO:CD[1_556]  | 2.07                     | 0.13              |
| 4:2:187:ASP:C   | 4:Z:191:LYS:CB[1_556]  | 2.07                     | 0.13              |
| 4:0:16:LEU:CD2  | 4:X:213:LYS:CA[1_556]  | 2.07                     | 0.13              |
| 4:3:197:GLY:N   | 4:Z:75:ILE:CD1[1_556]  | 2.07                     | 0.13              |
| 4:2:213:LYS:CA  | 4:Z:253:GLU:OE1[1_556] | 2.07                     | 0.13              |
| 4:1:292:ASP:CA  | 4:Y:318:THR:O[1_556]   | 2.07                     | 0.13              |
| 4:2:292:ASP:CA  | 4:Z:321:ALA:CA[1_556]  | 2.07                     | 0.13              |
| 4:0:251:GLY:CA  | 4:W:114:ALA:CB[1_556]  | 2.07                     | 0.13              |
| 4:0:202:THR:O   | 4:X:201:VAL:CG2[1_556] | 2.07                     | 0.13              |
| 4:0:129:VAL:CG2 | 4:X:25:ASP:C[1_556]    | 2.07                     | 0.13              |
| 4:1:203:THR:C   | 4:Y:205:GLU:OE2[1_556] | 2.07                     | 0.13              |
| 4:1:108:ALA:C   | 4:Y:154:ASP:OD1[1_556] | 2.07                     | 0.13              |
| 4:0:78:ASN:C    | 4:X:17:VAL:N[1_556]    | 2.07                     | 0.13              |
| 4:2:186:THR:CA  | 4:Z:190:MET:C[1_556]   | 2.07                     | 0.13              |
| 4:1:294:TYR:C   | 4:Y:319:ALA:CA[1_556]  | 2.07                     | 0.13              |
| 4:1:337:TYR:O   | 4:Y:307:PRO:CA[1_556]  | 2.07                     | 0.13              |
| 4:2:269:MET:CB  | 4:Z:268:GLY:O[1_556]   | 2.07                     | 0.13              |
| 4:2:78:ASN:C    | 4:Z:17:VAL:N[1_556]    | 2.07                     | 0.13              |
| 4:0:294:TYR:O   | 4:X:319:ALA:O[1_556]   | 2.07                     | 0.13              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:137:GLN:N   | 4:X:299:MET:CB[1_556]  | 2.07                     | 0.13              |
| 4:1:260:THR:C   | 4:Y:266:PHE:C[1_556]   | 2.07                     | 0.13              |
| 4:0:209:VAL:CB  | 4:X:194:THR:N[1_556]   | 2.07                     | 0.13              |
| 4:0:203:THR:C   | 4:X:205:GLU:OE2[1_556] | 2.07                     | 0.13              |
| 4:0:206:ARG:CZ  | 4:X:190:MET:SD[1_556]  | 2.07                     | 0.13              |
| 4:1:338:SER:CA  | 4:Y:307:PRO:C[1_556]   | 2.07                     | 0.13              |
| 4:2:196:ARG:NH1 | 4:Y:115:ASN:CB[1_556]  | 2.07                     | 0.13              |
| 4:3:232:SER:CB  | 4:Z:369:ILE:CB[1_556]  | 2.08                     | 0.12              |
| 4:0:264:PRO:CB  | 4:X:268:GLY:N[1_556]   | 2.08                     | 0.12              |
| 4:2:265:SER:C   | 4:Y:173:HIS:NE2[1_556] | 2.08                     | 0.12              |
| 4:1:166:TYR:CZ  | 4:Y:325:MET:CG[1_556]  | 2.08                     | 0.12              |
| 4:1:116:ARG:NH1 | 4:Y:140:LEU:O[1_556]   | 2.08                     | 0.12              |
| 4:3:62:ARG:O    | 4:Y:288:ASP:N[1_556]   | 2.08                     | 0.12              |
| 4:1:266:PHE:C   | 4:X:173:HIS:CA[1_556]  | 2.08                     | 0.12              |
| 4:2:79:TRP:N    | 4:Z:31:PHE:O[1_556]    | 2.08                     | 0.12              |
| 4:2:139:VAL:CG2 | 4:Z:297:ASN:C[1_556]   | 2.08                     | 0.12              |
| 4:0:33:SER:CB   | 4:X:214:GLU:CD[1_556]  | 2.08                     | 0.12              |
| 4:0:76:ILE:CD1  | 4:X:18:LYS:CE[1_556]   | 2.08                     | 0.12              |
| 4:0:170:ALA:CA  | 4:X:151:ILE:O[1_556]   | 2.08                     | 0.12              |
| 4:0:39:ARG:NH1  | 4:V:289:ILE:CG2[1_556] | 2.08                     | 0.12              |
| 4:0:86:TRP:CD2  | 4:X:337:TYR:OH[1_556]  | 2.08                     | 0.12              |
| 4:1:252:ASN:CB  | 4:X:113:LYS:CA[1_556]  | 2.08                     | 0.12              |
| 4:2:11:ASP:CG   | 4:Z:305:MET:CE[1_556]  | 2.08                     | 0.12              |
| 4:2:177:ARG:CG  | 4:Z:178:LEU:C[1_556]   | 2.08                     | 0.12              |
| 4:3:45:VAL:CG2  | 4:Y:328:LYS:CD[1_556]  | 2.08                     | 0.12              |
| 4:1:213:LYS:NZ  | 4:Y:189:LEU:CA[1_556]  | 2.08                     | 0.12              |
| 4:2:306:TYR:C   | 4:Z:227:MET:CG[1_556]  | 2.08                     | 0.12              |
| 4:1:109:PRO:N   | 4:Y:154:ASP:N[1_556]   | 2.08                     | 0.12              |
| 4:1:159:VAL:CG2 | 4:Y:181:ALA:CA[1_556]  | 2.08                     | 0.12              |
| 4:2:198:TYR:N   | 4:Y:75:ILE:CG2[1_556]  | 2.08                     | 0.12              |
| 4:4:41:GLN:CA   | 4:Z:167:GLU:CD[1_556]  | 2.08                     | 0.12              |
| 4:1:303:THR:CA  | 4:Y:256:ARG:C[1_556]   | 2.08                     | 0.12              |
| 4:2:292:ASP:CB  | 4:Z:321:ALA:C[1_556]   | 2.08                     | 0.12              |
| 4:1:139:VAL:O   | 4:Y:329:ILE:C[1_556]   | 2.08                     | 0.12              |
| 4:0:191:LYS:CE  | 4:W:110:LEU:CD1[1_556] | 2.08                     | 0.12              |
| 4:2:172:PRO:CA  | 4:Z:162:ASN:O[1_556]   | 2.08                     | 0.12              |
| 4:2:73:HIS:CE1  | 4:Z:184:ASP:CG[1_556]  | 2.08                     | 0.12              |
| 4:1:232:SER:O   | 4:X:366:GLY:C[1_556]   | 2.08                     | 0.12              |
| 4:0:31:PHE:CB   | 4:X:215:LYS:CE[1_556]  | 2.08                     | 0.12              |
| 4:0:112:PRO:O   | 4:X:137:GLN:CD[1_556]  | 2.08                     | 0.12              |
| 4:1:73:HIS:C    | 4:Y:156:GLY:C[1_556]   | 2.08                     | 0.12              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:370:VAL:CG1 | 4:X:342:GLY:O[1_556]   | 2.08                     | 0.12              |
| 4:0:367:PRO:O   | 4:X:343:GLY:O[1_556]   | 2.08                     | 0.12              |
| 4:1:145:SER:CB  | 4:Y:311:ASP:CA[1_556]  | 2.08                     | 0.12              |
| 4:2:82:MET:C    | 4:Z:30:VAL:CA[1_556]   | 2.08                     | 0.12              |
| 4:2:147:ARG:CB  | 4:Z:314:GLN:NE2[1_556] | 2.08                     | 0.12              |
| 4:0:115:ASN:OD1 | 4:X:12:ASN:O[1_556]    | 2.08                     | 0.12              |
| 4:0:187:ASP:C   | 4:X:191:LYS:CB[1_556]  | 2.08                     | 0.12              |
| 4:0:67:LEU:C    | 4:X:207:GLU:OE2[1_556] | 2.08                     | 0.12              |
| 4:3:253:GLU:CG  | 4:Z:112:PRO:C[1_556]   | 2.08                     | 0.12              |
| 4:0:164:PRO:CB  | 4:X:278:THR:CB[1_556]  | 2.08                     | 0.12              |
| 4:1:79:TRP:CA   | 4:Y:17:VAL:O[1_556]    | 2.08                     | 0.12              |
| 4:0:301:GLY:CA  | 4:X:258:PRO:CB[1_556]  | 2.08                     | 0.12              |
| 4:1:272:ALA:N   | 4:Y:271:SER:N[1_556]   | 2.08                     | 0.12              |
| 4:0:160:THR:CB  | 4:X:180:LEU:CD1[1_556] | 2.08                     | 0.12              |
| 4:1:227:MET:SD  | 4:X:372:ARG:O[1_556]   | 2.08                     | 0.12              |
| 4:2:153:LEU:CA  | 4:Z:262:PHE:CG[1_556]  | 2.08                     | 0.12              |
| 4:1:261:LEU:N   | 4:Y:266:PHE:C[1_556]   | 2.08                     | 0.12              |
| 4:1:112:PRO:CB  | 4:Y:137:GLN:OE1[1_556] | 2.08                     | 0.12              |
| 4:2:41:GLN:CA   | 4:X:167:GLU:CD[1_556]  | 2.08                     | 0.12              |
| 4:1:124:PHE:O   | 4:Y:24:ASP:OD2[1_556]  | 2.08                     | 0.12              |
| 4:1:137:GLN:CD  | 4:Y:304:THR:OG1[1_556] | 2.08                     | 0.12              |
| 4:2:293:LEU:O   | 4:Z:320:LEU:N[1_556]   | 2.08                     | 0.12              |
| 4:1:109:PRO:CG  | 4:Y:153:LEU:CG[1_556]  | 2.08                     | 0.12              |
| 4:2:151:ILE:CB  | 4:Z:317:ILE:CG2[1_556] | 2.08                     | 0.12              |
| 4:0:274:ILE:CA  | 4:X:263:GLN:CA[1_556]  | 2.08                     | 0.12              |
| 4:2:308:GLY:CA  | 4:Z:224:GLU:O[1_556]   | 2.08                     | 0.12              |
| 4:1:209:VAL:C   | 4:Y:193:LEU:CA[1_556]  | 2.08                     | 0.12              |
| 4:2:114:ALA:O   | 4:Z:106:THR:OG1[1_556] | 2.08                     | 0.12              |
| 4:1:306:TYR:C   | 4:Y:227:MET:CG[1_556]  | 2.08                     | 0.12              |
| 4:0:337:TYR:CD2 | 4:X:218:TYR:OH[1_556]  | 2.08                     | 0.12              |
| 4:2:331:ALA:CB  | 4:Z:222:ASP:C[1_556]   | 2.08                     | 0.12              |
| 4:2:305:MET:CG  | 4:Z:255:PHE:CA[1_556]  | 2.08                     | 0.12              |
| 4:1:282:ILE:O   | 4:Y:279:TYR:CD2[1_556] | 2.08                     | 0.12              |
| 4:0:292:ASP:CA  | 4:X:321:ALA:CA[1_556]  | 2.08                     | 0.12              |
| 4:0:139:VAL:CG2 | 4:X:297:ASN:C[1_556]   | 2.08                     | 0.12              |
| 4:2:206:ARG:C   | 4:Z:200:PHE:N[1_556]   | 2.08                     | 0.12              |
| 4:2:11:ASP:OD1  | 4:Z:305:MET:SD[1_556]  | 2.08                     | 0.12              |
| 4:1:164:PRO:CB  | 4:Y:278:THR:CB[1_556]  | 2.08                     | 0.12              |
| 4:0:178:LEU:N   | 4:X:180:LEU:CG[1_556]  | 2.08                     | 0.12              |
| 4:1:82:MET:C    | 4:Y:30:VAL:C[1_556]    | 2.08                     | 0.12              |
| 4:1:106:THR:OG1 | 4:Y:305:MET:SD[1_556]  | 2.08                     | 0.12              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:184:ASP:N   | 4:X:187:ASP:O[1_556]   | 2.08                     | 0.12              |
| 4:1:195:GLU:CG  | 4:X:109:PRO:C[1_556]   | 2.08                     | 0.12              |
| 4:2:206:ARG:O   | 4:Z:200:PHE:CE2[1_556] | 2.08                     | 0.12              |
| 4:1:121:GLN:OE1 | 4:Y:20:GLY:N[1_556]    | 2.08                     | 0.12              |
| 4:2:115:ASN:OD1 | 4:Z:12:ASN:O[1_556]    | 2.08                     | 0.12              |
| 4:1:78:ASN:CA   | 4:Y:31:PHE:O[1_556]    | 2.08                     | 0.12              |
| 4:0:169:TYR:OH  | 4:X:164:PRO:C[1_556]   | 2.08                     | 0.12              |
| 4:2:174:ALA:C   | 4:Z:277:THR:C[1_556]   | 2.08                     | 0.12              |
| 4:2:270:GLU:OE2 | 4:Y:286:ASP:N[1_556]   | 2.08                     | 0.12              |
| 4:2:339:VAL:CG1 | 4:Z:304:THR:O[1_556]   | 2.08                     | 0.12              |
| 4:2:366:GLY:N   | 4:Z:347:ALA:CA[1_556]  | 2.08                     | 0.12              |
| 4:1:184:ASP:CA  | 4:Y:188:TYR:N[1_556]   | 2.08                     | 0.12              |
| 4:0:172:PRO:CA  | 4:X:162:ASN:O[1_556]   | 2.08                     | 0.12              |
| 4:1:157:ASP:O   | 4:Y:185:LEU:CB[1_556]  | 2.08                     | 0.12              |
| 4:2:371:HIS:CA  | 4:Z:140:LEU:CA[1_556]  | 2.08                     | 0.12              |
| 4:2:193:LEU:CA  | 4:Y:112:PRO:CG[1_556]  | 2.08                     | 0.12              |
| 4:2:175:ILE:CD1 | 4:Z:162:ASN:CG[1_556]  | 2.08                     | 0.12              |
| 4:0:32:PRO:N    | 4:X:211:ASP:CB[1_556]  | 2.08                     | 0.12              |
| 4:2:303:THR:CB  | 4:Z:257:CYS:N[1_556]   | 2.08                     | 0.12              |
| 4:2:153:LEU:CD2 | 4:Z:262:PHE:CD2[1_556] | 2.08                     | 0.12              |
| 4:1:306:TYR:CD2 | 4:Y:256:ARG:CA[1_556]  | 2.08                     | 0.12              |
| 4:0:115:ASN:C   | 4:X:11:ASP:OD2[1_556]  | 2.08                     | 0.12              |
| 4:2:362:TYR:CZ  | 4:Z:22:ALA:C[1_556]    | 2.08                     | 0.12              |
| 4:2:177:ARG:NH1 | 4:Z:160:THR:N[1_556]   | 2.08                     | 0.12              |
| 4:0:210:ARG:N   | 4:X:193:LEU:CG[1_556]  | 2.08                     | 0.12              |
| 4:1:175:ILE:C   | 4:Y:162:ASN:OD1[1_556] | 2.08                     | 0.12              |
| 4:1:372:ARG:N   | 4:Y:143:TYR:CG[1_556]  | 2.08                     | 0.12              |
| 4:0:365:ALA:CB  | 4:X:349:LEU:N[1_556]   | 2.08                     | 0.12              |
| 4:1:167:GLU:N   | 4:Y:294:TYR:CA[1_556]  | 2.08                     | 0.12              |
| 4:1:169:TYR:N   | 4:Y:297:ASN:N[1_556]   | 2.08                     | 0.12              |
| 4:1:12:ASN:O    | 4:Y:302:GLY:C[1_556]   | 2.08                     | 0.12              |
| 4:1:252:ASN:C   | 4:X:113:LYS:CD[1_556]  | 2.08                     | 0.12              |
| 4:1:191:LYS:CE  | 4:X:110:LEU:CD1[1_556] | 2.08                     | 0.12              |
| 4:0:196:ARG:NH1 | 4:W:115:ASN:CB[1_556]  | 2.08                     | 0.12              |
| 4:2:178:LEU:N   | 4:Z:180:LEU:CG[1_556]  | 2.08                     | 0.12              |
| 4:1:184:ASP:C   | 4:Y:188:TYR:CA[1_556]  | 2.08                     | 0.12              |
| 4:2:296:ASN:CB  | 4:Z:318:THR:CB[1_556]  | 2.08                     | 0.12              |
| 4:1:299:MET:CE  | 4:Y:312:ARG:NE[1_556]  | 2.08                     | 0.12              |
| 4:1:163:VAL:CB  | 4:Y:153:LEU:CD1[1_556] | 2.08                     | 0.12              |
| 4:1:172:PRO:CG  | 4:Y:163:VAL:C[1_556]   | 2.08                     | 0.12              |
| 4:1:125:GLU:OE1 | 4:Y:21:PHE:CA[1_556]   | 2.08                     | 0.12              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:161:HIS:C   | 4:X:274:ILE:N[1_556]   | 2.08                     | 0.12              |
| 4:2:78:ASN:N    | 4:Z:15:GLY:O[1_556]    | 2.08                     | 0.12              |
| 4:0:31:PHE:CA   | 4:X:215:LYS:CE[1_556]  | 2.08                     | 0.12              |
| 4:2:184:ASP:N   | 4:Z:187:ASP:O[1_556]   | 2.08                     | 0.12              |
| 4:2:204:ALA:O   | 4:Z:246:GLN:OE1[1_556] | 2.08                     | 0.12              |
| 4:1:232:SER:CA  | 4:X:369:ILE:CB[1_556]  | 2.08                     | 0.12              |
| 4:0:298:VAL:CB  | 4:X:312:ARG:CA[1_556]  | 2.08                     | 0.12              |
| 4:0:228:ALA:O   | 4:W:369:ILE:C[1_556]   | 2.08                     | 0.12              |
| 4:3:195:GLU:CG  | 4:Z:109:PRO:C[1_556]   | 2.08                     | 0.12              |
| 4:1:211:ASP:C   | 4:Y:196:ARG:NE[1_556]  | 2.08                     | 0.12              |
| 4:0:62:ARG:O    | 4:V:288:ASP:N[1_556]   | 2.08                     | 0.12              |
| 4:2:137:GLN:N   | 4:Z:299:MET:CB[1_556]  | 2.08                     | 0.12              |
| 4:0:41:GLN:CB   | 4:V:167:GLU:OE1[1_556] | 2.08                     | 0.12              |
| 4:2:31:PHE:CA   | 4:Z:215:LYS:CE[1_556]  | 2.08                     | 0.12              |
| 4:0:308:GLY:CA  | 4:X:224:GLU:O[1_556]   | 2.08                     | 0.12              |
| 4:1:110:LEU:CA  | 4:Y:161:HIS:CB[1_556]  | 2.08                     | 0.12              |
| 4:1:150:GLY:CA  | 4:Y:317:ILE:CA[1_556]  | 2.08                     | 0.12              |
| 4:2:261:LEU:O   | 4:Z:265:SER:CB[1_556]  | 2.08                     | 0.12              |
| 4:3:197:GLY:CA  | 4:Z:75:ILE:CB[1_556]   | 2.08                     | 0.12              |
| 4:2:33:SER:CB   | 4:Z:214:GLU:CD[1_556]  | 2.08                     | 0.12              |
| 4:1:78:ASN:N    | 4:Y:15:GLY:O[1_556]    | 2.08                     | 0.12              |
| 4:1:148:THR:C   | 4:Y:328:LYS:CA[1_556]  | 2.08                     | 0.12              |
| 4:3:192:ILE:O   | 4:Z:111:ASN:C[1_556]   | 2.08                     | 0.12              |
| 4:1:233:SER:C   | 4:X:367:PRO:CA[1_556]  | 2.08                     | 0.12              |
| 4:2:62:ARG:CA   | 4:Z:204:ALA:CB[1_556]  | 2.08                     | 0.12              |
| 4:2:160:THR:CG2 | 4:Z:260:THR:O[1_556]   | 2.08                     | 0.12              |
| 4:2:77:THR:CB   | 4:Z:15:GLY:C[1_556]    | 2.08                     | 0.12              |
| 4:1:153:LEU:C   | 4:Y:262:PHE:CE2[1_556] | 2.08                     | 0.12              |
| 4:2:120:THR:OG1 | 4:Z:341:ILE:C[1_556]   | 2.08                     | 0.12              |
| 4:1:62:ARG:C    | 4:W:288:ASP:C[1_556]   | 2.08                     | 0.12              |
| 4:0:120:THR:OG1 | 4:X:341:ILE:C[1_556]   | 2.08                     | 0.12              |
| 4:3:232:SER:CA  | 4:Z:369:ILE:CB[1_556]  | 2.08                     | 0.12              |
| 4:3:252:ASN:C   | 4:Z:113:LYS:CD[1_556]  | 2.08                     | 0.12              |
| 4:0:288:ASP:OD1 | 4:Z:205:GLU:OE2[1_556] | 2.09                     | 0.11              |
| 4:1:293:LEU:O   | 4:Y:320:LEU:N[1_556]   | 2.09                     | 0.11              |
| 4:1:124:PHE:CB  | 4:Y:24:ASP:C[1_556]    | 2.09                     | 0.11              |
| 4:1:112:PRO:CA  | 4:Y:137:GLN:OE1[1_556] | 2.09                     | 0.11              |
| 4:0:186:THR:C   | 4:X:190:MET:C[1_556]   | 2.09                     | 0.11              |
| 4:2:16:LEU:CD2  | 4:Z:213:LYS:CA[1_556]  | 2.09                     | 0.11              |
| 4:0:296:ASN:CB  | 4:X:318:THR:CB[1_556]  | 2.09                     | 0.11              |
| 4:0:214:GLU:O   | 4:X:253:GLU:N[1_556]   | 2.09                     | 0.11              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:82:MET:CA   | 4:X:30:VAL:CB[1_556]   | 2.09                     | 0.11              |
| 4:1:122:ILE:CG2 | 4:Y:27:PRO:CA[1_556]   | 2.09                     | 0.11              |
| 4:2:67:LEU:C    | 4:Z:207:GLU:OE2[1_556] | 2.09                     | 0.11              |
| 4:2:298:VAL:CB  | 4:Z:312:ARG:CA[1_556]  | 2.09                     | 0.11              |
| 4:2:215:LYS:CB  | 4:Z:237:GLU:OE2[1_556] | 2.09                     | 0.11              |
| 4:1:179:ASP:CA  | 4:Y:180:LEU:CB[1_556]  | 2.09                     | 0.11              |
| 4:0:180:LEU:CD1 | 4:X:267:ILE:CA[1_556]  | 2.09                     | 0.11              |
| 4:0:171:LEU:N   | 4:X:151:ILE:CB[1_556]  | 2.09                     | 0.11              |
| 4:3:253:GLU:OE2 | 4:Z:112:PRO:O[1_556]   | 2.09                     | 0.11              |
| 4:1:120:THR:C   | 4:Y:340:TRP:CZ2[1_556] | 2.09                     | 0.11              |
| 4:0:37:ARG:NH2  | 4:X:56:ASP:CB[1_556]   | 2.09                     | 0.11              |
| 4:2:173:HIS:CG  | 4:Z:174:ALA:CB[1_556]  | 2.09                     | 0.11              |
| 4:1:371:HIS:C   | 4:Y:140:LEU:CA[1_556]  | 2.09                     | 0.11              |
| 4:2:139:VAL:CG2 | 4:Z:297:ASN:O[1_556]   | 2.09                     | 0.11              |
| 4:1:118:LYS:CG  | 4:Y:10:CYS:CA[1_556]   | 2.09                     | 0.11              |
| 4:1:45:VAL:CG2  | 4:W:328:LYS:CD[1_556]  | 2.09                     | 0.11              |
| 4:1:76:ILE:O    | 4:Y:13:GLY:N[1_556]    | 2.09                     | 0.11              |
| 4:0:78:ASN:ND2  | 4:X:32:PRO:N[1_556]    | 2.09                     | 0.11              |
| 4:1:289:ILE:CB  | 4:Y:294:TYR:CE2[1_556] | 2.09                     | 0.11              |
| 4:2:175:ILE:CB  | 4:Z:162:ASN:CB[1_556]  | 2.09                     | 0.11              |
| 4:0:206:ARG:C   | 4:X:200:PHE:N[1_556]   | 2.09                     | 0.11              |
| 4:1:148:THR:OG1 | 4:Y:327:ILE:C[1_556]   | 2.09                     | 0.11              |
| 4:0:260:THR:C   | 4:X:266:PHE:C[1_556]   | 2.09                     | 0.11              |
| 4:1:16:LEU:O    | 4:Y:214:GLU:CG[1_556]  | 2.09                     | 0.11              |
| 4:0:215:LYS:CB  | 4:X:237:GLU:OE2[1_556] | 2.09                     | 0.11              |
| 4:2:301:GLY:CA  | 4:Z:258:PRO:CB[1_556]  | 2.09                     | 0.11              |
| 4:2:126:THR:N   | 4:Z:24:ASP:OD2[1_556]  | 2.09                     | 0.11              |
| 4:0:183:ARG:C   | 4:X:187:ASP:CA[1_556]  | 2.09                     | 0.11              |
| 4:0:173:HIS:C   | 4:X:174:ALA:O[1_556]   | 2.09                     | 0.11              |
| 4:1:294:TYR:O   | 4:Y:319:ALA:CB[1_556]  | 2.09                     | 0.11              |
| 4:1:298:VAL:CG1 | 4:Y:311:ASP:O[1_556]   | 2.09                     | 0.11              |
| 4:0:192:ILE:O   | 4:W:111:ASN:C[1_556]   | 2.09                     | 0.11              |
| 4:1:69:TYR:CE2  | 4:Y:210:ARG:CG[1_556]  | 2.09                     | 0.11              |
| 4:1:159:VAL:CA  | 4:Y:181:ALA:C[1_556]   | 2.09                     | 0.11              |
| 4:2:252:ASN:O   | 4:Y:113:LYS:NZ[1_556]  | 2.09                     | 0.11              |
| 4:1:297:ASN:C   | 4:Y:316:GLU:CA[1_556]  | 2.09                     | 0.11              |
| 4:1:113:LYS:CA  | 4:Y:136:ILE:O[1_556]   | 2.09                     | 0.11              |
| 4:1:365:ALA:CB  | 4:Y:349:LEU:N[1_556]   | 2.09                     | 0.11              |
| 4:0:252:ASN:C   | 4:W:113:LYS:CD[1_556]  | 2.09                     | 0.11              |
| 4:2:68:LYS:CG   | 4:Z:59:GLN:CA[1_556]   | 2.09                     | 0.11              |
| 4:0:139:VAL:CG2 | 4:X:297:ASN:O[1_556]   | 2.09                     | 0.11              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:370:VAL:O   | 4:X:140:LEU:O[1_556]   | 2.09                     | 0.11              |
| 4:2:228:ALA:O   | 4:Y:369:ILE:C[1_556]   | 2.09                     | 0.11              |
| 4:1:297:ASN:CA  | 4:Y:316:GLU:CG[1_556]  | 2.09                     | 0.11              |
| 4:2:298:VAL:CA  | 4:Z:312:ARG:CA[1_556]  | 2.09                     | 0.11              |
| 4:0:114:ALA:O   | 4:X:106:THR:CB[1_556]  | 2.09                     | 0.11              |
| 4:0:141:SER:CB  | 4:X:309:ILE:O[1_556]   | 2.09                     | 0.11              |
| 4:1:62:ARG:NE   | 4:Y:205:GLU:C[1_556]   | 2.09                     | 0.11              |
| 4:2:129:VAL:CG2 | 4:Z:25:ASP:C[1_556]    | 2.09                     | 0.11              |
| 4:0:77:THR:CB   | 4:X:15:GLY:C[1_556]    | 2.09                     | 0.11              |
| 4:1:253:GLU:OE2 | 4:X:112:PRO:O[1_556]   | 2.09                     | 0.11              |
| 4:2:252:ASN:C   | 4:Y:113:LYS:CD[1_556]  | 2.09                     | 0.11              |
| 4:0:213:LYS:CG  | 4:X:192:ILE:CG1[1_556] | 2.09                     | 0.11              |
| 4:1:160:THR:CG2 | 4:Y:260:THR:O[1_556]   | 2.09                     | 0.11              |
| 4:2:209:VAL:C   | 4:Z:193:LEU:CA[1_556]  | 2.09                     | 0.11              |
| 4:2:110:LEU:CD1 | 4:Z:161:HIS:CG[1_556]  | 2.09                     | 0.11              |
| 4:0:109:PRO:N   | 4:X:154:ASP:N[1_556]   | 2.09                     | 0.11              |
| 4:1:268:GLY:N   | 4:X:173:HIS:C[1_556]   | 2.09                     | 0.11              |
| 4:1:196:ARG:CB  | 4:X:112:PRO:CD[1_556]  | 2.09                     | 0.11              |
| 4:1:161:HIS:ND1 | 4:Y:160:THR:OG1[1_556] | 2.09                     | 0.11              |
| 4:1:365:ALA:O   | 4:Y:352:PHE:CB[1_556]  | 2.09                     | 0.11              |
| 4:2:112:PRO:O   | 4:Z:137:GLN:CD[1_556]  | 2.09                     | 0.11              |
| 4:0:206:ARG:O   | 4:X:200:PHE:CE2[1_556] | 2.09                     | 0.11              |
| 4:2:197:GLY:CA  | 4:Y:75:ILE:N[1_556]    | 2.09                     | 0.11              |
| 4:1:121:GLN:CG  | 4:Y:9:VAL:CA[1_556]    | 2.09                     | 0.11              |
| 4:2:126:THR:N   | 4:Z:28:ARG:NE[1_556]   | 2.09                     | 0.11              |
| 4:2:196:ARG:CB  | 4:Y:112:PRO:CD[1_556]  | 2.09                     | 0.11              |
| 4:0:270:GLU:OE2 | 4:W:286:ASP:N[1_556]   | 2.09                     | 0.11              |
| 4:0:304:THR:CG2 | 4:X:259:GLU:CA[1_556]  | 2.09                     | 0.11              |
| 4:0:303:THR:CA  | 4:X:256:ARG:C[1_556]   | 2.09                     | 0.11              |
| 4:0:265:SER:C   | 4:W:173:HIS:NE2[1_556] | 2.09                     | 0.11              |
| 4:1:12:ASN:ND2  | 4:Y:336:LYS:CD[1_556]  | 2.09                     | 0.11              |
| 4:0:364:GLU:C   | 4:X:349:LEU:O[1_556]   | 2.09                     | 0.11              |
| 4:2:197:GLY:N   | 4:Y:75:ILE:CD1[1_556]  | 2.09                     | 0.11              |
| 4:1:294:TYR:CA  | 4:Y:320:LEU:N[1_556]   | 2.09                     | 0.11              |
| 4:1:171:LEU:N   | 4:Y:151:ILE:CB[1_556]  | 2.09                     | 0.11              |
| 4:0:186:THR:CA  | 4:X:190:MET:C[1_556]   | 2.09                     | 0.11              |
| 4:2:282:ILE:CA  | 4:Z:279:TYR:CD2[1_556] | 2.09                     | 0.11              |
| 4:2:109:PRO:N   | 4:Z:154:ASP:N[1_556]   | 2.09                     | 0.11              |
| 4:0:62:ARG:NE   | 4:X:205:GLU:C[1_556]   | 2.09                     | 0.11              |
| 4:0:208:ILE:CB  | 4:X:198:TYR:CG[1_556]  | 2.09                     | 0.11              |
| 4:0:272:ALA:CB  | 4:X:270:GLU:CA[1_556]  | 2.09                     | 0.11              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:268:GLY:N   | 4:Z:173:HIS:C[1_556]   | 2.09                     | 0.11              |
| 4:1:306:TYR:CE2 | 4:Y:256:ARG:O[1_556]   | 2.09                     | 0.11              |
| 4:1:331:ALA:CB  | 4:Y:222:ASP:C[1_556]   | 2.09                     | 0.11              |
| 4:1:370:VAL:CG2 | 4:Y:342:GLY:CA[1_556]  | 2.09                     | 0.11              |
| 4:2:272:ALA:CB  | 4:Z:270:GLU:CA[1_556]  | 2.09                     | 0.11              |
| 4:1:14:SER:CB   | 4:Y:213:LYS:NZ[1_556]  | 2.09                     | 0.11              |
| 4:2:81:ASP:C    | 4:Z:30:VAL:O[1_556]    | 2.09                     | 0.11              |
| 4:3:232:SER:O   | 4:Z:366:GLY:C[1_556]   | 2.09                     | 0.11              |
| 4:1:59:GLN:CD   | 4:Y:208:ILE:CG2[1_556] | 2.09                     | 0.11              |
| 4:0:126:THR:N   | 4:X:24:ASP:OD2[1_556]  | 2.09                     | 0.11              |
| 4:2:309:ILE:CG2 | 4:Z:223:PHE:CA[1_556]  | 2.09                     | 0.11              |
| 4:0:11:ASP:CG   | 4:X:305:MET:CE[1_556]  | 2.09                     | 0.11              |
| 4:0:32:PRO:N    | 4:X:211:ASP:OD1[1_556] | 2.09                     | 0.11              |
| 4:0:82:MET:C    | 4:X:30:VAL:CA[1_556]   | 2.09                     | 0.11              |
| 4:1:153:LEU:CA  | 4:Y:262:PHE:CG[1_556]  | 2.09                     | 0.11              |
| 4:2:172:PRO:CD  | 4:Z:164:PRO:CB[1_556]  | 2.09                     | 0.11              |
| 4:4:62:ARG:C    | 4:Z:288:ASP:C[1_556]   | 2.09                     | 0.11              |
| 4:1:331:ALA:CB  | 4:Y:223:PHE:N[1_556]   | 2.09                     | 0.11              |
| 4:2:115:ASN:C   | 4:Z:11:ASP:OD2[1_556]  | 2.09                     | 0.11              |
| 4:0:230:ALA:CA  | 4:W:368:SER:O[1_556]   | 2.09                     | 0.11              |
| 4:3:233:SER:C   | 4:Z:367:PRO:CA[1_556]  | 2.09                     | 0.11              |
| 4:0:336:LYS:O   | 4:X:217:CYS:O[1_556]   | 2.09                     | 0.11              |
| 4:0:293:LEU:CA  | 4:X:320:LEU:N[1_556]   | 2.09                     | 0.11              |
| 4:2:31:PHE:CB   | 4:Z:215:LYS:CE[1_556]  | 2.09                     | 0.11              |
| 4:1:310:ALA:N   | 4:Y:224:GLU:N[1_556]   | 2.09                     | 0.11              |
| 4:0:203:THR:O   | 4:X:199:SER:O[1_556]   | 2.09                     | 0.11              |
| 4:2:62:ARG:CZ   | 4:Z:204:ALA:C[1_556]   | 2.09                     | 0.11              |
| 4:1:266:PHE:CA  | 4:X:173:HIS:ND1[1_556] | 2.09                     | 0.11              |
| 4:0:168:GLY:CA  | 4:X:328:LYS:O[1_556]   | 2.09                     | 0.11              |
| 4:0:364:GLU:O   | 4:X:350:SER:N[1_556]   | 2.09                     | 0.11              |
| 4:3:233:SER:OG  | 4:Z:367:PRO:CA[1_556]  | 2.09                     | 0.11              |
| 4:1:119:MET:C   | 4:Y:340:TRP:CD1[1_556] | 2.09                     | 0.11              |
| 4:3:191:LYS:CE  | 4:Z:110:LEU:CD1[1_556] | 2.09                     | 0.11              |
| 4:2:288:ASP:O   | 4:Z:322:PRO:CD[1_556]  | 2.09                     | 0.11              |
| 4:3:62:ARG:C    | 4:Y:288:ASP:C[1_556]   | 2.09                     | 0.11              |
| 4:2:117:GLU:OE1 | 4:Z:104:LEU:CG[1_556]  | 2.09                     | 0.11              |
| 4:0:362:TYR:CZ  | 4:X:22:ALA:C[1_556]    | 2.09                     | 0.11              |
| 4:0:76:ILE:CG2  | 4:X:18:LYS:NZ[1_556]   | 2.09                     | 0.11              |
| 4:1:161:HIS:CG  | 4:Y:160:THR:CG2[1_556] | 2.09                     | 0.11              |
| 4:1:62:ARG:O    | 4:W:288:ASP:N[1_556]   | 2.09                     | 0.11              |
| 4:2:299:MET:CE  | 4:Z:312:ARG:NE[1_556]  | 2.09                     | 0.11              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:367:PRO:C   | 4:Y:343:GLY:C[1_556]   | 2.09                     | 0.11              |
| 4:2:213:LYS:CA  | 4:Z:192:ILE:O[1_556]   | 2.09                     | 0.11              |
| 4:1:9:VAL:CG1   | 4:Y:333:PRO:CA[1_556]  | 2.09                     | 0.11              |
| 4:1:139:VAL:CG1 | 4:Y:330:ILE:N[1_556]   | 2.09                     | 0.11              |
| 4:1:272:ALA:C   | 4:Y:270:GLU:C[1_556]   | 2.09                     | 0.11              |
| 4:2:265:SER:CA  | 4:Y:173:HIS:NE2[1_556] | 2.09                     | 0.11              |
| 4:2:41:GLN:CB   | 4:X:167:GLU:OE1[1_556] | 2.09                     | 0.11              |
| 4:1:33:SER:N    | 4:Y:214:GLU:OE1[1_556] | 2.09                     | 0.11              |
| 4:1:253:GLU:CG  | 4:X:112:PRO:C[1_556]   | 2.09                     | 0.11              |
| 4:0:209:VAL:C   | 4:X:193:LEU:CA[1_556]  | 2.09                     | 0.11              |
| 4:1:108:ALA:C   | 4:Y:300:SER:O[1_556]   | 2.09                     | 0.11              |
| 4:2:260:THR:CB  | 4:Z:266:PHE:O[1_556]   | 2.09                     | 0.11              |
| 4:2:32:PRO:N    | 4:Z:211:ASP:CB[1_556]  | 2.10                     | 0.10              |
| 4:0:114:ALA:CB  | 4:X:106:THR:OG1[1_556] | 2.10                     | 0.10              |
| 4:0:213:LYS:N   | 4:X:196:ARG:CG[1_556]  | 2.10                     | 0.10              |
| 4:1:121:GLN:CB  | 4:Y:9:VAL:N[1_556]     | 2.10                     | 0.10              |
| 4:1:119:MET:N   | 4:Y:340:TRP:CB[1_556]  | 2.10                     | 0.10              |
| 4:0:336:LYS:CG  | 4:X:218:TYR:CB[1_556]  | 2.10                     | 0.10              |
| 4:0:126:THR:N   | 4:X:28:ARG:NE[1_556]   | 2.10                     | 0.10              |
| 4:2:116:ARG:CB  | 4:Z:339:VAL:C[1_556]   | 2.10                     | 0.10              |
| 4:1:175:ILE:CB  | 4:Y:162:ASN:CB[1_556]  | 2.10                     | 0.10              |
| 4:0:271:SER:O   | 4:X:270:GLU:CG[1_556]  | 2.10                     | 0.10              |
| 4:1:261:LEU:N   | 4:Y:266:PHE:N[1_556]   | 2.10                     | 0.10              |
| 4:2:364:GLU:C   | 4:Z:349:LEU:O[1_556]   | 2.10                     | 0.10              |
| 4:2:337:TYR:CD2 | 4:Z:218:TYR:OH[1_556]  | 2.10                     | 0.10              |
| 4:0:79:TRP:CB   | 4:X:17:VAL:CA[1_556]   | 2.10                     | 0.10              |
| 4:2:115:ASN:CB  | 4:Z:11:ASP:OD2[1_556]  | 2.10                     | 0.10              |
| 4:1:78:ASN:C    | 4:Y:17:VAL:N[1_556]    | 2.10                     | 0.10              |
| 4:0:303:THR:CG2 | 4:X:260:THR:OG1[1_556] | 2.10                     | 0.10              |
| 4:0:207:GLU:CA  | 4:X:200:PHE:CZ[1_556]  | 2.10                     | 0.10              |
| 4:0:371:HIS:CB  | 4:X:140:LEU:CG[1_556]  | 2.10                     | 0.10              |
| 4:2:289:ILE:CG1 | 4:Z:294:TYR:CZ[1_556]  | 2.10                     | 0.10              |
| 4:3:266:PHE:C   | 4:Z:173:HIS:CA[1_556]  | 2.10                     | 0.10              |
| 4:0:79:TRP:CZ3  | 4:X:18:LYS:CE[1_556]   | 2.10                     | 0.10              |
| 4:3:195:GLU:CA  | 4:Z:75:ILE:CD1[1_556]  | 2.10                     | 0.10              |
| 4:3:252:ASN:CB  | 4:Z:113:LYS:CA[1_556]  | 2.10                     | 0.10              |
| 4:1:294:TYR:C   | 4:Y:319:ALA:CB[1_556]  | 2.10                     | 0.10              |
| 4:0:172:PRO:CD  | 4:X:164:PRO:CB[1_556]  | 2.10                     | 0.10              |
| 4:1:67:LEU:CD1  | 4:Y:207:GLU:CD[1_556]  | 2.10                     | 0.10              |
| 4:2:86:TRP:CD2  | 4:Z:337:TYR:OH[1_556]  | 2.10                     | 0.10              |
| 4:0:369:ILE:N   | 4:X:346:LEU:CG[1_556]  | 2.10                     | 0.10              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:309:ILE:CG2 | 4:X:223:PHE:CA[1_556]  | 2.10                     | 0.10              |
| 4:2:67:LEU:CD1  | 4:Z:207:GLU:CD[1_556]  | 2.10                     | 0.10              |
| 4:1:177:ARG:CZ  | 4:Y:159:VAL:C[1_556]   | 2.10                     | 0.10              |
| 4:0:151:ILE:CB  | 4:X:317:ILE:CG2[1_556] | 2.10                     | 0.10              |
| 4:2:213:LYS:N   | 4:Z:196:ARG:CG[1_556]  | 2.10                     | 0.10              |
| 4:2:70:PRO:O    | 4:Z:15:GLY:O[1_556]    | 2.10                     | 0.10              |
| 4:2:74:GLY:CA   | 4:Z:157:ASP:N[1_556]   | 2.10                     | 0.10              |
| 4:0:174:ALA:N   | 4:X:281:SER:CA[1_556]  | 2.10                     | 0.10              |
| 4:0:131:ALA:N   | 4:X:25:ASP:CG[1_556]   | 2.10                     | 0.10              |
| 4:4:41:GLN:CB   | 4:Z:167:GLU:OE1[1_556] | 2.10                     | 0.10              |
| 4:0:147:ARG:CB  | 4:X:314:GLN:NE2[1_556] | 2.10                     | 0.10              |
| 4:3:195:GLU:OE1 | 4:Z:111:ASN:N[1_556]   | 2.10                     | 0.10              |
| 4:2:303:THR:CG2 | 4:Z:260:THR:OG1[1_556] | 2.10                     | 0.10              |
| 4:2:266:PHE:C   | 4:Y:173:HIS:CA[1_556]  | 2.10                     | 0.10              |
| 4:1:155:SER:O   | 4:Y:258:PRO:CG[1_556]  | 2.10                     | 0.10              |
| 4:0:119:MET:CE  | 4:X:337:TYR:N[1_556]   | 2.10                     | 0.10              |
| 4:3:231:ALA:N   | 4:Z:367:PRO:O[1_556]   | 2.10                     | 0.10              |
| 4:2:176:MET:C   | 4:Z:178:LEU:CB[1_556]  | 2.10                     | 0.10              |
| 4:2:108:ALA:C   | 4:Z:154:ASP:OD1[1_556] | 2.10                     | 0.10              |
| 4:1:185:LEU:CG  | 4:Y:188:TYR:CE2[1_556] | 2.10                     | 0.10              |
| 4:1:269:MET:CB  | 4:Y:268:GLY:O[1_556]   | 2.10                     | 0.10              |
| 4:2:113:LYS:CB  | 4:Z:135:ALA:C[1_556]   | 2.10                     | 0.10              |
| 4:1:109:PRO:CD  | 4:Y:155:SER:N[1_556]   | 2.10                     | 0.10              |
| 4:2:166:TYR:CD2 | 4:Z:290:ARG:O[1_556]   | 2.10                     | 0.10              |
| 4:2:213:LYS:CD  | 4:Z:192:ILE:CD1[1_556] | 2.10                     | 0.10              |
| 4:0:288:ASP:O   | 4:X:322:PRO:CD[1_556]  | 2.10                     | 0.10              |
| 4:2:336:LYS:O   | 4:Z:217:CYS:O[1_556]   | 2.10                     | 0.10              |
| 4:2:76:ILE:CG2  | 4:Z:18:LYS:NZ[1_556]   | 2.10                     | 0.10              |
| 4:0:166:TYR:CD2 | 4:X:290:ARG:O[1_556]   | 2.10                     | 0.10              |
| 4:2:32:PRO:CB   | 4:Z:211:ASP:CG[1_556]  | 2.10                     | 0.10              |
| 4:1:302:GLY:N   | 4:Y:258:PRO:CD[1_556]  | 2.10                     | 0.10              |
| 4:2:131:ALA:N   | 4:Z:25:ASP:CG[1_556]   | 2.10                     | 0.10              |
| 4:4:40:HIS:CD2  | 4:Z:167:GLU:N[1_556]   | 2.10                     | 0.10              |
| 4:0:11:ASP:OD1  | 4:X:305:MET:SD[1_556]  | 2.10                     | 0.10              |
| 4:0:213:LYS:CD  | 4:X:192:ILE:CD1[1_556] | 2.10                     | 0.10              |
| 4:0:153:LEU:CD2 | 4:X:262:PHE:CD2[1_556] | 2.10                     | 0.10              |
| 4:1:274:ILE:CG1 | 4:Y:264:PRO:N[1_556]   | 2.10                     | 0.10              |
| 4:1:336:LYS:N   | 4:Y:219:VAL:N[1_556]   | 2.10                     | 0.10              |
| 4:0:298:VAL:CA  | 4:X:312:ARG:CA[1_556]  | 2.10                     | 0.10              |
| 4:1:121:GLN:CB  | 4:Y:9:VAL:O[1_556]     | 2.10                     | 0.10              |
| 4:1:233:SER:O   | 4:X:367:PRO:CG[1_556]  | 2.10                     | 0.10              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:105:LEU:CA  | 4:Y:334:GLU:CB[1_556]  | 2.10                     | 0.10              |
| 4:2:208:ILE:CB  | 4:Z:198:TYR:CG[1_556]  | 2.10                     | 0.10              |
| 4:2:171:LEU:N   | 4:Z:151:ILE:CG2[1_556] | 2.10                     | 0.10              |
| 4:2:369:ILE:N   | 4:Z:346:LEU:CG[1_556]  | 2.10                     | 0.10              |
| 4:1:148:THR:O   | 4:Y:328:LYS:CA[1_556]  | 2.10                     | 0.10              |
| 4:0:79:TRP:CG   | 4:X:18:LYS:N[1_556]    | 2.10                     | 0.10              |
| 4:0:274:ILE:CD1 | 4:X:263:GLN:CA[1_556]  | 2.10                     | 0.10              |
| 4:1:79:TRP:CB   | 4:Y:17:VAL:CA[1_556]   | 2.10                     | 0.10              |
| 4:0:213:LYS:CA  | 4:X:192:ILE:O[1_556]   | 2.10                     | 0.10              |
| 4:1:298:VAL:CB  | 4:Y:312:ARG:CA[1_556]  | 2.10                     | 0.10              |
| 4:2:303:THR:CG2 | 4:Z:257:CYS:CA[1_556]  | 2.10                     | 0.10              |
| 4:0:12:ASN:O    | 4:X:302:GLY:C[1_556]   | 2.10                     | 0.10              |
| 4:1:298:VAL:CG2 | 4:Y:312:ARG:O[1_556]   | 2.10                     | 0.10              |
| 4:2:180:LEU:CD1 | 4:Z:267:ILE:CA[1_556]  | 2.10                     | 0.10              |
| 4:2:114:ALA:O   | 4:Z:106:THR:CB[1_556]  | 2.10                     | 0.10              |
| 4:1:372:ARG:CZ  | 4:Y:142:LEU:C[1_556]   | 2.10                     | 0.10              |
| 4:2:78:ASN:ND2  | 4:Z:32:PRO:N[1_556]    | 2.10                     | 0.10              |
| 4:2:157:ASP:CB  | 4:Z:213:LYS:CE[1_556]  | 2.10                     | 0.10              |
| 4:0:39:ARG:CA   | 4:V:166:TYR:CZ[1_556]  | 2.10                     | 0.10              |
| 4:2:215:LYS:O   | 4:Z:252:ASN:ND2[1_556] | 2.10                     | 0.10              |
| 4:2:66:THR:CB   | 4:Z:62:ARG:N[1_556]    | 2.10                     | 0.10              |
| 4:0:175:ILE:CB  | 4:X:162:ASN:CB[1_556]  | 2.10                     | 0.10              |
| 4:1:362:TYR:CE2 | 4:Y:22:ALA:N[1_556]    | 2.10                     | 0.10              |
| 4:1:212:ILE:CB  | 4:Y:196:ARG:CG[1_556]  | 2.10                     | 0.10              |
| 4:2:62:ARG:O    | 4:X:288:ASP:N[1_556]   | 2.10                     | 0.10              |
| 4:0:204:ALA:O   | 4:X:246:GLN:OE1[1_556] | 2.10                     | 0.10              |
| 4:1:207:GLU:CA  | 4:Y:200:PHE:CZ[1_556]  | 2.10                     | 0.10              |
| 4:0:148:THR:C   | 4:X:327:ILE:CA[1_556]  | 2.10                     | 0.10              |
| 4:1:231:ALA:N   | 4:X:367:PRO:O[1_556]   | 2.10                     | 0.10              |
| 4:0:86:TRP:CE2  | 4:X:337:TYR:CE2[1_556] | 2.10                     | 0.10              |
| 4:2:331:ALA:N   | 4:Z:221:LEU:C[1_556]   | 2.10                     | 0.10              |
| 4:2:86:TRP:CE2  | 4:Z:337:TYR:CE2[1_556] | 2.10                     | 0.10              |
| 4:2:252:ASN:CB  | 4:Y:113:LYS:CA[1_556]  | 2.10                     | 0.10              |
| 4:0:68:LYS:CG   | 4:X:59:GLN:CA[1_556]   | 2.10                     | 0.10              |
| 4:2:114:ALA:CB  | 4:Z:106:THR:OG1[1_556] | 2.10                     | 0.10              |
| 4:2:161:HIS:C   | 4:Z:274:ILE:N[1_556]   | 2.10                     | 0.10              |
| 4:0:260:THR:C   | 4:X:265:SER:O[1_556]   | 2.10                     | 0.10              |
| 4:2:79:TRP:CG   | 4:Z:18:LYS:N[1_556]    | 2.10                     | 0.10              |
| 4:0:173:HIS:CG  | 4:X:174:ALA:CB[1_556]  | 2.10                     | 0.10              |
| 4:1:61:LYS:CA   | 4:W:291:LYS:CD[1_556]  | 2.10                     | 0.10              |
| 4:0:197:GLY:CA  | 4:W:75:ILE:N[1_556]    | 2.10                     | 0.10              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:127:PHE:N   | 4:Z:28:ARG:NE[1_556]   | 2.10                     | 0.10              |
| 4:0:32:PRO:CB   | 4:X:211:ASP:CG[1_556]  | 2.10                     | 0.10              |
| 4:1:168:GLY:C   | 4:Y:296:ASN:O[1_556]   | 2.10                     | 0.10              |
| 4:0:282:ILE:CA  | 4:X:279:TYR:CD2[1_556] | 2.10                     | 0.10              |
| 4:1:195:GLU:CA  | 4:X:75:ILE:CD1[1_556]  | 2.10                     | 0.10              |
| 4:0:227:MET:SD  | 4:W:372:ARG:O[1_556]   | 2.10                     | 0.10              |
| 4:0:70:PRO:O    | 4:X:15:GLY:O[1_556]    | 2.10                     | 0.10              |
| 4:1:139:VAL:CG2 | 4:Y:297:ASN:C[1_556]   | 2.10                     | 0.10              |
| 4:1:62:ARG:CA   | 4:Y:204:ALA:CB[1_556]  | 2.10                     | 0.10              |
| 4:1:169:TYR:OH  | 4:Y:165:ILE:N[1_556]   | 2.10                     | 0.10              |
| 4:0:370:VAL:CG2 | 4:X:342:GLY:N[1_556]   | 2.10                     | 0.10              |
| 4:1:177:ARG:CZ  | 4:Y:158:GLY:O[1_556]   | 2.10                     | 0.10              |
| 4:1:80:ASP:CA   | 4:Y:31:PHE:CD2[1_556]  | 2.10                     | 0.10              |
| 4:0:197:GLY:N   | 4:W:75:ILE:CD1[1_556]  | 2.10                     | 0.10              |
| 4:1:115:ASN:C   | 4:Y:11:ASP:OD2[1_556]  | 2.10                     | 0.10              |
| 4:1:372:ARG:CA  | 4:Y:143:TYR:CG[1_556]  | 2.10                     | 0.10              |
| 4:2:370:VAL:CG2 | 4:Z:342:GLY:N[1_556]   | 2.10                     | 0.10              |
| 4:1:79:TRP:N    | 4:Y:31:PHE:O[1_556]    | 2.10                     | 0.10              |
| 4:2:207:GLU:CA  | 4:Z:200:PHE:CZ[1_556]  | 2.10                     | 0.10              |
| 4:2:174:ALA:N   | 4:Z:281:SER:CA[1_556]  | 2.10                     | 0.10              |
| 4:0:158:GLY:O   | 4:X:184:ASP:CB[1_556]  | 2.10                     | 0.10              |
| 4:1:205:GLU:O   | 4:Y:199:SER:CA[1_556]  | 2.10                     | 0.10              |
| 4:2:147:ARG:N   | 4:Z:314:GLN:NE2[1_556] | 2.10                     | 0.10              |
| 4:1:37:ARG:O    | 4:Y:60:SER:C[1_556]    | 2.10                     | 0.10              |
| 4:0:331:ALA:N   | 4:X:221:LEU:C[1_556]   | 2.10                     | 0.10              |
| 4:2:32:PRO:N    | 4:Z:211:ASP:OD1[1_556] | 2.10                     | 0.10              |
| 4:3:193:LEU:CA  | 4:Z:112:PRO:CG[1_556]  | 2.10                     | 0.10              |
| 4:2:62:ARG:NE   | 4:Z:205:GLU:C[1_556]   | 2.10                     | 0.10              |
| 4:1:159:VAL:CA  | 4:Y:181:ALA:CA[1_556]  | 2.10                     | 0.10              |
| 4:2:39:ARG:CA   | 4:X:166:TYR:CZ[1_556]  | 2.10                     | 0.10              |
| 4:0:167:GLU:CD  | 4:X:326:LYS:CG[1_556]  | 2.10                     | 0.10              |
| 4:0:155:SER:OG  | 4:X:260:THR:C[1_556]   | 2.10                     | 0.10              |
| 4:1:110:LEU:CG  | 4:Y:162:ASN:N[1_556]   | 2.10                     | 0.10              |
| 4:2:364:GLU:O   | 4:Z:350:SER:N[1_556]   | 2.10                     | 0.10              |
| 4:3:196:ARG:CB  | 4:Z:112:PRO:CD[1_556]  | 2.10                     | 0.10              |
| 4:2:62:ARG:C    | 4:X:288:ASP:C[1_556]   | 2.10                     | 0.10              |
| 4:1:299:MET:C   | 4:Y:219:VAL:CG1[1_556] | 2.10                     | 0.10              |
| 4:1:142:LEU:N   | 4:Y:310:ALA:CB[1_556]  | 2.10                     | 0.10              |
| 4:1:195:GLU:OE1 | 4:X:111:ASN:N[1_556]   | 2.10                     | 0.10              |
| 4:1:206:ARG:CA  | 4:Y:199:SER:N[1_556]   | 2.10                     | 0.10              |
| 4:0:197:GLY:O   | 4:W:76:ILE:C[1_556]    | 2.10                     | 0.10              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:261:LEU:CD1 | 4:X:266:PHE:CZ[1_556]  | 2.10                     | 0.10              |
| 4:1:136:ILE:O   | 4:Y:299:MET:C[1_556]   | 2.10                     | 0.10              |
| 4:1:274:ILE:CG1 | 4:Y:263:GLN:CB[1_556]  | 2.10                     | 0.10              |
| 4:0:133:TYR:O   | 4:X:334:GLU:CD[1_556]  | 2.10                     | 0.10              |
| 4:1:161:HIS:N   | 4:Y:274:ILE:CD1[1_556] | 2.10                     | 0.10              |
| 4:1:67:LEU:CB   | 4:Y:62:ARG:NH1[1_556]  | 2.10                     | 0.10              |
| 4:2:260:THR:C   | 4:Z:265:SER:O[1_556]   | 2.10                     | 0.10              |
| 4:0:196:ARG:CB  | 4:W:112:PRO:CD[1_556]  | 2.10                     | 0.10              |
| 4:0:105:LEU:N   | 4:X:334:GLU:N[1_556]   | 2.10                     | 0.10              |
| 4:1:291:LYS:CG  | 4:Y:322:PRO:CA[1_556]  | 2.10                     | 0.10              |
| 4:1:155:SER:N   | 4:Y:261:LEU:CB[1_556]  | 2.10                     | 0.10              |
| 4:0:122:ILE:C   | 4:X:26:ALA:O[1_556]    | 2.10                     | 0.10              |
| 4:2:304:THR:CG2 | 4:Z:259:GLU:CA[1_556]  | 2.10                     | 0.10              |
| 4:1:307:PRO:C   | 4:Y:227:MET:CA[1_556]  | 2.10                     | 0.10              |
| 4:2:37:ARG:NH2  | 4:Z:56:ASP:CB[1_556]   | 2.10                     | 0.10              |
| 4:1:140:LEU:N   | 4:Y:299:MET:CE[1_556]  | 2.10                     | 0.10              |
| 4:0:45:VAL:CG2  | 4:V:328:LYS:CD[1_556]  | 2.10                     | 0.10              |
| 4:1:192:ILE:O   | 4:X:111:ASN:C[1_556]   | 2.10                     | 0.10              |
| 4:1:137:GLN:CA  | 4:Y:304:THR:CB[1_556]  | 2.10                     | 0.10              |
| 4:2:370:VAL:O   | 4:Z:140:LEU:O[1_556]   | 2.11                     | 0.09              |
| 4:0:309:ILE:CG2 | 4:X:223:PHE:O[1_556]   | 2.11                     | 0.09              |
| 4:0:265:SER:CA  | 4:W:173:HIS:NE2[1_556] | 2.11                     | 0.09              |
| 4:0:252:ASN:O   | 4:W:113:LYS:NZ[1_556]  | 2.11                     | 0.09              |
| 4:3:227:MET:CB  | 4:Z:372:ARG:CA[1_556]  | 2.11                     | 0.09              |
| 4:1:178:LEU:CD1 | 4:Y:269:MET:CG[1_556]  | 2.11                     | 0.09              |
| 4:0:176:MET:C   | 4:X:178:LEU:CB[1_556]  | 2.11                     | 0.09              |
| 4:1:15:GLY:C    | 4:Y:214:GLU:CG[1_556]  | 2.11                     | 0.09              |
| 4:1:233:SER:OG  | 4:X:367:PRO:CA[1_556]  | 2.11                     | 0.09              |
| 4:2:252:ASN:CB  | 4:Y:113:LYS:CB[1_556]  | 2.11                     | 0.09              |
| 4:1:175:ILE:O   | 4:Y:176:MET:CB[1_556]  | 2.11                     | 0.09              |
| 4:2:79:TRP:N    | 4:Z:17:VAL:CG2[1_556]  | 2.11                     | 0.09              |
| 4:0:66:THR:CB   | 4:X:62:ARG:N[1_556]    | 2.11                     | 0.09              |
| 4:2:139:VAL:CG1 | 4:Z:330:ILE:C[1_556]   | 2.11                     | 0.09              |
| 4:1:298:VAL:C   | 4:Y:312:ARG:CB[1_556]  | 2.11                     | 0.09              |
| 4:0:115:ASN:CB  | 4:X:11:ASP:OD2[1_556]  | 2.11                     | 0.09              |
| 4:1:370:VAL:O   | 4:Y:144:ALA:N[1_556]   | 2.11                     | 0.09              |
| 4:1:215:LYS:CG  | 4:Y:196:ARG:CZ[1_556]  | 2.11                     | 0.09              |
| 4:2:167:GLU:CD  | 4:Z:326:LYS:CG[1_556]  | 2.11                     | 0.09              |
| 4:1:292:ASP:C   | 4:Y:317:ILE:O[1_556]   | 2.11                     | 0.09              |
| 4:2:153:LEU:CD2 | 4:Z:262:PHE:CA[1_556]  | 2.11                     | 0.09              |
| 4:1:279:TYR:C   | 4:Y:276:GLU:CD[1_556]  | 2.11                     | 0.09              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:80:ASP:O    | 4:Y:30:VAL:O[1_556]    | 2.11                     | 0.09              |
| 4:1:306:TYR:CE1 | 4:Y:256:ARG:CD[1_556]  | 2.11                     | 0.09              |
| 4:2:306:TYR:CE2 | 4:Z:256:ARG:O[1_556]   | 2.11                     | 0.09              |
| 4:0:74:GLY:CA   | 4:X:157:ASP:N[1_556]   | 2.11                     | 0.09              |
| 4:2:159:VAL:CA  | 4:Z:181:ALA:C[1_556]   | 2.11                     | 0.09              |
| 4:0:116:ARG:CB  | 4:X:339:VAL:C[1_556]   | 2.11                     | 0.09              |
| 4:2:290:ARG:CD  | 4:Z:279:TYR:OH[1_556]  | 2.11                     | 0.09              |
| 4:2:168:GLY:CA  | 4:Z:328:LYS:O[1_556]   | 2.11                     | 0.09              |
| 4:2:217:CYS:CB  | 4:Z:256:ARG:NE[1_556]  | 2.11                     | 0.09              |
| 4:1:253:GLU:OE2 | 4:X:113:LYS:N[1_556]   | 2.11                     | 0.09              |
| 4:1:185:LEU:CA  | 4:Y:188:TYR:CD1[1_556] | 2.11                     | 0.09              |
| 4:0:215:LYS:O   | 4:X:252:ASN:ND2[1_556] | 2.11                     | 0.09              |
| 4:2:173:HIS:ND1 | 4:Z:174:ALA:CB[1_556]  | 2.11                     | 0.09              |
| 4:1:206:ARG:C   | 4:Y:199:SER:CA[1_556]  | 2.11                     | 0.09              |
| 4:0:111:ASN:CB  | 4:X:154:ASP:OD1[1_556] | 2.11                     | 0.09              |
| 4:2:371:HIS:CB  | 4:Z:140:LEU:CG[1_556]  | 2.11                     | 0.09              |
| 4:3:198:TYR:N   | 4:Z:75:ILE:CG2[1_556]  | 2.11                     | 0.09              |
| 4:2:336:LYS:N   | 4:Z:218:TYR:CA[1_556]  | 2.11                     | 0.09              |
| 4:0:289:ILE:CG1 | 4:X:294:TYR:CZ[1_556]  | 2.11                     | 0.09              |
| 4:1:148:THR:C   | 4:Y:327:ILE:CA[1_556]  | 2.11                     | 0.09              |
| 4:0:41:GLN:N    | 4:V:167:GLU:CG[1_556]  | 2.11                     | 0.09              |
| 4:0:59:GLN:CB   | 4:X:208:ILE:CD1[1_556] | 2.11                     | 0.09              |
| 4:2:124:PHE:C   | 4:Z:24:ASP:N[1_556]    | 2.11                     | 0.09              |
| 4:0:306:TYR:CD1 | 4:X:256:ARG:NE[1_556]  | 2.11                     | 0.09              |
| 4:1:303:THR:O   | 4:Y:255:PHE:O[1_556]   | 2.11                     | 0.09              |
| 4:2:203:THR:O   | 4:Z:199:SER:O[1_556]   | 2.11                     | 0.09              |
| 4:2:164:PRO:CB  | 4:Z:278:THR:CA[1_556]  | 2.11                     | 0.09              |
| 4:1:76:ILE:CG2  | 4:Y:18:LYS:NZ[1_556]   | 2.11                     | 0.09              |
| 4:1:277:THR:CA  | 4:Y:272:ALA:CB[1_556]  | 2.11                     | 0.09              |
| 4:0:148:THR:CG2 | 4:X:328:LYS:CA[1_556]  | 2.11                     | 0.09              |
| 4:2:336:LYS:CG  | 4:Z:218:TYR:CB[1_556]  | 2.11                     | 0.09              |
| 4:2:141:SER:CB  | 4:Z:309:ILE:O[1_556]   | 2.11                     | 0.09              |
| 4:0:110:LEU:CD1 | 4:X:161:HIS:CG[1_556]  | 2.11                     | 0.09              |
| 4:0:338:SER:CA  | 4:X:307:PRO:C[1_556]   | 2.11                     | 0.09              |
| 4:2:122:ILE:C   | 4:Z:26:ALA:O[1_556]    | 2.11                     | 0.09              |
| 4:2:230:ALA:CA  | 4:Y:368:SER:O[1_556]   | 2.11                     | 0.09              |
| 4:1:289:ILE:CD1 | 4:Y:282:ILE:CG2[1_556] | 2.11                     | 0.09              |
| 4:1:155:SER:CA  | 4:Y:261:LEU:CG[1_556]  | 2.11                     | 0.09              |
| 4:3:266:PHE:CA  | 4:Z:173:HIS:ND1[1_556] | 2.11                     | 0.09              |
| 4:2:124:PHE:CG  | 4:Z:23:GLY:C[1_556]    | 2.11                     | 0.09              |
| 4:0:311:ASP:N   | 4:X:224:GLU:CG[1_556]  | 2.11                     | 0.09              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:147:ARG:N   | 4:X:314:GLN:NE2[1_556] | 2.11                     | 0.09              |
| 4:1:306:TYR:CD1 | 4:Y:256:ARG:NE[1_556]  | 2.11                     | 0.09              |
| 4:0:124:PHE:C   | 4:X:24:ASP:N[1_556]    | 2.11                     | 0.09              |
| 4:0:122:ILE:CB  | 4:X:27:PRO:CA[1_556]   | 2.11                     | 0.09              |
| 4:1:124:PHE:CG  | 4:Y:23:GLY:O[1_556]    | 2.11                     | 0.09              |
| 4:1:79:TRP:CZ3  | 4:Y:18:LYS:CE[1_556]   | 2.11                     | 0.09              |
| 4:0:81:ASP:C    | 4:X:30:VAL:O[1_556]    | 2.11                     | 0.09              |
| 4:2:192:ILE:O   | 4:Y:111:ASN:C[1_556]   | 2.11                     | 0.09              |
| 4:0:336:LYS:N   | 4:X:218:TYR:CA[1_556]  | 2.11                     | 0.09              |
| 4:4:39:ARG:CA   | 4:Z:166:TYR:CZ[1_556]  | 2.11                     | 0.09              |
| 4:1:214:GLU:N   | 4:Y:253:GLU:CB[1_556]  | 2.11                     | 0.09              |
| 4:1:77:THR:N    | 4:Y:15:GLY:N[1_556]    | 2.11                     | 0.09              |
| 4:0:173:HIS:ND1 | 4:X:174:ALA:CB[1_556]  | 2.11                     | 0.09              |
| 4:2:185:LEU:CA  | 4:Z:188:TYR:CD1[1_556] | 2.11                     | 0.09              |
| 4:0:171:LEU:N   | 4:X:151:ILE:CG2[1_556] | 2.11                     | 0.09              |
| 4:2:303:THR:CA  | 4:Z:256:ARG:C[1_556]   | 2.11                     | 0.09              |
| 4:0:185:LEU:CA  | 4:X:188:TYR:CD1[1_556] | 2.11                     | 0.09              |
| 4:1:207:GLU:C   | 4:Y:200:PHE:CE1[1_556] | 2.11                     | 0.09              |
| 4:0:79:TRP:CB   | 4:X:17:VAL:C[1_556]    | 2.11                     | 0.09              |
| 4:3:253:GLU:OE2 | 4:Z:113:LYS:N[1_556]   | 2.11                     | 0.09              |
| 4:2:119:MET:CE  | 4:Z:337:TYR:N[1_556]   | 2.11                     | 0.09              |
| 4:2:306:TYR:CE2 | 4:Z:256:ARG:C[1_556]   | 2.11                     | 0.09              |
| 4:2:40:HIS:CD2  | 4:X:167:GLU:N[1_556]   | 2.11                     | 0.09              |
| 4:1:134:VAL:O   | 4:Y:338:SER:OG[1_556]  | 2.11                     | 0.09              |
| 4:1:166:TYR:CD1 | 4:Y:294:TYR:CE2[1_556] | 2.11                     | 0.09              |
| 4:2:133:TYR:O   | 4:Z:334:GLU:CD[1_556]  | 2.11                     | 0.09              |
| 4:0:134:VAL:CB  | 4:X:338:SER:OG[1_556]  | 2.11                     | 0.09              |
| 4:0:16:LEU:CB   | 4:X:215:LYS:N[1_556]   | 2.11                     | 0.09              |
| 4:0:62:ARG:CZ   | 4:X:204:ALA:C[1_556]   | 2.11                     | 0.09              |
| 4:1:264:PRO:CG  | 4:Y:268:GLY:C[1_556]   | 2.11                     | 0.09              |
| 4:0:303:THR:CG2 | 4:X:257:CYS:CA[1_556]  | 2.11                     | 0.09              |
| 4:0:335:ARG:CG  | 4:X:220:ALA:CB[1_556]  | 2.11                     | 0.09              |
| 4:2:271:SER:O   | 4:Z:270:GLU:CG[1_556]  | 2.11                     | 0.09              |
| 4:2:140:LEU:CD1 | 4:Z:332:PRO:O[1_556]   | 2.11                     | 0.09              |
| 4:2:79:TRP:C    | 4:Z:31:PHE:CG[1_556]   | 2.11                     | 0.09              |
| 4:1:30:VAL:C    | 4:Y:215:LYS:CD[1_556]  | 2.11                     | 0.09              |
| 4:1:169:TYR:C   | 4:Y:296:ASN:O[1_556]   | 2.11                     | 0.09              |
| 4:1:62:ARG:NE   | 4:Y:204:ALA:O[1_556]   | 2.11                     | 0.09              |
| 4:0:252:ASN:OD1 | 4:W:117:GLU:N[1_556]   | 2.11                     | 0.09              |
| 4:1:337:TYR:O   | 4:Y:307:PRO:CB[1_556]  | 2.11                     | 0.09              |
| 4:0:153:LEU:CD2 | 4:X:262:PHE:CA[1_556]  | 2.11                     | 0.09              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:79:TRP:N    | 4:X:17:VAL:CG2[1_556]  | 2.11                     | 0.09              |
| 4:3:61:LYS:CA   | 4:Y:291:LYS:CD[1_556]  | 2.11                     | 0.09              |
| 4:2:293:LEU:CA  | 4:Z:320:LEU:N[1_556]   | 2.11                     | 0.09              |
| 4:0:139:VAL:CG1 | 4:X:330:ILE:C[1_556]   | 2.11                     | 0.09              |
| 4:0:62:ARG:C    | 4:V:288:ASP:C[1_556]   | 2.11                     | 0.09              |
| 4:1:119:MET:CG  | 4:Y:340:TRP:N[1_556]   | 2.11                     | 0.09              |
| 4:2:197:GLY:C   | 4:Y:75:ILE:CG2[1_556]  | 2.11                     | 0.09              |
| 4:0:132:MET:CE  | 4:X:341:ILE:CD1[1_556] | 2.11                     | 0.09              |
| 4:2:148:THR:C   | 4:Z:327:ILE:CA[1_556]  | 2.11                     | 0.09              |
| 4:2:169:TYR:OH  | 4:Z:165:ILE:N[1_556]   | 2.11                     | 0.09              |
| 4:1:186:THR:C   | 4:Y:190:MET:C[1_556]   | 2.11                     | 0.09              |
| 4:0:79:TRP:C    | 4:X:31:PHE:CG[1_556]   | 2.11                     | 0.09              |
| 4:1:228:ALA:O   | 4:X:369:ILE:O[1_556]   | 2.11                     | 0.09              |
| 4:1:362:TYR:CE1 | 4:Y:344:SER:O[1_556]   | 2.11                     | 0.09              |
| 4:2:138:ALA:O   | 4:Z:299:MET:SD[1_556]  | 2.11                     | 0.09              |
| 4:2:306:TYR:CD1 | 4:Z:256:ARG:NE[1_556]  | 2.11                     | 0.09              |
| 4:1:76:ILE:O    | 4:Y:13:GLY:C[1_556]    | 2.11                     | 0.09              |
| 4:0:260:THR:CB  | 4:X:266:PHE:O[1_556]   | 2.11                     | 0.09              |
| 4:0:123:MET:CA  | 4:X:26:ALA:N[1_556]    | 2.11                     | 0.09              |
| 4:0:278:THR:CA  | 4:X:276:GLU:OE2[1_556] | 2.11                     | 0.09              |
| 4:3:228:ALA:O   | 4:Z:369:ILE:O[1_556]   | 2.11                     | 0.09              |
| 4:2:158:GLY:O   | 4:Z:184:ASP:CB[1_556]  | 2.12                     | 0.08              |
| 4:3:195:GLU:CG  | 4:Z:108:ALA:C[1_556]   | 2.12                     | 0.08              |
| 4:1:73:HIS:O    | 4:Y:156:GLY:O[1_556]   | 2.12                     | 0.08              |
| 4:2:291:LYS:CG  | 4:Z:322:PRO:CA[1_556]  | 2.12                     | 0.08              |
| 4:1:211:ASP:CA  | 4:Y:249:THR:O[1_556]   | 2.12                     | 0.08              |
| 4:1:109:PRO:CA  | 4:Y:154:ASP:O[1_556]   | 2.12                     | 0.08              |
| 4:0:299:MET:CE  | 4:X:312:ARG:NE[1_556]  | 2.12                     | 0.08              |
| 4:2:189:LEU:CA  | 4:Z:195:GLU:CB[1_556]  | 2.12                     | 0.08              |
| 4:2:148:THR:CG2 | 4:Z:328:LYS:CA[1_556]  | 2.12                     | 0.08              |
| 4:1:77:THR:C    | 4:Y:33:SER:OG[1_556]   | 2.12                     | 0.08              |
| 4:0:67:LEU:CD1  | 4:X:207:GLU:CD[1_556]  | 2.12                     | 0.08              |
| 4:0:117:GLU:OE1 | 4:X:104:LEU:CG[1_556]  | 2.12                     | 0.08              |
| 4:1:187:ASP:CA  | 4:Y:191:LYS:CB[1_556]  | 2.12                     | 0.08              |
| 4:1:105:LEU:N   | 4:Y:334:GLU:CG[1_556]  | 2.12                     | 0.08              |
| 4:0:304:THR:CG2 | 4:X:223:PHE:CE2[1_556] | 2.12                     | 0.08              |
| 4:1:213:LYS:CD  | 4:Y:192:ILE:CD1[1_556] | 2.12                     | 0.08              |
| 4:2:153:LEU:CG  | 4:Z:262:PHE:CD1[1_556] | 2.12                     | 0.08              |
| 4:2:311:ASP:N   | 4:Z:224:GLU:CG[1_556]  | 2.12                     | 0.08              |
| 4:1:335:ARG:NE  | 4:Y:223:PHE:CD1[1_556] | 2.12                     | 0.08              |
| 4:1:86:TRP:CH2  | 4:Y:337:TYR:CE1[1_556] | 2.12                     | 0.08              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:189:LEU:CA  | 4:X:195:GLU:CB[1_556]  | 2.12                     | 0.08              |
| 4:2:278:THR:CB  | 4:Z:275:HIS:NE2[1_556] | 2.12                     | 0.08              |
| 4:2:274:ILE:CD1 | 4:Z:263:GLN:CA[1_556]  | 2.12                     | 0.08              |
| 4:2:45:VAL:CG2  | 4:X:328:LYS:CD[1_556]  | 2.12                     | 0.08              |
| 4:2:137:GLN:N   | 4:Z:299:MET:C[1_556]   | 2.12                     | 0.08              |
| 4:1:206:ARG:O   | 4:Y:200:PHE:CE2[1_556] | 2.12                     | 0.08              |
| 4:2:138:ALA:CB  | 4:Z:299:MET:SD[1_556]  | 2.12                     | 0.08              |
| 4:1:330:ILE:CG1 | 4:Y:315:LYS:CB[1_556]  | 2.12                     | 0.08              |
| 4:0:183:ARG:CA  | 4:X:187:ASP:C[1_556]   | 2.12                     | 0.08              |
| 4:4:62:ARG:O    | 4:Z:288:ASP:N[1_556]   | 2.12                     | 0.08              |
| 4:2:116:ARG:NH1 | 4:Z:140:LEU:O[1_556]   | 2.12                     | 0.08              |
| 4:2:195:GLU:CG  | 4:Y:109:PRO:C[1_556]   | 2.12                     | 0.08              |
| 4:2:79:TRP:CZ3  | 4:Z:18:LYS:CE[1_556]   | 2.12                     | 0.08              |
| 4:0:113:LYS:CB  | 4:X:135:ALA:C[1_556]   | 2.12                     | 0.08              |
| 4:1:298:VAL:C   | 4:Y:312:ARG:CA[1_556]  | 2.12                     | 0.08              |
| 4:0:195:GLU:CG  | 4:W:109:PRO:C[1_556]   | 2.12                     | 0.08              |
| 4:3:252:ASN:OD1 | 4:Z:117:GLU:N[1_556]   | 2.12                     | 0.08              |
| 4:2:155:SER:OG  | 4:Z:260:THR:C[1_556]   | 2.12                     | 0.08              |
| 4:2:16:LEU:CB   | 4:Z:215:LYS:N[1_556]   | 2.12                     | 0.08              |
| 4:0:218:TYR:OH  | 4:X:231:ALA:CB[1_556]  | 2.12                     | 0.08              |
| 4:1:137:GLN:N   | 4:Y:299:MET:C[1_556]   | 2.12                     | 0.08              |
| 4:1:274:ILE:CD1 | 4:Y:264:PRO:CD[1_556]  | 2.12                     | 0.08              |
| 4:0:197:GLY:C   | 4:W:75:ILE:CG2[1_556]  | 2.12                     | 0.08              |
| 4:1:17:VAL:N    | 4:Y:214:GLU:CB[1_556]  | 2.12                     | 0.08              |
| 4:1:86:TRP:CD2  | 4:Y:337:TYR:OH[1_556]  | 2.12                     | 0.08              |
| 4:1:210:ARG:N   | 4:Y:193:LEU:CG[1_556]  | 2.12                     | 0.08              |
| 4:0:266:PHE:C   | 4:W:173:HIS:CA[1_556]  | 2.12                     | 0.08              |
| 4:0:119:MET:O   | 4:X:340:TRP:CG[1_556]  | 2.12                     | 0.08              |
| 4:1:116:ARG:CD  | 4:Y:140:LEU:O[1_556]   | 2.12                     | 0.08              |
| 4:2:122:ILE:CB  | 4:Z:27:PRO:CA[1_556]   | 2.12                     | 0.08              |
| 4:0:177:ARG:CB  | 4:X:178:LEU:CA[1_556]  | 2.12                     | 0.08              |
| 4:2:12:ASN:O    | 4:Z:302:GLY:C[1_556]   | 2.12                     | 0.08              |
| 4:1:301:GLY:N   | 4:Y:219:VAL:CA[1_556]  | 2.12                     | 0.08              |
| 4:2:79:TRP:CB   | 4:Z:17:VAL:CA[1_556]   | 2.12                     | 0.08              |
| 4:2:122:ILE:CB  | 4:Z:19:ALA:C[1_556]    | 2.12                     | 0.08              |
| 4:2:163:VAL:O   | 4:Z:278:THR:OG1[1_556] | 2.12                     | 0.08              |
| 4:2:210:ARG:NH2 | 4:Z:212:ILE:CD1[1_556] | 2.12                     | 0.08              |
| 4:1:372:ARG:NH1 | 4:Y:145:SER:OG[1_556]  | 2.12                     | 0.08              |
| 4:2:120:THR:C   | 4:Z:340:TRP:CZ2[1_556] | 2.12                     | 0.08              |
| 4:2:338:SER:CA  | 4:Z:307:PRO:C[1_556]   | 2.12                     | 0.08              |
| 4:0:136:ILE:CD1 | 4:X:152:VAL:CG1[1_556] | 2.12                     | 0.08              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:309:ILE:CG2 | 4:Z:223:PHE:O[1_556]   | 2.12                     | 0.08              |
| 4:1:63:GLY:C    | 4:W:288:ASP:O[1_556]   | 2.12                     | 0.08              |
| 4:0:205:GLU:O   | 4:X:198:TYR:CA[1_556]  | 2.12                     | 0.08              |
| 4:4:41:GLN:N    | 4:Z:167:GLU:CG[1_556]  | 2.12                     | 0.08              |
| 4:0:164:PRO:CB  | 4:X:278:THR:CA[1_556]  | 2.12                     | 0.08              |
| 4:2:136:ILE:CD1 | 4:Z:152:VAL:CG1[1_556] | 2.12                     | 0.08              |
| 4:0:196:ARG:NH1 | 4:W:116:ARG:N[1_556]   | 2.12                     | 0.08              |
| 4:1:116:ARG:CG  | 4:Y:339:VAL:C[1_556]   | 2.12                     | 0.08              |
| 4:1:177:ARG:NH1 | 4:Y:160:THR:N[1_556]   | 2.12                     | 0.08              |
| 4:0:127:PHE:N   | 4:X:28:ARG:NE[1_556]   | 2.12                     | 0.08              |
| 4:0:176:MET:N   | 4:X:277:THR:CB[1_556]  | 2.12                     | 0.08              |
| 4:2:105:LEU:N   | 4:Z:334:GLU:N[1_556]   | 2.12                     | 0.08              |
| 4:1:227:MET:CB  | 4:X:372:ARG:CA[1_556]  | 2.12                     | 0.08              |
| 4:3:233:SER:O   | 4:Z:367:PRO:CG[1_556]  | 2.12                     | 0.08              |
| 4:2:197:GLY:O   | 4:Y:76:ILE:C[1_556]    | 2.12                     | 0.08              |
| 4:0:130:PRO:CA  | 4:X:25:ASP:OD2[1_556]  | 2.12                     | 0.08              |
| 4:1:120:THR:C   | 4:Y:340:TRP:CD2[1_556] | 2.12                     | 0.08              |
| 4:1:161:HIS:O   | 4:Y:274:ILE:CG1[1_556] | 2.12                     | 0.08              |
| 4:2:41:GLN:N    | 4:X:167:GLU:CG[1_556]  | 2.12                     | 0.08              |
| 4:0:108:ALA:C   | 4:X:154:ASP:OD1[1_556] | 2.12                     | 0.08              |
| 4:2:183:ARG:CA  | 4:Z:187:ASP:N[1_556]   | 2.12                     | 0.08              |
| 4:1:79:TRP:CD1  | 4:Y:17:VAL:CG2[1_556]  | 2.12                     | 0.08              |
| 4:1:305:MET:C   | 4:Y:255:PHE:CZ[1_556]  | 2.12                     | 0.08              |
| 4:1:206:ARG:CZ  | 4:Y:190:MET:SD[1_556]  | 2.12                     | 0.08              |
| 4:0:230:ALA:C   | 4:W:367:PRO:C[1_556]   | 2.12                     | 0.08              |
| 4:2:261:LEU:N   | 4:Z:266:PHE:N[1_556]   | 2.12                     | 0.08              |
| 4:1:124:PHE:CG  | 4:Y:23:GLY:C[1_556]    | 2.12                     | 0.08              |
| 4:2:161:HIS:N   | 4:Z:274:ILE:CD1[1_556] | 2.12                     | 0.08              |
| 4:1:126:THR:N   | 4:Y:24:ASP:OD2[1_556]  | 2.12                     | 0.08              |
| 4:0:163:VAL:O   | 4:X:278:THR:OG1[1_556] | 2.12                     | 0.08              |
| 4:2:118:LYS:CD  | 4:Z:10:CYS:CB[1_556]   | 2.12                     | 0.08              |
| 4:1:198:TYR:N   | 4:X:75:ILE:CG2[1_556]  | 2.12                     | 0.08              |
| 4:2:123:MET:CA  | 4:Z:26:ALA:N[1_556]    | 2.12                     | 0.08              |
| 4:2:227:MET:SD  | 4:Y:372:ARG:O[1_556]   | 2.12                     | 0.08              |
| 4:1:197:GLY:N   | 4:X:75:ILE:CG2[1_556]  | 2.12                     | 0.08              |
| 4:1:337:TYR:CG  | 4:Y:307:PRO:CG[1_556]  | 2.12                     | 0.08              |
| 4:1:309:ILE:CB  | 4:Y:259:GLU:OE1[1_556] | 2.12                     | 0.08              |
| 4:2:261:LEU:CD1 | 4:Z:266:PHE:CZ[1_556]  | 2.12                     | 0.08              |
| 4:1:290:ARG:CA  | 4:Y:279:TYR:OH[1_556]  | 2.12                     | 0.08              |
| 4:1:260:THR:CB  | 4:Y:266:PHE:O[1_556]   | 2.12                     | 0.08              |
| 4:1:252:ASN:CB  | 4:X:113:LYS:CB[1_556]  | 2.12                     | 0.08              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:300:SER:CA  | 4:Y:219:VAL:CG2[1_556] | 2.12                     | 0.08              |
| 4:2:299:MET:C   | 4:Z:219:VAL:CG1[1_556] | 2.12                     | 0.08              |
| 4:2:119:MET:O   | 4:Z:340:TRP:CG[1_556]  | 2.12                     | 0.08              |
| 4:0:157:ASP:CB  | 4:X:213:LYS:CE[1_556]  | 2.12                     | 0.08              |
| 4:1:123:MET:CG  | 4:Y:27:PRO:CD[1_556]   | 2.12                     | 0.08              |
| 4:1:39:ARG:NH1  | 4:W:289:ILE:CG2[1_556] | 2.12                     | 0.08              |
| 4:4:61:LYS:CA   | 4:Z:291:LYS:CD[1_556]  | 2.12                     | 0.08              |
| 4:1:157:ASP:OD2 | 4:Y:186:THR:CA[1_556]  | 2.12                     | 0.08              |
| 4:1:337:TYR:CD2 | 4:Y:218:TYR:OH[1_556]  | 2.12                     | 0.08              |
| 4:0:252:ASN:CB  | 4:W:113:LYS:CA[1_556]  | 2.12                     | 0.08              |
| 4:0:371:HIS:C   | 4:X:140:LEU:CA[1_556]  | 2.12                     | 0.08              |
| 4:1:126:THR:OG1 | 4:Y:28:ARG:C[1_556]    | 2.12                     | 0.08              |
| 4:2:166:TYR:CG  | 4:Z:294:TYR:CA[1_556]  | 2.12                     | 0.08              |
| 4:2:78:ASN:OD1  | 4:Z:31:PHE:CD2[1_556]  | 2.12                     | 0.08              |
| 4:0:183:ARG:CA  | 4:X:189:LEU:N[1_556]   | 2.12                     | 0.08              |
| 4:2:292:ASP:C   | 4:Z:317:ILE:O[1_556]   | 2.12                     | 0.08              |
| 4:0:78:ASN:CA   | 4:X:33:SER:N[1_556]    | 2.12                     | 0.08              |
| 4:3:39:ARG:NH1  | 4:Y:289:ILE:CG2[1_556] | 2.12                     | 0.08              |
| 4:4:61:LYS:O    | 4:Z:288:ASP:O[1_556]   | 2.12                     | 0.08              |
| 4:1:174:ALA:N   | 4:Y:281:SER:CA[1_556]  | 2.12                     | 0.08              |
| 4:0:120:THR:C   | 4:X:340:TRP:CZ2[1_556] | 2.12                     | 0.08              |
| 4:2:125:GLU:O   | 4:Z:21:PHE:CD1[1_556]  | 2.12                     | 0.08              |
| 4:0:30:VAL:C    | 4:X:215:LYS:CD[1_556]  | 2.12                     | 0.08              |
| 4:0:61:LYS:O    | 4:V:288:ASP:O[1_556]   | 2.12                     | 0.08              |
| 4:0:290:ARG:CD  | 4:X:279:TYR:OH[1_556]  | 2.12                     | 0.08              |
| 4:2:124:PHE:N   | 4:Z:24:ASP:C[1_556]    | 2.12                     | 0.08              |
| 4:1:83:GLU:OE2  | 4:Y:28:ARG:O[1_556]    | 2.12                     | 0.08              |
| 4:3:40:HIS:CG   | 4:Y:166:TYR:CB[1_556]  | 2.12                     | 0.08              |
| 4:1:193:LEU:CA  | 4:X:112:PRO:CG[1_556]  | 2.12                     | 0.08              |
| 4:0:197:GLY:C   | 4:W:76:ILE:N[1_556]    | 2.12                     | 0.08              |
| 4:1:117:GLU:OE1 | 4:Y:104:LEU:CG[1_556]  | 2.12                     | 0.08              |
| 4:2:370:VAL:CB  | 4:Z:341:ILE:O[1_556]   | 2.12                     | 0.08              |
| 4:2:59:GLN:CB   | 4:Z:208:ILE:CD1[1_556] | 2.12                     | 0.08              |
| 4:2:177:ARG:CB  | 4:Z:178:LEU:CA[1_556]  | 2.12                     | 0.08              |
| 4:0:133:TYR:OH  | 4:X:145:SER:OG[1_556]  | 2.12                     | 0.08              |
| 4:1:363:ASP:C   | 4:Y:348:SER:O[1_556]   | 2.12                     | 0.08              |
| 4:0:159:VAL:CA  | 4:X:181:ALA:C[1_556]   | 2.12                     | 0.08              |
| 4:0:33:SER:CB   | 4:X:210:ARG:CZ[1_556]  | 2.12                     | 0.08              |
| 4:0:120:THR:N   | 4:X:340:TRP:C[1_556]   | 2.13                     | 0.07              |
| 4:0:331:ALA:CB  | 4:X:223:PHE:N[1_556]   | 2.13                     | 0.07              |
| 4:0:269:MET:N   | 4:W:173:HIS:CD2[1_556] | 2.13                     | 0.07              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:63:GLY:C    | 4:Y:288:ASP:O[1_556]   | 2.13                     | 0.07              |
| 4:0:125:GLU:O   | 4:X:21:PHE:CD1[1_556]  | 2.13                     | 0.07              |
| 4:2:116:ARG:CG  | 4:Z:339:VAL:C[1_556]   | 2.13                     | 0.07              |
| 4:4:45:VAL:CG2  | 4:Z:328:LYS:CD[1_556]  | 2.13                     | 0.07              |
| 4:0:217:CYS:CB  | 4:X:256:ARG:NE[1_556]  | 2.13                     | 0.07              |
| 4:1:368:SER:O   | 4:Y:346:LEU:CG[1_556]  | 2.13                     | 0.07              |
| 4:2:111:ASN:CB  | 4:Z:154:ASP:OD1[1_556] | 2.13                     | 0.07              |
| 4:1:292:ASP:O   | 4:Y:317:ILE:O[1_556]   | 2.13                     | 0.07              |
| 4:1:110:LEU:CD1 | 4:Y:161:HIS:N[1_556]   | 2.13                     | 0.07              |
| 4:0:63:GLY:CA   | 4:V:287:ILE:O[1_556]   | 2.13                     | 0.07              |
| 4:1:370:VAL:CB  | 4:Y:341:ILE:O[1_556]   | 2.13                     | 0.07              |
| 4:2:304:THR:CG2 | 4:Z:223:PHE:CE2[1_556] | 2.13                     | 0.07              |
| 4:0:278:THR:N   | 4:X:276:GLU:OE2[1_556] | 2.13                     | 0.07              |
| 4:1:331:ALA:N   | 4:Y:221:LEU:C[1_556]   | 2.13                     | 0.07              |
| 4:2:297:ASN:C   | 4:Z:316:GLU:CA[1_556]  | 2.13                     | 0.07              |
| 4:2:66:THR:OG1  | 4:Z:60:SER:CA[1_556]   | 2.13                     | 0.07              |
| 4:0:306:TYR:CE2 | 4:X:256:ARG:O[1_556]   | 2.13                     | 0.07              |
| 4:0:124:PHE:O   | 4:X:24:ASP:CA[1_556]   | 2.13                     | 0.07              |
| 4:2:183:ARG:CA  | 4:Z:187:ASP:C[1_556]   | 2.13                     | 0.07              |
| 4:0:167:GLU:O   | 4:X:296:ASN:N[1_556]   | 2.13                     | 0.07              |
| 4:0:234:SER:CA  | 4:W:367:PRO:CD[1_556]  | 2.13                     | 0.07              |
| 4:2:297:ASN:CA  | 4:Z:316:GLU:CG[1_556]  | 2.13                     | 0.07              |
| 4:0:208:ILE:C   | 4:X:198:TYR:CE2[1_556] | 2.13                     | 0.07              |
| 4:2:33:SER:CB   | 4:Z:210:ARG:CZ[1_556]  | 2.13                     | 0.07              |
| 4:1:82:MET:CA   | 4:Y:30:VAL:CB[1_556]   | 2.13                     | 0.07              |
| 4:2:185:LEU:N   | 4:Z:188:TYR:O[1_556]   | 2.13                     | 0.07              |
| 4:1:165:ILE:CG2 | 4:Y:297:ASN:CG[1_556]  | 2.13                     | 0.07              |
| 4:1:185:LEU:C   | 4:Y:192:ILE:N[1_556]   | 2.13                     | 0.07              |
| 4:0:196:ARG:CZ  | 4:W:115:ASN:CB[1_556]  | 2.13                     | 0.07              |
| 4:0:305:MET:N   | 4:X:255:PHE:CD1[1_556] | 2.13                     | 0.07              |
| 4:2:62:ARG:NH2  | 4:Z:205:GLU:C[1_556]   | 2.13                     | 0.07              |
| 4:1:123:MET:CA  | 4:Y:27:PRO:N[1_556]    | 2.13                     | 0.07              |
| 4:1:330:ILE:CD1 | 4:Y:315:LYS:CE[1_556]  | 2.13                     | 0.07              |
| 4:1:137:GLN:N   | 4:Y:299:MET:CB[1_556]  | 2.13                     | 0.07              |
| 4:2:61:LYS:O    | 4:X:288:ASP:O[1_556]   | 2.13                     | 0.07              |
| 4:3:197:GLY:C   | 4:Z:76:ILE:N[1_556]    | 2.13                     | 0.07              |
| 4:0:299:MET:C   | 4:X:219:VAL:CG1[1_556] | 2.13                     | 0.07              |
| 4:0:121:GLN:CG  | 4:X:9:VAL:CA[1_556]    | 2.13                     | 0.07              |
| 4:0:161:HIS:N   | 4:X:274:ILE:CD1[1_556] | 2.13                     | 0.07              |
| 4:0:252:ASN:CB  | 4:W:113:LYS:CB[1_556]  | 2.13                     | 0.07              |
| 4:1:81:ASP:CA   | 4:Y:31:PHE:CB[1_556]   | 2.13                     | 0.07              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:217:CYS:CB  | 4:Y:256:ARG:NE[1_556]  | 2.13                     | 0.07              |
| 4:1:227:MET:C   | 4:X:372:ARG:N[1_556]   | 2.13                     | 0.07              |
| 4:0:253:GLU:CG  | 4:W:112:PRO:C[1_556]   | 2.13                     | 0.07              |
| 4:2:79:TRP:CB   | 4:Z:17:VAL:C[1_556]    | 2.13                     | 0.07              |
| 4:1:303:THR:CB  | 4:Y:257:CYS:N[1_556]   | 2.13                     | 0.07              |
| 4:2:196:ARG:CZ  | 4:Y:115:ASN:CB[1_556]  | 2.13                     | 0.07              |
| 4:2:252:ASN:OD1 | 4:Y:117:GLU:N[1_556]   | 2.13                     | 0.07              |
| 4:1:302:GLY:O   | 4:Y:255:PHE:N[1_556]   | 2.13                     | 0.07              |
| 4:0:37:ARG:NH1  | 4:X:56:ASP:O[1_556]    | 2.13                     | 0.07              |
| 4:2:118:LYS:CG  | 4:Z:10:CYS:CA[1_556]   | 2.13                     | 0.07              |
| 4:2:213:LYS:O   | 4:Z:253:GLU:CD[1_556]  | 2.13                     | 0.07              |
| 4:0:337:TYR:O   | 4:X:307:PRO:CB[1_556]  | 2.13                     | 0.07              |
| 4:3:267:ILE:CA  | 4:Z:173:HIS:CG[1_556]  | 2.13                     | 0.07              |
| 4:1:110:LEU:CD2 | 4:Y:161:HIS:CB[1_556]  | 2.13                     | 0.07              |
| 4:0:165:ILE:N   | 4:X:278:THR:CG2[1_556] | 2.13                     | 0.07              |
| 4:2:208:ILE:C   | 4:Z:198:TYR:CE2[1_556] | 2.13                     | 0.07              |
| 4:1:288:ASP:O   | 4:Y:322:PRO:CD[1_556]  | 2.13                     | 0.07              |
| 4:1:195:GLU:CG  | 4:X:108:ALA:C[1_556]   | 2.13                     | 0.07              |
| 4:0:120:THR:C   | 4:X:340:TRP:CD2[1_556] | 2.13                     | 0.07              |
| 4:0:138:ALA:O   | 4:X:299:MET:SD[1_556]  | 2.13                     | 0.07              |
| 4:1:125:GLU:CA  | 4:Y:24:ASP:CG[1_556]   | 2.13                     | 0.07              |
| 4:2:119:MET:CG  | 4:Z:340:TRP:N[1_556]   | 2.13                     | 0.07              |
| 4:0:153:LEU:CG  | 4:X:262:PHE:CD1[1_556] | 2.13                     | 0.07              |
| 4:0:119:MET:CG  | 4:X:340:TRP:N[1_556]   | 2.13                     | 0.07              |
| 4:1:157:ASP:CB  | 4:Y:213:LYS:CE[1_556]  | 2.13                     | 0.07              |
| 4:3:194:THR:O   | 4:Z:75:ILE:CB[1_556]   | 2.13                     | 0.07              |
| 4:1:59:GLN:OE1  | 4:Y:208:ILE:CB[1_556]  | 2.13                     | 0.07              |
| 4:3:227:MET:C   | 4:Z:372:ARG:N[1_556]   | 2.13                     | 0.07              |
| 4:0:118:LYS:CD  | 4:X:10:CYS:CB[1_556]   | 2.13                     | 0.07              |
| 4:1:178:LEU:N   | 4:Y:180:LEU:CG[1_556]  | 2.13                     | 0.07              |
| 4:2:167:GLU:O   | 4:Z:296:ASN:N[1_556]   | 2.13                     | 0.07              |
| 4:1:368:SER:O   | 4:Y:346:LEU:CD2[1_556] | 2.13                     | 0.07              |
| 4:1:34:ILE:CD1  | 4:Y:207:GLU:O[1_556]   | 2.13                     | 0.07              |
| 4:2:132:MET:CE  | 4:Z:341:ILE:CD1[1_556] | 2.13                     | 0.07              |
| 4:0:40:HIS:CD2  | 4:V:167:GLU:N[1_556]   | 2.13                     | 0.07              |
| 4:1:267:ILE:CA  | 4:X:173:HIS:O[1_556]   | 2.13                     | 0.07              |
| 4:0:261:LEU:N   | 4:X:266:PHE:N[1_556]   | 2.13                     | 0.07              |
| 4:0:124:PHE:N   | 4:X:24:ASP:C[1_556]    | 2.13                     | 0.07              |
| 4:0:66:THR:C    | 4:X:62:ARG:NH1[1_556]  | 2.13                     | 0.07              |
| 4:2:233:SER:O   | 4:Y:367:PRO:CG[1_556]  | 2.13                     | 0.07              |
| 4:3:197:GLY:N   | 4:Z:75:ILE:CG2[1_556]  | 2.13                     | 0.07              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:261:LEU:N   | 4:Z:266:PHE:C[1_556]   | 2.13                     | 0.07              |
| 4:0:278:THR:CB  | 4:X:275:HIS:NE2[1_556] | 2.13                     | 0.07              |
| 4:2:218:TYR:OH  | 4:Z:231:ALA:CB[1_556]  | 2.13                     | 0.07              |
| 4:2:136:ILE:C   | 4:Z:300:SER:N[1_556]   | 2.13                     | 0.07              |
| 4:0:338:SER:OG  | 4:X:308:GLY:O[1_556]   | 2.13                     | 0.07              |
| 4:2:73:HIS:CB   | 4:Z:158:GLY:CA[1_556]  | 2.13                     | 0.07              |
| 4:2:278:THR:CA  | 4:Z:276:GLU:OE2[1_556] | 2.13                     | 0.07              |
| 4:2:130:PRO:CA  | 4:Z:25:ASP:OD2[1_556]  | 2.13                     | 0.07              |
| 4:0:292:ASP:CA  | 4:X:321:ALA:N[1_556]   | 2.13                     | 0.07              |
| 4:3:39:ARG:CA   | 4:Y:166:TYR:CZ[1_556]  | 2.13                     | 0.07              |
| 4:2:230:ALA:C   | 4:Y:367:PRO:C[1_556]   | 2.13                     | 0.07              |
| 4:1:76:ILE:CD1  | 4:Y:18:LYS:NZ[1_556]   | 2.13                     | 0.07              |
| 4:0:138:ALA:CB  | 4:X:299:MET:SD[1_556]  | 2.13                     | 0.07              |
| 4:0:185:LEU:N   | 4:X:188:TYR:O[1_556]   | 2.13                     | 0.07              |
| 4:2:234:SER:CA  | 4:Y:367:PRO:CD[1_556]  | 2.13                     | 0.07              |
| 4:1:81:ASP:OD1  | 4:Y:56:ASP:N[1_556]    | 2.13                     | 0.07              |
| 4:1:331:ALA:C   | 4:Y:222:ASP:N[1_556]   | 2.13                     | 0.07              |
| 4:2:292:ASP:CA  | 4:Z:321:ALA:N[1_556]   | 2.13                     | 0.07              |
| 4:0:124:PHE:CG  | 4:X:23:GLY:C[1_556]    | 2.13                     | 0.07              |
| 4:0:304:THR:CA  | 4:X:259:GLU:CB[1_556]  | 2.13                     | 0.07              |
| 4:2:134:VAL:CB  | 4:Z:338:SER:OG[1_556]  | 2.13                     | 0.07              |
| 4:0:122:ILE:CB  | 4:X:19:ALA:C[1_556]    | 2.13                     | 0.07              |
| 4:2:297:ASN:C   | 4:Z:316:GLU:N[1_556]   | 2.13                     | 0.07              |
| 4:1:173:HIS:O   | 4:Y:176:MET:CG[1_556]  | 2.13                     | 0.07              |
| 4:1:309:ILE:CD1 | 4:Y:259:GLU:CB[1_556]  | 2.13                     | 0.07              |
| 4:0:310:ALA:CB  | 4:X:224:GLU:CB[1_556]  | 2.13                     | 0.07              |
| 4:1:11:ASP:OD1  | 4:Y:305:MET:SD[1_556]  | 2.13                     | 0.07              |
| 4:2:186:THR:OG1 | 4:Z:190:MET:N[1_556]   | 2.13                     | 0.07              |
| 4:2:161:HIS:O   | 4:Z:274:ILE:CG1[1_556] | 2.13                     | 0.07              |
| 4:0:110:LEU:CB  | 4:X:161:HIS:CA[1_556]  | 2.13                     | 0.07              |
| 4:2:371:HIS:C   | 4:Z:140:LEU:CA[1_556]  | 2.13                     | 0.07              |
| 4:0:297:ASN:C   | 4:X:316:GLU:CA[1_556]  | 2.13                     | 0.07              |
| 4:1:125:GLU:N   | 4:Y:24:ASP:CB[1_556]   | 2.13                     | 0.07              |
| 4:2:178:LEU:CG  | 4:Z:180:LEU:CD2[1_556] | 2.13                     | 0.07              |
| 4:0:169:TYR:OH  | 4:X:165:ILE:N[1_556]   | 2.13                     | 0.07              |
| 4:0:140:LEU:CD1 | 4:X:332:PRO:O[1_556]   | 2.13                     | 0.07              |
| 4:0:60:SER:CA   | 4:X:243:PRO:CA[1_556]  | 2.13                     | 0.07              |
| 4:2:165:ILE:N   | 4:Z:278:THR:CG2[1_556] | 2.13                     | 0.07              |
| 4:0:370:VAL:CB  | 4:X:341:ILE:O[1_556]   | 2.13                     | 0.07              |
| 4:0:137:GLN:N   | 4:X:299:MET:C[1_556]   | 2.13                     | 0.07              |
| 4:1:306:TYR:CA  | 4:Y:255:PHE:CE1[1_556] | 2.13                     | 0.07              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:369:ILE:CA  | 4:Y:346:LEU:CB[1_556]  | 2.13                     | 0.07              |
| 4:2:78:ASN:CA   | 4:Z:33:SER:N[1_556]    | 2.13                     | 0.07              |
| 4:0:110:LEU:CA  | 4:X:161:HIS:CB[1_556]  | 2.13                     | 0.07              |
| 4:2:335:ARG:CG  | 4:Z:220:ALA:CB[1_556]  | 2.13                     | 0.07              |
| 4:1:175:ILE:O   | 4:Y:277:THR:CG2[1_556] | 2.13                     | 0.07              |
| 4:1:252:ASN:OD1 | 4:X:117:GLU:N[1_556]   | 2.13                     | 0.07              |
| 4:0:210:ARG:NH2 | 4:X:212:ILE:CD1[1_556] | 2.13                     | 0.07              |
| 4:3:253:GLU:CG  | 4:Z:113:LYS:N[1_556]   | 2.13                     | 0.07              |
| 4:1:195:GLU:OE1 | 4:X:110:LEU:C[1_556]   | 2.13                     | 0.07              |
| 4:2:205:GLU:O   | 4:Z:198:TYR:CA[1_556]  | 2.13                     | 0.07              |
| 4:0:116:ARG:NH1 | 4:X:140:LEU:O[1_556]   | 2.13                     | 0.07              |
| 4:0:306:TYR:CE2 | 4:X:256:ARG:C[1_556]   | 2.13                     | 0.07              |
| 4:0:181:ALA:O   | 4:X:188:TYR:CD2[1_556] | 2.13                     | 0.07              |
| 4:0:134:VAL:O   | 4:X:338:SER:OG[1_556]  | 2.13                     | 0.07              |
| 4:1:82:MET:SD   | 4:Y:16:LEU:CG[1_556]   | 2.14                     | 0.06              |
| 4:2:9:VAL:CG1   | 4:Z:333:PRO:CA[1_556]  | 2.14                     | 0.06              |
| 4:2:61:LYS:CA   | 4:X:291:LYS:CD[1_556]  | 2.14                     | 0.06              |
| 4:1:298:VAL:CA  | 4:Y:312:ARG:CA[1_556]  | 2.14                     | 0.06              |
| 4:1:81:ASP:C    | 4:Y:30:VAL:O[1_556]    | 2.14                     | 0.06              |
| 4:2:30:VAL:C    | 4:Z:215:LYS:CD[1_556]  | 2.14                     | 0.06              |
| 4:0:16:LEU:O    | 4:X:214:GLU:CG[1_556]  | 2.14                     | 0.06              |
| 4:0:62:ARG:NH2  | 4:X:205:GLU:C[1_556]   | 2.14                     | 0.06              |
| 4:2:176:MET:N   | 4:Z:277:THR:CB[1_556]  | 2.14                     | 0.06              |
| 4:2:133:TYR:OH  | 4:Z:145:SER:OG[1_556]  | 2.14                     | 0.06              |
| 4:1:278:THR:N   | 4:Y:276:GLU:OE2[1_556] | 2.14                     | 0.06              |
| 4:0:104:LEU:CB  | 4:X:333:PRO:CG[1_556]  | 2.14                     | 0.06              |
| 4:0:160:THR:OG1 | 4:X:261:LEU:N[1_556]   | 2.14                     | 0.06              |
| 4:0:297:ASN:CA  | 4:X:316:GLU:CG[1_556]  | 2.14                     | 0.06              |
| 4:0:166:TYR:CG  | 4:X:294:TYR:CA[1_556]  | 2.14                     | 0.06              |
| 4:1:264:PRO:CB  | 4:Y:268:GLY:N[1_556]   | 2.14                     | 0.06              |
| 4:1:33:SER:C    | 4:Y:210:ARG:NE[1_556]  | 2.14                     | 0.06              |
| 4:0:183:ARG:CA  | 4:X:187:ASP:N[1_556]   | 2.14                     | 0.06              |
| 4:1:216:LEU:N   | 4:Y:252:ASN:OD1[1_556] | 2.14                     | 0.06              |
| 4:0:291:LYS:CG  | 4:X:322:PRO:CA[1_556]  | 2.14                     | 0.06              |
| 4:0:292:ASP:C   | 4:X:317:ILE:O[1_556]   | 2.14                     | 0.06              |
| 4:2:37:ARG:NH1  | 4:Z:56:ASP:O[1_556]    | 2.14                     | 0.06              |
| 4:2:120:THR:N   | 4:Z:340:TRP:C[1_556]   | 2.14                     | 0.06              |
| 4:2:134:VAL:O   | 4:Z:338:SER:OG[1_556]  | 2.14                     | 0.06              |
| 4:2:196:ARG:NH1 | 4:Y:116:ARG:N[1_556]   | 2.14                     | 0.06              |
| 4:1:39:ARG:CA   | 4:W:166:TYR:CZ[1_556]  | 2.14                     | 0.06              |
| 4:1:129:VAL:C   | 4:Y:25:ASP:CG[1_556]   | 2.14                     | 0.06              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:118:LYS:CB  | 4:X:11:ASP:CB[1_556]   | 2.14                     | 0.06              |
| 4:1:267:ILE:CA  | 4:X:173:HIS:CG[1_556]  | 2.14                     | 0.06              |
| 4:2:185:LEU:N   | 4:Z:188:TYR:C[1_556]   | 2.14                     | 0.06              |
| 4:0:185:LEU:CD1 | 4:X:188:TYR:CZ[1_556]  | 2.14                     | 0.06              |
| 4:0:166:TYR:OH  | 4:X:325:MET:CG[1_556]  | 2.14                     | 0.06              |
| 4:0:363:ASP:C   | 4:X:348:SER:O[1_556]   | 2.14                     | 0.06              |
| 4:2:183:ARG:CA  | 4:Z:189:LEU:N[1_556]   | 2.14                     | 0.06              |
| 4:2:309:ILE:CD1 | 4:Z:259:GLU:CB[1_556]  | 2.14                     | 0.06              |
| 4:0:232:SER:CA  | 4:W:369:ILE:CB[1_556]  | 2.14                     | 0.06              |
| 4:0:116:ARG:CG  | 4:X:339:VAL:C[1_556]   | 2.14                     | 0.06              |
| 4:0:371:HIS:O   | 4:X:140:LEU:C[1_556]   | 2.14                     | 0.06              |
| 4:1:113:LYS:CB  | 4:Y:135:ALA:O[1_556]   | 2.14                     | 0.06              |
| 4:0:195:GLU:CD  | 4:W:109:PRO:CA[1_556]  | 2.14                     | 0.06              |
| 4:1:140:LEU:CD1 | 4:Y:332:PRO:O[1_556]   | 2.14                     | 0.06              |
| 4:1:194:THR:O   | 4:X:75:ILE:CB[1_556]   | 2.14                     | 0.06              |
| 4:0:60:SER:O    | 4:X:243:PRO:CB[1_556]  | 2.14                     | 0.06              |
| 4:2:173:HIS:O   | 4:Z:176:MET:CG[1_556]  | 2.14                     | 0.06              |
| 4:2:76:ILE:O    | 4:Z:13:GLY:N[1_556]    | 2.14                     | 0.06              |
| 4:1:170:ALA:O   | 4:Y:151:ILE:CG2[1_556] | 2.14                     | 0.06              |
| 4:1:186:THR:N   | 4:Y:191:LYS:N[1_556]   | 2.14                     | 0.06              |
| 4:1:82:MET:CA   | 4:Y:30:VAL:C[1_556]    | 2.14                     | 0.06              |
| 4:1:168:GLY:CA  | 4:Y:328:LYS:O[1_556]   | 2.14                     | 0.06              |
| 4:0:66:THR:OG1  | 4:X:60:SER:CA[1_556]   | 2.14                     | 0.06              |
| 4:2:365:ALA:O   | 4:Z:352:PHE:CB[1_556]  | 2.14                     | 0.06              |
| 4:2:196:ARG:O   | 4:Y:115:ASN:ND2[1_556] | 2.14                     | 0.06              |
| 4:1:40:HIS:CG   | 4:W:166:TYR:CB[1_556]  | 2.14                     | 0.06              |
| 4:2:278:THR:N   | 4:Z:276:GLU:OE2[1_556] | 2.14                     | 0.06              |
| 4:0:116:ARG:N   | 4:X:339:VAL:CB[1_556]  | 2.14                     | 0.06              |
| 4:1:66:THR:C    | 4:Y:62:ARG:NH1[1_556]  | 2.14                     | 0.06              |
| 4:0:140:LEU:CD1 | 4:X:335:ARG:NH1[1_556] | 2.14                     | 0.06              |
| 4:4:61:LYS:O    | 4:Z:291:LYS:CE[1_556]  | 2.14                     | 0.06              |
| 4:0:9:VAL:CG1   | 4:X:333:PRO:CA[1_556]  | 2.14                     | 0.06              |
| 4:2:337:TYR:O   | 4:Z:307:PRO:CB[1_556]  | 2.14                     | 0.06              |
| 4:0:139:VAL:CB  | 4:X:297:ASN:O[1_556]   | 2.14                     | 0.06              |
| 4:2:121:GLN:CG  | 4:Z:9:VAL:CA[1_556]    | 2.14                     | 0.06              |
| 4:0:136:ILE:C   | 4:X:300:SER:N[1_556]   | 2.14                     | 0.06              |
| 4:1:124:PHE:C   | 4:Y:24:ASP:N[1_556]    | 2.14                     | 0.06              |
| 4:1:282:ILE:CA  | 4:Y:279:TYR:CD2[1_556] | 2.14                     | 0.06              |
| 4:0:17:VAL:N    | 4:X:214:GLU:CB[1_556]  | 2.14                     | 0.06              |
| 4:1:302:GLY:N   | 4:Y:218:TYR:O[1_556]   | 2.14                     | 0.06              |
| 4:1:303:THR:C   | 4:Y:256:ARG:C[1_556]   | 2.14                     | 0.06              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:337:TYR:O   | 4:X:307:PRO:CA[1_556]  | 2.14                     | 0.06              |
| 4:2:232:SER:CA  | 4:Y:369:ILE:CB[1_556]  | 2.14                     | 0.06              |
| 4:3:269:MET:N   | 4:Z:173:HIS:CD2[1_556] | 2.14                     | 0.06              |
| 4:2:331:ALA:CB  | 4:Z:223:PHE:N[1_556]   | 2.14                     | 0.06              |
| 4:0:173:HIS:O   | 4:X:176:MET:CG[1_556]  | 2.14                     | 0.06              |
| 4:0:304:THR:CB  | 4:X:223:PHE:CD2[1_556] | 2.14                     | 0.06              |
| 4:2:110:LEU:CD2 | 4:Z:161:HIS:CB[1_556]  | 2.14                     | 0.06              |
| 4:2:139:VAL:CB  | 4:Z:297:ASN:O[1_556]   | 2.14                     | 0.06              |
| 4:0:206:ARG:NE  | 4:X:200:PHE:CG[1_556]  | 2.14                     | 0.06              |
| 4:1:336:LYS:CA  | 4:Y:218:TYR:C[1_556]   | 2.14                     | 0.06              |
| 4:2:337:TYR:CA  | 4:Z:307:PRO:N[1_556]   | 2.14                     | 0.06              |
| 4:1:184:ASP:CA  | 4:Y:188:TYR:CA[1_556]  | 2.14                     | 0.06              |
| 4:1:151:ILE:CB  | 4:Y:317:ILE:CG2[1_556] | 2.14                     | 0.06              |
| 4:1:147:ARG:CA  | 4:Y:314:GLN:OE1[1_556] | 2.14                     | 0.06              |
| 4:2:185:LEU:CD1 | 4:Z:188:TYR:CZ[1_556]  | 2.14                     | 0.06              |
| 4:1:278:THR:C   | 4:Y:276:GLU:OE1[1_556] | 2.14                     | 0.06              |
| 4:2:309:ILE:CB  | 4:Z:259:GLU:OE1[1_556] | 2.14                     | 0.06              |
| 4:1:232:SER:O   | 4:X:362:TYR:CE1[1_556] | 2.14                     | 0.06              |
| 4:2:16:LEU:O    | 4:Z:214:GLU:CG[1_556]  | 2.14                     | 0.06              |
| 4:2:214:GLU:N   | 4:Z:253:GLU:CB[1_556]  | 2.14                     | 0.06              |
| 4:0:162:ASN:CB  | 4:X:275:HIS:N[1_556]   | 2.14                     | 0.06              |
| 4:1:134:VAL:CA  | 4:Y:338:SER:CA[1_556]  | 2.14                     | 0.06              |
| 4:0:115:ASN:N   | 4:X:11:ASP:OD1[1_556]  | 2.14                     | 0.06              |
| 4:0:150:GLY:CA  | 4:X:317:ILE:CA[1_556]  | 2.14                     | 0.06              |
| 4:0:214:GLU:CA  | 4:X:253:GLU:N[1_556]   | 2.14                     | 0.06              |
| 4:1:133:TYR:CB  | 4:Y:334:GLU:OE1[1_556] | 2.14                     | 0.06              |
| 4:2:124:PHE:O   | 4:Z:24:ASP:CA[1_556]   | 2.14                     | 0.06              |
| 4:0:78:ASN:OD1  | 4:X:31:PHE:CD2[1_556]  | 2.14                     | 0.06              |
| 4:1:155:SER:OG  | 4:Y:260:THR:CA[1_556]  | 2.14                     | 0.06              |
| 4:2:281:SER:CA  | 4:Z:276:GLU:C[1_556]   | 2.14                     | 0.06              |
| 4:3:195:GLU:OE1 | 4:Z:110:LEU:C[1_556]   | 2.14                     | 0.06              |
| 4:1:15:GLY:O    | 4:Y:210:ARG:C[1_556]   | 2.14                     | 0.06              |
| 4:0:196:ARG:O   | 4:W:115:ASN:ND2[1_556] | 2.14                     | 0.06              |
| 4:0:34:ILE:CD1  | 4:X:207:GLU:O[1_556]   | 2.14                     | 0.06              |
| 4:1:15:GLY:CA   | 4:Y:213:LYS:CE[1_556]  | 2.14                     | 0.06              |
| 4:2:232:SER:O   | 4:Y:362:TYR:CE1[1_556] | 2.14                     | 0.06              |
| 4:0:151:ILE:CG1 | 4:X:275:HIS:CB[1_556]  | 2.14                     | 0.06              |
| 4:1:133:TYR:CZ  | 4:Y:145:SER:CB[1_556]  | 2.14                     | 0.06              |
| 4:0:337:TYR:CA  | 4:X:307:PRO:N[1_556]   | 2.14                     | 0.06              |
| 4:1:171:LEU:C   | 4:Y:151:ILE:CG1[1_556] | 2.14                     | 0.06              |
| 4:0:129:VAL:C   | 4:X:25:ASP:CG[1_556]   | 2.14                     | 0.06              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:268:GLY:N   | 4:Z:173:HIS:CG[1_556]  | 2.14                     | 0.06              |
| 4:1:293:LEU:CA  | 4:Y:320:LEU:N[1_556]   | 2.14                     | 0.06              |
| 4:2:160:THR:OG1 | 4:Z:261:LEU:N[1_556]   | 2.14                     | 0.06              |
| 4:1:272:ALA:C   | 4:Y:270:GLU:N[1_556]   | 2.14                     | 0.06              |
| 4:2:162:ASN:CB  | 4:Z:275:HIS:N[1_556]   | 2.14                     | 0.06              |
| 4:1:296:ASN:CB  | 4:Y:318:THR:CB[1_556]  | 2.14                     | 0.06              |
| 4:3:232:SER:O   | 4:Z:362:TYR:CE1[1_556] | 2.14                     | 0.06              |
| 4:1:309:ILE:CG2 | 4:Y:223:PHE:C[1_556]   | 2.14                     | 0.06              |
| 4:3:252:ASN:CB  | 4:Z:113:LYS:CB[1_556]  | 2.14                     | 0.06              |
| 4:2:269:MET:N   | 4:Y:173:HIS:CD2[1_556] | 2.14                     | 0.06              |
| 4:2:206:ARG:NE  | 4:Z:200:PHE:CG[1_556]  | 2.14                     | 0.06              |
| 4:2:33:SER:N    | 4:Z:210:ARG:NH2[1_556] | 2.14                     | 0.06              |
| 4:2:105:LEU:CD2 | 4:Z:337:TYR:CD2[1_556] | 2.14                     | 0.06              |
| 4:2:63:GLY:CA   | 4:X:287:ILE:O[1_556]   | 2.14                     | 0.06              |
| 4:2:140:LEU:CD1 | 4:Z:335:ARG:NH1[1_556] | 2.14                     | 0.06              |
| 4:2:305:MET:N   | 4:Z:255:PHE:CD1[1_556] | 2.14                     | 0.06              |
| 4:2:338:SER:OG  | 4:Z:308:GLY:O[1_556]   | 2.14                     | 0.06              |
| 4:0:169:TYR:CD2 | 4:X:293:LEU:CB[1_556]  | 2.14                     | 0.06              |
| 4:1:140:LEU:CA  | 4:Y:331:ALA:CA[1_556]  | 2.14                     | 0.06              |
| 4:1:105:LEU:N   | 4:Y:334:GLU:O[1_556]   | 2.14                     | 0.06              |
| 4:0:213:LYS:O   | 4:X:253:GLU:CD[1_556]  | 2.14                     | 0.06              |
| 4:2:266:PHE:CA  | 4:Y:173:HIS:ND1[1_556] | 2.14                     | 0.06              |
| 4:1:274:ILE:CA  | 4:Y:263:GLN:CA[1_556]  | 2.14                     | 0.06              |
| 4:0:61:LYS:CA   | 4:V:291:LYS:CD[1_556]  | 2.14                     | 0.06              |
| 4:2:371:HIS:O   | 4:Z:140:LEU:C[1_556]   | 2.14                     | 0.06              |
| 4:2:277:THR:CG2 | 4:Z:273:GLY:CA[1_556]  | 2.14                     | 0.06              |
| 4:0:364:GLU:C   | 4:X:348:SER:C[1_556]   | 2.14                     | 0.06              |
| 4:0:336:LYS:CE  | 4:X:254:ARG:CZ[1_556]  | 2.15                     | 0.05              |
| 4:1:262:PHE:N   | 4:Y:265:SER:C[1_556]   | 2.15                     | 0.05              |
| 4:2:304:THR:CA  | 4:Z:259:GLU:CB[1_556]  | 2.15                     | 0.05              |
| 4:2:368:SER:C   | 4:Z:346:LEU:CA[1_556]  | 2.15                     | 0.05              |
| 4:1:336:LYS:CE  | 4:Y:254:ARG:CZ[1_556]  | 2.15                     | 0.05              |
| 4:0:184:ASP:O   | 4:X:191:LYS:CG[1_556]  | 2.15                     | 0.05              |
| 4:2:195:GLU:CD  | 4:Y:109:PRO:CA[1_556]  | 2.15                     | 0.05              |
| 4:2:73:HIS:O    | 4:Z:156:GLY:C[1_556]   | 2.15                     | 0.05              |
| 4:1:296:ASN:CB  | 4:Y:318:THR:CA[1_556]  | 2.15                     | 0.05              |
| 4:0:161:HIS:CE1 | 4:X:160:THR:CB[1_556]  | 2.15                     | 0.05              |
| 4:0:232:SER:O   | 4:W:362:TYR:CE1[1_556] | 2.15                     | 0.05              |
| 4:1:112:PRO:CG  | 4:Y:137:GLN:OE1[1_556] | 2.15                     | 0.05              |
| 4:0:118:LYS:CG  | 4:X:10:CYS:CA[1_556]   | 2.15                     | 0.05              |
| 4:1:237:GLU:OE2 | 4:X:114:ALA:C[1_556]   | 2.15                     | 0.05              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:73:HIS:CB   | 4:X:158:GLY:CA[1_556]  | 2.15                     | 0.05              |
| 4:0:365:ALA:O   | 4:X:352:PHE:CB[1_556]  | 2.15                     | 0.05              |
| 4:1:168:GLY:O   | 4:Y:297:ASN:CA[1_556]  | 2.15                     | 0.05              |
| 4:2:197:GLY:C   | 4:Y:76:ILE:N[1_556]    | 2.15                     | 0.05              |
| 4:1:209:VAL:CA  | 4:Y:193:LEU:C[1_556]   | 2.15                     | 0.05              |
| 4:2:60:SER:CA   | 4:Z:243:PRO:CA[1_556]  | 2.15                     | 0.05              |
| 4:2:151:ILE:CG1 | 4:Z:275:HIS:CB[1_556]  | 2.15                     | 0.05              |
| 4:3:61:LYS:CB   | 4:Y:291:LYS:CD[1_556]  | 2.15                     | 0.05              |
| 4:3:267:ILE:CA  | 4:Z:173:HIS:O[1_556]   | 2.15                     | 0.05              |
| 4:1:40:HIS:CD2  | 4:W:167:GLU:N[1_556]   | 2.15                     | 0.05              |
| 4:0:297:ASN:C   | 4:X:316:GLU:N[1_556]   | 2.15                     | 0.05              |
| 4:2:277:THR:CA  | 4:Z:272:ALA:CB[1_556]  | 2.15                     | 0.05              |
| 4:1:126:THR:N   | 4:Y:28:ARG:NE[1_556]   | 2.15                     | 0.05              |
| 4:2:120:THR:C   | 4:Z:340:TRP:CD2[1_556] | 2.15                     | 0.05              |
| 4:0:103:THR:O   | 4:X:334:GLU:CG[1_556]  | 2.15                     | 0.05              |
| 4:0:77:THR:N    | 4:X:15:GLY:N[1_556]    | 2.15                     | 0.05              |
| 4:1:304:THR:C   | 4:Y:255:PHE:O[1_556]   | 2.15                     | 0.05              |
| 4:1:306:TYR:CE2 | 4:Y:256:ARG:C[1_556]   | 2.15                     | 0.05              |
| 4:2:185:LEU:CD1 | 4:Z:188:TYR:CG[1_556]  | 2.15                     | 0.05              |
| 4:0:110:LEU:CD2 | 4:X:161:HIS:CB[1_556]  | 2.15                     | 0.05              |
| 4:0:177:ARG:CZ  | 4:X:158:GLY:O[1_556]   | 2.15                     | 0.05              |
| 4:0:261:LEU:N   | 4:X:266:PHE:C[1_556]   | 2.15                     | 0.05              |
| 4:2:214:GLU:CA  | 4:Z:253:GLU:N[1_556]   | 2.15                     | 0.05              |
| 4:0:292:ASP:CG  | 4:X:322:PRO:O[1_556]   | 2.15                     | 0.05              |
| 4:1:135:ALA:CB  | 4:Y:332:PRO:N[1_556]   | 2.15                     | 0.05              |
| 4:0:186:THR:OG1 | 4:X:190:MET:N[1_556]   | 2.15                     | 0.05              |
| 4:2:253:GLU:CG  | 4:Y:112:PRO:C[1_556]   | 2.15                     | 0.05              |
| 4:2:60:SER:O    | 4:Z:243:PRO:CB[1_556]  | 2.15                     | 0.05              |
| 4:2:62:ARG:CD   | 4:Z:204:ALA:N[1_556]   | 2.15                     | 0.05              |
| 4:2:66:THR:C    | 4:Z:62:ARG:NH1[1_556]  | 2.15                     | 0.05              |
| 4:0:261:LEU:CB  | 4:X:266:PHE:CA[1_556]  | 2.15                     | 0.05              |
| 4:0:227:MET:CB  | 4:W:372:ARG:CA[1_556]  | 2.15                     | 0.05              |
| 4:0:214:GLU:N   | 4:X:253:GLU:CB[1_556]  | 2.15                     | 0.05              |
| 4:2:261:LEU:CB  | 4:Z:266:PHE:CA[1_556]  | 2.15                     | 0.05              |
| 4:3:194:THR:CA  | 4:Z:75:ILE:CG1[1_556]  | 2.15                     | 0.05              |
| 4:1:287:ILE:N   | 4:Y:283:MET:CG[1_556]  | 2.15                     | 0.05              |
| 4:0:15:GLY:CA   | 4:X:213:LYS:CE[1_556]  | 2.15                     | 0.05              |
| 4:0:178:LEU:CD1 | 4:X:269:MET:CG[1_556]  | 2.15                     | 0.05              |
| 4:1:61:LYS:CB   | 4:W:291:LYS:CD[1_556]  | 2.15                     | 0.05              |
| 4:0:233:SER:O   | 4:W:367:PRO:CG[1_556]  | 2.15                     | 0.05              |
| 4:2:177:ARG:CZ  | 4:Z:158:GLY:O[1_556]   | 2.15                     | 0.05              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:181:ALA:O   | 4:Z:188:TYR:CD2[1_556] | 2.15                     | 0.05              |
| 4:1:126:THR:CA  | 4:Y:28:ARG:CB[1_556]   | 2.15                     | 0.05              |
| 4:2:163:VAL:CB  | 4:Z:153:LEU:CD1[1_556] | 2.15                     | 0.05              |
| 4:0:281:SER:CA  | 4:X:276:GLU:C[1_556]   | 2.15                     | 0.05              |
| 4:2:161:HIS:CE1 | 4:Z:160:THR:CB[1_556]  | 2.15                     | 0.05              |
| 4:2:363:ASP:C   | 4:Z:348:SER:O[1_556]   | 2.15                     | 0.05              |
| 4:0:267:ILE:CA  | 4:W:173:HIS:CG[1_556]  | 2.15                     | 0.05              |
| 4:1:11:ASP:CG   | 4:Y:305:MET:CE[1_556]  | 2.15                     | 0.05              |
| 4:0:364:GLU:C   | 4:X:349:LEU:CA[1_556]  | 2.15                     | 0.05              |
| 4:2:61:LYS:O    | 4:X:291:LYS:CE[1_556]  | 2.15                     | 0.05              |
| 4:1:289:ILE:C   | 4:Y:322:PRO:CD[1_556]  | 2.15                     | 0.05              |
| 4:1:153:LEU:CD2 | 4:Y:262:PHE:CD2[1_556] | 2.15                     | 0.05              |
| 4:2:115:ASN:N   | 4:Z:11:ASP:OD1[1_556]  | 2.15                     | 0.05              |
| 4:1:197:GLY:C   | 4:X:76:ILE:N[1_556]    | 2.15                     | 0.05              |
| 4:1:103:THR:O   | 4:Y:334:GLU:CG[1_556]  | 2.15                     | 0.05              |
| 4:2:166:TYR:OH  | 4:Z:325:MET:CG[1_556]  | 2.15                     | 0.05              |
| 4:0:155:SER:OG  | 4:X:260:THR:N[1_556]   | 2.15                     | 0.05              |
| 4:0:32:PRO:CA   | 4:X:211:ASP:CG[1_556]  | 2.15                     | 0.05              |
| 4:1:125:GLU:CA  | 4:Y:21:PHE:CB[1_556]   | 2.15                     | 0.05              |
| 4:1:179:ASP:CB  | 4:Y:179:ASP:O[1_556]   | 2.15                     | 0.05              |
| 4:2:104:LEU:CB  | 4:Z:333:PRO:CG[1_556]  | 2.15                     | 0.05              |
| 4:0:306:TYR:CE1 | 4:X:256:ARG:NE[1_556]  | 2.15                     | 0.05              |
| 4:1:299:MET:CE  | 4:Y:312:ARG:CZ[1_556]  | 2.15                     | 0.05              |
| 4:2:159:VAL:CA  | 4:Z:181:ALA:CA[1_556]  | 2.15                     | 0.05              |
| 4:1:120:THR:N   | 4:Y:340:TRP:C[1_556]   | 2.15                     | 0.05              |
| 4:0:230:ALA:C   | 4:W:368:SER:C[1_556]   | 2.15                     | 0.05              |
| 4:2:188:TYR:CB  | 4:Z:191:LYS:CD[1_556]  | 2.15                     | 0.05              |
| 4:2:178:LEU:CD1 | 4:Z:269:MET:CG[1_556]  | 2.15                     | 0.05              |
| 4:2:110:LEU:CA  | 4:Z:161:HIS:CB[1_556]  | 2.15                     | 0.05              |
| 4:2:310:ALA:CB  | 4:Z:224:GLU:CB[1_556]  | 2.15                     | 0.05              |
| 4:1:154:ASP:O   | 4:Y:261:LEU:CD2[1_556] | 2.15                     | 0.05              |
| 4:0:369:ILE:CG2 | 4:X:345:ILE:CB[1_556]  | 2.15                     | 0.05              |
| 4:4:39:ARG:CB   | 4:Z:166:TYR:CZ[1_556]  | 2.15                     | 0.05              |
| 4:1:139:VAL:CB  | 4:Y:297:ASN:O[1_556]   | 2.15                     | 0.05              |
| 4:0:76:ILE:O    | 4:X:13:GLY:N[1_556]    | 2.15                     | 0.05              |
| 4:2:207:GLU:C   | 4:Z:200:PHE:CE1[1_556] | 2.15                     | 0.05              |
| 4:2:168:GLY:N   | 4:Z:295:ALA:O[1_556]   | 2.15                     | 0.05              |
| 4:1:120:THR:OG1 | 4:Y:341:ILE:C[1_556]   | 2.15                     | 0.05              |
| 4:0:274:ILE:CD1 | 4:X:264:PRO:CA[1_556]  | 2.15                     | 0.05              |
| 4:1:272:ALA:C   | 4:Y:269:MET:C[1_556]   | 2.15                     | 0.05              |
| 4:1:166:TYR:CG  | 4:Y:294:TYR:CA[1_556]  | 2.15                     | 0.05              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:185:LEU:N   | 4:X:188:TYR:C[1_556]   | 2.15                     | 0.05              |
| 4:0:15:GLY:O    | 4:X:210:ARG:C[1_556]   | 2.15                     | 0.05              |
| 4:0:206:ARG:C   | 4:X:199:SER:CA[1_556]  | 2.15                     | 0.05              |
| 4:0:178:LEU:CG  | 4:X:180:LEU:CD2[1_556] | 2.15                     | 0.05              |
| 4:2:209:VAL:CG2 | 4:Z:194:THR:N[1_556]   | 2.15                     | 0.05              |
| 4:0:161:HIS:O   | 4:X:274:ILE:CG1[1_556] | 2.15                     | 0.05              |
| 4:2:112:PRO:CG  | 4:Z:137:GLN:NE2[1_556] | 2.15                     | 0.05              |
| 4:1:285:CYS:CA  | 4:Y:283:MET:CA[1_556]  | 2.15                     | 0.05              |
| 4:2:292:ASP:CG  | 4:Z:322:PRO:O[1_556]   | 2.15                     | 0.05              |
| 4:2:145:SER:CB  | 4:Z:311:ASP:CA[1_556]  | 2.15                     | 0.05              |
| 4:2:272:ALA:C   | 4:Z:270:GLU:C[1_556]   | 2.15                     | 0.05              |
| 4:0:277:THR:CG2 | 4:X:273:GLY:CA[1_556]  | 2.15                     | 0.05              |
| 4:1:138:ALA:CA  | 4:Y:299:MET:CG[1_556]  | 2.15                     | 0.05              |
| 4:1:335:ARG:CG  | 4:Y:220:ALA:CB[1_556]  | 2.15                     | 0.05              |
| 4:1:142:LEU:CD1 | 4:Y:313:MET:O[1_556]   | 2.15                     | 0.05              |
| 4:1:253:GLU:CG  | 4:X:113:LYS:N[1_556]   | 2.15                     | 0.05              |
| 4:1:268:GLY:N   | 4:X:173:HIS:CG[1_556]  | 2.15                     | 0.05              |
| 4:1:37:ARG:NH2  | 4:Y:56:ASP:CB[1_556]   | 2.15                     | 0.05              |
| 4:1:285:CYS:SG  | 4:Y:280:ASN:N[1_556]   | 2.15                     | 0.05              |
| 4:2:274:ILE:CD1 | 4:Z:264:PRO:CA[1_556]  | 2.15                     | 0.05              |
| 4:0:62:ARG:CD   | 4:X:204:ALA:N[1_556]   | 2.15                     | 0.05              |
| 4:0:309:ILE:CB  | 4:X:259:GLU:OE1[1_556] | 2.15                     | 0.05              |
| 4:0:196:ARG:CG  | 4:W:115:ASN:ND2[1_556] | 2.15                     | 0.05              |
| 4:2:232:SER:O   | 4:Y:366:GLY:O[1_556]   | 2.15                     | 0.05              |
| 4:1:206:ARG:CB  | 4:Y:201:VAL:N[1_556]   | 2.15                     | 0.05              |
| 4:1:187:ASP:C   | 4:Y:191:LYS:CB[1_556]  | 2.15                     | 0.05              |
| 4:1:109:PRO:CB  | 4:Y:154:ASP:O[1_556]   | 2.15                     | 0.05              |
| 4:2:196:ARG:CG  | 4:Y:115:ASN:ND2[1_556] | 2.15                     | 0.05              |
| 4:2:79:TRP:CD1  | 4:Z:17:VAL:CG2[1_556]  | 2.15                     | 0.05              |
| 4:3:254:ARG:CB  | 4:Z:113:LYS:NZ[1_556]  | 2.15                     | 0.05              |
| 4:0:79:TRP:CD1  | 4:X:17:VAL:CG2[1_556]  | 2.15                     | 0.05              |
| 4:1:32:PRO:N    | 4:Y:211:ASP:OD1[1_556] | 2.15                     | 0.05              |
| 4:2:337:TYR:O   | 4:Z:307:PRO:CA[1_556]  | 2.15                     | 0.05              |
| 4:2:296:ASN:CB  | 4:Z:318:THR:CA[1_556]  | 2.15                     | 0.05              |
| 4:2:73:HIS:CG   | 4:Z:157:ASP:O[1_556]   | 2.15                     | 0.05              |
| 4:1:337:TYR:CD1 | 4:Y:307:PRO:CG[1_556]  | 2.16                     | 0.04              |
| 4:2:116:ARG:N   | 4:Z:339:VAL:CB[1_556]  | 2.16                     | 0.04              |
| 4:2:336:LYS:CE  | 4:Z:254:ARG:CZ[1_556]  | 2.16                     | 0.04              |
| 4:1:237:GLU:OE1 | 4:X:114:ALA:O[1_556]   | 2.16                     | 0.04              |
| 4:2:32:PRO:CA   | 4:Z:211:ASP:CG[1_556]  | 2.16                     | 0.04              |
| 4:0:105:LEU:CD2 | 4:X:337:TYR:CD2[1_556] | 2.16                     | 0.04              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:33:SER:N    | 4:X:210:ARG:NH2[1_556] | 2.16                     | 0.04              |
| 4:0:64:ILE:CG2  | 4:V:289:ILE:O[1_556]   | 2.16                     | 0.04              |
| 4:1:364:GLU:C   | 4:Y:348:SER:C[1_556]   | 2.16                     | 0.04              |
| 4:2:177:ARG:NE  | 4:Z:159:VAL:CA[1_556]  | 2.16                     | 0.04              |
| 4:1:72:GLU:CG   | 4:Y:183:ARG:NH2[1_556] | 2.16                     | 0.04              |
| 4:0:163:VAL:CB  | 4:X:153:LEU:CD1[1_556] | 2.16                     | 0.04              |
| 4:0:72:GLU:O    | 4:X:157:ASP:O[1_556]   | 2.16                     | 0.04              |
| 4:1:254:ARG:CB  | 4:X:113:LYS:NZ[1_556]  | 2.16                     | 0.04              |
| 4:1:31:PHE:CB   | 4:Y:215:LYS:CE[1_556]  | 2.16                     | 0.04              |
| 4:0:306:TYR:CG  | 4:X:256:ARG:CD[1_556]  | 2.16                     | 0.04              |
| 4:2:214:GLU:O   | 4:Z:252:ASN:C[1_556]   | 2.16                     | 0.04              |
| 4:2:304:THR:CB  | 4:Z:223:PHE:CD2[1_556] | 2.16                     | 0.04              |
| 4:2:39:ARG:CB   | 4:X:166:TYR:CZ[1_556]  | 2.16                     | 0.04              |
| 4:1:214:GLU:CA  | 4:Y:253:GLU:N[1_556]   | 2.16                     | 0.04              |
| 4:1:232:SER:O   | 4:X:366:GLY:O[1_556]   | 2.16                     | 0.04              |
| 4:0:126:THR:CB  | 4:X:28:ARG:CA[1_556]   | 2.16                     | 0.04              |
| 4:0:266:PHE:CA  | 4:W:173:HIS:ND1[1_556] | 2.16                     | 0.04              |
| 4:1:252:ASN:O   | 4:X:113:LYS:NZ[1_556]  | 2.16                     | 0.04              |
| 4:1:214:GLU:O   | 4:Y:252:ASN:C[1_556]   | 2.16                     | 0.04              |
| 4:1:174:ALA:C   | 4:Y:277:THR:C[1_556]   | 2.16                     | 0.04              |
| 4:1:362:TYR:CZ  | 4:Y:22:ALA:C[1_556]    | 2.16                     | 0.04              |
| 4:0:80:ASP:C    | 4:X:31:PHE:CA[1_556]   | 2.16                     | 0.04              |
| 4:3:231:ALA:N   | 4:Z:370:VAL:N[1_556]   | 2.16                     | 0.04              |
| 4:2:122:ILE:N   | 4:Z:340:TRP:CH2[1_556] | 2.16                     | 0.04              |
| 4:1:78:ASN:ND2  | 4:Y:32:PRO:C[1_556]    | 2.16                     | 0.04              |
| 4:0:357:ILE:CG2 | 4:X:345:ILE:CB[1_556]  | 2.16                     | 0.04              |
| 4:1:116:ARG:CB  | 4:Y:339:VAL:C[1_556]   | 2.16                     | 0.04              |
| 4:2:109:PRO:CD  | 4:Z:155:SER:N[1_556]   | 2.16                     | 0.04              |
| 4:1:78:ASN:CA   | 4:Y:32:PRO:C[1_556]    | 2.16                     | 0.04              |
| 4:1:296:ASN:ND2 | 4:Y:319:ALA:N[1_556]   | 2.16                     | 0.04              |
| 4:1:336:LYS:CD  | 4:Y:218:TYR:CG[1_556]  | 2.16                     | 0.04              |
| 4:1:197:GLY:C   | 4:X:75:ILE:CG2[1_556]  | 2.16                     | 0.04              |
| 4:1:310:ALA:CB  | 4:Y:224:GLU:CB[1_556]  | 2.16                     | 0.04              |
| 4:2:150:GLY:CA  | 4:Z:317:ILE:CA[1_556]  | 2.16                     | 0.04              |
| 4:2:110:LEU:CB  | 4:Z:161:HIS:CA[1_556]  | 2.16                     | 0.04              |
| 4:2:364:GLU:C   | 4:Z:348:SER:C[1_556]   | 2.16                     | 0.04              |
| 4:3:229:THR:C   | 4:Z:369:ILE:N[1_556]   | 2.16                     | 0.04              |
| 4:2:175:ILE:O   | 4:Z:176:MET:CB[1_556]  | 2.16                     | 0.04              |
| 4:0:122:ILE:N   | 4:X:340:TRP:CH2[1_556] | 2.16                     | 0.04              |
| 4:1:157:ASP:O   | 4:Y:185:LEU:N[1_556]   | 2.16                     | 0.04              |
| 4:0:303:THR:OG1 | 4:X:257:CYS:N[1_556]   | 2.16                     | 0.04              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:145:SER:CB  | 4:X:311:ASP:CA[1_556]  | 2.16                     | 0.04              |
| 4:0:188:TYR:CB  | 4:X:191:LYS:CD[1_556]  | 2.16                     | 0.04              |
| 4:0:336:LYS:CD  | 4:X:218:TYR:CG[1_556]  | 2.16                     | 0.04              |
| 4:1:117:GLU:CD  | 4:Y:135:ALA:CB[1_556]  | 2.16                     | 0.04              |
| 4:0:296:ASN:CB  | 4:X:318:THR:CA[1_556]  | 2.16                     | 0.04              |
| 4:2:118:LYS:CB  | 4:Z:11:ASP:CB[1_556]   | 2.16                     | 0.04              |
| 4:3:197:GLY:C   | 4:Z:75:ILE:CG2[1_556]  | 2.16                     | 0.04              |
| 4:1:166:TYR:OH  | 4:Y:325:MET:CG[1_556]  | 2.16                     | 0.04              |
| 4:0:272:ALA:C   | 4:X:270:GLU:C[1_556]   | 2.16                     | 0.04              |
| 4:1:303:THR:CG2 | 4:Y:257:CYS:CA[1_556]  | 2.16                     | 0.04              |
| 4:0:76:ILE:C    | 4:X:16:LEU:N[1_556]    | 2.16                     | 0.04              |
| 4:1:134:VAL:CB  | 4:Y:338:SER:OG[1_556]  | 2.16                     | 0.04              |
| 4:0:137:GLN:CA  | 4:X:304:THR:CB[1_556]  | 2.16                     | 0.04              |
| 4:1:64:ILE:CG1  | 4:W:292:ASP:OD2[1_556] | 2.16                     | 0.04              |
| 4:1:297:ASN:C   | 4:Y:316:GLU:N[1_556]   | 2.16                     | 0.04              |
| 4:2:161:HIS:CG  | 4:Z:160:THR:CG2[1_556] | 2.16                     | 0.04              |
| 4:2:189:LEU:CD1 | 4:Z:195:GLU:CA[1_556]  | 2.16                     | 0.04              |
| 4:0:277:THR:CA  | 4:X:272:ALA:CB[1_556]  | 2.16                     | 0.04              |
| 4:2:129:VAL:C   | 4:Z:25:ASP:CG[1_556]   | 2.16                     | 0.04              |
| 4:2:213:LYS:NZ  | 4:Z:189:LEU:CA[1_556]  | 2.16                     | 0.04              |
| 4:0:367:PRO:CG  | 4:X:9:VAL:CG2[1_556]   | 2.16                     | 0.04              |
| 4:1:134:VAL:CG2 | 4:Y:338:SER:N[1_556]   | 2.16                     | 0.04              |
| 4:1:204:ALA:O   | 4:Y:246:GLN:OE1[1_556] | 2.16                     | 0.04              |
| 4:0:309:ILE:CD1 | 4:X:259:GLU:CB[1_556]  | 2.16                     | 0.04              |
| 4:2:300:SER:CA  | 4:Z:219:VAL:CG2[1_556] | 2.16                     | 0.04              |
| 4:1:67:LEU:N    | 4:Y:62:ARG:CZ[1_556]   | 2.16                     | 0.04              |
| 4:1:269:MET:N   | 4:X:173:HIS:CD2[1_556] | 2.16                     | 0.04              |
| 4:2:140:LEU:CA  | 4:Z:331:ALA:CA[1_556]  | 2.16                     | 0.04              |
| 4:1:33:SER:CB   | 4:Y:214:GLU:CD[1_556]  | 2.16                     | 0.04              |
| 4:2:290:ARG:CG  | 4:Z:279:TYR:CZ[1_556]  | 2.16                     | 0.04              |
| 4:1:139:VAL:N   | 4:Y:299:MET:CG[1_556]  | 2.16                     | 0.04              |
| 4:3:196:ARG:CG  | 4:Z:115:ASN:ND2[1_556] | 2.16                     | 0.04              |
| 4:2:357:ILE:CG2 | 4:Z:345:ILE:CB[1_556]  | 2.16                     | 0.04              |
| 4:3:237:GLU:OE1 | 4:Z:114:ALA:O[1_556]   | 2.16                     | 0.04              |
| 4:2:267:ILE:CA  | 4:Y:173:HIS:CG[1_556]  | 2.16                     | 0.04              |
| 4:1:110:LEU:CB  | 4:Y:161:HIS:CA[1_556]  | 2.16                     | 0.04              |
| 4:1:205:GLU:O   | 4:Y:198:TYR:CA[1_556]  | 2.16                     | 0.04              |
| 4:0:227:MET:O   | 4:W:368:SER:O[1_556]   | 2.16                     | 0.04              |
| 4:2:209:VAL:CA  | 4:Z:193:LEU:C[1_556]   | 2.16                     | 0.04              |
| 4:0:121:GLN:CB  | 4:X:9:VAL:O[1_556]     | 2.16                     | 0.04              |
| 4:1:189:LEU:CD1 | 4:Y:195:GLU:CA[1_556]  | 2.16                     | 0.04              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:366:GLY:CA  | 4:X:347:ALA:N[1_556]   | 2.16                     | 0.04              |
| 4:1:147:ARG:N   | 4:Y:314:GLN:CD[1_556]  | 2.16                     | 0.04              |
| 4:0:233:SER:CA  | 4:W:366:GLY:C[1_556]   | 2.16                     | 0.04              |
| 4:2:111:ASN:C   | 4:Z:137:GLN:CB[1_556]  | 2.16                     | 0.04              |
| 4:2:184:ASP:O   | 4:Z:191:LYS:CG[1_556]  | 2.16                     | 0.04              |
| 4:2:17:VAL:N    | 4:Z:214:GLU:CB[1_556]  | 2.16                     | 0.04              |
| 4:2:76:ILE:C    | 4:Z:16:LEU:N[1_556]    | 2.16                     | 0.04              |
| 4:2:306:TYR:CG  | 4:Z:256:ARG:CD[1_556]  | 2.16                     | 0.04              |
| 4:0:303:THR:N   | 4:X:257:CYS:C[1_556]   | 2.16                     | 0.04              |
| 4:3:40:HIS:CD2  | 4:Y:167:GLU:N[1_556]   | 2.16                     | 0.04              |
| 4:0:124:PHE:O   | 4:X:24:ASP:OD2[1_556]  | 2.16                     | 0.04              |
| 4:0:185:LEU:CG  | 4:X:188:TYR:OH[1_556]  | 2.16                     | 0.04              |
| 4:2:208:ILE:O   | 4:Z:198:TYR:CZ[1_556]  | 2.16                     | 0.04              |
| 4:1:111:ASN:C   | 4:Y:137:GLN:CB[1_556]  | 2.16                     | 0.04              |
| 4:1:297:ASN:CA  | 4:Y:316:GLU:OE1[1_556] | 2.16                     | 0.04              |
| 4:2:160:THR:C   | 4:Z:261:LEU:CD2[1_556] | 2.16                     | 0.04              |
| 4:0:123:MET:CA  | 4:X:27:PRO:N[1_556]    | 2.16                     | 0.04              |
| 4:2:299:MET:CG  | 4:Z:312:ARG:CD[1_556]  | 2.16                     | 0.04              |
| 4:2:289:ILE:CD1 | 4:Z:282:ILE:CG2[1_556] | 2.16                     | 0.04              |
| 4:0:126:THR:OG1 | 4:X:28:ARG:C[1_556]    | 2.16                     | 0.04              |
| 4:1:37:ARG:NH2  | 4:Y:57:GLU:N[1_556]    | 2.16                     | 0.04              |
| 4:2:15:GLY:CA   | 4:Z:213:LYS:CE[1_556]  | 2.16                     | 0.04              |
| 4:2:166:TYR:CA  | 4:Z:294:TYR:O[1_556]   | 2.16                     | 0.04              |
| 4:1:196:ARG:CG  | 4:X:115:ASN:ND2[1_556] | 2.16                     | 0.04              |
| 4:0:194:THR:CA  | 4:W:75:ILE:CG1[1_556]  | 2.16                     | 0.04              |
| 4:2:287:ILE:N   | 4:Z:283:MET:CG[1_556]  | 2.16                     | 0.04              |
| 4:2:34:ILE:CD1  | 4:Z:207:GLU:O[1_556]   | 2.16                     | 0.04              |
| 4:0:73:HIS:O    | 4:X:156:GLY:C[1_556]   | 2.16                     | 0.04              |
| 4:0:133:TYR:CB  | 4:X:334:GLU:OE1[1_556] | 2.16                     | 0.04              |
| 4:1:292:ASP:CG  | 4:Y:322:PRO:O[1_556]   | 2.16                     | 0.04              |
| 4:1:140:LEU:CD1 | 4:Y:335:ARG:NH1[1_556] | 2.16                     | 0.04              |
| 4:3:197:GLY:O   | 4:Z:76:ILE:C[1_556]    | 2.16                     | 0.04              |
| 4:1:139:VAL:CG2 | 4:Y:297:ASN:O[1_556]   | 2.16                     | 0.04              |
| 4:0:368:SER:C   | 4:X:346:LEU:CA[1_556]  | 2.16                     | 0.04              |
| 4:0:111:ASN:N   | 4:X:154:ASP:CB[1_556]  | 2.16                     | 0.04              |
| 4:2:286:ASP:C   | 4:Z:283:MET:CE[1_556]  | 2.16                     | 0.04              |
| 4:2:113:LYS:N   | 4:Z:136:ILE:C[1_556]   | 2.16                     | 0.04              |
| 4:2:230:ALA:C   | 4:Y:368:SER:C[1_556]   | 2.16                     | 0.04              |
| 4:0:286:ASP:C   | 4:X:283:MET:CE[1_556]  | 2.16                     | 0.04              |
| 4:4:63:GLY:CA   | 4:Z:287:ILE:O[1_556]   | 2.16                     | 0.04              |
| 4:2:112:PRO:N   | 4:Z:137:GLN:CB[1_556]  | 2.16                     | 0.04              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:80:ASP:C    | 4:Y:31:PHE:CA[1_556]   | 2.16                     | 0.04              |
| 4:2:117:GLU:CD  | 4:Z:104:LEU:CD2[1_556] | 2.16                     | 0.04              |
| 4:1:364:GLU:O   | 4:Y:350:SER:N[1_556]   | 2.16                     | 0.04              |
| 4:1:304:THR:CA  | 4:Y:223:PHE:CE1[1_556] | 2.16                     | 0.04              |
| 4:2:303:THR:N   | 4:Z:257:CYS:C[1_556]   | 2.16                     | 0.04              |
| 4:1:213:LYS:N   | 4:Y:196:ARG:CG[1_556]  | 2.16                     | 0.04              |
| 4:2:285:CYS:CA  | 4:Z:283:MET:CA[1_556]  | 2.16                     | 0.04              |
| 4:1:118:LYS:CB  | 4:Y:11:ASP:CB[1_556]   | 2.16                     | 0.04              |
| 4:2:336:LYS:CD  | 4:Z:218:TYR:CG[1_556]  | 2.16                     | 0.04              |
| 4:2:232:SER:CB  | 4:Y:369:ILE:CB[1_556]  | 2.16                     | 0.04              |
| 4:0:253:GLU:CG  | 4:W:113:LYS:N[1_556]   | 2.16                     | 0.04              |
| 4:0:230:ALA:C   | 4:W:368:SER:CA[1_556]  | 2.16                     | 0.04              |
| 4:1:307:PRO:CD  | 4:Y:227:MET:SD[1_556]  | 2.16                     | 0.04              |
| 4:2:169:TYR:CD2 | 4:Z:293:LEU:CB[1_556]  | 2.16                     | 0.04              |
| 4:2:227:MET:CB  | 4:Y:372:ARG:CA[1_556]  | 2.16                     | 0.04              |
| 4:2:206:ARG:C   | 4:Z:199:SER:CA[1_556]  | 2.16                     | 0.04              |
| 4:0:167:GLU:CG  | 4:X:326:LYS:O[1_556]   | 2.16                     | 0.04              |
| 4:2:368:SER:O   | 4:Z:346:LEU:CG[1_556]  | 2.16                     | 0.04              |
| 4:2:121:GLN:CB  | 4:Z:9:VAL:N[1_556]     | 2.16                     | 0.04              |
| 4:1:124:PHE:O   | 4:Y:24:ASP:CA[1_556]   | 2.17                     | 0.03              |
| 4:2:306:TYR:CE1 | 4:Z:256:ARG:NE[1_556]  | 2.17                     | 0.03              |
| 4:0:208:ILE:O   | 4:X:198:TYR:CZ[1_556]  | 2.17                     | 0.03              |
| 4:2:185:LEU:N   | 4:Z:188:TYR:CB[1_556]  | 2.17                     | 0.03              |
| 4:1:165:ILE:CD1 | 4:Y:297:ASN:CG[1_556]  | 2.17                     | 0.03              |
| 4:0:232:SER:CB  | 4:W:369:ILE:CB[1_556]  | 2.17                     | 0.03              |
| 4:1:183:ARG:N   | 4:Y:188:TYR:N[1_556]   | 2.17                     | 0.03              |
| 4:0:232:SER:O   | 4:W:366:GLY:O[1_556]   | 2.17                     | 0.03              |
| 4:2:115:ASN:OD1 | 4:Z:11:ASP:OD1[1_556]  | 2.17                     | 0.03              |
| 4:0:155:SER:OG  | 4:X:260:THR:CA[1_556]  | 2.17                     | 0.03              |
| 4:0:140:LEU:N   | 4:X:299:MET:CE[1_556]  | 2.17                     | 0.03              |
| 4:2:285:CYS:O   | 4:Z:283:MET:CA[1_556]  | 2.17                     | 0.03              |
| 4:2:124:PHE:O   | 4:Z:24:ASP:OD2[1_556]  | 2.17                     | 0.03              |
| 4:0:175:ILE:O   | 4:X:176:MET:CB[1_556]  | 2.17                     | 0.03              |
| 4:1:169:TYR:CD2 | 4:Y:293:LEU:CB[1_556]  | 2.17                     | 0.03              |
| 4:0:302:GLY:N   | 4:X:258:PRO:CD[1_556]  | 2.17                     | 0.03              |
| 4:2:138:ALA:CA  | 4:Z:299:MET:CG[1_556]  | 2.17                     | 0.03              |
| 4:0:214:GLU:O   | 4:X:252:ASN:C[1_556]   | 2.17                     | 0.03              |
| 4:2:82:MET:C    | 4:Z:30:VAL:C[1_556]    | 2.17                     | 0.03              |
| 4:0:209:VAL:CA  | 4:X:193:LEU:C[1_556]   | 2.17                     | 0.03              |
| 4:1:261:LEU:CA  | 4:Y:265:SER:C[1_556]   | 2.17                     | 0.03              |
| 4:3:237:GLU:OE2 | 4:Z:114:ALA:C[1_556]   | 2.17                     | 0.03              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:31:PHE:CA   | 4:Y:215:LYS:CE[1_556]  | 2.17                     | 0.03              |
| 4:2:367:PRO:CG  | 4:Z:9:VAL:CG2[1_556]   | 2.17                     | 0.03              |
| 4:0:78:ASN:N    | 4:X:16:LEU:CA[1_556]   | 2.17                     | 0.03              |
| 4:2:369:ILE:CG2 | 4:Z:345:ILE:CB[1_556]  | 2.17                     | 0.03              |
| 4:2:77:THR:N    | 4:Z:15:GLY:N[1_556]    | 2.17                     | 0.03              |
| 4:0:300:SER:CA  | 4:X:219:VAL:CG2[1_556] | 2.17                     | 0.03              |
| 4:0:274:ILE:CD1 | 4:X:264:PRO:CD[1_556]  | 2.17                     | 0.03              |
| 4:1:114:ALA:CB  | 4:Y:106:THR:OG1[1_556] | 2.17                     | 0.03              |
| 4:0:185:LEU:CD1 | 4:X:188:TYR:CG[1_556]  | 2.17                     | 0.03              |
| 4:2:230:ALA:C   | 4:Y:368:SER:CA[1_556]  | 2.17                     | 0.03              |
| 4:0:171:LEU:CB  | 4:X:282:ILE:CG1[1_556] | 2.17                     | 0.03              |
| 4:1:338:SER:N   | 4:Y:307:PRO:O[1_556]   | 2.17                     | 0.03              |
| 4:0:167:GLU:OE1 | 4:X:326:LYS:CD[1_556]  | 2.17                     | 0.03              |
| 4:2:15:GLY:O    | 4:Z:210:ARG:C[1_556]   | 2.17                     | 0.03              |
| 4:2:137:GLN:CA  | 4:Z:304:THR:CB[1_556]  | 2.17                     | 0.03              |
| 4:0:159:VAL:CG2 | 4:X:181:ALA:CA[1_556]  | 2.17                     | 0.03              |
| 4:1:215:LYS:O   | 4:Y:252:ASN:ND2[1_556] | 2.17                     | 0.03              |
| 4:1:117:GLU:CD  | 4:Y:104:LEU:CD2[1_556] | 2.17                     | 0.03              |
| 4:0:39:ARG:CB   | 4:V:166:TYR:CZ[1_556]  | 2.17                     | 0.03              |
| 4:2:155:SER:CA  | 4:Z:261:LEU:CG[1_556]  | 2.17                     | 0.03              |
| 4:1:213:LYS:CA  | 4:Y:253:GLU:OE1[1_556] | 2.17                     | 0.03              |
| 4:0:134:VAL:CG2 | 4:X:338:SER:N[1_556]   | 2.17                     | 0.03              |
| 4:1:293:LEU:CA  | 4:Y:320:LEU:CB[1_556]  | 2.17                     | 0.03              |
| 4:2:362:TYR:CE2 | 4:Z:22:ALA:N[1_556]    | 2.17                     | 0.03              |
| 4:4:64:ILE:CG1  | 4:Z:292:ASP:OD2[1_556] | 2.17                     | 0.03              |
| 4:0:116:ARG:CG  | 4:X:339:VAL:N[1_556]   | 2.17                     | 0.03              |
| 4:0:61:LYS:O    | 4:V:291:LYS:CE[1_556]  | 2.17                     | 0.03              |
| 4:1:303:THR:C   | 4:Y:259:GLU:N[1_556]   | 2.17                     | 0.03              |
| 4:0:159:VAL:CA  | 4:X:181:ALA:CA[1_556]  | 2.17                     | 0.03              |
| 4:2:103:THR:O   | 4:Z:334:GLU:CG[1_556]  | 2.17                     | 0.03              |
| 4:3:232:SER:O   | 4:Z:366:GLY:O[1_556]   | 2.17                     | 0.03              |
| 4:0:299:MET:CG  | 4:X:312:ARG:CD[1_556]  | 2.17                     | 0.03              |
| 4:0:207:GLU:C   | 4:X:200:PHE:CE1[1_556] | 2.17                     | 0.03              |
| 4:2:167:GLU:OE1 | 4:Z:326:LYS:CD[1_556]  | 2.17                     | 0.03              |
| 4:2:337:TYR:CD1 | 4:Z:307:PRO:CG[1_556]  | 2.17                     | 0.03              |
| 4:0:362:TYR:CE2 | 4:X:22:ALA:N[1_556]    | 2.17                     | 0.03              |
| 4:3:252:ASN:O   | 4:Z:113:LYS:NZ[1_556]  | 2.17                     | 0.03              |
| 4:0:161:HIS:CG  | 4:X:160:THR:CG2[1_556] | 2.17                     | 0.03              |
| 4:1:161:HIS:O   | 4:Y:261:LEU:O[1_556]   | 2.17                     | 0.03              |
| 4:0:183:ARG:CZ  | 4:X:186:THR:OG1[1_556] | 2.17                     | 0.03              |
| 4:0:168:GLY:N   | 4:X:295:ALA:O[1_556]   | 2.17                     | 0.03              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:184:ASP:CA  | 4:Z:187:ASP:C[1_556]   | 2.17                     | 0.03              |
| 4:0:209:VAL:CG2 | 4:X:194:THR:N[1_556]   | 2.17                     | 0.03              |
| 4:0:160:THR:C   | 4:X:261:LEU:CD2[1_556] | 2.17                     | 0.03              |
| 4:0:368:SER:N   | 4:X:346:LEU:CB[1_556]  | 2.17                     | 0.03              |
| 4:1:194:THR:CA  | 4:X:75:ILE:CG1[1_556]  | 2.17                     | 0.03              |
| 4:0:287:ILE:N   | 4:X:283:MET:CG[1_556]  | 2.17                     | 0.03              |
| 4:2:296:ASN:CG  | 4:Z:318:THR:CG2[1_556] | 2.17                     | 0.03              |
| 4:0:60:SER:N    | 4:X:243:PRO:CG[1_556]  | 2.17                     | 0.03              |
| 4:2:82:MET:CA   | 4:Z:30:VAL:C[1_556]    | 2.17                     | 0.03              |
| 4:1:62:ARG:CZ   | 4:Y:205:GLU:C[1_556]   | 2.17                     | 0.03              |
| 4:1:132:MET:CB  | 4:Y:25:ASP:O[1_556]    | 2.17                     | 0.03              |
| 4:0:337:TYR:CD1 | 4:X:307:PRO:CG[1_556]  | 2.17                     | 0.03              |
| 4:1:16:LEU:CD1  | 4:Y:211:ASP:C[1_556]   | 2.17                     | 0.03              |
| 4:1:176:MET:N   | 4:Y:277:THR:CB[1_556]  | 2.17                     | 0.03              |
| 4:1:181:ALA:CB  | 4:Y:185:LEU:CA[1_556]  | 2.17                     | 0.03              |
| 4:1:266:PHE:CG  | 4:X:172:PRO:CG[1_556]  | 2.17                     | 0.03              |
| 4:0:230:ALA:O   | 4:W:368:SER:N[1_556]   | 2.17                     | 0.03              |
| 4:0:113:LYS:N   | 4:X:136:ILE:C[1_556]   | 2.17                     | 0.03              |
| 4:1:123:MET:O   | 4:Y:24:ASP:CB[1_556]   | 2.17                     | 0.03              |
| 4:1:293:LEU:N   | 4:Y:321:ALA:CA[1_556]  | 2.17                     | 0.03              |
| 4:1:112:PRO:CG  | 4:Y:137:GLN:NE2[1_556] | 2.17                     | 0.03              |
| 4:0:213:LYS:NZ  | 4:X:189:LEU:CA[1_556]  | 2.17                     | 0.03              |
| 4:0:109:PRO:CD  | 4:X:155:SER:N[1_556]   | 2.17                     | 0.03              |
| 4:2:364:GLU:C   | 4:Z:349:LEU:CA[1_556]  | 2.17                     | 0.03              |
| 4:1:303:THR:OG1 | 4:Y:257:CYS:O[1_556]   | 2.17                     | 0.03              |
| 4:0:166:TYR:CA  | 4:X:294:TYR:O[1_556]   | 2.17                     | 0.03              |
| 4:1:261:LEU:CD1 | 4:Y:266:PHE:CZ[1_556]  | 2.17                     | 0.03              |
| 4:1:207:GLU:O   | 4:Y:200:PHE:CE1[1_556] | 2.17                     | 0.03              |
| 4:1:371:HIS:O   | 4:Y:140:LEU:C[1_556]   | 2.17                     | 0.03              |
| 4:1:82:MET:C    | 4:Y:30:VAL:O[1_556]    | 2.17                     | 0.03              |
| 4:2:78:ASN:N    | 4:Z:16:LEU:CA[1_556]   | 2.17                     | 0.03              |
| 4:2:164:PRO:CB  | 4:Z:278:THR:CG2[1_556] | 2.17                     | 0.03              |
| 4:1:78:ASN:ND2  | 4:Y:32:PRO:N[1_556]    | 2.17                     | 0.03              |
| 4:1:125:GLU:OE1 | 4:Y:7:ALA:O[1_556]     | 2.17                     | 0.03              |
| 4:0:179:ASP:CG  | 4:X:179:ASP:C[1_556]   | 2.17                     | 0.03              |
| 4:1:231:ALA:N   | 4:X:370:VAL:N[1_556]   | 2.17                     | 0.03              |
| 4:2:274:ILE:CD1 | 4:Z:264:PRO:CD[1_556]  | 2.17                     | 0.03              |
| 4:0:285:CYS:CA  | 4:X:283:MET:CA[1_556]  | 2.17                     | 0.03              |
| 4:2:155:SER:OG  | 4:Z:260:THR:N[1_556]   | 2.17                     | 0.03              |
| 4:2:186:THR:N   | 4:Z:191:LYS:N[1_556]   | 2.17                     | 0.03              |
| 4:2:121:GLN:CB  | 4:Z:9:VAL:O[1_556]     | 2.17                     | 0.03              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:362:TYR:CZ  | 4:Y:22:ALA:N[1_556]    | 2.17                     | 0.03              |
| 4:0:195:GLU:CG  | 4:W:108:ALA:C[1_556]   | 2.17                     | 0.03              |
| 4:2:227:MET:O   | 4:Y:368:SER:O[1_556]   | 2.17                     | 0.03              |
| 4:1:104:LEU:CG  | 4:Y:334:GLU:CD[1_556]  | 2.17                     | 0.03              |
| 4:0:40:HIS:CG   | 4:V:166:TYR:CB[1_556]  | 2.17                     | 0.03              |
| 4:1:151:ILE:CG1 | 4:Y:275:HIS:CB[1_556]  | 2.17                     | 0.03              |
| 4:1:115:ASN:N   | 4:Y:11:ASP:OD1[1_556]  | 2.17                     | 0.03              |
| 4:1:229:THR:C   | 4:X:369:ILE:N[1_556]   | 2.17                     | 0.03              |
| 4:2:215:LYS:C   | 4:Z:252:ASN:CG[1_556]  | 2.17                     | 0.03              |
| 4:0:290:ARG:CG  | 4:X:279:TYR:CZ[1_556]  | 2.17                     | 0.03              |
| 4:2:274:ILE:N   | 4:Z:264:PRO:N[1_556]   | 2.17                     | 0.03              |
| 4:0:215:LYS:CG  | 4:X:237:GLU:OE2[1_556] | 2.17                     | 0.03              |
| 4:0:157:ASP:OD2 | 4:X:186:THR:CA[1_556]  | 2.17                     | 0.03              |
| 4:1:364:GLU:C   | 4:Y:349:LEU:CA[1_556]  | 2.17                     | 0.03              |
| 4:2:159:VAL:CG2 | 4:Z:181:ALA:CA[1_556]  | 2.17                     | 0.03              |
| 4:2:330:ILE:CG1 | 4:Z:315:LYS:CB[1_556]  | 2.17                     | 0.03              |
| 4:0:73:HIS:CG   | 4:X:157:ASP:O[1_556]   | 2.17                     | 0.03              |
| 4:2:181:ALA:CB  | 4:Z:185:LEU:CA[1_556]  | 2.17                     | 0.03              |
| 4:0:118:LYS:C   | 4:X:340:TRP:CG[1_556]  | 2.17                     | 0.03              |
| 4:3:64:ILE:CG2  | 4:Y:289:ILE:O[1_556]   | 2.17                     | 0.03              |
| 4:1:163:VAL:CG1 | 4:Y:153:LEU:CB[1_556]  | 2.17                     | 0.03              |
| 4:2:64:ILE:CG2  | 4:X:289:ILE:O[1_556]   | 2.17                     | 0.03              |
| 4:1:179:ASP:CG  | 4:Y:179:ASP:C[1_556]   | 2.17                     | 0.03              |
| 4:2:271:SER:O   | 4:Z:270:GLU:CA[1_556]  | 2.17                     | 0.03              |
| 4:3:266:PHE:CG  | 4:Z:172:PRO:CG[1_556]  | 2.17                     | 0.03              |
| 4:0:253:GLU:OE2 | 4:W:112:PRO:O[1_556]   | 2.18                     | 0.02              |
| 4:0:122:ILE:CB  | 4:X:27:PRO:CB[1_556]   | 2.18                     | 0.02              |
| 4:2:81:ASP:CA   | 4:Z:31:PHE:CB[1_556]   | 2.18                     | 0.02              |
| 4:0:117:GLU:CG  | 4:X:140:LEU:CD1[1_556] | 2.18                     | 0.02              |
| 4:2:233:SER:CA  | 4:Y:366:GLY:C[1_556]   | 2.18                     | 0.02              |
| 4:2:185:LEU:CG  | 4:Z:188:TYR:OH[1_556]  | 2.18                     | 0.02              |
| 4:2:303:THR:OG1 | 4:Z:257:CYS:N[1_556]   | 2.18                     | 0.02              |
| 4:3:230:ALA:C   | 4:Z:368:SER:C[1_556]   | 2.18                     | 0.02              |
| 4:0:253:GLU:OE2 | 4:W:113:LYS:N[1_556]   | 2.18                     | 0.02              |
| 4:2:183:ARG:CZ  | 4:Z:186:THR:OG1[1_556] | 2.18                     | 0.02              |
| 4:2:183:ARG:NE  | 4:Z:186:THR:OG1[1_556] | 2.18                     | 0.02              |
| 4:1:308:GLY:CA  | 4:Y:224:GLU:O[1_556]   | 2.18                     | 0.02              |
| 4:2:73:HIS:C    | 4:Z:157:ASP:N[1_556]   | 2.18                     | 0.02              |
| 4:2:156:GLY:CA  | 4:Z:306:TYR:CZ[1_556]  | 2.18                     | 0.02              |
| 4:0:112:PRO:CG  | 4:X:137:GLN:NE2[1_556] | 2.18                     | 0.02              |
| 4:1:177:ARG:NE  | 4:Y:159:VAL:CA[1_556]  | 2.18                     | 0.02              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:167:GLU:N   | 4:X:294:TYR:CA[1_556]  | 2.18                     | 0.02              |
| 4:1:274:ILE:CD1 | 4:Y:263:GLN:CA[1_556]  | 2.18                     | 0.02              |
| 4:1:209:VAL:CG2 | 4:Y:194:THR:N[1_556]   | 2.18                     | 0.02              |
| 4:1:77:THR:CB   | 4:Y:15:GLY:C[1_556]    | 2.18                     | 0.02              |
| 4:3:64:ILE:CG1  | 4:Y:292:ASP:OD2[1_556] | 2.18                     | 0.02              |
| 4:1:76:ILE:C    | 4:Y:16:LEU:N[1_556]    | 2.18                     | 0.02              |
| 4:2:133:TYR:CB  | 4:Z:334:GLU:OE1[1_556] | 2.18                     | 0.02              |
| 4:1:60:SER:N    | 4:Y:243:PRO:CG[1_556]  | 2.18                     | 0.02              |
| 4:0:215:LYS:C   | 4:X:252:ASN:CG[1_556]  | 2.18                     | 0.02              |
| 4:0:82:MET:C    | 4:X:30:VAL:C[1_556]    | 2.18                     | 0.02              |
| 4:0:115:ASN:OD1 | 4:X:11:ASP:OD1[1_556]  | 2.18                     | 0.02              |
| 4:2:173:HIS:ND1 | 4:Z:164:PRO:CG[1_556]  | 2.18                     | 0.02              |
| 4:2:368:SER:N   | 4:Z:346:LEU:CB[1_556]  | 2.18                     | 0.02              |
| 4:2:253:GLU:OE2 | 4:Y:113:LYS:N[1_556]   | 2.18                     | 0.02              |
| 4:0:206:ARG:C   | 4:X:199:SER:N[1_556]   | 2.18                     | 0.02              |
| 4:0:33:SER:C    | 4:X:210:ARG:NE[1_556]  | 2.18                     | 0.02              |
| 4:0:271:SER:O   | 4:X:270:GLU:CA[1_556]  | 2.18                     | 0.02              |
| 4:2:292:ASP:O   | 4:Z:317:ILE:O[1_556]   | 2.18                     | 0.02              |
| 4:1:178:LEU:N   | 4:Y:178:LEU:CG[1_556]  | 2.18                     | 0.02              |
| 4:1:167:GLU:CG  | 4:Y:326:LYS:O[1_556]   | 2.18                     | 0.02              |
| 4:0:117:GLU:CD  | 4:X:104:LEU:CD2[1_556] | 2.18                     | 0.02              |
| 4:2:162:ASN:CB  | 4:Z:274:ILE:O[1_556]   | 2.18                     | 0.02              |
| 4:1:110:LEU:CG  | 4:Y:161:HIS:CG[1_556]  | 2.18                     | 0.02              |
| 4:0:175:ILE:CD1 | 4:X:162:ASN:ND2[1_556] | 2.18                     | 0.02              |
| 4:0:281:SER:CB  | 4:X:276:GLU:CB[1_556]  | 2.18                     | 0.02              |
| 4:1:126:THR:CB  | 4:Y:28:ARG:CA[1_556]   | 2.18                     | 0.02              |
| 4:1:67:LEU:C    | 4:Y:207:GLU:OE2[1_556] | 2.18                     | 0.02              |
| 4:1:111:ASN:CB  | 4:Y:154:ASP:OD1[1_556] | 2.18                     | 0.02              |
| 4:2:179:ASP:CG  | 4:Z:179:ASP:C[1_556]   | 2.18                     | 0.02              |
| 4:2:116:ARG:CG  | 4:Z:339:VAL:N[1_556]   | 2.18                     | 0.02              |
| 4:1:207:GLU:N   | 4:Y:199:SER:C[1_556]   | 2.18                     | 0.02              |
| 4:0:306:TYR:CA  | 4:X:227:MET:SD[1_556]  | 2.18                     | 0.02              |
| 4:0:189:LEU:CD1 | 4:X:195:GLU:CA[1_556]  | 2.18                     | 0.02              |
| 4:0:185:LEU:N   | 4:X:188:TYR:CB[1_556]  | 2.18                     | 0.02              |
| 4:2:126:THR:OG1 | 4:Z:28:ARG:C[1_556]    | 2.18                     | 0.02              |
| 4:2:293:LEU:N   | 4:Z:321:ALA:CA[1_556]  | 2.18                     | 0.02              |
| 4:0:148:THR:OG1 | 4:X:327:ILE:C[1_556]   | 2.18                     | 0.02              |
| 4:2:233:SER:C   | 4:Y:367:PRO:CA[1_556]  | 2.18                     | 0.02              |
| 4:2:80:ASP:C    | 4:Z:31:PHE:CA[1_556]   | 2.18                     | 0.02              |
| 4:2:302:GLY:N   | 4:Z:258:PRO:CD[1_556]  | 2.18                     | 0.02              |
| 4:2:136:ILE:O   | 4:Z:299:MET:C[1_556]   | 2.18                     | 0.02              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:123:MET:CA  | 4:Z:27:PRO:N[1_556]    | 2.18                     | 0.02              |
| 4:1:197:GLY:O   | 4:X:76:ILE:C[1_556]    | 2.18                     | 0.02              |
| 4:2:111:ASN:N   | 4:Z:154:ASP:CB[1_556]  | 2.18                     | 0.02              |
| 4:0:177:ARG:NE  | 4:X:159:VAL:CA[1_556]  | 2.18                     | 0.02              |
| 4:1:289:ILE:CG1 | 4:Y:294:TYR:CZ[1_556]  | 2.18                     | 0.02              |
| 4:2:72:GLU:O    | 4:Z:157:ASP:O[1_556]   | 2.18                     | 0.02              |
| 4:3:64:ILE:CA   | 4:Y:289:ILE:CA[1_556]  | 2.18                     | 0.02              |
| 4:1:297:ASN:CG  | 4:Y:316:GLU:OE2[1_556] | 2.18                     | 0.02              |
| 4:3:230:ALA:C   | 4:Z:367:PRO:C[1_556]   | 2.18                     | 0.02              |
| 4:0:121:GLN:CB  | 4:X:9:VAL:N[1_556]     | 2.18                     | 0.02              |
| 4:0:289:ILE:CD1 | 4:X:282:ILE:CG2[1_556] | 2.18                     | 0.02              |
| 4:0:112:PRO:N   | 4:X:137:GLN:CB[1_556]  | 2.18                     | 0.02              |
| 4:2:230:ALA:O   | 4:Y:368:SER:N[1_556]   | 2.18                     | 0.02              |
| 4:2:126:THR:CB  | 4:Z:28:ARG:CA[1_556]   | 2.18                     | 0.02              |
| 4:2:118:LYS:C   | 4:Z:340:TRP:CG[1_556]  | 2.18                     | 0.02              |
| 4:0:155:SER:CA  | 4:X:261:LEU:CG[1_556]  | 2.18                     | 0.02              |
| 4:1:132:MET:CE  | 4:Y:341:ILE:CD1[1_556] | 2.18                     | 0.02              |
| 4:1:213:LYS:O   | 4:Y:253:GLU:CD[1_556]  | 2.18                     | 0.02              |
| 4:0:331:ALA:C   | 4:X:222:ASP:N[1_556]   | 2.18                     | 0.02              |
| 4:1:141:SER:C   | 4:Y:310:ALA:O[1_556]   | 2.18                     | 0.02              |
| 4:1:139:VAL:CG1 | 4:Y:330:ILE:C[1_556]   | 2.18                     | 0.02              |
| 4:1:79:TRP:CB   | 4:Y:17:VAL:C[1_556]    | 2.18                     | 0.02              |
| 4:2:32:PRO:CA   | 4:Z:211:ASP:OD2[1_556] | 2.18                     | 0.02              |
| 4:1:115:ASN:CB  | 4:Y:11:ASP:OD2[1_556]  | 2.18                     | 0.02              |
| 4:0:68:LYS:N    | 4:X:207:GLU:OE2[1_556] | 2.18                     | 0.02              |
| 4:2:264:PRO:CG  | 4:Z:268:GLY:C[1_556]   | 2.18                     | 0.02              |
| 4:2:171:LEU:CB  | 4:Z:282:ILE:CG1[1_556] | 2.18                     | 0.02              |
| 4:0:150:GLY:C   | 4:X:317:ILE:N[1_556]   | 2.18                     | 0.02              |
| 4:0:196:ARG:NE  | 4:W:115:ASN:N[1_556]   | 2.18                     | 0.02              |
| 4:1:76:ILE:CG2  | 4:Y:16:LEU:CA[1_556]   | 2.18                     | 0.02              |
| 4:2:190:MET:SD  | 4:Z:194:THR:CG2[1_556] | 2.18                     | 0.02              |
| 4:0:160:THR:OG1 | 4:X:260:THR:C[1_556]   | 2.18                     | 0.02              |
| 4:0:183:ARG:NE  | 4:X:186:THR:OG1[1_556] | 2.18                     | 0.02              |
| 4:0:78:ASN:ND2  | 4:X:32:PRO:C[1_556]    | 2.18                     | 0.02              |
| 4:2:167:GLU:N   | 4:Z:294:TYR:CA[1_556]  | 2.18                     | 0.02              |
| 4:2:140:LEU:N   | 4:Z:299:MET:CE[1_556]  | 2.18                     | 0.02              |
| 4:3:195:GLU:CG  | 4:Z:109:PRO:N[1_556]   | 2.18                     | 0.02              |
| 4:1:290:ARG:CD  | 4:Y:279:TYR:OH[1_556]  | 2.18                     | 0.02              |
| 4:1:122:ILE:CG2 | 4:Y:29:ALA:N[1_556]    | 2.18                     | 0.02              |
| 4:2:253:GLU:OE2 | 4:Y:112:PRO:O[1_556]   | 2.18                     | 0.02              |
| 4:0:186:THR:N   | 4:X:191:LYS:N[1_556]   | 2.18                     | 0.02              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:286:ASP:OD1 | 4:Y:290:ARG:NH2[1_556] | 2.18                     | 0.02              |
| 4:1:66:THR:C    | 4:Y:59:GLN:O[1_556]    | 2.18                     | 0.02              |
| 4:1:171:LEU:N   | 4:Y:151:ILE:CG2[1_556] | 2.18                     | 0.02              |
| 4:0:211:ASP:OD2 | 4:X:250:ILE:N[1_556]   | 2.18                     | 0.02              |
| 4:1:120:THR:C   | 4:Y:340:TRP:CE2[1_556] | 2.18                     | 0.02              |
| 4:0:140:LEU:CA  | 4:X:331:ALA:CA[1_556]  | 2.18                     | 0.02              |
| 4:0:298:VAL:CG2 | 4:X:312:ARG:O[1_556]   | 2.18                     | 0.02              |
| 4:0:293:LEU:N   | 4:X:321:ALA:CA[1_556]  | 2.18                     | 0.02              |
| 4:1:231:ALA:CA  | 4:X:371:HIS:N[1_556]   | 2.18                     | 0.02              |
| 4:0:111:ASN:C   | 4:X:137:GLN:CB[1_556]  | 2.18                     | 0.02              |
| 4:0:303:THR:C   | 4:X:256:ARG:C[1_556]   | 2.18                     | 0.02              |
| 4:1:126:THR:C   | 4:Y:28:ARG:CZ[1_556]   | 2.18                     | 0.02              |
| 4:0:121:GLN:CD  | 4:X:20:GLY:N[1_556]    | 2.18                     | 0.02              |
| 4:2:125:GLU:OE1 | 4:Z:7:ALA:O[1_556]     | 2.18                     | 0.02              |
| 4:1:86:TRP:CE2  | 4:Y:337:TYR:CE2[1_556] | 2.18                     | 0.02              |
| 4:2:170:ALA:C   | 4:Z:151:ILE:CA[1_556]  | 2.18                     | 0.02              |
| 4:2:228:ALA:O   | 4:Y:369:ILE:N[1_556]   | 2.18                     | 0.02              |
| 4:2:194:THR:CA  | 4:Y:75:ILE:CG1[1_556]  | 2.18                     | 0.02              |
| 4:0:253:GLU:CA  | 4:W:113:LYS:CG[1_556]  | 2.18                     | 0.02              |
| 4:2:366:GLY:CA  | 4:Z:347:ALA:N[1_556]   | 2.18                     | 0.02              |
| 4:2:167:GLU:CG  | 4:Z:326:LYS:O[1_556]   | 2.18                     | 0.02              |
| 4:1:149:THR:O   | 4:Y:327:ILE:CG1[1_556] | 2.18                     | 0.02              |
| 4:1:153:LEU:CG  | 4:Y:262:PHE:CD1[1_556] | 2.18                     | 0.02              |
| 4:0:64:ILE:CA   | 4:V:289:ILE:CA[1_556]  | 2.18                     | 0.02              |
| 4:1:169:TYR:OH  | 4:Y:164:PRO:CB[1_556]  | 2.18                     | 0.02              |
| 4:1:72:GLU:O    | 4:Y:157:ASP:O[1_556]   | 2.18                     | 0.02              |
| 4:2:152:VAL:C   | 4:Z:313:MET:SD[1_556]  | 2.18                     | 0.02              |
| 4:1:113:LYS:N   | 4:Y:136:ILE:C[1_556]   | 2.18                     | 0.02              |
| 4:1:166:TYR:CA  | 4:Y:294:TYR:N[1_556]   | 2.18                     | 0.02              |
| 4:1:105:LEU:N   | 4:Y:334:GLU:N[1_556]   | 2.18                     | 0.02              |
| 4:2:166:TYR:N   | 4:Z:294:TYR:CA[1_556]  | 2.18                     | 0.02              |
| 4:2:67:LEU:CB   | 4:Z:62:ARG:NH1[1_556]  | 2.18                     | 0.02              |
| 4:0:228:ALA:O   | 4:W:369:ILE:N[1_556]   | 2.18                     | 0.02              |
| 4:1:61:LYS:CB   | 4:W:291:LYS:CE[1_556]  | 2.18                     | 0.02              |
| 4:0:233:SER:C   | 4:W:367:PRO:CA[1_556]  | 2.18                     | 0.02              |
| 4:1:123:MET:N   | 4:Y:27:PRO:CA[1_556]   | 2.18                     | 0.02              |
| 4:2:64:ILE:CG1  | 4:X:292:ASP:OD2[1_556] | 2.18                     | 0.02              |
| 4:1:285:CYS:O   | 4:Y:283:MET:CA[1_556]  | 2.18                     | 0.02              |
| 4:0:336:LYS:N   | 4:X:219:VAL:N[1_556]   | 2.18                     | 0.02              |
| 4:2:272:ALA:C   | 4:Z:269:MET:C[1_556]   | 2.18                     | 0.02              |
| 4:1:306:TYR:CG  | 4:Y:256:ARG:CD[1_556]  | 2.18                     | 0.02              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:179:ASP:OD1 | 4:Y:179:ASP:O[1_556]   | 2.18                     | 0.02              |
| 4:0:37:ARG:O    | 4:X:60:SER:C[1_556]    | 2.18                     | 0.02              |
| 4:0:368:SER:O   | 4:X:346:LEU:CG[1_556]  | 2.18                     | 0.02              |
| 4:2:116:ARG:CB  | 4:Z:339:VAL:O[1_556]   | 2.18                     | 0.02              |
| 4:1:309:ILE:CG2 | 4:Y:223:PHE:CA[1_556]  | 2.18                     | 0.02              |
| 4:1:309:ILE:CG2 | 4:Y:223:PHE:O[1_556]   | 2.18                     | 0.02              |
| 4:3:253:GLU:CA  | 4:Z:113:LYS:CG[1_556]  | 2.18                     | 0.02              |
| 4:2:278:THR:OG1 | 4:Z:275:HIS:NE2[1_556] | 2.18                     | 0.02              |
| 4:2:148:THR:OG1 | 4:Z:327:ILE:C[1_556]   | 2.18                     | 0.02              |
| 4:0:155:SER:CA  | 4:X:258:PRO:O[1_556]   | 2.18                     | 0.02              |
| 4:2:201:VAL:O   | 4:Z:201:VAL:CG1[1_556] | 2.18                     | 0.02              |
| 4:2:253:GLU:CG  | 4:Y:113:LYS:N[1_556]   | 2.18                     | 0.02              |
| 4:1:68:LYS:NZ   | 4:Y:56:ASP:O[1_556]    | 2.18                     | 0.02              |
| 4:1:195:GLU:OE2 | 4:X:109:PRO:CB[1_556]  | 2.19                     | 0.01              |
| 4:0:141:SER:C   | 4:X:310:ALA:O[1_556]   | 2.19                     | 0.01              |
| 4:2:211:ASP:OD2 | 4:Z:250:ILE:N[1_556]   | 2.19                     | 0.01              |
| 4:2:161:HIS:ND1 | 4:Z:160:THR:OG1[1_556] | 2.19                     | 0.01              |
| 4:0:104:LEU:CA  | 4:X:334:GLU:OE2[1_556] | 2.19                     | 0.01              |
| 4:2:149:THR:N   | 4:Z:328:LYS:N[1_556]   | 2.19                     | 0.01              |
| 4:2:168:GLY:C   | 4:Z:296:ASN:O[1_556]   | 2.19                     | 0.01              |
| 4:2:205:GLU:O   | 4:Z:199:SER:CA[1_556]  | 2.19                     | 0.01              |
| 4:0:293:LEU:C   | 4:X:319:ALA:C[1_556]   | 2.19                     | 0.01              |
| 4:2:163:VAL:CG1 | 4:Z:153:LEU:CB[1_556]  | 2.19                     | 0.01              |
| 4:0:184:ASP:CA  | 4:X:187:ASP:C[1_556]   | 2.19                     | 0.01              |
| 4:2:134:VAL:CG2 | 4:Z:338:SER:N[1_556]   | 2.19                     | 0.01              |
| 4:2:166:TYR:CE2 | 4:Z:291:LYS:O[1_556]   | 2.19                     | 0.01              |
| 4:2:37:ARG:O    | 4:Z:60:SER:C[1_556]    | 2.19                     | 0.01              |
| 4:1:195:GLU:CG  | 4:X:109:PRO:N[1_556]   | 2.19                     | 0.01              |
| 4:0:132:MET:CG  | 4:X:25:ASP:O[1_556]    | 2.19                     | 0.01              |
| 4:1:119:MET:CE  | 4:Y:337:TYR:N[1_556]   | 2.19                     | 0.01              |
| 4:0:166:TYR:N   | 4:X:294:TYR:CA[1_556]  | 2.19                     | 0.01              |
| 4:0:141:SER:N   | 4:X:310:ALA:CA[1_556]  | 2.19                     | 0.01              |
| 4:0:166:TYR:CD1 | 4:X:294:TYR:CE2[1_556] | 2.19                     | 0.01              |
| 4:1:215:LYS:CB  | 4:Y:237:GLU:OE2[1_556] | 2.19                     | 0.01              |
| 4:0:285:CYS:O   | 4:X:283:MET:CA[1_556]  | 2.19                     | 0.01              |
| 4:1:218:TYR:OH  | 4:Y:231:ALA:CB[1_556]  | 2.19                     | 0.01              |
| 4:3:233:SER:CA  | 4:Z:366:GLY:C[1_556]   | 2.19                     | 0.01              |
| 4:0:296:ASN:CG  | 4:X:318:THR:CG2[1_556] | 2.19                     | 0.01              |
| 4:1:332:PRO:N   | 4:Y:221:LEU:C[1_556]   | 2.19                     | 0.01              |
| 4:1:230:ALA:C   | 4:X:368:SER:C[1_556]   | 2.19                     | 0.01              |
| 4:3:63:GLY:CA   | 4:Y:287:ILE:O[1_556]   | 2.19                     | 0.01              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:168:GLY:O   | 4:X:297:ASN:CA[1_556]  | 2.19                     | 0.01              |
| 4:0:138:ALA:CA  | 4:X:299:MET:CG[1_556]  | 2.19                     | 0.01              |
| 4:0:32:PRO:CA   | 4:X:211:ASP:OD2[1_556] | 2.19                     | 0.01              |
| 4:2:362:TYR:CZ  | 4:Z:22:ALA:N[1_556]    | 2.19                     | 0.01              |
| 4:0:78:ASN:CA   | 4:X:32:PRO:C[1_556]    | 2.19                     | 0.01              |
| 4:0:181:ALA:CB  | 4:X:185:LEU:CA[1_556]  | 2.19                     | 0.01              |
| 4:2:178:LEU:N   | 4:Z:178:LEU:CG[1_556]  | 2.19                     | 0.01              |
| 4:2:40:HIS:NE2  | 4:X:166:TYR:CA[1_556]  | 2.19                     | 0.01              |
| 4:2:215:LYS:CG  | 4:Z:237:GLU:OE2[1_556] | 2.19                     | 0.01              |
| 4:1:290:ARG:CG  | 4:Y:279:TYR:CZ[1_556]  | 2.19                     | 0.01              |
| 4:2:184:ASP:OD1 | 4:Z:184:ASP:C[1_556]   | 2.19                     | 0.01              |
| 4:3:195:GLU:OE2 | 4:Z:109:PRO:CB[1_556]  | 2.19                     | 0.01              |
| 4:0:72:GLU:CB   | 4:X:157:ASP:CG[1_556]  | 2.19                     | 0.01              |
| 4:2:298:VAL:CG2 | 4:Z:312:ARG:O[1_556]   | 2.19                     | 0.01              |
| 4:2:337:TYR:CG  | 4:Z:307:PRO:CG[1_556]  | 2.19                     | 0.01              |
| 4:1:78:ASN:OD1  | 4:Y:31:PHE:CD2[1_556]  | 2.19                     | 0.01              |
| 4:1:305:MET:N   | 4:Y:255:PHE:CD1[1_556] | 2.19                     | 0.01              |
| 4:0:155:SER:N   | 4:X:261:LEU:CB[1_556]  | 2.19                     | 0.01              |
| 4:0:80:ASP:CA   | 4:X:31:PHE:CD2[1_556]  | 2.19                     | 0.01              |
| 4:2:372:ARG:NH1 | 4:Z:145:SER:N[1_556]   | 2.19                     | 0.01              |
| 4:2:190:MET:N   | 4:Z:194:THR:OG1[1_556] | 2.19                     | 0.01              |
| 4:0:161:HIS:O   | 4:X:261:LEU:O[1_556]   | 2.19                     | 0.01              |
| 4:0:169:TYR:CD2 | 4:X:293:LEU:CA[1_556]  | 2.19                     | 0.01              |
| 4:2:123:MET:O   | 4:Z:24:ASP:CB[1_556]   | 2.19                     | 0.01              |
| 4:1:170:ALA:C   | 4:Y:151:ILE:CA[1_556]  | 2.19                     | 0.01              |
| 4:2:336:LYS:N   | 4:Z:219:VAL:N[1_556]   | 2.19                     | 0.01              |
| 4:0:372:ARG:CZ  | 4:X:142:LEU:C[1_556]   | 2.19                     | 0.01              |
| 4:2:179:ASP:CB  | 4:Z:179:ASP:O[1_556]   | 2.19                     | 0.01              |
| 4:0:125:GLU:OE1 | 4:X:7:ALA:O[1_556]     | 2.19                     | 0.01              |
| 4:0:107:GLU:CA  | 4:X:300:SER:C[1_556]   | 2.19                     | 0.01              |
| 4:0:67:LEU:N    | 4:X:62:ARG:CZ[1_556]   | 2.19                     | 0.01              |
| 4:2:155:SER:OG  | 4:Z:260:THR:CA[1_556]  | 2.19                     | 0.01              |
| 4:0:330:ILE:CG1 | 4:X:315:LYS:CB[1_556]  | 2.19                     | 0.01              |
| 4:2:370:VAL:CG2 | 4:Z:342:GLY:CA[1_556]  | 2.19                     | 0.01              |
| 4:0:161:HIS:ND1 | 4:X:160:THR:OG1[1_556] | 2.19                     | 0.01              |
| 4:4:40:HIS:NE2  | 4:Z:166:TYR:CA[1_556]  | 2.19                     | 0.01              |
| 4:1:367:PRO:CG  | 4:Y:9:VAL:CG2[1_556]   | 2.19                     | 0.01              |
| 4:1:31:PHE:C    | 4:Y:211:ASP:OD2[1_556] | 2.19                     | 0.01              |
| 4:0:370:VAL:CG2 | 4:X:342:GLY:CA[1_556]  | 2.19                     | 0.01              |
| 4:1:137:GLN:NE2 | 4:Y:301:GLY:CA[1_556]  | 2.19                     | 0.01              |
| 4:0:366:GLY:C   | 4:X:346:LEU:C[1_556]   | 2.19                     | 0.01              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:179:ASP:CB  | 4:X:179:ASP:O[1_556]   | 2.19                     | 0.01              |
| 4:2:132:MET:CG  | 4:Z:25:ASP:O[1_556]    | 2.19                     | 0.01              |
| 4:0:164:PRO:CB  | 4:X:278:THR:CG2[1_556] | 2.19                     | 0.01              |
| 4:1:59:GLN:CB   | 4:Y:208:ILE:CD1[1_556] | 2.19                     | 0.01              |
| 4:0:215:LYS:CG  | 4:X:196:ARG:CZ[1_556]  | 2.19                     | 0.01              |
| 4:2:303:THR:C   | 4:Z:256:ARG:C[1_556]   | 2.19                     | 0.01              |
| 4:1:185:LEU:CD1 | 4:Y:188:TYR:CG[1_556]  | 2.19                     | 0.01              |
| 4:2:72:GLU:CB   | 4:Z:157:ASP:CG[1_556]  | 2.19                     | 0.01              |
| 4:0:79:TRP:CZ3  | 4:X:18:LYS:CG[1_556]   | 2.19                     | 0.01              |
| 4:0:264:PRO:CG  | 4:X:268:GLY:C[1_556]   | 2.19                     | 0.01              |
| 4:2:60:SER:N    | 4:Z:243:PRO:CG[1_556]  | 2.19                     | 0.01              |
| 4:2:121:GLN:CD  | 4:Z:20:GLY:N[1_556]    | 2.19                     | 0.01              |
| 4:0:81:ASP:CA   | 4:X:31:PHE:CB[1_556]   | 2.19                     | 0.01              |
| 4:2:165:ILE:CD1 | 4:Z:297:ASN:CG[1_556]  | 2.19                     | 0.01              |
| 4:2:40:HIS:CG   | 4:X:166:TYR:CB[1_556]  | 2.19                     | 0.01              |
| 4:2:335:ARG:NE  | 4:Z:220:ALA:C[1_556]   | 2.19                     | 0.01              |
| 4:1:210:ARG:CG  | 4:Y:193:LEU:CB[1_556]  | 2.19                     | 0.01              |
| 4:1:104:LEU:CG  | 4:Y:334:GLU:N[1_556]   | 2.19                     | 0.01              |
| 4:0:274:ILE:N   | 4:X:264:PRO:N[1_556]   | 2.19                     | 0.01              |
| 4:2:78:ASN:CA   | 4:Z:32:PRO:C[1_556]    | 2.19                     | 0.01              |
| 4:2:157:ASP:OD2 | 4:Z:186:THR:CA[1_556]  | 2.19                     | 0.01              |
| 4:2:195:GLU:CG  | 4:Y:108:ALA:C[1_556]   | 2.19                     | 0.01              |
| 4:0:173:HIS:ND1 | 4:X:164:PRO:CG[1_556]  | 2.19                     | 0.01              |
| 4:0:364:GLU:C   | 4:X:350:SER:N[1_556]   | 2.19                     | 0.01              |
| 4:2:119:MET:C   | 4:Z:340:TRP:CD1[1_556] | 2.19                     | 0.01              |
| 4:3:61:LYS:CB   | 4:Y:291:LYS:CE[1_556]  | 2.19                     | 0.01              |
| 4:1:299:MET:CE  | 4:Y:312:ARG:NH2[1_556] | 2.19                     | 0.01              |
| 4:2:113:LYS:CB  | 4:Z:135:ALA:O[1_556]   | 2.19                     | 0.01              |
| 4:0:178:LEU:N   | 4:X:178:LEU:CG[1_556]  | 2.19                     | 0.01              |
| 4:0:201:VAL:O   | 4:X:201:VAL:CG1[1_556] | 2.19                     | 0.01              |
| 4:0:82:MET:CA   | 4:X:30:VAL:C[1_556]    | 2.19                     | 0.01              |
| 4:2:104:LEU:CA  | 4:Z:334:GLU:OE2[1_556] | 2.19                     | 0.01              |
| 4:0:261:LEU:CD2 | 4:X:266:PHE:CG[1_556]  | 2.19                     | 0.01              |
| 4:3:192:ILE:N   | 4:Z:110:LEU:CB[1_556]  | 2.19                     | 0.01              |
| 4:1:361:GLU:O   | 4:Y:349:LEU:N[1_556]   | 2.19                     | 0.01              |
| 4:1:67:LEU:O    | 4:Y:59:GLN:CD[1_556]   | 2.19                     | 0.01              |
| 4:0:292:ASP:O   | 4:X:317:ILE:O[1_556]   | 2.19                     | 0.01              |
| 4:0:337:TYR:CG  | 4:X:307:PRO:CG[1_556]  | 2.19                     | 0.01              |
| 4:2:212:ILE:O   | 4:Z:253:GLU:OE1[1_556] | 2.19                     | 0.01              |
| 4:0:278:THR:OG1 | 4:X:275:HIS:NE2[1_556] | 2.19                     | 0.01              |
| 4:0:117:GLU:CD  | 4:X:135:ALA:CB[1_556]  | 2.19                     | 0.01              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:0:136:ILE:O   | 4:X:299:MET:C[1_556]   | 2.19                     | 0.01              |
| 4:2:82:MET:CB   | 4:Z:30:VAL:CB[1_556]   | 2.19                     | 0.01              |
| 4:0:147:ARG:CA  | 4:X:314:GLN:OE1[1_556] | 2.19                     | 0.01              |
| 4:2:68:LYS:N    | 4:Z:207:GLU:OE2[1_556] | 2.19                     | 0.01              |
| 4:1:73:HIS:C    | 4:Y:157:ASP:N[1_556]   | 2.19                     | 0.01              |
| 4:0:162:ASN:CB  | 4:X:274:ILE:O[1_556]   | 2.19                     | 0.01              |
| 4:2:196:ARG:NE  | 4:Y:115:ASN:N[1_556]   | 2.19                     | 0.01              |
| 4:3:196:ARG:NE  | 4:Z:115:ASN:N[1_556]   | 2.19                     | 0.01              |
| 4:1:183:ARG:O   | 4:Y:188:TYR:N[1_556]   | 2.19                     | 0.01              |
| 4:1:79:TRP:CG   | 4:Y:18:LYS:N[1_556]    | 2.19                     | 0.01              |
| 4:1:147:ARG:CG  | 4:Y:314:GLN:CG[1_556]  | 2.19                     | 0.01              |
| 4:0:272:ALA:C   | 4:X:269:MET:C[1_556]   | 2.19                     | 0.01              |
| 4:2:303:THR:C   | 4:Z:259:GLU:N[1_556]   | 2.19                     | 0.01              |
| 4:0:67:LEU:CB   | 4:X:62:ARG:NH1[1_556]  | 2.19                     | 0.01              |
| 4:2:140:LEU:CD1 | 4:Z:331:ALA:C[1_556]   | 2.19                     | 0.01              |
| 4:1:158:GLY:CA  | 4:Y:181:ALA:O[1_556]   | 2.19                     | 0.01              |
| 4:4:64:ILE:CG2  | 4:Z:289:ILE:O[1_556]   | 2.19                     | 0.01              |
| 4:1:230:ALA:CA  | 4:X:371:HIS:CB[1_556]  | 2.19                     | 0.01              |
| 4:2:153:LEU:CB  | 4:Z:262:PHE:CE1[1_556] | 2.19                     | 0.01              |
| 4:0:119:MET:C   | 4:X:340:TRP:CD1[1_556] | 2.19                     | 0.01              |
| 4:2:122:ILE:CB  | 4:Z:27:PRO:CB[1_556]   | 2.19                     | 0.01              |
| 4:2:155:SER:N   | 4:Z:261:LEU:CB[1_556]  | 2.19                     | 0.01              |
| 4:1:206:ARG:C   | 4:Y:199:SER:N[1_556]   | 2.19                     | 0.01              |
| 4:0:31:PHE:CA   | 4:X:215:LYS:CG[1_556]  | 2.19                     | 0.01              |
| 4:0:158:GLY:C   | 4:X:185:LEU:N[1_556]   | 2.19                     | 0.01              |
| 4:2:211:ASP:O   | 4:Z:249:THR:O[1_556]   | 2.19                     | 0.01              |
| 4:0:152:VAL:C   | 4:X:262:PHE:CE1[1_556] | 2.19                     | 0.01              |
| 4:1:230:ALA:C   | 4:X:367:PRO:C[1_556]   | 2.19                     | 0.01              |
| 4:2:237:GLU:OE2 | 4:Y:114:ALA:C[1_556]   | 2.19                     | 0.01              |
| 4:2:372:ARG:CZ  | 4:Z:142:LEU:C[1_556]   | 2.19                     | 0.01              |
| 4:0:40:HIS:NE2  | 4:V:166:TYR:CA[1_556]  | 2.19                     | 0.01              |
| 4:1:304:THR:CB  | 4:Y:223:PHE:CD2[1_556] | 2.19                     | 0.01              |
| 4:2:160:THR:CG2 | 4:Z:261:LEU:O[1_556]   | 2.19                     | 0.01              |
| 4:1:105:LEU:CD1 | 4:Y:337:TYR:CG[1_556]  | 2.19                     | 0.01              |

## 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 PDB entries followed by that with respect to all EM

entries.

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

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 1   | A     | 789/840 (94%)   | 650 (82%)  | 113 (14%) | 26 (3%)  | 4           | 35  |
| 1   | D     | 789/840 (94%)   | 651 (82%)  | 112 (14%) | 26 (3%)  | 4           | 35  |
| 1   | G     | 789/840 (94%)   | 649 (82%)  | 113 (14%) | 27 (3%)  | 4           | 35  |
| 1   | J     | 791/840 (94%)   | 651 (82%)  | 112 (14%) | 28 (4%)  | 4           | 34  |
| 2   | B     | 143/145 (99%)   | 126 (88%)  | 9 (6%)    | 8 (6%)   | 2           | 25  |
| 2   | E     | 143/145 (99%)   | 126 (88%)  | 9 (6%)    | 8 (6%)   | 2           | 25  |
| 2   | H     | 143/145 (99%)   | 126 (88%)  | 9 (6%)    | 8 (6%)   | 2           | 25  |
| 2   | K     | 143/145 (99%)   | 126 (88%)  | 9 (6%)    | 8 (6%)   | 2           | 25  |
| 3   | C     | 143/147 (97%)   | 133 (93%)  | 10 (7%)   | 0        | 100         | 100 |
| 3   | F     | 143/147 (97%)   | 133 (93%)  | 10 (7%)   | 0        | 100         | 100 |
| 3   | I     | 143/147 (97%)   | 133 (93%)  | 10 (7%)   | 0        | 100         | 100 |
| 3   | L     | 143/147 (97%)   | 133 (93%)  | 10 (7%)   | 0        | 100         | 100 |
| 4   | 0     | 370/375 (99%)   | 334 (90%)  | 30 (8%)   | 6 (2%)   | 11          | 51  |
| 4   | 1     | 370/375 (99%)   | 335 (90%)  | 29 (8%)   | 6 (2%)   | 11          | 51  |
| 4   | 2     | 370/375 (99%)   | 334 (90%)  | 30 (8%)   | 6 (2%)   | 11          | 51  |
| 4   | 3     | 370/375 (99%)   | 335 (90%)  | 29 (8%)   | 6 (2%)   | 11          | 51  |
| 4   | 4     | 370/375 (99%)   | 334 (90%)  | 30 (8%)   | 6 (2%)   | 11          | 51  |
| 4   | 5     | 370/375 (99%)   | 335 (90%)  | 29 (8%)   | 6 (2%)   | 11          | 51  |
| 4   | 6     | 370/375 (99%)   | 335 (90%)  | 29 (8%)   | 6 (2%)   | 11          | 51  |
| 4   | 7     | 370/375 (99%)   | 334 (90%)  | 30 (8%)   | 6 (2%)   | 11          | 51  |
| 4   | 8     | 370/375 (99%)   | 335 (90%)  | 29 (8%)   | 6 (2%)   | 11          | 51  |
| 4   | V     | 370/375 (99%)   | 334 (90%)  | 30 (8%)   | 6 (2%)   | 11          | 51  |
| 4   | W     | 370/375 (99%)   | 334 (90%)  | 30 (8%)   | 6 (2%)   | 11          | 51  |
| 4   | X     | 370/375 (99%)   | 334 (90%)  | 30 (8%)   | 6 (2%)   | 11          | 51  |
| 4   | Y     | 370/375 (99%)   | 334 (90%)  | 30 (8%)   | 6 (2%)   | 11          | 51  |
| 4   | Z     | 370/375 (99%)   | 335 (90%)  | 29 (8%)   | 6 (2%)   | 11          | 51  |
| All | All   | 9482/9778 (97%) | 8319 (88%) | 940 (10%) | 223 (2%) | 11          | 42  |

All (223) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 73  | LYS  |
| 1   | A     | 202 | SER  |
| 1   | A     | 572 | LYS  |
| 1   | A     | 712 | PRO  |
| 1   | A     | 729 | ALA  |
| 1   | A     | 757 | GLN  |
| 1   | A     | 762 | HIS  |
| 2   | B     | 131 | GLU  |
| 2   | B     | 141 | PRO  |
| 1   | D     | 73  | LYS  |
| 1   | D     | 202 | SER  |
| 1   | D     | 572 | LYS  |
| 1   | D     | 712 | PRO  |
| 1   | D     | 729 | ALA  |
| 1   | D     | 757 | GLN  |
| 1   | D     | 762 | HIS  |
| 2   | E     | 131 | GLU  |
| 2   | E     | 141 | PRO  |
| 1   | G     | 73  | LYS  |
| 1   | G     | 202 | SER  |
| 1   | G     | 572 | LYS  |
| 1   | G     | 712 | PRO  |
| 1   | G     | 729 | ALA  |
| 1   | G     | 757 | GLN  |
| 1   | G     | 762 | HIS  |
| 2   | H     | 131 | GLU  |
| 2   | H     | 141 | PRO  |
| 1   | J     | 73  | LYS  |
| 1   | J     | 202 | SER  |
| 1   | J     | 572 | LYS  |
| 1   | J     | 712 | PRO  |
| 1   | J     | 729 | ALA  |
| 1   | J     | 757 | GLN  |
| 1   | J     | 762 | HIS  |
| 1   | J     | 785 | GLU  |
| 2   | K     | 131 | GLU  |
| 2   | K     | 141 | PRO  |
| 4   | 0     | 246 | GLN  |
| 4   | 1     | 246 | GLN  |
| 4   | 2     | 246 | GLN  |
| 4   | 3     | 246 | GLN  |
| 4   | 4     | 246 | GLN  |
| 4   | 5     | 246 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 6     | 246 | GLN  |
| 4   | 7     | 246 | GLN  |
| 4   | 8     | 246 | GLN  |
| 4   | V     | 246 | GLN  |
| 4   | W     | 246 | GLN  |
| 4   | X     | 246 | GLN  |
| 4   | Y     | 246 | GLN  |
| 4   | Z     | 246 | GLN  |
| 1   | A     | 11  | GLY  |
| 1   | A     | 21  | GLU  |
| 1   | A     | 219 | GLU  |
| 1   | A     | 517 | MET  |
| 1   | A     | 532 | ILE  |
| 1   | A     | 637 | LYS  |
| 2   | B     | 130 | PRO  |
| 2   | B     | 147 | ASN  |
| 2   | B     | 151 | LYS  |
| 2   | B     | 161 | GLU  |
| 1   | D     | 11  | GLY  |
| 1   | D     | 21  | GLU  |
| 1   | D     | 219 | GLU  |
| 1   | D     | 517 | MET  |
| 1   | D     | 532 | ILE  |
| 1   | D     | 637 | LYS  |
| 2   | E     | 130 | PRO  |
| 2   | E     | 147 | ASN  |
| 2   | E     | 151 | LYS  |
| 2   | E     | 161 | GLU  |
| 1   | G     | 11  | GLY  |
| 1   | G     | 21  | GLU  |
| 1   | G     | 219 | GLU  |
| 1   | G     | 517 | MET  |
| 1   | G     | 532 | ILE  |
| 1   | G     | 637 | LYS  |
| 1   | G     | 785 | GLU  |
| 2   | H     | 130 | PRO  |
| 2   | H     | 147 | ASN  |
| 2   | H     | 151 | LYS  |
| 1   | J     | 11  | GLY  |
| 1   | J     | 21  | GLU  |
| 1   | J     | 219 | GLU  |
| 1   | J     | 517 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 637 | LYS  |
| 2   | K     | 130 | PRO  |
| 2   | K     | 147 | ASN  |
| 2   | K     | 151 | LYS  |
| 2   | K     | 161 | GLU  |
| 4   | 0     | 274 | ILE  |
| 4   | 1     | 274 | ILE  |
| 4   | 2     | 274 | ILE  |
| 4   | 3     | 274 | ILE  |
| 4   | 4     | 274 | ILE  |
| 4   | 5     | 274 | ILE  |
| 4   | 6     | 274 | ILE  |
| 4   | 7     | 274 | ILE  |
| 4   | 8     | 274 | ILE  |
| 4   | V     | 274 | ILE  |
| 4   | W     | 274 | ILE  |
| 4   | X     | 274 | ILE  |
| 4   | Y     | 274 | ILE  |
| 4   | Z     | 274 | ILE  |
| 1   | A     | 58  | GLY  |
| 1   | A     | 294 | ASN  |
| 1   | A     | 644 | SER  |
| 1   | D     | 58  | GLY  |
| 1   | D     | 294 | ASN  |
| 1   | D     | 644 | SER  |
| 1   | G     | 58  | GLY  |
| 1   | G     | 294 | ASN  |
| 1   | G     | 644 | SER  |
| 2   | H     | 161 | GLU  |
| 1   | J     | 58  | GLY  |
| 1   | J     | 294 | ASN  |
| 1   | J     | 532 | ILE  |
| 1   | J     | 644 | SER  |
| 4   | 0     | 233 | SER  |
| 4   | 1     | 233 | SER  |
| 4   | 2     | 233 | SER  |
| 4   | 3     | 233 | SER  |
| 4   | 4     | 233 | SER  |
| 4   | 5     | 233 | SER  |
| 4   | 6     | 233 | SER  |
| 4   | 7     | 233 | SER  |
| 4   | 8     | 233 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | V     | 233 | SER  |
| 4   | W     | 233 | SER  |
| 4   | X     | 233 | SER  |
| 4   | Y     | 233 | SER  |
| 4   | Z     | 233 | SER  |
| 1   | A     | 435 | GLU  |
| 1   | A     | 817 | GLN  |
| 1   | D     | 269 | LEU  |
| 1   | D     | 435 | GLU  |
| 1   | D     | 817 | GLN  |
| 1   | G     | 269 | LEU  |
| 1   | G     | 435 | GLU  |
| 1   | G     | 817 | GLN  |
| 1   | J     | 435 | GLU  |
| 1   | J     | 817 | GLN  |
| 4   | 0     | 2   | GLU  |
| 4   | 0     | 253 | GLU  |
| 4   | 1     | 2   | GLU  |
| 4   | 1     | 253 | GLU  |
| 4   | 2     | 2   | GLU  |
| 4   | 2     | 253 | GLU  |
| 4   | 3     | 2   | GLU  |
| 4   | 3     | 253 | GLU  |
| 4   | 4     | 2   | GLU  |
| 4   | 4     | 253 | GLU  |
| 4   | 5     | 2   | GLU  |
| 4   | 6     | 2   | GLU  |
| 4   | 6     | 253 | GLU  |
| 4   | 7     | 2   | GLU  |
| 4   | 7     | 253 | GLU  |
| 4   | 8     | 2   | GLU  |
| 4   | V     | 2   | GLU  |
| 4   | V     | 253 | GLU  |
| 4   | W     | 2   | GLU  |
| 4   | X     | 2   | GLU  |
| 4   | X     | 253 | GLU  |
| 4   | Y     | 2   | GLU  |
| 4   | Y     | 253 | GLU  |
| 4   | Z     | 2   | GLU  |
| 1   | A     | 8   | ALA  |
| 1   | A     | 269 | LEU  |
| 1   | A     | 578 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 140 | PHE  |
| 1   | D     | 8   | ALA  |
| 1   | D     | 578 | HIS  |
| 2   | E     | 140 | PHE  |
| 1   | G     | 8   | ALA  |
| 1   | G     | 79  | SER  |
| 1   | G     | 578 | HIS  |
| 2   | H     | 140 | PHE  |
| 1   | J     | 8   | ALA  |
| 1   | J     | 269 | LEU  |
| 1   | J     | 578 | HIS  |
| 2   | K     | 140 | PHE  |
| 4   | 5     | 253 | GLU  |
| 4   | 8     | 253 | GLU  |
| 4   | W     | 253 | GLU  |
| 4   | Z     | 253 | GLU  |
| 1   | A     | 79  | SER  |
| 1   | A     | 199 | ILE  |
| 1   | A     | 556 | ASP  |
| 2   | B     | 142 | PRO  |
| 1   | D     | 79  | SER  |
| 1   | D     | 199 | ILE  |
| 1   | D     | 556 | ASP  |
| 2   | E     | 142 | PRO  |
| 1   | G     | 199 | ILE  |
| 1   | G     | 556 | ASP  |
| 2   | H     | 142 | PRO  |
| 1   | J     | 79  | SER  |
| 1   | J     | 199 | ILE  |
| 1   | J     | 556 | ASP  |
| 1   | J     | 822 | SER  |
| 2   | K     | 142 | PRO  |
| 1   | A     | 840 | PRO  |
| 1   | D     | 287 | ILE  |
| 1   | D     | 840 | PRO  |
| 1   | G     | 840 | PRO  |
| 1   | J     | 287 | ILE  |
| 1   | J     | 840 | PRO  |
| 4   | 0     | 242 | LEU  |
| 4   | 1     | 242 | LEU  |
| 4   | 2     | 242 | LEU  |
| 4   | 3     | 242 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 4     | 242 | LEU  |
| 4   | 5     | 242 | LEU  |
| 4   | 6     | 242 | LEU  |
| 4   | 7     | 242 | LEU  |
| 4   | 8     | 242 | LEU  |
| 4   | V     | 242 | LEU  |
| 4   | W     | 242 | LEU  |
| 4   | X     | 242 | LEU  |
| 4   | Y     | 242 | LEU  |
| 4   | Z     | 242 | LEU  |
| 1   | A     | 287 | ILE  |
| 1   | G     | 287 | ILE  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric | Outliers  | Percentiles |    |
|-----|-------|----------------|-----------|-----------|-------------|----|
| 1   | A     | 672/672 (100%) | 512 (76%) | 160 (24%) | 1           | 5  |
| 1   | D     | 672/672 (100%) | 515 (77%) | 157 (23%) | 1           | 5  |
| 1   | G     | 672/672 (100%) | 514 (76%) | 158 (24%) | 1           | 5  |
| 1   | J     | 672/672 (100%) | 514 (76%) | 158 (24%) | 1           | 5  |
| 2   | B     | 120/120 (100%) | 119 (99%) | 1 (1%)    | 85          | 92 |
| 2   | E     | 120/120 (100%) | 119 (99%) | 1 (1%)    | 85          | 92 |
| 2   | H     | 120/120 (100%) | 119 (99%) | 1 (1%)    | 85          | 92 |
| 2   | K     | 120/120 (100%) | 119 (99%) | 1 (1%)    | 85          | 92 |
| 3   | C     | 117/117 (100%) | 112 (96%) | 5 (4%)    | 33          | 64 |
| 3   | F     | 117/117 (100%) | 112 (96%) | 5 (4%)    | 33          | 64 |
| 3   | I     | 117/117 (100%) | 112 (96%) | 5 (4%)    | 33          | 64 |
| 3   | L     | 117/117 (100%) | 112 (96%) | 5 (4%)    | 33          | 64 |
| 4   | 0     | 315/318 (99%)  | 269 (85%) | 46 (15%)  | 3           | 21 |
| 4   | 1     | 315/318 (99%)  | 268 (85%) | 47 (15%)  | 3           | 20 |

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| Mol | Chain | Analysed         | Rotameric  | Outliers   | Percentiles |    |
|-----|-------|------------------|------------|------------|-------------|----|
| 4   | 2     | 315/318 (99%)    | 268 (85%)  | 47 (15%)   | 3           | 20 |
| 4   | 3     | 315/318 (99%)    | 268 (85%)  | 47 (15%)   | 3           | 20 |
| 4   | 4     | 315/318 (99%)    | 268 (85%)  | 47 (15%)   | 3           | 20 |
| 4   | 5     | 315/318 (99%)    | 269 (85%)  | 46 (15%)   | 3           | 21 |
| 4   | 6     | 315/318 (99%)    | 268 (85%)  | 47 (15%)   | 3           | 20 |
| 4   | 7     | 315/318 (99%)    | 269 (85%)  | 46 (15%)   | 3           | 21 |
| 4   | 8     | 315/318 (99%)    | 268 (85%)  | 47 (15%)   | 3           | 20 |
| 4   | V     | 315/318 (99%)    | 269 (85%)  | 46 (15%)   | 3           | 21 |
| 4   | W     | 315/318 (99%)    | 269 (85%)  | 46 (15%)   | 3           | 21 |
| 4   | X     | 315/318 (99%)    | 269 (85%)  | 46 (15%)   | 3           | 21 |
| 4   | Y     | 315/318 (99%)    | 268 (85%)  | 47 (15%)   | 3           | 20 |
| 4   | Z     | 315/318 (99%)    | 268 (85%)  | 47 (15%)   | 3           | 20 |
| All | All   | 8046/8088 (100%) | 6737 (84%) | 1309 (16%) | 6           | 17 |

All (1309) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 4   | ASP  |
| 1   | A     | 7   | MET  |
| 1   | A     | 12  | GLU  |
| 1   | A     | 15  | PRO  |
| 1   | A     | 17  | LEU  |
| 1   | A     | 20  | SER  |
| 1   | A     | 22  | LYS  |
| 1   | A     | 36  | SER  |
| 1   | A     | 37  | SER  |
| 1   | A     | 46  | SER  |
| 1   | A     | 61  | THR  |
| 1   | A     | 69  | THR  |
| 1   | A     | 70  | LEU  |
| 1   | A     | 72  | VAL  |
| 1   | A     | 73  | LYS  |
| 1   | A     | 75  | ASP  |
| 1   | A     | 76  | GLN  |
| 1   | A     | 97  | LEU  |
| 1   | A     | 106 | LEU  |
| 1   | A     | 109 | ARG  |
| 1   | A     | 114 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 117 | THR  |
| 1   | A     | 121 | LEU  |
| 1   | A     | 126 | VAL  |
| 1   | A     | 127 | ASN  |
| 1   | A     | 135 | TYR  |
| 1   | A     | 136 | ASN  |
| 1   | A     | 146 | LYS  |
| 1   | A     | 149 | GLN  |
| 1   | A     | 155 | ILE  |
| 1   | A     | 157 | SER  |
| 1   | A     | 158 | ILE  |
| 1   | A     | 159 | SER  |
| 1   | A     | 165 | PHE  |
| 1   | A     | 167 | LEU  |
| 1   | A     | 169 | ASP  |
| 1   | A     | 173 | GLN  |
| 1   | A     | 178 | THR  |
| 1   | A     | 185 | LYS  |
| 1   | A     | 186 | THR  |
| 1   | A     | 187 | VAL  |
| 1   | A     | 189 | THR  |
| 1   | A     | 191 | ARG  |
| 1   | A     | 193 | ILE  |
| 1   | A     | 194 | GLN  |
| 1   | A     | 198 | THR  |
| 1   | A     | 199 | ILE  |
| 1   | A     | 218 | LEU  |
| 1   | A     | 219 | GLU  |
| 1   | A     | 221 | GLN  |
| 1   | A     | 223 | ILE  |
| 1   | A     | 227 | PRO  |
| 1   | A     | 229 | LEU  |
| 1   | A     | 244 | SER  |
| 1   | A     | 245 | ARG  |
| 1   | A     | 251 | ARG  |
| 1   | A     | 264 | ASP  |
| 1   | A     | 273 | SER  |
| 1   | A     | 274 | ARG  |
| 1   | A     | 278 | GLN  |
| 1   | A     | 282 | GLU  |
| 1   | A     | 287 | ILE  |
| 1   | A     | 290 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 294 | ASN  |
| 1   | A     | 298 | GLU  |
| 1   | A     | 300 | ILE  |
| 1   | A     | 325 | ILE  |
| 1   | A     | 331 | LEU  |
| 1   | A     | 336 | SER  |
| 1   | A     | 351 | ILE  |
| 1   | A     | 354 | LEU  |
| 1   | A     | 364 | LEU  |
| 1   | A     | 365 | LYS  |
| 1   | A     | 372 | GLU  |
| 1   | A     | 376 | GLU  |
| 1   | A     | 381 | GLU  |
| 1   | A     | 389 | LEU  |
| 1   | A     | 392 | LEU  |
| 1   | A     | 394 | SER  |
| 1   | A     | 399 | LYS  |
| 1   | A     | 405 | ARG  |
| 1   | A     | 410 | ASN  |
| 1   | A     | 439 | LEU  |
| 1   | A     | 447 | GLN  |
| 1   | A     | 448 | GLN  |
| 1   | A     | 449 | LEU  |
| 1   | A     | 453 | GLN  |
| 1   | A     | 455 | ARG  |
| 1   | A     | 457 | TYR  |
| 1   | A     | 462 | LEU  |
| 1   | A     | 471 | ASP  |
| 1   | A     | 474 | SER  |
| 1   | A     | 480 | ILE  |
| 1   | A     | 487 | LEU  |
| 1   | A     | 495 | MET  |
| 1   | A     | 499 | GLU  |
| 1   | A     | 506 | GLU  |
| 1   | A     | 513 | ILE  |
| 1   | A     | 518 | ASP  |
| 1   | A     | 524 | GLU  |
| 1   | A     | 532 | ILE  |
| 1   | A     | 534 | SER  |
| 1   | A     | 537 | GLU  |
| 1   | A     | 543 | PRO  |
| 1   | A     | 549 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 561 | LYS  |
| 1   | A     | 562 | SER  |
| 1   | A     | 563 | ASN  |
| 1   | A     | 569 | LYS  |
| 1   | A     | 580 | SER  |
| 1   | A     | 593 | SER  |
| 1   | A     | 597 | GLU  |
| 1   | A     | 604 | ASN  |
| 1   | A     | 608 | ILE  |
| 1   | A     | 610 | LEU  |
| 1   | A     | 615 | SER  |
| 1   | A     | 621 | LEU  |
| 1   | A     | 625 | THR  |
| 1   | A     | 664 | LEU  |
| 1   | A     | 666 | SER  |
| 1   | A     | 673 | ARG  |
| 1   | A     | 675 | ILE  |
| 1   | A     | 676 | ILE  |
| 1   | A     | 686 | MET  |
| 1   | A     | 689 | GLU  |
| 1   | A     | 690 | LEU  |
| 1   | A     | 693 | HIS  |
| 1   | A     | 698 | ASN  |
| 1   | A     | 701 | LEU  |
| 1   | A     | 702 | GLU  |
| 1   | A     | 704 | ILE  |
| 1   | A     | 708 | ARG  |
| 1   | A     | 713 | SER  |
| 1   | A     | 714 | ARG  |
| 1   | A     | 716 | LEU  |
| 1   | A     | 719 | ASP  |
| 1   | A     | 722 | GLN  |
| 1   | A     | 723 | ARG  |
| 1   | A     | 727 | LEU  |
| 1   | A     | 728 | ASN  |
| 1   | A     | 745 | GLU  |
| 1   | A     | 752 | ASP  |
| 1   | A     | 753 | VAL  |
| 1   | A     | 754 | ASP  |
| 1   | A     | 762 | HIS  |
| 1   | A     | 774 | LEU  |
| 1   | A     | 785 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 787 | ILE  |
| 1   | A     | 793 | ARG  |
| 1   | A     | 799 | MET  |
| 1   | A     | 802 | GLU  |
| 1   | A     | 804 | ARG  |
| 1   | A     | 810 | ARG  |
| 1   | A     | 816 | ILE  |
| 1   | A     | 822 | SER  |
| 1   | A     | 832 | MET  |
| 1   | A     | 834 | LEU  |
| 1   | A     | 838 | ILE  |
| 1   | A     | 842 | LEU  |
| 1   | A     | 843 | LYS  |
| 2   | B     | 142 | PRO  |
| 3   | C     | 48  | LYS  |
| 3   | C     | 68  | PHE  |
| 3   | C     | 83  | THR  |
| 3   | C     | 95  | ASP  |
| 3   | C     | 96  | LYS  |
| 1   | D     | 4   | ASP  |
| 1   | D     | 7   | MET  |
| 1   | D     | 12  | GLU  |
| 1   | D     | 15  | PRO  |
| 1   | D     | 17  | LEU  |
| 1   | D     | 20  | SER  |
| 1   | D     | 22  | LYS  |
| 1   | D     | 36  | SER  |
| 1   | D     | 37  | SER  |
| 1   | D     | 46  | SER  |
| 1   | D     | 61  | THR  |
| 1   | D     | 69  | THR  |
| 1   | D     | 70  | LEU  |
| 1   | D     | 72  | VAL  |
| 1   | D     | 73  | LYS  |
| 1   | D     | 75  | ASP  |
| 1   | D     | 76  | GLN  |
| 1   | D     | 97  | LEU  |
| 1   | D     | 106 | LEU  |
| 1   | D     | 109 | ARG  |
| 1   | D     | 114 | MET  |
| 1   | D     | 117 | THR  |
| 1   | D     | 121 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 126 | VAL  |
| 1   | D     | 127 | ASN  |
| 1   | D     | 135 | TYR  |
| 1   | D     | 136 | ASN  |
| 1   | D     | 146 | LYS  |
| 1   | D     | 149 | GLN  |
| 1   | D     | 155 | ILE  |
| 1   | D     | 157 | SER  |
| 1   | D     | 158 | ILE  |
| 1   | D     | 159 | SER  |
| 1   | D     | 165 | PHE  |
| 1   | D     | 167 | LEU  |
| 1   | D     | 169 | ASP  |
| 1   | D     | 173 | GLN  |
| 1   | D     | 178 | THR  |
| 1   | D     | 185 | LYS  |
| 1   | D     | 186 | THR  |
| 1   | D     | 187 | VAL  |
| 1   | D     | 191 | ARG  |
| 1   | D     | 193 | ILE  |
| 1   | D     | 194 | GLN  |
| 1   | D     | 198 | THR  |
| 1   | D     | 199 | ILE  |
| 1   | D     | 218 | LEU  |
| 1   | D     | 219 | GLU  |
| 1   | D     | 221 | GLN  |
| 1   | D     | 223 | ILE  |
| 1   | D     | 229 | LEU  |
| 1   | D     | 244 | SER  |
| 1   | D     | 245 | ARG  |
| 1   | D     | 251 | ARG  |
| 1   | D     | 264 | ASP  |
| 1   | D     | 273 | SER  |
| 1   | D     | 274 | ARG  |
| 1   | D     | 278 | GLN  |
| 1   | D     | 282 | GLU  |
| 1   | D     | 287 | ILE  |
| 1   | D     | 290 | GLN  |
| 1   | D     | 294 | ASN  |
| 1   | D     | 298 | GLU  |
| 1   | D     | 300 | ILE  |
| 1   | D     | 325 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 331 | LEU  |
| 1   | D     | 336 | SER  |
| 1   | D     | 351 | ILE  |
| 1   | D     | 354 | LEU  |
| 1   | D     | 364 | LEU  |
| 1   | D     | 365 | LYS  |
| 1   | D     | 372 | GLU  |
| 1   | D     | 376 | GLU  |
| 1   | D     | 381 | GLU  |
| 1   | D     | 389 | LEU  |
| 1   | D     | 392 | LEU  |
| 1   | D     | 394 | SER  |
| 1   | D     | 399 | LYS  |
| 1   | D     | 405 | ARG  |
| 1   | D     | 410 | ASN  |
| 1   | D     | 439 | LEU  |
| 1   | D     | 447 | GLN  |
| 1   | D     | 448 | GLN  |
| 1   | D     | 449 | LEU  |
| 1   | D     | 453 | GLN  |
| 1   | D     | 455 | ARG  |
| 1   | D     | 457 | TYR  |
| 1   | D     | 462 | LEU  |
| 1   | D     | 471 | ASP  |
| 1   | D     | 474 | SER  |
| 1   | D     | 480 | ILE  |
| 1   | D     | 487 | LEU  |
| 1   | D     | 495 | MET  |
| 1   | D     | 499 | GLU  |
| 1   | D     | 506 | GLU  |
| 1   | D     | 513 | ILE  |
| 1   | D     | 518 | ASP  |
| 1   | D     | 524 | GLU  |
| 1   | D     | 532 | ILE  |
| 1   | D     | 534 | SER  |
| 1   | D     | 537 | GLU  |
| 1   | D     | 549 | SER  |
| 1   | D     | 561 | LYS  |
| 1   | D     | 562 | SER  |
| 1   | D     | 563 | ASN  |
| 1   | D     | 569 | LYS  |
| 1   | D     | 580 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 593 | SER  |
| 1   | D     | 597 | GLU  |
| 1   | D     | 604 | ASN  |
| 1   | D     | 608 | ILE  |
| 1   | D     | 610 | LEU  |
| 1   | D     | 615 | SER  |
| 1   | D     | 621 | LEU  |
| 1   | D     | 625 | THR  |
| 1   | D     | 664 | LEU  |
| 1   | D     | 666 | SER  |
| 1   | D     | 673 | ARG  |
| 1   | D     | 675 | ILE  |
| 1   | D     | 676 | ILE  |
| 1   | D     | 686 | MET  |
| 1   | D     | 689 | GLU  |
| 1   | D     | 690 | LEU  |
| 1   | D     | 693 | HIS  |
| 1   | D     | 698 | ASN  |
| 1   | D     | 701 | LEU  |
| 1   | D     | 702 | GLU  |
| 1   | D     | 704 | ILE  |
| 1   | D     | 708 | ARG  |
| 1   | D     | 713 | SER  |
| 1   | D     | 714 | ARG  |
| 1   | D     | 716 | LEU  |
| 1   | D     | 719 | ASP  |
| 1   | D     | 722 | GLN  |
| 1   | D     | 723 | ARG  |
| 1   | D     | 727 | LEU  |
| 1   | D     | 728 | ASN  |
| 1   | D     | 745 | GLU  |
| 1   | D     | 752 | ASP  |
| 1   | D     | 753 | VAL  |
| 1   | D     | 754 | ASP  |
| 1   | D     | 762 | HIS  |
| 1   | D     | 774 | LEU  |
| 1   | D     | 785 | GLU  |
| 1   | D     | 787 | ILE  |
| 1   | D     | 793 | ARG  |
| 1   | D     | 799 | MET  |
| 1   | D     | 802 | GLU  |
| 1   | D     | 804 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 810 | ARG  |
| 1   | D     | 816 | ILE  |
| 1   | D     | 822 | SER  |
| 1   | D     | 832 | MET  |
| 1   | D     | 834 | LEU  |
| 1   | D     | 838 | ILE  |
| 1   | D     | 842 | LEU  |
| 1   | D     | 843 | LYS  |
| 2   | E     | 142 | PRO  |
| 3   | F     | 48  | LYS  |
| 3   | F     | 68  | PHE  |
| 3   | F     | 83  | THR  |
| 3   | F     | 95  | ASP  |
| 3   | F     | 96  | LYS  |
| 1   | G     | 4   | ASP  |
| 1   | G     | 7   | MET  |
| 1   | G     | 12  | GLU  |
| 1   | G     | 15  | PRO  |
| 1   | G     | 17  | LEU  |
| 1   | G     | 20  | SER  |
| 1   | G     | 22  | LYS  |
| 1   | G     | 36  | SER  |
| 1   | G     | 37  | SER  |
| 1   | G     | 46  | SER  |
| 1   | G     | 61  | THR  |
| 1   | G     | 69  | THR  |
| 1   | G     | 70  | LEU  |
| 1   | G     | 72  | VAL  |
| 1   | G     | 73  | LYS  |
| 1   | G     | 75  | ASP  |
| 1   | G     | 76  | GLN  |
| 1   | G     | 97  | LEU  |
| 1   | G     | 106 | LEU  |
| 1   | G     | 109 | ARG  |
| 1   | G     | 114 | MET  |
| 1   | G     | 117 | THR  |
| 1   | G     | 121 | LEU  |
| 1   | G     | 126 | VAL  |
| 1   | G     | 127 | ASN  |
| 1   | G     | 135 | TYR  |
| 1   | G     | 136 | ASN  |
| 1   | G     | 146 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 149 | GLN  |
| 1   | G     | 155 | ILE  |
| 1   | G     | 157 | SER  |
| 1   | G     | 158 | ILE  |
| 1   | G     | 159 | SER  |
| 1   | G     | 165 | PHE  |
| 1   | G     | 167 | LEU  |
| 1   | G     | 169 | ASP  |
| 1   | G     | 173 | GLN  |
| 1   | G     | 178 | THR  |
| 1   | G     | 185 | LYS  |
| 1   | G     | 186 | THR  |
| 1   | G     | 187 | VAL  |
| 1   | G     | 189 | THR  |
| 1   | G     | 191 | ARG  |
| 1   | G     | 193 | ILE  |
| 1   | G     | 194 | GLN  |
| 1   | G     | 198 | THR  |
| 1   | G     | 199 | ILE  |
| 1   | G     | 218 | LEU  |
| 1   | G     | 219 | GLU  |
| 1   | G     | 221 | GLN  |
| 1   | G     | 223 | ILE  |
| 1   | G     | 229 | LEU  |
| 1   | G     | 244 | SER  |
| 1   | G     | 245 | ARG  |
| 1   | G     | 251 | ARG  |
| 1   | G     | 264 | ASP  |
| 1   | G     | 273 | SER  |
| 1   | G     | 274 | ARG  |
| 1   | G     | 278 | GLN  |
| 1   | G     | 282 | GLU  |
| 1   | G     | 287 | ILE  |
| 1   | G     | 290 | GLN  |
| 1   | G     | 294 | ASN  |
| 1   | G     | 298 | GLU  |
| 1   | G     | 300 | ILE  |
| 1   | G     | 325 | ILE  |
| 1   | G     | 331 | LEU  |
| 1   | G     | 336 | SER  |
| 1   | G     | 351 | ILE  |
| 1   | G     | 354 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 364 | LEU  |
| 1   | G     | 365 | LYS  |
| 1   | G     | 372 | GLU  |
| 1   | G     | 376 | GLU  |
| 1   | G     | 381 | GLU  |
| 1   | G     | 389 | LEU  |
| 1   | G     | 392 | LEU  |
| 1   | G     | 394 | SER  |
| 1   | G     | 399 | LYS  |
| 1   | G     | 405 | ARG  |
| 1   | G     | 410 | ASN  |
| 1   | G     | 439 | LEU  |
| 1   | G     | 447 | GLN  |
| 1   | G     | 448 | GLN  |
| 1   | G     | 449 | LEU  |
| 1   | G     | 453 | GLN  |
| 1   | G     | 455 | ARG  |
| 1   | G     | 457 | TYR  |
| 1   | G     | 462 | LEU  |
| 1   | G     | 471 | ASP  |
| 1   | G     | 474 | SER  |
| 1   | G     | 480 | ILE  |
| 1   | G     | 487 | LEU  |
| 1   | G     | 495 | MET  |
| 1   | G     | 499 | GLU  |
| 1   | G     | 506 | GLU  |
| 1   | G     | 513 | ILE  |
| 1   | G     | 518 | ASP  |
| 1   | G     | 524 | GLU  |
| 1   | G     | 532 | ILE  |
| 1   | G     | 534 | SER  |
| 1   | G     | 537 | GLU  |
| 1   | G     | 549 | SER  |
| 1   | G     | 561 | LYS  |
| 1   | G     | 562 | SER  |
| 1   | G     | 563 | ASN  |
| 1   | G     | 569 | LYS  |
| 1   | G     | 580 | SER  |
| 1   | G     | 593 | SER  |
| 1   | G     | 597 | GLU  |
| 1   | G     | 604 | ASN  |
| 1   | G     | 608 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 610 | LEU  |
| 1   | G     | 615 | SER  |
| 1   | G     | 621 | LEU  |
| 1   | G     | 625 | THR  |
| 1   | G     | 664 | LEU  |
| 1   | G     | 666 | SER  |
| 1   | G     | 673 | ARG  |
| 1   | G     | 675 | ILE  |
| 1   | G     | 676 | ILE  |
| 1   | G     | 686 | MET  |
| 1   | G     | 689 | GLU  |
| 1   | G     | 690 | LEU  |
| 1   | G     | 693 | HIS  |
| 1   | G     | 698 | ASN  |
| 1   | G     | 701 | LEU  |
| 1   | G     | 702 | GLU  |
| 1   | G     | 704 | ILE  |
| 1   | G     | 708 | ARG  |
| 1   | G     | 713 | SER  |
| 1   | G     | 714 | ARG  |
| 1   | G     | 716 | LEU  |
| 1   | G     | 719 | ASP  |
| 1   | G     | 722 | GLN  |
| 1   | G     | 723 | ARG  |
| 1   | G     | 727 | LEU  |
| 1   | G     | 728 | ASN  |
| 1   | G     | 745 | GLU  |
| 1   | G     | 752 | ASP  |
| 1   | G     | 753 | VAL  |
| 1   | G     | 754 | ASP  |
| 1   | G     | 762 | HIS  |
| 1   | G     | 774 | LEU  |
| 1   | G     | 785 | GLU  |
| 1   | G     | 787 | ILE  |
| 1   | G     | 793 | ARG  |
| 1   | G     | 799 | MET  |
| 1   | G     | 802 | GLU  |
| 1   | G     | 804 | ARG  |
| 1   | G     | 810 | ARG  |
| 1   | G     | 816 | ILE  |
| 1   | G     | 822 | SER  |
| 1   | G     | 832 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 834 | LEU  |
| 1   | G     | 838 | ILE  |
| 1   | G     | 842 | LEU  |
| 1   | G     | 843 | LYS  |
| 2   | H     | 142 | PRO  |
| 3   | I     | 48  | LYS  |
| 3   | I     | 68  | PHE  |
| 3   | I     | 83  | THR  |
| 3   | I     | 95  | ASP  |
| 3   | I     | 96  | LYS  |
| 1   | J     | 4   | ASP  |
| 1   | J     | 7   | MET  |
| 1   | J     | 12  | GLU  |
| 1   | J     | 15  | PRO  |
| 1   | J     | 17  | LEU  |
| 1   | J     | 20  | SER  |
| 1   | J     | 22  | LYS  |
| 1   | J     | 36  | SER  |
| 1   | J     | 37  | SER  |
| 1   | J     | 46  | SER  |
| 1   | J     | 61  | THR  |
| 1   | J     | 69  | THR  |
| 1   | J     | 70  | LEU  |
| 1   | J     | 72  | VAL  |
| 1   | J     | 73  | LYS  |
| 1   | J     | 75  | ASP  |
| 1   | J     | 76  | GLN  |
| 1   | J     | 97  | LEU  |
| 1   | J     | 106 | LEU  |
| 1   | J     | 109 | ARG  |
| 1   | J     | 114 | MET  |
| 1   | J     | 117 | THR  |
| 1   | J     | 121 | LEU  |
| 1   | J     | 126 | VAL  |
| 1   | J     | 127 | ASN  |
| 1   | J     | 135 | TYR  |
| 1   | J     | 136 | ASN  |
| 1   | J     | 146 | LYS  |
| 1   | J     | 149 | GLN  |
| 1   | J     | 155 | ILE  |
| 1   | J     | 157 | SER  |
| 1   | J     | 158 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 159 | SER  |
| 1   | J     | 165 | PHE  |
| 1   | J     | 167 | LEU  |
| 1   | J     | 169 | ASP  |
| 1   | J     | 173 | GLN  |
| 1   | J     | 178 | THR  |
| 1   | J     | 185 | LYS  |
| 1   | J     | 186 | THR  |
| 1   | J     | 187 | VAL  |
| 1   | J     | 189 | THR  |
| 1   | J     | 191 | ARG  |
| 1   | J     | 193 | ILE  |
| 1   | J     | 194 | GLN  |
| 1   | J     | 198 | THR  |
| 1   | J     | 199 | ILE  |
| 1   | J     | 218 | LEU  |
| 1   | J     | 219 | GLU  |
| 1   | J     | 221 | GLN  |
| 1   | J     | 223 | ILE  |
| 1   | J     | 229 | LEU  |
| 1   | J     | 244 | SER  |
| 1   | J     | 245 | ARG  |
| 1   | J     | 251 | ARG  |
| 1   | J     | 264 | ASP  |
| 1   | J     | 273 | SER  |
| 1   | J     | 274 | ARG  |
| 1   | J     | 278 | GLN  |
| 1   | J     | 282 | GLU  |
| 1   | J     | 287 | ILE  |
| 1   | J     | 290 | GLN  |
| 1   | J     | 294 | ASN  |
| 1   | J     | 298 | GLU  |
| 1   | J     | 300 | ILE  |
| 1   | J     | 325 | ILE  |
| 1   | J     | 331 | LEU  |
| 1   | J     | 336 | SER  |
| 1   | J     | 351 | ILE  |
| 1   | J     | 354 | LEU  |
| 1   | J     | 364 | LEU  |
| 1   | J     | 365 | LYS  |
| 1   | J     | 372 | GLU  |
| 1   | J     | 376 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 381 | GLU  |
| 1   | J     | 389 | LEU  |
| 1   | J     | 392 | LEU  |
| 1   | J     | 394 | SER  |
| 1   | J     | 399 | LYS  |
| 1   | J     | 405 | ARG  |
| 1   | J     | 410 | ASN  |
| 1   | J     | 439 | LEU  |
| 1   | J     | 447 | GLN  |
| 1   | J     | 448 | GLN  |
| 1   | J     | 449 | LEU  |
| 1   | J     | 453 | GLN  |
| 1   | J     | 455 | ARG  |
| 1   | J     | 457 | TYR  |
| 1   | J     | 462 | LEU  |
| 1   | J     | 471 | ASP  |
| 1   | J     | 474 | SER  |
| 1   | J     | 480 | ILE  |
| 1   | J     | 487 | LEU  |
| 1   | J     | 495 | MET  |
| 1   | J     | 499 | GLU  |
| 1   | J     | 506 | GLU  |
| 1   | J     | 513 | ILE  |
| 1   | J     | 518 | ASP  |
| 1   | J     | 524 | GLU  |
| 1   | J     | 532 | ILE  |
| 1   | J     | 534 | SER  |
| 1   | J     | 537 | GLU  |
| 1   | J     | 543 | PRO  |
| 1   | J     | 549 | SER  |
| 1   | J     | 561 | LYS  |
| 1   | J     | 562 | SER  |
| 1   | J     | 563 | ASN  |
| 1   | J     | 569 | LYS  |
| 1   | J     | 580 | SER  |
| 1   | J     | 593 | SER  |
| 1   | J     | 597 | GLU  |
| 1   | J     | 604 | ASN  |
| 1   | J     | 608 | ILE  |
| 1   | J     | 610 | LEU  |
| 1   | J     | 615 | SER  |
| 1   | J     | 621 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 625 | THR  |
| 1   | J     | 664 | LEU  |
| 1   | J     | 666 | SER  |
| 1   | J     | 673 | ARG  |
| 1   | J     | 675 | ILE  |
| 1   | J     | 676 | ILE  |
| 1   | J     | 686 | MET  |
| 1   | J     | 689 | GLU  |
| 1   | J     | 690 | LEU  |
| 1   | J     | 693 | HIS  |
| 1   | J     | 698 | ASN  |
| 1   | J     | 701 | LEU  |
| 1   | J     | 702 | GLU  |
| 1   | J     | 708 | ARG  |
| 1   | J     | 713 | SER  |
| 1   | J     | 714 | ARG  |
| 1   | J     | 716 | LEU  |
| 1   | J     | 719 | ASP  |
| 1   | J     | 722 | GLN  |
| 1   | J     | 723 | ARG  |
| 1   | J     | 727 | LEU  |
| 1   | J     | 728 | ASN  |
| 1   | J     | 745 | GLU  |
| 1   | J     | 752 | ASP  |
| 1   | J     | 753 | VAL  |
| 1   | J     | 754 | ASP  |
| 1   | J     | 762 | HIS  |
| 1   | J     | 774 | LEU  |
| 1   | J     | 785 | GLU  |
| 1   | J     | 787 | ILE  |
| 1   | J     | 793 | ARG  |
| 1   | J     | 799 | MET  |
| 1   | J     | 802 | GLU  |
| 1   | J     | 804 | ARG  |
| 1   | J     | 810 | ARG  |
| 1   | J     | 816 | ILE  |
| 1   | J     | 822 | SER  |
| 1   | J     | 832 | MET  |
| 1   | J     | 834 | LEU  |
| 1   | J     | 838 | ILE  |
| 1   | J     | 842 | LEU  |
| 1   | J     | 843 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | K     | 142 | PRO  |
| 3   | L     | 48  | LYS  |
| 3   | L     | 68  | PHE  |
| 3   | L     | 83  | THR  |
| 3   | L     | 95  | ASP  |
| 3   | L     | 96  | LYS  |
| 4   | 0     | 33  | SER  |
| 4   | 0     | 34  | ILE  |
| 4   | 0     | 37  | ARG  |
| 4   | 0     | 66  | THR  |
| 4   | 0     | 72  | GLU  |
| 4   | 0     | 80  | ASP  |
| 4   | 0     | 100 | GLU  |
| 4   | 0     | 109 | PRO  |
| 4   | 0     | 116 | ARG  |
| 4   | 0     | 145 | SER  |
| 4   | 0     | 153 | LEU  |
| 4   | 0     | 159 | VAL  |
| 4   | 0     | 180 | LEU  |
| 4   | 0     | 191 | LYS  |
| 4   | 0     | 196 | ARG  |
| 4   | 0     | 199 | SER  |
| 4   | 0     | 201 | VAL  |
| 4   | 0     | 206 | ARG  |
| 4   | 0     | 221 | LEU  |
| 4   | 0     | 223 | PHE  |
| 4   | 0     | 229 | THR  |
| 4   | 0     | 239 | SER  |
| 4   | 0     | 242 | LEU  |
| 4   | 0     | 246 | GLN  |
| 4   | 0     | 263 | GLN  |
| 4   | 0     | 281 | SER  |
| 4   | 0     | 283 | MET  |
| 4   | 0     | 287 | ILE  |
| 4   | 0     | 291 | LYS  |
| 4   | 0     | 293 | LEU  |
| 4   | 0     | 297 | ASN  |
| 4   | 0     | 299 | MET  |
| 4   | 0     | 312 | ARG  |
| 4   | 0     | 315 | LYS  |
| 4   | 0     | 318 | THR  |
| 4   | 0     | 320 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 0     | 327 | ILE  |
| 4   | 0     | 334 | GLU  |
| 4   | 0     | 349 | LEU  |
| 4   | 0     | 350 | SER  |
| 4   | 0     | 351 | THR  |
| 4   | 0     | 354 | GLN  |
| 4   | 0     | 359 | LYS  |
| 4   | 0     | 360 | GLN  |
| 4   | 0     | 361 | GLU  |
| 4   | 0     | 368 | SER  |
| 4   | 1     | 16  | LEU  |
| 4   | 1     | 33  | SER  |
| 4   | 1     | 34  | ILE  |
| 4   | 1     | 37  | ARG  |
| 4   | 1     | 66  | THR  |
| 4   | 1     | 72  | GLU  |
| 4   | 1     | 80  | ASP  |
| 4   | 1     | 100 | GLU  |
| 4   | 1     | 109 | PRO  |
| 4   | 1     | 116 | ARG  |
| 4   | 1     | 145 | SER  |
| 4   | 1     | 153 | LEU  |
| 4   | 1     | 159 | VAL  |
| 4   | 1     | 180 | LEU  |
| 4   | 1     | 191 | LYS  |
| 4   | 1     | 196 | ARG  |
| 4   | 1     | 199 | SER  |
| 4   | 1     | 201 | VAL  |
| 4   | 1     | 206 | ARG  |
| 4   | 1     | 221 | LEU  |
| 4   | 1     | 223 | PHE  |
| 4   | 1     | 229 | THR  |
| 4   | 1     | 239 | SER  |
| 4   | 1     | 242 | LEU  |
| 4   | 1     | 246 | GLN  |
| 4   | 1     | 263 | GLN  |
| 4   | 1     | 281 | SER  |
| 4   | 1     | 283 | MET  |
| 4   | 1     | 287 | ILE  |
| 4   | 1     | 291 | LYS  |
| 4   | 1     | 293 | LEU  |
| 4   | 1     | 297 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 1     | 299 | MET  |
| 4   | 1     | 312 | ARG  |
| 4   | 1     | 315 | LYS  |
| 4   | 1     | 318 | THR  |
| 4   | 1     | 320 | LEU  |
| 4   | 1     | 327 | ILE  |
| 4   | 1     | 334 | GLU  |
| 4   | 1     | 349 | LEU  |
| 4   | 1     | 350 | SER  |
| 4   | 1     | 351 | THR  |
| 4   | 1     | 354 | GLN  |
| 4   | 1     | 359 | LYS  |
| 4   | 1     | 360 | GLN  |
| 4   | 1     | 361 | GLU  |
| 4   | 1     | 368 | SER  |
| 4   | 2     | 16  | LEU  |
| 4   | 2     | 33  | SER  |
| 4   | 2     | 34  | ILE  |
| 4   | 2     | 37  | ARG  |
| 4   | 2     | 66  | THR  |
| 4   | 2     | 72  | GLU  |
| 4   | 2     | 80  | ASP  |
| 4   | 2     | 100 | GLU  |
| 4   | 2     | 109 | PRO  |
| 4   | 2     | 116 | ARG  |
| 4   | 2     | 145 | SER  |
| 4   | 2     | 153 | LEU  |
| 4   | 2     | 159 | VAL  |
| 4   | 2     | 180 | LEU  |
| 4   | 2     | 191 | LYS  |
| 4   | 2     | 196 | ARG  |
| 4   | 2     | 199 | SER  |
| 4   | 2     | 201 | VAL  |
| 4   | 2     | 206 | ARG  |
| 4   | 2     | 221 | LEU  |
| 4   | 2     | 223 | PHE  |
| 4   | 2     | 229 | THR  |
| 4   | 2     | 239 | SER  |
| 4   | 2     | 242 | LEU  |
| 4   | 2     | 246 | GLN  |
| 4   | 2     | 263 | GLN  |
| 4   | 2     | 281 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 2     | 283 | MET  |
| 4   | 2     | 287 | ILE  |
| 4   | 2     | 291 | LYS  |
| 4   | 2     | 293 | LEU  |
| 4   | 2     | 297 | ASN  |
| 4   | 2     | 299 | MET  |
| 4   | 2     | 312 | ARG  |
| 4   | 2     | 315 | LYS  |
| 4   | 2     | 318 | THR  |
| 4   | 2     | 320 | LEU  |
| 4   | 2     | 327 | ILE  |
| 4   | 2     | 334 | GLU  |
| 4   | 2     | 349 | LEU  |
| 4   | 2     | 350 | SER  |
| 4   | 2     | 351 | THR  |
| 4   | 2     | 354 | GLN  |
| 4   | 2     | 359 | LYS  |
| 4   | 2     | 360 | GLN  |
| 4   | 2     | 361 | GLU  |
| 4   | 2     | 368 | SER  |
| 4   | 3     | 16  | LEU  |
| 4   | 3     | 33  | SER  |
| 4   | 3     | 34  | ILE  |
| 4   | 3     | 37  | ARG  |
| 4   | 3     | 66  | THR  |
| 4   | 3     | 72  | GLU  |
| 4   | 3     | 80  | ASP  |
| 4   | 3     | 100 | GLU  |
| 4   | 3     | 109 | PRO  |
| 4   | 3     | 116 | ARG  |
| 4   | 3     | 145 | SER  |
| 4   | 3     | 153 | LEU  |
| 4   | 3     | 159 | VAL  |
| 4   | 3     | 180 | LEU  |
| 4   | 3     | 191 | LYS  |
| 4   | 3     | 196 | ARG  |
| 4   | 3     | 199 | SER  |
| 4   | 3     | 201 | VAL  |
| 4   | 3     | 206 | ARG  |
| 4   | 3     | 221 | LEU  |
| 4   | 3     | 223 | PHE  |
| 4   | 3     | 229 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 3     | 239 | SER  |
| 4   | 3     | 242 | LEU  |
| 4   | 3     | 246 | GLN  |
| 4   | 3     | 263 | GLN  |
| 4   | 3     | 281 | SER  |
| 4   | 3     | 283 | MET  |
| 4   | 3     | 287 | ILE  |
| 4   | 3     | 291 | LYS  |
| 4   | 3     | 293 | LEU  |
| 4   | 3     | 297 | ASN  |
| 4   | 3     | 299 | MET  |
| 4   | 3     | 312 | ARG  |
| 4   | 3     | 315 | LYS  |
| 4   | 3     | 318 | THR  |
| 4   | 3     | 320 | LEU  |
| 4   | 3     | 327 | ILE  |
| 4   | 3     | 334 | GLU  |
| 4   | 3     | 349 | LEU  |
| 4   | 3     | 350 | SER  |
| 4   | 3     | 351 | THR  |
| 4   | 3     | 354 | GLN  |
| 4   | 3     | 359 | LYS  |
| 4   | 3     | 360 | GLN  |
| 4   | 3     | 361 | GLU  |
| 4   | 3     | 368 | SER  |
| 4   | 4     | 16  | LEU  |
| 4   | 4     | 33  | SER  |
| 4   | 4     | 34  | ILE  |
| 4   | 4     | 37  | ARG  |
| 4   | 4     | 66  | THR  |
| 4   | 4     | 72  | GLU  |
| 4   | 4     | 80  | ASP  |
| 4   | 4     | 100 | GLU  |
| 4   | 4     | 109 | PRO  |
| 4   | 4     | 116 | ARG  |
| 4   | 4     | 145 | SER  |
| 4   | 4     | 153 | LEU  |
| 4   | 4     | 159 | VAL  |
| 4   | 4     | 180 | LEU  |
| 4   | 4     | 191 | LYS  |
| 4   | 4     | 196 | ARG  |
| 4   | 4     | 199 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 4     | 201 | VAL  |
| 4   | 4     | 206 | ARG  |
| 4   | 4     | 221 | LEU  |
| 4   | 4     | 223 | PHE  |
| 4   | 4     | 229 | THR  |
| 4   | 4     | 239 | SER  |
| 4   | 4     | 242 | LEU  |
| 4   | 4     | 246 | GLN  |
| 4   | 4     | 263 | GLN  |
| 4   | 4     | 281 | SER  |
| 4   | 4     | 283 | MET  |
| 4   | 4     | 287 | ILE  |
| 4   | 4     | 291 | LYS  |
| 4   | 4     | 293 | LEU  |
| 4   | 4     | 297 | ASN  |
| 4   | 4     | 299 | MET  |
| 4   | 4     | 312 | ARG  |
| 4   | 4     | 315 | LYS  |
| 4   | 4     | 318 | THR  |
| 4   | 4     | 320 | LEU  |
| 4   | 4     | 327 | ILE  |
| 4   | 4     | 334 | GLU  |
| 4   | 4     | 349 | LEU  |
| 4   | 4     | 350 | SER  |
| 4   | 4     | 351 | THR  |
| 4   | 4     | 354 | GLN  |
| 4   | 4     | 359 | LYS  |
| 4   | 4     | 360 | GLN  |
| 4   | 4     | 361 | GLU  |
| 4   | 4     | 368 | SER  |
| 4   | 5     | 33  | SER  |
| 4   | 5     | 34  | ILE  |
| 4   | 5     | 37  | ARG  |
| 4   | 5     | 66  | THR  |
| 4   | 5     | 72  | GLU  |
| 4   | 5     | 80  | ASP  |
| 4   | 5     | 100 | GLU  |
| 4   | 5     | 109 | PRO  |
| 4   | 5     | 116 | ARG  |
| 4   | 5     | 145 | SER  |
| 4   | 5     | 153 | LEU  |
| 4   | 5     | 159 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 5     | 180 | LEU  |
| 4   | 5     | 191 | LYS  |
| 4   | 5     | 196 | ARG  |
| 4   | 5     | 199 | SER  |
| 4   | 5     | 201 | VAL  |
| 4   | 5     | 206 | ARG  |
| 4   | 5     | 221 | LEU  |
| 4   | 5     | 223 | PHE  |
| 4   | 5     | 229 | THR  |
| 4   | 5     | 239 | SER  |
| 4   | 5     | 242 | LEU  |
| 4   | 5     | 246 | GLN  |
| 4   | 5     | 263 | GLN  |
| 4   | 5     | 281 | SER  |
| 4   | 5     | 283 | MET  |
| 4   | 5     | 287 | ILE  |
| 4   | 5     | 291 | LYS  |
| 4   | 5     | 293 | LEU  |
| 4   | 5     | 297 | ASN  |
| 4   | 5     | 299 | MET  |
| 4   | 5     | 312 | ARG  |
| 4   | 5     | 315 | LYS  |
| 4   | 5     | 318 | THR  |
| 4   | 5     | 320 | LEU  |
| 4   | 5     | 327 | ILE  |
| 4   | 5     | 334 | GLU  |
| 4   | 5     | 349 | LEU  |
| 4   | 5     | 350 | SER  |
| 4   | 5     | 351 | THR  |
| 4   | 5     | 354 | GLN  |
| 4   | 5     | 359 | LYS  |
| 4   | 5     | 360 | GLN  |
| 4   | 5     | 361 | GLU  |
| 4   | 5     | 368 | SER  |
| 4   | 6     | 16  | LEU  |
| 4   | 6     | 33  | SER  |
| 4   | 6     | 34  | ILE  |
| 4   | 6     | 37  | ARG  |
| 4   | 6     | 66  | THR  |
| 4   | 6     | 72  | GLU  |
| 4   | 6     | 80  | ASP  |
| 4   | 6     | 100 | GLU  |

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*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 6     | 109 | PRO  |
| 4   | 6     | 116 | ARG  |
| 4   | 6     | 145 | SER  |
| 4   | 6     | 153 | LEU  |
| 4   | 6     | 159 | VAL  |
| 4   | 6     | 180 | LEU  |
| 4   | 6     | 191 | LYS  |
| 4   | 6     | 196 | ARG  |
| 4   | 6     | 199 | SER  |
| 4   | 6     | 201 | VAL  |
| 4   | 6     | 206 | ARG  |
| 4   | 6     | 221 | LEU  |
| 4   | 6     | 223 | PHE  |
| 4   | 6     | 229 | THR  |
| 4   | 6     | 239 | SER  |
| 4   | 6     | 242 | LEU  |
| 4   | 6     | 246 | GLN  |
| 4   | 6     | 263 | GLN  |
| 4   | 6     | 281 | SER  |
| 4   | 6     | 283 | MET  |
| 4   | 6     | 287 | ILE  |
| 4   | 6     | 291 | LYS  |
| 4   | 6     | 293 | LEU  |
| 4   | 6     | 297 | ASN  |
| 4   | 6     | 299 | MET  |
| 4   | 6     | 312 | ARG  |
| 4   | 6     | 315 | LYS  |
| 4   | 6     | 318 | THR  |
| 4   | 6     | 320 | LEU  |
| 4   | 6     | 327 | ILE  |
| 4   | 6     | 334 | GLU  |
| 4   | 6     | 349 | LEU  |
| 4   | 6     | 350 | SER  |
| 4   | 6     | 351 | THR  |
| 4   | 6     | 354 | GLN  |
| 4   | 6     | 359 | LYS  |
| 4   | 6     | 360 | GLN  |
| 4   | 6     | 361 | GLU  |
| 4   | 6     | 368 | SER  |
| 4   | 7     | 33  | SER  |
| 4   | 7     | 34  | ILE  |
| 4   | 7     | 37  | ARG  |

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*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 7     | 66  | THR  |
| 4   | 7     | 72  | GLU  |
| 4   | 7     | 80  | ASP  |
| 4   | 7     | 100 | GLU  |
| 4   | 7     | 109 | PRO  |
| 4   | 7     | 116 | ARG  |
| 4   | 7     | 145 | SER  |
| 4   | 7     | 153 | LEU  |
| 4   | 7     | 159 | VAL  |
| 4   | 7     | 180 | LEU  |
| 4   | 7     | 191 | LYS  |
| 4   | 7     | 196 | ARG  |
| 4   | 7     | 199 | SER  |
| 4   | 7     | 201 | VAL  |
| 4   | 7     | 206 | ARG  |
| 4   | 7     | 221 | LEU  |
| 4   | 7     | 223 | PHE  |
| 4   | 7     | 229 | THR  |
| 4   | 7     | 239 | SER  |
| 4   | 7     | 242 | LEU  |
| 4   | 7     | 246 | GLN  |
| 4   | 7     | 263 | GLN  |
| 4   | 7     | 281 | SER  |
| 4   | 7     | 283 | MET  |
| 4   | 7     | 287 | ILE  |
| 4   | 7     | 291 | LYS  |
| 4   | 7     | 293 | LEU  |
| 4   | 7     | 297 | ASN  |
| 4   | 7     | 299 | MET  |
| 4   | 7     | 312 | ARG  |
| 4   | 7     | 315 | LYS  |
| 4   | 7     | 318 | THR  |
| 4   | 7     | 320 | LEU  |
| 4   | 7     | 327 | ILE  |
| 4   | 7     | 334 | GLU  |
| 4   | 7     | 349 | LEU  |
| 4   | 7     | 350 | SER  |
| 4   | 7     | 351 | THR  |
| 4   | 7     | 354 | GLN  |
| 4   | 7     | 359 | LYS  |
| 4   | 7     | 360 | GLN  |
| 4   | 7     | 361 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 7     | 368 | SER  |
| 4   | 8     | 16  | LEU  |
| 4   | 8     | 33  | SER  |
| 4   | 8     | 34  | ILE  |
| 4   | 8     | 37  | ARG  |
| 4   | 8     | 66  | THR  |
| 4   | 8     | 72  | GLU  |
| 4   | 8     | 80  | ASP  |
| 4   | 8     | 100 | GLU  |
| 4   | 8     | 109 | PRO  |
| 4   | 8     | 116 | ARG  |
| 4   | 8     | 145 | SER  |
| 4   | 8     | 153 | LEU  |
| 4   | 8     | 159 | VAL  |
| 4   | 8     | 180 | LEU  |
| 4   | 8     | 191 | LYS  |
| 4   | 8     | 196 | ARG  |
| 4   | 8     | 199 | SER  |
| 4   | 8     | 201 | VAL  |
| 4   | 8     | 206 | ARG  |
| 4   | 8     | 221 | LEU  |
| 4   | 8     | 223 | PHE  |
| 4   | 8     | 229 | THR  |
| 4   | 8     | 239 | SER  |
| 4   | 8     | 242 | LEU  |
| 4   | 8     | 246 | GLN  |
| 4   | 8     | 263 | GLN  |
| 4   | 8     | 281 | SER  |
| 4   | 8     | 283 | MET  |
| 4   | 8     | 287 | ILE  |
| 4   | 8     | 291 | LYS  |
| 4   | 8     | 293 | LEU  |
| 4   | 8     | 297 | ASN  |
| 4   | 8     | 299 | MET  |
| 4   | 8     | 312 | ARG  |
| 4   | 8     | 315 | LYS  |
| 4   | 8     | 318 | THR  |
| 4   | 8     | 320 | LEU  |
| 4   | 8     | 327 | ILE  |
| 4   | 8     | 334 | GLU  |
| 4   | 8     | 349 | LEU  |
| 4   | 8     | 350 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 8     | 351 | THR  |
| 4   | 8     | 354 | GLN  |
| 4   | 8     | 359 | LYS  |
| 4   | 8     | 360 | GLN  |
| 4   | 8     | 361 | GLU  |
| 4   | 8     | 368 | SER  |
| 4   | V     | 33  | SER  |
| 4   | V     | 34  | ILE  |
| 4   | V     | 37  | ARG  |
| 4   | V     | 66  | THR  |
| 4   | V     | 72  | GLU  |
| 4   | V     | 80  | ASP  |
| 4   | V     | 100 | GLU  |
| 4   | V     | 109 | PRO  |
| 4   | V     | 116 | ARG  |
| 4   | V     | 145 | SER  |
| 4   | V     | 153 | LEU  |
| 4   | V     | 159 | VAL  |
| 4   | V     | 180 | LEU  |
| 4   | V     | 191 | LYS  |
| 4   | V     | 196 | ARG  |
| 4   | V     | 199 | SER  |
| 4   | V     | 201 | VAL  |
| 4   | V     | 206 | ARG  |
| 4   | V     | 221 | LEU  |
| 4   | V     | 223 | PHE  |
| 4   | V     | 229 | THR  |
| 4   | V     | 239 | SER  |
| 4   | V     | 242 | LEU  |
| 4   | V     | 246 | GLN  |
| 4   | V     | 263 | GLN  |
| 4   | V     | 281 | SER  |
| 4   | V     | 283 | MET  |
| 4   | V     | 287 | ILE  |
| 4   | V     | 291 | LYS  |
| 4   | V     | 293 | LEU  |
| 4   | V     | 297 | ASN  |
| 4   | V     | 299 | MET  |
| 4   | V     | 312 | ARG  |
| 4   | V     | 315 | LYS  |
| 4   | V     | 318 | THR  |
| 4   | V     | 320 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | V     | 327 | ILE  |
| 4   | V     | 334 | GLU  |
| 4   | V     | 349 | LEU  |
| 4   | V     | 350 | SER  |
| 4   | V     | 351 | THR  |
| 4   | V     | 354 | GLN  |
| 4   | V     | 359 | LYS  |
| 4   | V     | 360 | GLN  |
| 4   | V     | 361 | GLU  |
| 4   | V     | 368 | SER  |
| 4   | W     | 33  | SER  |
| 4   | W     | 34  | ILE  |
| 4   | W     | 37  | ARG  |
| 4   | W     | 66  | THR  |
| 4   | W     | 72  | GLU  |
| 4   | W     | 80  | ASP  |
| 4   | W     | 100 | GLU  |
| 4   | W     | 109 | PRO  |
| 4   | W     | 116 | ARG  |
| 4   | W     | 145 | SER  |
| 4   | W     | 153 | LEU  |
| 4   | W     | 159 | VAL  |
| 4   | W     | 180 | LEU  |
| 4   | W     | 191 | LYS  |
| 4   | W     | 196 | ARG  |
| 4   | W     | 199 | SER  |
| 4   | W     | 201 | VAL  |
| 4   | W     | 206 | ARG  |
| 4   | W     | 221 | LEU  |
| 4   | W     | 223 | PHE  |
| 4   | W     | 229 | THR  |
| 4   | W     | 239 | SER  |
| 4   | W     | 242 | LEU  |
| 4   | W     | 246 | GLN  |
| 4   | W     | 263 | GLN  |
| 4   | W     | 281 | SER  |
| 4   | W     | 283 | MET  |
| 4   | W     | 287 | ILE  |
| 4   | W     | 291 | LYS  |
| 4   | W     | 293 | LEU  |
| 4   | W     | 297 | ASN  |
| 4   | W     | 299 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | W     | 312 | ARG  |
| 4   | W     | 315 | LYS  |
| 4   | W     | 318 | THR  |
| 4   | W     | 320 | LEU  |
| 4   | W     | 327 | ILE  |
| 4   | W     | 334 | GLU  |
| 4   | W     | 349 | LEU  |
| 4   | W     | 350 | SER  |
| 4   | W     | 351 | THR  |
| 4   | W     | 354 | GLN  |
| 4   | W     | 359 | LYS  |
| 4   | W     | 360 | GLN  |
| 4   | W     | 361 | GLU  |
| 4   | W     | 368 | SER  |
| 4   | X     | 33  | SER  |
| 4   | X     | 34  | ILE  |
| 4   | X     | 37  | ARG  |
| 4   | X     | 66  | THR  |
| 4   | X     | 72  | GLU  |
| 4   | X     | 80  | ASP  |
| 4   | X     | 100 | GLU  |
| 4   | X     | 109 | PRO  |
| 4   | X     | 116 | ARG  |
| 4   | X     | 145 | SER  |
| 4   | X     | 153 | LEU  |
| 4   | X     | 159 | VAL  |
| 4   | X     | 180 | LEU  |
| 4   | X     | 191 | LYS  |
| 4   | X     | 196 | ARG  |
| 4   | X     | 199 | SER  |
| 4   | X     | 201 | VAL  |
| 4   | X     | 206 | ARG  |
| 4   | X     | 221 | LEU  |
| 4   | X     | 223 | PHE  |
| 4   | X     | 229 | THR  |
| 4   | X     | 239 | SER  |
| 4   | X     | 242 | LEU  |
| 4   | X     | 246 | GLN  |
| 4   | X     | 263 | GLN  |
| 4   | X     | 281 | SER  |
| 4   | X     | 283 | MET  |
| 4   | X     | 287 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | X     | 291 | LYS  |
| 4   | X     | 293 | LEU  |
| 4   | X     | 297 | ASN  |
| 4   | X     | 299 | MET  |
| 4   | X     | 312 | ARG  |
| 4   | X     | 315 | LYS  |
| 4   | X     | 318 | THR  |
| 4   | X     | 320 | LEU  |
| 4   | X     | 327 | ILE  |
| 4   | X     | 334 | GLU  |
| 4   | X     | 349 | LEU  |
| 4   | X     | 350 | SER  |
| 4   | X     | 351 | THR  |
| 4   | X     | 354 | GLN  |
| 4   | X     | 359 | LYS  |
| 4   | X     | 360 | GLN  |
| 4   | X     | 361 | GLU  |
| 4   | X     | 368 | SER  |
| 4   | Y     | 16  | LEU  |
| 4   | Y     | 33  | SER  |
| 4   | Y     | 34  | ILE  |
| 4   | Y     | 37  | ARG  |
| 4   | Y     | 66  | THR  |
| 4   | Y     | 72  | GLU  |
| 4   | Y     | 80  | ASP  |
| 4   | Y     | 100 | GLU  |
| 4   | Y     | 109 | PRO  |
| 4   | Y     | 116 | ARG  |
| 4   | Y     | 145 | SER  |
| 4   | Y     | 153 | LEU  |
| 4   | Y     | 159 | VAL  |
| 4   | Y     | 180 | LEU  |
| 4   | Y     | 191 | LYS  |
| 4   | Y     | 196 | ARG  |
| 4   | Y     | 199 | SER  |
| 4   | Y     | 201 | VAL  |
| 4   | Y     | 206 | ARG  |
| 4   | Y     | 221 | LEU  |
| 4   | Y     | 223 | PHE  |
| 4   | Y     | 229 | THR  |
| 4   | Y     | 239 | SER  |
| 4   | Y     | 242 | LEU  |

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*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | Y     | 246 | GLN  |
| 4   | Y     | 263 | GLN  |
| 4   | Y     | 281 | SER  |
| 4   | Y     | 283 | MET  |
| 4   | Y     | 287 | ILE  |
| 4   | Y     | 291 | LYS  |
| 4   | Y     | 293 | LEU  |
| 4   | Y     | 297 | ASN  |
| 4   | Y     | 299 | MET  |
| 4   | Y     | 312 | ARG  |
| 4   | Y     | 315 | LYS  |
| 4   | Y     | 318 | THR  |
| 4   | Y     | 320 | LEU  |
| 4   | Y     | 327 | ILE  |
| 4   | Y     | 334 | GLU  |
| 4   | Y     | 349 | LEU  |
| 4   | Y     | 350 | SER  |
| 4   | Y     | 351 | THR  |
| 4   | Y     | 354 | GLN  |
| 4   | Y     | 359 | LYS  |
| 4   | Y     | 360 | GLN  |
| 4   | Y     | 361 | GLU  |
| 4   | Y     | 368 | SER  |
| 4   | Z     | 16  | LEU  |
| 4   | Z     | 33  | SER  |
| 4   | Z     | 34  | ILE  |
| 4   | Z     | 37  | ARG  |
| 4   | Z     | 66  | THR  |
| 4   | Z     | 72  | GLU  |
| 4   | Z     | 80  | ASP  |
| 4   | Z     | 100 | GLU  |
| 4   | Z     | 109 | PRO  |
| 4   | Z     | 116 | ARG  |
| 4   | Z     | 145 | SER  |
| 4   | Z     | 153 | LEU  |
| 4   | Z     | 159 | VAL  |
| 4   | Z     | 180 | LEU  |
| 4   | Z     | 191 | LYS  |
| 4   | Z     | 196 | ARG  |
| 4   | Z     | 199 | SER  |
| 4   | Z     | 201 | VAL  |
| 4   | Z     | 206 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | Z     | 221 | LEU  |
| 4   | Z     | 223 | PHE  |
| 4   | Z     | 229 | THR  |
| 4   | Z     | 239 | SER  |
| 4   | Z     | 242 | LEU  |
| 4   | Z     | 246 | GLN  |
| 4   | Z     | 263 | GLN  |
| 4   | Z     | 281 | SER  |
| 4   | Z     | 283 | MET  |
| 4   | Z     | 287 | ILE  |
| 4   | Z     | 291 | LYS  |
| 4   | Z     | 293 | LEU  |
| 4   | Z     | 297 | ASN  |
| 4   | Z     | 299 | MET  |
| 4   | Z     | 312 | ARG  |
| 4   | Z     | 315 | LYS  |
| 4   | Z     | 318 | THR  |
| 4   | Z     | 320 | LEU  |
| 4   | Z     | 327 | ILE  |
| 4   | Z     | 334 | GLU  |
| 4   | Z     | 349 | LEU  |
| 4   | Z     | 350 | SER  |
| 4   | Z     | 351 | THR  |
| 4   | Z     | 354 | GLN  |
| 4   | Z     | 359 | LYS  |
| 4   | Z     | 360 | GLN  |
| 4   | Z     | 361 | GLU  |
| 4   | Z     | 368 | SER  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (184) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 29  | ASN  |
| 1   | A     | 127 | ASN  |
| 1   | A     | 149 | GLN  |
| 1   | A     | 164 | GLN  |
| 1   | A     | 188 | ASN  |
| 1   | A     | 194 | GLN  |
| 1   | A     | 221 | GLN  |
| 1   | A     | 253 | HIS  |
| 1   | A     | 290 | GLN  |
| 1   | A     | 368 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 424 | ASN  |
| 1   | A     | 453 | GLN  |
| 1   | A     | 481 | ASN  |
| 1   | A     | 484 | ASN  |
| 1   | A     | 563 | ASN  |
| 1   | A     | 564 | ASN  |
| 1   | A     | 578 | HIS  |
| 1   | A     | 612 | GLN  |
| 1   | A     | 656 | ASN  |
| 1   | A     | 670 | HIS  |
| 1   | A     | 762 | HIS  |
| 2   | B     | 159 | HIS  |
| 3   | C     | 52  | ASN  |
| 1   | D     | 29  | ASN  |
| 1   | D     | 127 | ASN  |
| 1   | D     | 149 | GLN  |
| 1   | D     | 164 | GLN  |
| 1   | D     | 188 | ASN  |
| 1   | D     | 194 | GLN  |
| 1   | D     | 221 | GLN  |
| 1   | D     | 253 | HIS  |
| 1   | D     | 290 | GLN  |
| 1   | D     | 368 | GLN  |
| 1   | D     | 424 | ASN  |
| 1   | D     | 447 | GLN  |
| 1   | D     | 453 | GLN  |
| 1   | D     | 481 | ASN  |
| 1   | D     | 484 | ASN  |
| 1   | D     | 563 | ASN  |
| 1   | D     | 564 | ASN  |
| 1   | D     | 578 | HIS  |
| 1   | D     | 612 | GLN  |
| 1   | D     | 656 | ASN  |
| 1   | D     | 670 | HIS  |
| 1   | D     | 698 | ASN  |
| 1   | D     | 757 | GLN  |
| 1   | D     | 762 | HIS  |
| 1   | D     | 817 | GLN  |
| 2   | E     | 159 | HIS  |
| 3   | F     | 39  | GLN  |
| 3   | F     | 52  | ASN  |
| 3   | F     | 81  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 29  | ASN  |
| 1   | G     | 127 | ASN  |
| 1   | G     | 164 | GLN  |
| 1   | G     | 188 | ASN  |
| 1   | G     | 194 | GLN  |
| 1   | G     | 221 | GLN  |
| 1   | G     | 253 | HIS  |
| 1   | G     | 290 | GLN  |
| 1   | G     | 368 | GLN  |
| 1   | G     | 424 | ASN  |
| 1   | G     | 447 | GLN  |
| 1   | G     | 453 | GLN  |
| 1   | G     | 481 | ASN  |
| 1   | G     | 484 | ASN  |
| 1   | G     | 563 | ASN  |
| 1   | G     | 564 | ASN  |
| 1   | G     | 578 | HIS  |
| 1   | G     | 612 | GLN  |
| 1   | G     | 656 | ASN  |
| 1   | G     | 670 | HIS  |
| 1   | G     | 728 | ASN  |
| 1   | G     | 762 | HIS  |
| 3   | I     | 39  | GLN  |
| 3   | I     | 40  | ASN  |
| 3   | I     | 52  | ASN  |
| 3   | I     | 81  | GLN  |
| 3   | I     | 109 | HIS  |
| 1   | J     | 29  | ASN  |
| 1   | J     | 127 | ASN  |
| 1   | J     | 164 | GLN  |
| 1   | J     | 188 | ASN  |
| 1   | J     | 194 | GLN  |
| 1   | J     | 221 | GLN  |
| 1   | J     | 253 | HIS  |
| 1   | J     | 290 | GLN  |
| 1   | J     | 368 | GLN  |
| 1   | J     | 424 | ASN  |
| 1   | J     | 447 | GLN  |
| 1   | J     | 453 | GLN  |
| 1   | J     | 481 | ASN  |
| 1   | J     | 484 | ASN  |
| 1   | J     | 563 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 564 | ASN  |
| 1   | J     | 578 | HIS  |
| 1   | J     | 612 | GLN  |
| 1   | J     | 656 | ASN  |
| 1   | J     | 670 | HIS  |
| 1   | J     | 698 | ASN  |
| 1   | J     | 762 | HIS  |
| 2   | K     | 159 | HIS  |
| 3   | L     | 39  | GLN  |
| 3   | L     | 52  | ASN  |
| 4   | 0     | 41  | GLN  |
| 4   | 0     | 92  | ASN  |
| 4   | 0     | 137 | GLN  |
| 4   | 0     | 252 | ASN  |
| 4   | 0     | 263 | GLN  |
| 4   | 0     | 354 | GLN  |
| 4   | 1     | 41  | GLN  |
| 4   | 1     | 92  | ASN  |
| 4   | 1     | 137 | GLN  |
| 4   | 1     | 252 | ASN  |
| 4   | 1     | 263 | GLN  |
| 4   | 1     | 354 | GLN  |
| 4   | 2     | 41  | GLN  |
| 4   | 2     | 92  | ASN  |
| 4   | 2     | 137 | GLN  |
| 4   | 2     | 252 | ASN  |
| 4   | 2     | 263 | GLN  |
| 4   | 2     | 354 | GLN  |
| 4   | 3     | 41  | GLN  |
| 4   | 3     | 92  | ASN  |
| 4   | 3     | 137 | GLN  |
| 4   | 3     | 252 | ASN  |
| 4   | 3     | 263 | GLN  |
| 4   | 3     | 354 | GLN  |
| 4   | 4     | 41  | GLN  |
| 4   | 4     | 92  | ASN  |
| 4   | 4     | 137 | GLN  |
| 4   | 4     | 252 | ASN  |
| 4   | 4     | 263 | GLN  |
| 4   | 5     | 41  | GLN  |
| 4   | 5     | 92  | ASN  |
| 4   | 5     | 137 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 5     | 252 | ASN  |
| 4   | 5     | 263 | GLN  |
| 4   | 6     | 41  | GLN  |
| 4   | 6     | 92  | ASN  |
| 4   | 6     | 137 | GLN  |
| 4   | 6     | 252 | ASN  |
| 4   | 6     | 263 | GLN  |
| 4   | 7     | 41  | GLN  |
| 4   | 7     | 92  | ASN  |
| 4   | 7     | 137 | GLN  |
| 4   | 7     | 252 | ASN  |
| 4   | 7     | 263 | GLN  |
| 4   | 8     | 41  | GLN  |
| 4   | 8     | 92  | ASN  |
| 4   | 8     | 137 | GLN  |
| 4   | 8     | 252 | ASN  |
| 4   | 8     | 263 | GLN  |
| 4   | 8     | 354 | GLN  |
| 4   | V     | 41  | GLN  |
| 4   | V     | 92  | ASN  |
| 4   | V     | 137 | GLN  |
| 4   | V     | 252 | ASN  |
| 4   | V     | 263 | GLN  |
| 4   | V     | 354 | GLN  |
| 4   | W     | 41  | GLN  |
| 4   | W     | 92  | ASN  |
| 4   | W     | 137 | GLN  |
| 4   | W     | 252 | ASN  |
| 4   | W     | 263 | GLN  |
| 4   | W     | 354 | GLN  |
| 4   | X     | 41  | GLN  |
| 4   | X     | 92  | ASN  |
| 4   | X     | 137 | GLN  |
| 4   | X     | 252 | ASN  |
| 4   | X     | 263 | GLN  |
| 4   | X     | 354 | GLN  |
| 4   | Y     | 41  | GLN  |
| 4   | Y     | 92  | ASN  |
| 4   | Y     | 137 | GLN  |
| 4   | Y     | 252 | ASN  |
| 4   | Y     | 263 | GLN  |
| 4   | Y     | 354 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | Z     | 41  | GLN  |
| 4   | Z     | 92  | ASN  |
| 4   | Z     | 137 | GLN  |
| 4   | Z     | 252 | ASN  |
| 4   | Z     | 263 | GLN  |
| 4   | Z     | 354 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 1   | MLY  | A     | 107 | 1    | 10,10,11     | 0.46 | 0           | 8,11,13     | 1.02 | 1 (12%)     |
| 1   | MLY  | A     | 130 | 1    | 10,10,11     | 0.99 | 1 (10%)     | 8,11,13     | 1.33 | 2 (25%)     |
| 1   | MLY  | A     | 138 | 1    | 10,10,11     | 1.36 | 1 (10%)     | 8,11,13     | 2.72 | 1 (12%)     |
| 1   | MLY  | A     | 19  | 1    | 10,10,11     | 1.19 | 1 (10%)     | 8,11,13     | 0.62 | 0           |
| 1   | MLY  | A     | 190 | 1    | 10,10,11     | 1.18 | 1 (10%)     | 8,11,13     | 1.31 | 1 (12%)     |
| 1   | MLY  | A     | 236 | 1    | 10,10,11     | 1.10 | 1 (10%)     | 8,11,13     | 1.56 | 2 (25%)     |
| 1   | MLY  | A     | 248 | 1    | 10,10,11     | 0.77 | 0           | 8,11,13     | 0.85 | 0           |
| 1   | MLY  | A     | 272 | 1    | 10,10,11     | 1.08 | 1 (10%)     | 8,11,13     | 1.32 | 1 (12%)     |
| 1   | MLY  | A     | 295 | 1    | 10,10,11     | 1.16 | 1 (10%)     | 8,11,13     | 0.31 | 0           |
| 1   | MLY  | A     | 296 | 1    | 10,10,11     | 0.84 | 1 (10%)     | 8,11,13     | 1.20 | 1 (12%)     |
| 1   | MLY  | A     | 30  | 1    | 10,10,11     | 0.88 | 0           | 8,11,13     | 0.91 | 0           |
| 1   | MLY  | A     | 348 | 1    | 10,10,11     | 0.79 | 0           | 8,11,13     | 1.10 | 1 (12%)     |
| 1   | MLY  | A     | 35  | 1    | 10,10,11     | 0.72 | 0           | 8,11,13     | 0.65 | 0           |
| 1   | MLY  | A     | 353 | 1    | 10,10,11     | 0.98 | 0           | 8,11,13     | 1.03 | 1 (12%)     |
| 1   | MLY  | A     | 367 | 1    | 10,10,11     | 0.89 | 1 (10%)     | 8,11,13     | 0.42 | 0           |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | MLY  | A     | 369 | 1    | 10,10,11     | 0.85 | 0        | 8,11,13     | 0.77 | 0        |
| 1   | MLY  | A     | 385 | 1    | 10,10,11     | 0.94 | 1 (10%)  | 8,11,13     | 0.52 | 0        |
| 1   | MLY  | A     | 415 | 1    | 10,10,11     | 0.71 | 0        | 8,11,13     | 0.73 | 0        |
| 1   | MLY  | A     | 431 | 1    | 10,10,11     | 0.49 | 0        | 8,11,13     | 1.19 | 1 (12%)  |
| 1   | MLY  | A     | 436 | 1    | 10,10,11     | 1.02 | 1 (10%)  | 8,11,13     | 1.79 | 1 (12%)  |
| 1   | MLY  | A     | 486 | 1    | 10,10,11     | 0.57 | 0        | 8,11,13     | 0.54 | 0        |
| 1   | MLY  | A     | 49  | 1    | 10,10,11     | 1.10 | 1 (10%)  | 8,11,13     | 1.24 | 1 (12%)  |
| 1   | MLY  | A     | 504 | 1    | 10,10,11     | 0.83 | 0        | 8,11,13     | 0.46 | 0        |
| 1   | MLY  | A     | 505 | 1    | 10,10,11     | 1.44 | 2 (20%)  | 8,11,13     | 0.51 | 0        |
| 1   | MLY  | A     | 528 | 1    | 10,10,11     | 0.84 | 0        | 8,11,13     | 1.12 | 1 (12%)  |
| 1   | MLY  | A     | 55  | 1    | 10,10,11     | 0.94 | 1 (10%)  | 8,11,13     | 1.09 | 0        |
| 1   | MLY  | A     | 551 | 1    | 10,10,11     | 0.61 | 0        | 8,11,13     | 0.72 | 0        |
| 1   | MLY  | A     | 553 | 1,4  | 10,10,11     | 0.65 | 0        | 8,11,13     | 0.65 | 0        |
| 1   | MLY  | A     | 59  | 1    | 10,10,11     | 0.80 | 0        | 8,11,13     | 1.13 | 1 (12%)  |
| 1   | MLY  | A     | 598 | 1    | 10,10,11     | 1.15 | 2 (20%)  | 8,11,13     | 1.31 | 1 (12%)  |
| 1   | MLY  | A     | 600 | 1    | 10,10,11     | 0.59 | 0        | 8,11,13     | 0.98 | 1 (12%)  |
| 1   | MLY  | A     | 613 | 1    | 10,10,11     | 0.63 | 0        | 8,11,13     | 1.10 | 1 (12%)  |
| 1   | MLY  | A     | 617 | 1    | 10,10,11     | 0.88 | 1 (10%)  | 8,11,13     | 0.60 | 0        |
| 1   | MLY  | A     | 63  | 1    | 10,10,11     | 0.91 | 0        | 8,11,13     | 0.79 | 0        |
| 1   | MLY  | A     | 659 | 1    | 10,10,11     | 0.73 | 0        | 8,11,13     | 0.85 | 0        |
| 1   | MLY  | A     | 681 | 1    | 10,10,11     | 0.99 | 1 (10%)  | 8,11,13     | 1.44 | 1 (12%)  |
| 1   | MLY  | A     | 764 | 1    | 10,10,11     | 0.81 | 0        | 8,11,13     | 0.50 | 0        |
| 1   | MLY  | A     | 768 | 1    | 10,10,11     | 0.86 | 0        | 8,11,13     | 1.96 | 1 (12%)  |
| 1   | MLY  | A     | 782 | 1    | 10,10,11     | 0.74 | 0        | 8,11,13     | 1.54 | 1 (12%)  |
| 1   | MLY  | A     | 827 | 1    | 10,10,11     | 1.00 | 1 (10%)  | 8,11,13     | 0.93 | 1 (12%)  |
| 1   | MLY  | A     | 833 | 1    | 10,10,11     | 1.08 | 1 (10%)  | 8,11,13     | 1.13 | 1 (12%)  |
| 1   | MLY  | A     | 837 | 1    | 10,10,11     | 0.68 | 0        | 8,11,13     | 0.54 | 0        |
| 1   | MLY  | A     | 839 | 1,2  | 10,10,11     | 0.65 | 0        | 8,11,13     | 1.50 | 1 (12%)  |
| 1   | MLY  | A     | 84  | 1    | 10,10,11     | 0.56 | 0        | 8,11,13     | 0.79 | 0        |
| 1   | MLY  | A     | 87  | 1    | 10,10,11     | 1.11 | 1 (10%)  | 8,11,13     | 0.59 | 0        |
| 1   | MLY  | D     | 107 | 1    | 10,10,11     | 0.49 | 0        | 8,11,13     | 1.03 | 1 (12%)  |
| 1   | MLY  | D     | 130 | 1    | 10,10,11     | 0.98 | 1 (10%)  | 8,11,13     | 1.34 | 2 (25%)  |
| 1   | MLY  | D     | 138 | 1    | 10,10,11     | 1.39 | 1 (10%)  | 8,11,13     | 2.70 | 1 (12%)  |
| 1   | MLY  | D     | 19  | 1    | 10,10,11     | 1.28 | 1 (10%)  | 8,11,13     | 0.63 | 0        |
| 1   | MLY  | D     | 190 | 1    | 10,10,11     | 1.15 | 1 (10%)  | 8,11,13     | 1.33 | 1 (12%)  |
| 1   | MLY  | D     | 236 | 1    | 10,10,11     | 1.12 | 1 (10%)  | 8,11,13     | 1.55 | 2 (25%)  |
| 1   | MLY  | D     | 248 | 1    | 10,10,11     | 0.77 | 0        | 8,11,13     | 0.85 | 0        |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | MLY  | D     | 272 | 1    | 10,10,11     | 1.07 | 1 (10%)  | 8,11,13     | 1.32 | 1 (12%)  |
| 1   | MLY  | D     | 295 | 1    | 10,10,11     | 1.13 | 1 (10%)  | 8,11,13     | 0.33 | 0        |
| 1   | MLY  | D     | 296 | 1    | 10,10,11     | 0.86 | 0        | 8,11,13     | 1.20 | 1 (12%)  |
| 1   | MLY  | D     | 30  | 1    | 10,10,11     | 0.88 | 0        | 8,11,13     | 0.94 | 0        |
| 1   | MLY  | D     | 348 | 1    | 10,10,11     | 0.76 | 0        | 8,11,13     | 1.07 | 1 (12%)  |
| 1   | MLY  | D     | 35  | 1    | 10,10,11     | 0.76 | 0        | 8,11,13     | 0.63 | 0        |
| 1   | MLY  | D     | 353 | 1    | 10,10,11     | 0.96 | 0        | 8,11,13     | 1.01 | 1 (12%)  |
| 1   | MLY  | D     | 367 | 1    | 10,10,11     | 0.90 | 1 (10%)  | 8,11,13     | 0.42 | 0        |
| 1   | MLY  | D     | 369 | 1    | 10,10,11     | 0.85 | 0        | 8,11,13     | 0.77 | 0        |
| 1   | MLY  | D     | 385 | 1    | 10,10,11     | 0.93 | 1 (10%)  | 8,11,13     | 0.54 | 0        |
| 1   | MLY  | D     | 415 | 1    | 10,10,11     | 0.73 | 0        | 8,11,13     | 0.77 | 0        |
| 1   | MLY  | D     | 431 | 1    | 10,10,11     | 0.48 | 0        | 8,11,13     | 1.20 | 1 (12%)  |
| 1   | MLY  | D     | 436 | 1    | 10,10,11     | 1.07 | 1 (10%)  | 8,11,13     | 1.76 | 1 (12%)  |
| 1   | MLY  | D     | 486 | 1    | 10,10,11     | 0.57 | 0        | 8,11,13     | 0.56 | 0        |
| 1   | MLY  | D     | 49  | 1    | 10,10,11     | 1.11 | 1 (10%)  | 8,11,13     | 1.24 | 1 (12%)  |
| 1   | MLY  | D     | 504 | 1    | 10,10,11     | 0.82 | 0        | 8,11,13     | 0.46 | 0        |
| 1   | MLY  | D     | 505 | 1    | 10,10,11     | 1.42 | 2 (20%)  | 8,11,13     | 0.51 | 0        |
| 1   | MLY  | D     | 528 | 1    | 10,10,11     | 0.86 | 0        | 8,11,13     | 1.12 | 1 (12%)  |
| 1   | MLY  | D     | 55  | 1    | 10,10,11     | 0.96 | 1 (10%)  | 8,11,13     | 1.07 | 0        |
| 1   | MLY  | D     | 551 | 1    | 10,10,11     | 0.60 | 0        | 8,11,13     | 0.74 | 0        |
| 1   | MLY  | D     | 553 | 1,4  | 10,10,11     | 0.64 | 0        | 8,11,13     | 0.67 | 0        |
| 1   | MLY  | D     | 59  | 1    | 10,10,11     | 0.80 | 0        | 8,11,13     | 1.13 | 1 (12%)  |
| 1   | MLY  | D     | 598 | 1    | 10,10,11     | 1.18 | 2 (20%)  | 8,11,13     | 1.28 | 1 (12%)  |
| 1   | MLY  | D     | 600 | 1    | 10,10,11     | 0.58 | 0        | 8,11,13     | 0.98 | 1 (12%)  |
| 1   | MLY  | D     | 613 | 1    | 10,10,11     | 0.61 | 0        | 8,11,13     | 1.08 | 1 (12%)  |
| 1   | MLY  | D     | 617 | 1    | 10,10,11     | 0.90 | 1 (10%)  | 8,11,13     | 0.61 | 0        |
| 1   | MLY  | D     | 63  | 1    | 10,10,11     | 0.91 | 0        | 8,11,13     | 0.79 | 0        |
| 1   | MLY  | D     | 659 | 1    | 10,10,11     | 0.74 | 0        | 8,11,13     | 0.84 | 0        |
| 1   | MLY  | D     | 681 | 1    | 10,10,11     | 0.96 | 1 (10%)  | 8,11,13     | 1.43 | 1 (12%)  |
| 1   | MLY  | D     | 764 | 1    | 10,10,11     | 0.78 | 0        | 8,11,13     | 0.50 | 0        |
| 1   | MLY  | D     | 768 | 1    | 10,10,11     | 0.85 | 0        | 8,11,13     | 1.96 | 1 (12%)  |
| 1   | MLY  | D     | 782 | 1    | 10,10,11     | 0.76 | 0        | 8,11,13     | 1.53 | 1 (12%)  |
| 1   | MLY  | D     | 827 | 1    | 10,10,11     | 0.98 | 1 (10%)  | 8,11,13     | 0.93 | 1 (12%)  |
| 1   | MLY  | D     | 833 | 1    | 10,10,11     | 1.06 | 1 (10%)  | 8,11,13     | 1.11 | 1 (12%)  |
| 1   | MLY  | D     | 837 | 1    | 10,10,11     | 0.67 | 0        | 8,11,13     | 0.56 | 0        |
| 1   | MLY  | D     | 839 | 1    | 10,10,11     | 0.66 | 0        | 8,11,13     | 1.49 | 1 (12%)  |
| 1   | MLY  | D     | 84  | 1    | 10,10,11     | 0.60 | 0        | 8,11,13     | 0.80 | 0        |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | MLY  | D     | 87  | 1    | 10,10,11     | 1.07 | 1 (10%)  | 8,11,13     | 0.61 | 0        |
| 1   | MLY  | G     | 107 | 1    | 10,10,11     | 0.46 | 0        | 8,11,13     | 1.01 | 1 (12%)  |
| 1   | MLY  | G     | 130 | 1    | 10,10,11     | 0.98 | 1 (10%)  | 8,11,13     | 1.34 | 2 (25%)  |
| 1   | MLY  | G     | 138 | 1    | 10,10,11     | 1.31 | 1 (10%)  | 8,11,13     | 2.74 | 1 (12%)  |
| 1   | MLY  | G     | 19  | 1    | 10,10,11     | 1.23 | 1 (10%)  | 8,11,13     | 0.65 | 0        |
| 1   | MLY  | G     | 190 | 1    | 10,10,11     | 1.19 | 1 (10%)  | 8,11,13     | 1.33 | 1 (12%)  |
| 1   | MLY  | G     | 236 | 1    | 10,10,11     | 1.09 | 1 (10%)  | 8,11,13     | 1.55 | 2 (25%)  |
| 1   | MLY  | G     | 248 | 1    | 10,10,11     | 0.74 | 0        | 8,11,13     | 0.87 | 0        |
| 1   | MLY  | G     | 272 | 1    | 10,10,11     | 1.07 | 1 (10%)  | 8,11,13     | 1.32 | 1 (12%)  |
| 1   | MLY  | G     | 295 | 1    | 10,10,11     | 1.15 | 1 (10%)  | 8,11,13     | 0.31 | 0        |
| 1   | MLY  | G     | 296 | 1    | 10,10,11     | 0.85 | 0        | 8,11,13     | 1.19 | 1 (12%)  |
| 1   | MLY  | G     | 30  | 1    | 10,10,11     | 0.88 | 0        | 8,11,13     | 0.92 | 0        |
| 1   | MLY  | G     | 348 | 1    | 10,10,11     | 0.80 | 1 (10%)  | 8,11,13     | 1.09 | 1 (12%)  |
| 1   | MLY  | G     | 35  | 1    | 10,10,11     | 0.74 | 0        | 8,11,13     | 0.64 | 0        |
| 1   | MLY  | G     | 353 | 1    | 10,10,11     | 0.99 | 0        | 8,11,13     | 1.01 | 1 (12%)  |
| 1   | MLY  | G     | 367 | 1    | 10,10,11     | 0.92 | 1 (10%)  | 8,11,13     | 0.43 | 0        |
| 1   | MLY  | G     | 369 | 1    | 10,10,11     | 0.83 | 0        | 8,11,13     | 0.78 | 0        |
| 1   | MLY  | G     | 385 | 1    | 10,10,11     | 0.93 | 1 (10%)  | 8,11,13     | 0.55 | 0        |
| 1   | MLY  | G     | 415 | 1    | 10,10,11     | 0.70 | 0        | 8,11,13     | 0.75 | 0        |
| 1   | MLY  | G     | 431 | 1    | 10,10,11     | 0.50 | 0        | 8,11,13     | 1.17 | 1 (12%)  |
| 1   | MLY  | G     | 436 | 1    | 10,10,11     | 1.03 | 1 (10%)  | 8,11,13     | 1.78 | 1 (12%)  |
| 1   | MLY  | G     | 486 | 1    | 10,10,11     | 0.56 | 0        | 8,11,13     | 0.55 | 0        |
| 1   | MLY  | G     | 49  | 1    | 10,10,11     | 1.10 | 1 (10%)  | 8,11,13     | 1.23 | 1 (12%)  |
| 1   | MLY  | G     | 504 | 1    | 10,10,11     | 0.81 | 0        | 8,11,13     | 0.45 | 0        |
| 1   | MLY  | G     | 505 | 1    | 10,10,11     | 1.44 | 2 (20%)  | 8,11,13     | 0.51 | 0        |
| 1   | MLY  | G     | 528 | 1    | 10,10,11     | 0.83 | 0        | 8,11,13     | 1.13 | 1 (12%)  |
| 1   | MLY  | G     | 55  | 1    | 10,10,11     | 0.98 | 1 (10%)  | 8,11,13     | 1.10 | 0        |
| 1   | MLY  | G     | 551 | 1    | 10,10,11     | 0.60 | 0        | 8,11,13     | 0.73 | 0        |
| 1   | MLY  | G     | 553 | 1,4  | 10,10,11     | 0.64 | 0        | 8,11,13     | 0.66 | 0        |
| 1   | MLY  | G     | 59  | 1    | 10,10,11     | 0.77 | 0        | 8,11,13     | 1.17 | 1 (12%)  |
| 1   | MLY  | G     | 598 | 1    | 10,10,11     | 1.12 | 2 (20%)  | 8,11,13     | 1.31 | 1 (12%)  |
| 1   | MLY  | G     | 600 | 1    | 10,10,11     | 0.63 | 0        | 8,11,13     | 0.97 | 1 (12%)  |
| 1   | MLY  | G     | 613 | 1    | 10,10,11     | 0.65 | 0        | 8,11,13     | 1.10 | 1 (12%)  |
| 1   | MLY  | G     | 617 | 1    | 10,10,11     | 0.88 | 1 (10%)  | 8,11,13     | 0.61 | 0        |
| 1   | MLY  | G     | 63  | 1    | 10,10,11     | 0.92 | 1 (10%)  | 8,11,13     | 0.79 | 0        |
| 1   | MLY  | G     | 659 | 1    | 10,10,11     | 0.75 | 0        | 8,11,13     | 0.82 | 0        |
| 1   | MLY  | G     | 681 | 1    | 10,10,11     | 0.98 | 1 (10%)  | 8,11,13     | 1.42 | 1 (12%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | MLY  | G     | 764 | 1    | 10,10,11     | 0.76 | 0        | 8,11,13     | 0.51 | 0        |
| 1   | MLY  | G     | 768 | 1    | 10,10,11     | 0.88 | 0        | 8,11,13     | 1.95 | 1 (12%)  |
| 1   | MLY  | G     | 782 | 1    | 10,10,11     | 0.72 | 0        | 8,11,13     | 1.54 | 1 (12%)  |
| 1   | MLY  | G     | 827 | 1    | 10,10,11     | 1.02 | 1 (10%)  | 8,11,13     | 0.93 | 1 (12%)  |
| 1   | MLY  | G     | 833 | 1    | 10,10,11     | 1.09 | 1 (10%)  | 8,11,13     | 1.15 | 1 (12%)  |
| 1   | MLY  | G     | 837 | 1    | 10,10,11     | 0.65 | 0        | 8,11,13     | 0.52 | 0        |
| 1   | MLY  | G     | 839 | 1    | 10,10,11     | 0.68 | 0        | 8,11,13     | 1.51 | 1 (12%)  |
| 1   | MLY  | G     | 84  | 1    | 10,10,11     | 0.61 | 0        | 8,11,13     | 0.80 | 0        |
| 1   | MLY  | G     | 87  | 1    | 10,10,11     | 1.12 | 1 (10%)  | 8,11,13     | 0.59 | 0        |
| 1   | MLY  | J     | 107 | 1    | 10,10,11     | 0.48 | 0        | 8,11,13     | 1.03 | 1 (12%)  |
| 1   | MLY  | J     | 130 | 1    | 10,10,11     | 0.93 | 0        | 8,11,13     | 1.34 | 2 (25%)  |
| 1   | MLY  | J     | 138 | 1    | 10,10,11     | 1.35 | 1 (10%)  | 8,11,13     | 2.73 | 1 (12%)  |
| 1   | MLY  | J     | 19  | 1    | 10,10,11     | 1.24 | 1 (10%)  | 8,11,13     | 0.64 | 0        |
| 1   | MLY  | J     | 190 | 1    | 10,10,11     | 1.19 | 1 (10%)  | 8,11,13     | 1.30 | 1 (12%)  |
| 1   | MLY  | J     | 236 | 1    | 10,10,11     | 1.12 | 1 (10%)  | 8,11,13     | 1.55 | 2 (25%)  |
| 1   | MLY  | J     | 248 | 1    | 10,10,11     | 0.76 | 0        | 8,11,13     | 0.86 | 0        |
| 1   | MLY  | J     | 272 | 1    | 10,10,11     | 1.11 | 1 (10%)  | 8,11,13     | 1.31 | 1 (12%)  |
| 1   | MLY  | J     | 295 | 1    | 10,10,11     | 1.14 | 1 (10%)  | 8,11,13     | 0.33 | 0        |
| 1   | MLY  | J     | 296 | 1    | 10,10,11     | 0.90 | 1 (10%)  | 8,11,13     | 1.18 | 1 (12%)  |
| 1   | MLY  | J     | 30  | 1    | 10,10,11     | 0.85 | 0        | 8,11,13     | 0.93 | 0        |
| 1   | MLY  | J     | 348 | 1    | 10,10,11     | 0.76 | 0        | 8,11,13     | 1.06 | 1 (12%)  |
| 1   | MLY  | J     | 35  | 1    | 10,10,11     | 0.74 | 0        | 8,11,13     | 0.64 | 0        |
| 1   | MLY  | J     | 353 | 1    | 10,10,11     | 0.96 | 0        | 8,11,13     | 1.02 | 1 (12%)  |
| 1   | MLY  | J     | 367 | 1    | 10,10,11     | 0.88 | 1 (10%)  | 8,11,13     | 0.42 | 0        |
| 1   | MLY  | J     | 369 | 1    | 10,10,11     | 0.85 | 0        | 8,11,13     | 0.77 | 0        |
| 1   | MLY  | J     | 385 | 1    | 10,10,11     | 0.95 | 1 (10%)  | 8,11,13     | 0.52 | 0        |
| 1   | MLY  | J     | 415 | 1    | 10,10,11     | 0.74 | 0        | 8,11,13     | 0.75 | 0        |
| 1   | MLY  | J     | 431 | 1    | 10,10,11     | 0.49 | 0        | 8,11,13     | 1.19 | 1 (12%)  |
| 1   | MLY  | J     | 436 | 1    | 10,10,11     | 1.02 | 1 (10%)  | 8,11,13     | 1.76 | 1 (12%)  |
| 1   | MLY  | J     | 486 | 1    | 10,10,11     | 0.56 | 0        | 8,11,13     | 0.55 | 0        |
| 1   | MLY  | J     | 49  | 1    | 10,10,11     | 1.12 | 1 (10%)  | 8,11,13     | 1.25 | 1 (12%)  |
| 1   | MLY  | J     | 504 | 1    | 10,10,11     | 0.79 | 0        | 8,11,13     | 0.45 | 0        |
| 1   | MLY  | J     | 505 | 1    | 10,10,11     | 1.47 | 2 (20%)  | 8,11,13     | 0.50 | 0        |
| 1   | MLY  | J     | 528 | 1    | 10,10,11     | 0.82 | 0        | 8,11,13     | 1.12 | 1 (12%)  |
| 1   | MLY  | J     | 55  | 1    | 10,10,11     | 0.93 | 1 (10%)  | 8,11,13     | 1.10 | 0        |
| 1   | MLY  | J     | 551 | 1    | 10,10,11     | 0.61 | 0        | 8,11,13     | 0.74 | 0        |
| 1   | MLY  | J     | 553 | 1,4  | 10,10,11     | 0.64 | 0        | 8,11,13     | 0.63 | 0        |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | MLY  | J     | 59  | 1    | 10,10,11     | 0.80 | 0        | 8,11,13     | 1.15 | 1 (12%)  |
| 1   | MLY  | J     | 598 | 1    | 10,10,11     | 1.16 | 2 (20%)  | 8,11,13     | 1.29 | 1 (12%)  |
| 1   | MLY  | J     | 600 | 1    | 10,10,11     | 0.64 | 0        | 8,11,13     | 0.97 | 1 (12%)  |
| 1   | MLY  | J     | 613 | 1    | 10,10,11     | 0.67 | 0        | 8,11,13     | 1.09 | 1 (12%)  |
| 1   | MLY  | J     | 617 | 1    | 10,10,11     | 0.90 | 1 (10%)  | 8,11,13     | 0.59 | 0        |
| 1   | MLY  | J     | 63  | 1    | 10,10,11     | 0.91 | 0        | 8,11,13     | 0.79 | 0        |
| 1   | MLY  | J     | 659 | 1    | 10,10,11     | 0.71 | 0        | 8,11,13     | 0.84 | 0        |
| 1   | MLY  | J     | 681 | 1    | 10,10,11     | 0.94 | 1 (10%)  | 8,11,13     | 1.43 | 1 (12%)  |
| 1   | MLY  | J     | 764 | 1    | 10,10,11     | 0.76 | 0        | 8,11,13     | 0.52 | 0        |
| 1   | MLY  | J     | 768 | 1    | 10,10,11     | 0.88 | 0        | 8,11,13     | 1.93 | 1 (12%)  |
| 1   | MLY  | J     | 782 | 1    | 10,10,11     | 0.73 | 0        | 8,11,13     | 1.55 | 1 (12%)  |
| 1   | MLY  | J     | 827 | 1    | 10,10,11     | 1.04 | 1 (10%)  | 8,11,13     | 0.92 | 1 (12%)  |
| 1   | MLY  | J     | 833 | 1    | 10,10,11     | 1.13 | 1 (10%)  | 8,11,13     | 1.07 | 1 (12%)  |
| 1   | MLY  | J     | 837 | 1    | 10,10,11     | 0.66 | 0        | 8,11,13     | 0.55 | 0        |
| 1   | MLY  | J     | 839 | 1    | 10,10,11     | 0.67 | 0        | 8,11,13     | 1.50 | 1 (12%)  |
| 1   | MLY  | J     | 84  | 1    | 10,10,11     | 0.58 | 0        | 8,11,13     | 0.80 | 0        |
| 1   | MLY  | J     | 87  | 1    | 10,10,11     | 1.13 | 1 (10%)  | 8,11,13     | 0.61 | 0        |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings   |
|-----|------|-------|-----|------|---------|----------|---------|
| 1   | MLY  | A     | 107 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 130 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 138 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 19  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 190 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 236 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 248 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 272 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 295 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 296 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 30  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 348 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 35  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 353 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 367 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 369 | 1    | -       | 0/7/9/11 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings   |
|-----|------|-------|-----|------|---------|----------|---------|
| 1   | MLY  | A     | 385 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 415 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 431 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 436 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 486 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 49  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 504 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 505 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 528 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 55  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 551 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 553 | 1,4  | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 59  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 598 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 600 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 613 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 617 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 63  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 659 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 681 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 764 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 768 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 782 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 827 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 833 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 837 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 839 | 1,2  | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 84  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 87  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 107 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 130 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 138 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 19  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 190 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 236 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 248 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 272 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 295 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 296 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 30  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 348 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 35  | 1    | -       | 0/7/9/11 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings   |
|-----|------|-------|-----|------|---------|----------|---------|
| 1   | MLY  | D     | 353 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 367 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 369 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 385 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 415 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 431 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 436 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 486 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 49  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 504 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 505 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 528 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 55  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 551 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 553 | 1,4  | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 59  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 598 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 600 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 613 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 617 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 63  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 659 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 681 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 764 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 768 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 782 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 827 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 833 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 837 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 839 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 84  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 87  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 107 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 130 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 138 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 19  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 190 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 236 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 248 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 272 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 295 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 296 | 1    | -       | 0/7/9/11 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings   |
|-----|------|-------|-----|------|---------|----------|---------|
| 1   | MLY  | G     | 30  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 348 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 35  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 353 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 367 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 369 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 385 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 415 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 431 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 436 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 486 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 49  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 504 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 505 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 528 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 55  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 551 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 553 | 1,4  | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 59  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 598 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 600 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 613 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 617 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 63  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 659 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 681 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 764 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 768 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 782 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 827 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 833 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 837 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 839 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 84  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 87  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 107 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 130 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 138 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 19  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 190 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 236 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 248 | 1    | -       | 0/7/9/11 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings   |
|-----|------|-------|-----|------|---------|----------|---------|
| 1   | MLY  | J     | 272 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 295 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 296 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 30  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 348 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 35  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 353 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 367 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 369 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 385 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 415 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 431 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 436 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 486 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 49  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 504 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 505 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 528 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 55  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 551 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 553 | 1,4  | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 59  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 598 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 600 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 613 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 617 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 63  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 659 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 681 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 764 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 768 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 782 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 827 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 833 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 837 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 839 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 84  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 87  | 1    | -       | 0/7/9/11 | 0/0/0/0 |

All (87) bond length outliers are listed below:

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|---|-------------|----------|
|-----|-------|-----|------|-------|---|-------------|----------|

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | D     | 138 | MLY  | CB-CA | -3.76 | 1.48        | 1.53     |
| 1   | J     | 138 | MLY  | CB-CA | -3.62 | 1.48        | 1.53     |
| 1   | A     | 138 | MLY  | CB-CA | -3.57 | 1.48        | 1.53     |
| 1   | G     | 138 | MLY  | CB-CA | -3.52 | 1.48        | 1.53     |
| 1   | D     | 19  | MLY  | CB-CA | -3.20 | 1.49        | 1.53     |
| 1   | J     | 19  | MLY  | CB-CA | -3.13 | 1.49        | 1.53     |
| 1   | G     | 87  | MLY  | CB-CA | -3.11 | 1.49        | 1.53     |
| 1   | J     | 87  | MLY  | CB-CA | -3.10 | 1.49        | 1.53     |
| 1   | D     | 436 | MLY  | CB-CA | -3.07 | 1.49        | 1.53     |
| 1   | G     | 19  | MLY  | CB-CA | -3.03 | 1.49        | 1.53     |
| 1   | A     | 87  | MLY  | CB-CA | -3.03 | 1.49        | 1.53     |
| 1   | A     | 19  | MLY  | CB-CA | -2.96 | 1.49        | 1.53     |
| 1   | D     | 87  | MLY  | CB-CA | -2.95 | 1.49        | 1.53     |
| 1   | G     | 436 | MLY  | CB-CA | -2.89 | 1.49        | 1.53     |
| 1   | J     | 436 | MLY  | CB-CA | -2.88 | 1.49        | 1.53     |
| 1   | A     | 436 | MLY  | CB-CA | -2.82 | 1.49        | 1.53     |
| 1   | J     | 236 | MLY  | CA-C  | -2.82 | 1.46        | 1.50     |
| 1   | D     | 236 | MLY  | CA-C  | -2.81 | 1.46        | 1.50     |
| 1   | D     | 49  | MLY  | CB-CA | -2.81 | 1.49        | 1.53     |
| 1   | J     | 49  | MLY  | CB-CA | -2.80 | 1.49        | 1.53     |
| 1   | J     | 272 | MLY  | CB-CA | -2.79 | 1.49        | 1.53     |
| 1   | G     | 49  | MLY  | CB-CA | -2.78 | 1.49        | 1.53     |
| 1   | A     | 49  | MLY  | CB-CA | -2.75 | 1.49        | 1.53     |
| 1   | A     | 272 | MLY  | CB-CA | -2.74 | 1.49        | 1.53     |
| 1   | A     | 236 | MLY  | CA-C  | -2.70 | 1.46        | 1.50     |
| 1   | G     | 236 | MLY  | CA-C  | -2.69 | 1.46        | 1.50     |
| 1   | G     | 272 | MLY  | CB-CA | -2.68 | 1.50        | 1.53     |
| 1   | D     | 272 | MLY  | CB-CA | -2.67 | 1.50        | 1.53     |
| 1   | J     | 598 | MLY  | CA-C  | -2.59 | 1.46        | 1.50     |
| 1   | G     | 190 | MLY  | CB-CA | -2.57 | 1.50        | 1.53     |
| 1   | J     | 190 | MLY  | CB-CA | -2.54 | 1.50        | 1.53     |
| 1   | D     | 598 | MLY  | CA-C  | -2.53 | 1.46        | 1.50     |
| 1   | A     | 190 | MLY  | CB-CA | -2.53 | 1.50        | 1.53     |
| 1   | A     | 598 | MLY  | CA-C  | -2.48 | 1.47        | 1.50     |
| 1   | G     | 598 | MLY  | CA-C  | -2.48 | 1.47        | 1.50     |
| 1   | J     | 833 | MLY  | CB-CA | -2.48 | 1.50        | 1.53     |
| 1   | J     | 385 | MLY  | CB-CA | -2.46 | 1.50        | 1.53     |
| 1   | D     | 190 | MLY  | CB-CA | -2.45 | 1.50        | 1.53     |
| 1   | A     | 385 | MLY  | CB-CA | -2.43 | 1.50        | 1.53     |
| 1   | G     | 385 | MLY  | CB-CA | -2.40 | 1.50        | 1.53     |
| 1   | D     | 385 | MLY  | CB-CA | -2.36 | 1.50        | 1.53     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | D     | 598 | MLY  | CB-CA | -2.33 | 1.50        | 1.53     |
| 1   | A     | 833 | MLY  | CB-CA | -2.28 | 1.50        | 1.53     |
| 1   | J     | 505 | MLY  | CB-CA | -2.28 | 1.50        | 1.53     |
| 1   | A     | 598 | MLY  | CB-CA | -2.26 | 1.50        | 1.53     |
| 1   | D     | 617 | MLY  | CB-CA | -2.25 | 1.50        | 1.53     |
| 1   | J     | 598 | MLY  | CB-CA | -2.23 | 1.50        | 1.53     |
| 1   | G     | 833 | MLY  | CB-CA | -2.22 | 1.50        | 1.53     |
| 1   | J     | 617 | MLY  | CB-CA | -2.22 | 1.50        | 1.53     |
| 1   | A     | 505 | MLY  | CB-CA | -2.19 | 1.50        | 1.53     |
| 1   | G     | 598 | MLY  | CB-CA | -2.16 | 1.50        | 1.53     |
| 1   | D     | 833 | MLY  | CB-CA | -2.16 | 1.50        | 1.53     |
| 1   | G     | 505 | MLY  | CB-CA | -2.15 | 1.50        | 1.53     |
| 1   | A     | 617 | MLY  | CB-CA | -2.14 | 1.50        | 1.53     |
| 1   | G     | 617 | MLY  | CB-CA | -2.12 | 1.50        | 1.53     |
| 1   | D     | 505 | MLY  | CB-CA | -2.06 | 1.50        | 1.53     |
| 1   | G     | 348 | MLY  | CB-CA | -2.02 | 1.50        | 1.53     |
| 1   | G     | 63  | MLY  | CB-CA | -2.02 | 1.50        | 1.53     |
| 1   | A     | 296 | MLY  | CA-C  | 2.02  | 1.52        | 1.50     |
| 1   | J     | 296 | MLY  | CA-C  | 2.07  | 1.53        | 1.50     |
| 1   | J     | 367 | MLY  | CA-C  | 2.08  | 1.53        | 1.50     |
| 1   | J     | 55  | MLY  | CA-C  | 2.11  | 1.53        | 1.50     |
| 1   | A     | 367 | MLY  | CA-C  | 2.12  | 1.53        | 1.50     |
| 1   | D     | 130 | MLY  | CA-C  | 2.13  | 1.53        | 1.50     |
| 1   | A     | 55  | MLY  | CA-C  | 2.14  | 1.53        | 1.50     |
| 1   | G     | 130 | MLY  | CA-C  | 2.15  | 1.53        | 1.50     |
| 1   | A     | 130 | MLY  | CA-C  | 2.16  | 1.53        | 1.50     |
| 1   | G     | 367 | MLY  | CA-C  | 2.17  | 1.53        | 1.50     |
| 1   | D     | 367 | MLY  | CA-C  | 2.21  | 1.53        | 1.50     |
| 1   | D     | 55  | MLY  | CA-C  | 2.23  | 1.53        | 1.50     |
| 1   | G     | 55  | MLY  | CA-C  | 2.28  | 1.53        | 1.50     |
| 1   | D     | 827 | MLY  | CA-C  | 2.37  | 1.53        | 1.50     |
| 1   | A     | 827 | MLY  | CA-C  | 2.40  | 1.53        | 1.50     |
| 1   | J     | 681 | MLY  | CA-C  | 2.42  | 1.53        | 1.50     |
| 1   | G     | 681 | MLY  | CA-C  | 2.46  | 1.53        | 1.50     |
| 1   | J     | 827 | MLY  | CA-C  | 2.50  | 1.53        | 1.50     |
| 1   | D     | 681 | MLY  | CA-C  | 2.51  | 1.53        | 1.50     |
| 1   | G     | 827 | MLY  | CA-C  | 2.55  | 1.53        | 1.50     |
| 1   | A     | 681 | MLY  | CA-C  | 2.57  | 1.53        | 1.50     |
| 1   | D     | 295 | MLY  | CA-C  | 2.74  | 1.53        | 1.50     |
| 1   | A     | 295 | MLY  | CA-C  | 2.74  | 1.53        | 1.50     |
| 1   | J     | 295 | MLY  | CA-C  | 2.81  | 1.53        | 1.50     |
| 1   | G     | 295 | MLY  | CA-C  | 2.81  | 1.53        | 1.50     |

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| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | A     | 505 | MLY  | CA-C  | 3.71 | 1.55        | 1.50     |
| 1   | D     | 505 | MLY  | CA-C  | 3.73 | 1.55        | 1.50     |
| 1   | J     | 505 | MLY  | CA-C  | 3.77 | 1.55        | 1.50     |
| 1   | G     | 505 | MLY  | CA-C  | 3.78 | 1.55        | 1.50     |

All (100) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | G     | 138 | MLY  | CB-CA-C | -7.47 | 99.33       | 111.65   |
| 1   | J     | 138 | MLY  | CB-CA-C | -7.45 | 99.38       | 111.65   |
| 1   | A     | 138 | MLY  | CB-CA-C | -7.40 | 99.45       | 111.65   |
| 1   | D     | 138 | MLY  | CB-CA-C | -7.34 | 99.56       | 111.65   |
| 1   | A     | 768 | MLY  | CB-CA-C | -5.21 | 103.06      | 111.65   |
| 1   | D     | 768 | MLY  | CB-CA-C | -5.19 | 103.09      | 111.65   |
| 1   | G     | 768 | MLY  | CB-CA-C | -5.15 | 103.16      | 111.65   |
| 1   | J     | 768 | MLY  | CB-CA-C | -5.10 | 103.24      | 111.65   |
| 1   | A     | 436 | MLY  | CB-CA-C | -4.83 | 103.69      | 111.65   |
| 1   | G     | 436 | MLY  | CB-CA-C | -4.80 | 103.74      | 111.65   |
| 1   | D     | 436 | MLY  | CB-CA-C | -4.76 | 103.81      | 111.65   |
| 1   | J     | 436 | MLY  | CB-CA-C | -4.74 | 103.83      | 111.65   |
| 1   | A     | 681 | MLY  | CB-CA-C | -3.75 | 105.47      | 111.65   |
| 1   | J     | 839 | MLY  | CB-CA-C | -3.72 | 105.53      | 111.65   |
| 1   | D     | 681 | MLY  | CB-CA-C | -3.70 | 105.55      | 111.65   |
| 1   | G     | 681 | MLY  | CB-CA-C | -3.70 | 105.55      | 111.65   |
| 1   | J     | 681 | MLY  | CB-CA-C | -3.70 | 105.56      | 111.65   |
| 1   | G     | 839 | MLY  | CB-CA-C | -3.69 | 105.58      | 111.65   |
| 1   | A     | 839 | MLY  | CB-CA-C | -3.68 | 105.59      | 111.65   |
| 1   | D     | 839 | MLY  | CB-CA-C | -3.63 | 105.67      | 111.65   |
| 1   | D     | 272 | MLY  | CB-CA-C | -3.43 | 105.99      | 111.65   |
| 1   | G     | 272 | MLY  | CB-CA-C | -3.43 | 105.99      | 111.65   |
| 1   | A     | 272 | MLY  | CB-CA-C | -3.43 | 106.00      | 111.65   |
| 1   | J     | 272 | MLY  | CB-CA-C | -3.40 | 106.05      | 111.65   |
| 1   | D     | 190 | MLY  | CB-CA-C | -3.27 | 106.26      | 111.65   |
| 1   | G     | 190 | MLY  | CB-CA-C | -3.26 | 106.28      | 111.65   |
| 1   | G     | 598 | MLY  | CB-CA-C | -3.22 | 106.35      | 111.65   |
| 1   | A     | 190 | MLY  | CB-CA-C | -3.20 | 106.38      | 111.65   |
| 1   | A     | 598 | MLY  | CB-CA-C | -3.19 | 106.39      | 111.65   |
| 1   | J     | 190 | MLY  | CB-CA-C | -3.18 | 106.41      | 111.65   |
| 1   | J     | 598 | MLY  | CB-CA-C | -3.15 | 106.45      | 111.65   |
| 1   | J     | 236 | MLY  | CB-CA-C | -3.15 | 106.47      | 111.65   |
| 1   | G     | 236 | MLY  | CB-CA-C | -3.13 | 106.49      | 111.65   |
| 1   | D     | 598 | MLY  | CB-CA-C | -3.13 | 106.49      | 111.65   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | D     | 236 | MLY  | CB-CA-C | -3.11 | 106.52      | 111.65   |
| 1   | A     | 236 | MLY  | CB-CA-C | -3.11 | 106.53      | 111.65   |
| 1   | A     | 431 | MLY  | CB-CA-C | -3.02 | 106.67      | 111.65   |
| 1   | D     | 431 | MLY  | CB-CA-C | -3.02 | 106.67      | 111.65   |
| 1   | J     | 431 | MLY  | CB-CA-C | -3.01 | 106.69      | 111.65   |
| 1   | G     | 833 | MLY  | CB-CA-C | -3.01 | 106.70      | 111.65   |
| 1   | A     | 833 | MLY  | CB-CA-C | -2.95 | 106.78      | 111.65   |
| 1   | G     | 431 | MLY  | CB-CA-C | -2.95 | 106.79      | 111.65   |
| 1   | D     | 49  | MLY  | CB-CA-C | -2.91 | 106.86      | 111.65   |
| 1   | J     | 49  | MLY  | CB-CA-C | -2.91 | 106.86      | 111.65   |
| 1   | A     | 49  | MLY  | CB-CA-C | -2.90 | 106.87      | 111.65   |
| 1   | A     | 236 | MLY  | O-C-CA  | -2.90 | 117.01      | 125.02   |
| 1   | D     | 833 | MLY  | CB-CA-C | -2.90 | 106.87      | 111.65   |
| 1   | D     | 236 | MLY  | O-C-CA  | -2.88 | 117.06      | 125.02   |
| 1   | A     | 296 | MLY  | CB-CA-C | -2.86 | 106.93      | 111.65   |
| 1   | G     | 236 | MLY  | O-C-CA  | -2.86 | 117.11      | 125.02   |
| 1   | G     | 49  | MLY  | CB-CA-C | -2.86 | 106.94      | 111.65   |
| 1   | J     | 236 | MLY  | O-C-CA  | -2.84 | 117.17      | 125.02   |
| 1   | D     | 296 | MLY  | CB-CA-C | -2.82 | 107.01      | 111.65   |
| 1   | G     | 296 | MLY  | CB-CA-C | -2.80 | 107.04      | 111.65   |
| 1   | J     | 833 | MLY  | CB-CA-C | -2.80 | 107.04      | 111.65   |
| 1   | G     | 59  | MLY  | CB-CA-C | -2.78 | 107.07      | 111.65   |
| 1   | D     | 528 | MLY  | O-C-CA  | -2.75 | 117.42      | 125.02   |
| 1   | G     | 528 | MLY  | O-C-CA  | -2.75 | 117.42      | 125.02   |
| 1   | J     | 296 | MLY  | CB-CA-C | -2.75 | 107.12      | 111.65   |
| 1   | J     | 528 | MLY  | O-C-CA  | -2.72 | 117.52      | 125.02   |
| 1   | A     | 528 | MLY  | O-C-CA  | -2.72 | 117.52      | 125.02   |
| 1   | J     | 59  | MLY  | CB-CA-C | -2.69 | 107.22      | 111.65   |
| 1   | D     | 59  | MLY  | CB-CA-C | -2.65 | 107.28      | 111.65   |
| 1   | A     | 59  | MLY  | CB-CA-C | -2.65 | 107.29      | 111.65   |
| 1   | A     | 613 | MLY  | CB-CA-C | -2.51 | 107.51      | 111.65   |
| 1   | G     | 613 | MLY  | CB-CA-C | -2.51 | 107.52      | 111.65   |
| 1   | A     | 600 | MLY  | CB-CA-C | -2.50 | 107.53      | 111.65   |
| 1   | D     | 600 | MLY  | CB-CA-C | -2.49 | 107.54      | 111.65   |
| 1   | G     | 600 | MLY  | CB-CA-C | -2.48 | 107.56      | 111.65   |
| 1   | J     | 600 | MLY  | CB-CA-C | -2.48 | 107.56      | 111.65   |
| 1   | D     | 107 | MLY  | CB-CA-C | -2.45 | 107.61      | 111.65   |
| 1   | J     | 107 | MLY  | CB-CA-C | -2.44 | 107.62      | 111.65   |
| 1   | J     | 613 | MLY  | CB-CA-C | -2.44 | 107.63      | 111.65   |
| 1   | D     | 613 | MLY  | CB-CA-C | -2.42 | 107.67      | 111.65   |
| 1   | A     | 107 | MLY  | CB-CA-C | -2.42 | 107.67      | 111.65   |
| 1   | G     | 107 | MLY  | CB-CA-C | -2.37 | 107.74      | 111.65   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | D     | 827 | MLY  | O-C-CA  | -2.23 | 118.85      | 125.02   |
| 1   | A     | 827 | MLY  | O-C-CA  | -2.23 | 118.85      | 125.02   |
| 1   | G     | 827 | MLY  | O-C-CA  | -2.21 | 118.91      | 125.02   |
| 1   | J     | 827 | MLY  | O-C-CA  | -2.18 | 118.99      | 125.02   |
| 1   | G     | 130 | MLY  | O-C-CA  | -2.18 | 119.01      | 125.02   |
| 1   | J     | 130 | MLY  | O-C-CA  | -2.15 | 119.08      | 125.02   |
| 1   | D     | 130 | MLY  | O-C-CA  | -2.15 | 119.08      | 125.02   |
| 1   | A     | 130 | MLY  | O-C-CA  | -2.13 | 119.13      | 125.02   |
| 1   | A     | 353 | MLY  | CB-CA-C | -2.11 | 108.17      | 111.65   |
| 1   | J     | 353 | MLY  | CB-CA-C | -2.11 | 108.17      | 111.65   |
| 1   | D     | 353 | MLY  | CB-CA-C | -2.07 | 108.23      | 111.65   |
| 1   | G     | 353 | MLY  | CB-CA-C | -2.05 | 108.28      | 111.65   |
| 1   | A     | 130 | MLY  | CB-CA-C | 2.51  | 115.78      | 111.65   |
| 1   | G     | 130 | MLY  | CB-CA-C | 2.51  | 115.79      | 111.65   |
| 1   | J     | 130 | MLY  | CB-CA-C | 2.52  | 115.80      | 111.65   |
| 1   | J     | 348 | MLY  | CB-CA-C | 2.55  | 115.86      | 111.65   |
| 1   | D     | 130 | MLY  | CB-CA-C | 2.55  | 115.86      | 111.65   |
| 1   | D     | 348 | MLY  | CB-CA-C | 2.57  | 115.89      | 111.65   |
| 1   | G     | 348 | MLY  | CB-CA-C | 2.62  | 115.97      | 111.65   |
| 1   | A     | 348 | MLY  | CB-CA-C | 2.68  | 116.06      | 111.65   |
| 1   | D     | 782 | MLY  | CB-CA-C | 4.12  | 118.45      | 111.65   |
| 1   | A     | 782 | MLY  | CB-CA-C | 4.16  | 118.51      | 111.65   |
| 1   | G     | 782 | MLY  | CB-CA-C | 4.16  | 118.51      | 111.65   |
| 1   | J     | 782 | MLY  | CB-CA-C | 4.18  | 118.53      | 111.65   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

124 monomers are involved in 525 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1   | A     | 107 | MLY  | 3       | 0            |
| 1   | A     | 138 | MLY  | 1       | 0            |
| 1   | A     | 190 | MLY  | 2       | 0            |
| 1   | A     | 248 | MLY  | 2       | 0            |
| 1   | A     | 272 | MLY  | 1       | 0            |
| 1   | A     | 295 | MLY  | 6       | 0            |
| 1   | A     | 296 | MLY  | 2       | 0            |
| 1   | A     | 30  | MLY  | 1       | 0            |
| 1   | A     | 348 | MLY  | 5       | 0            |
| 1   | A     | 369 | MLY  | 1       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1   | A     | 415 | MLY  | 1       | 0            |
| 1   | A     | 436 | MLY  | 2       | 0            |
| 1   | A     | 486 | MLY  | 3       | 0            |
| 1   | A     | 49  | MLY  | 3       | 0            |
| 1   | A     | 504 | MLY  | 4       | 0            |
| 1   | A     | 505 | MLY  | 11      | 0            |
| 1   | A     | 528 | MLY  | 2       | 0            |
| 1   | A     | 55  | MLY  | 1       | 0            |
| 1   | A     | 551 | MLY  | 2       | 0            |
| 1   | A     | 553 | MLY  | 17      | 0            |
| 1   | A     | 59  | MLY  | 2       | 0            |
| 1   | A     | 598 | MLY  | 1       | 0            |
| 1   | A     | 600 | MLY  | 1       | 0            |
| 1   | A     | 617 | MLY  | 1       | 0            |
| 1   | A     | 63  | MLY  | 3       | 0            |
| 1   | A     | 659 | MLY  | 2       | 0            |
| 1   | A     | 764 | MLY  | 7       | 0            |
| 1   | A     | 768 | MLY  | 14      | 0            |
| 1   | A     | 782 | MLY  | 1       | 0            |
| 1   | A     | 837 | MLY  | 1       | 0            |
| 1   | A     | 839 | MLY  | 15      | 0            |
| 1   | A     | 87  | MLY  | 3       | 0            |
| 1   | D     | 107 | MLY  | 2       | 0            |
| 1   | D     | 138 | MLY  | 1       | 0            |
| 1   | D     | 190 | MLY  | 2       | 0            |
| 1   | D     | 248 | MLY  | 2       | 0            |
| 1   | D     | 272 | MLY  | 1       | 0            |
| 1   | D     | 295 | MLY  | 6       | 0            |
| 1   | D     | 296 | MLY  | 3       | 0            |
| 1   | D     | 30  | MLY  | 1       | 0            |
| 1   | D     | 348 | MLY  | 6       | 0            |
| 1   | D     | 415 | MLY  | 1       | 0            |
| 1   | D     | 436 | MLY  | 2       | 0            |
| 1   | D     | 486 | MLY  | 3       | 0            |
| 1   | D     | 49  | MLY  | 3       | 0            |
| 1   | D     | 528 | MLY  | 3       | 0            |
| 1   | D     | 55  | MLY  | 1       | 0            |
| 1   | D     | 551 | MLY  | 1       | 0            |
| 1   | D     | 553 | MLY  | 16      | 0            |
| 1   | D     | 59  | MLY  | 2       | 0            |
| 1   | D     | 598 | MLY  | 1       | 0            |
| 1   | D     | 600 | MLY  | 1       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1   | D     | 617 | MLY  | 1       | 0            |
| 1   | D     | 63  | MLY  | 3       | 0            |
| 1   | D     | 659 | MLY  | 2       | 0            |
| 1   | D     | 764 | MLY  | 2       | 0            |
| 1   | D     | 768 | MLY  | 6       | 0            |
| 1   | D     | 782 | MLY  | 32      | 0            |
| 1   | D     | 837 | MLY  | 1       | 0            |
| 1   | D     | 839 | MLY  | 16      | 0            |
| 1   | D     | 87  | MLY  | 3       | 0            |
| 1   | G     | 107 | MLY  | 3       | 0            |
| 1   | G     | 138 | MLY  | 1       | 0            |
| 1   | G     | 190 | MLY  | 2       | 0            |
| 1   | G     | 248 | MLY  | 2       | 0            |
| 1   | G     | 272 | MLY  | 1       | 0            |
| 1   | G     | 295 | MLY  | 5       | 0            |
| 1   | G     | 296 | MLY  | 2       | 0            |
| 1   | G     | 30  | MLY  | 1       | 0            |
| 1   | G     | 348 | MLY  | 4       | 0            |
| 1   | G     | 369 | MLY  | 1       | 0            |
| 1   | G     | 415 | MLY  | 1       | 0            |
| 1   | G     | 436 | MLY  | 2       | 0            |
| 1   | G     | 486 | MLY  | 3       | 0            |
| 1   | G     | 49  | MLY  | 2       | 0            |
| 1   | G     | 528 | MLY  | 3       | 0            |
| 1   | G     | 55  | MLY  | 1       | 0            |
| 1   | G     | 551 | MLY  | 2       | 0            |
| 1   | G     | 553 | MLY  | 16      | 0            |
| 1   | G     | 59  | MLY  | 3       | 0            |
| 1   | G     | 598 | MLY  | 1       | 0            |
| 1   | G     | 600 | MLY  | 1       | 0            |
| 1   | G     | 617 | MLY  | 1       | 0            |
| 1   | G     | 63  | MLY  | 3       | 0            |
| 1   | G     | 659 | MLY  | 2       | 0            |
| 1   | G     | 764 | MLY  | 12      | 0            |
| 1   | G     | 768 | MLY  | 15      | 0            |
| 1   | G     | 782 | MLY  | 1       | 0            |
| 1   | G     | 827 | MLY  | 1       | 0            |
| 1   | G     | 837 | MLY  | 1       | 0            |
| 1   | G     | 839 | MLY  | 4       | 0            |
| 1   | G     | 84  | MLY  | 18      | 0            |
| 1   | G     | 87  | MLY  | 2       | 0            |
| 1   | J     | 107 | MLY  | 3       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1   | J     | 138 | MLY  | 1       | 0            |
| 1   | J     | 190 | MLY  | 2       | 0            |
| 1   | J     | 248 | MLY  | 2       | 0            |
| 1   | J     | 272 | MLY  | 1       | 0            |
| 1   | J     | 295 | MLY  | 6       | 0            |
| 1   | J     | 296 | MLY  | 3       | 0            |
| 1   | J     | 30  | MLY  | 1       | 0            |
| 1   | J     | 348 | MLY  | 5       | 0            |
| 1   | J     | 415 | MLY  | 1       | 0            |
| 1   | J     | 436 | MLY  | 2       | 0            |
| 1   | J     | 486 | MLY  | 3       | 0            |
| 1   | J     | 49  | MLY  | 2       | 0            |
| 1   | J     | 528 | MLY  | 3       | 0            |
| 1   | J     | 55  | MLY  | 1       | 0            |
| 1   | J     | 551 | MLY  | 1       | 0            |
| 1   | J     | 553 | MLY  | 17      | 0            |
| 1   | J     | 59  | MLY  | 3       | 0            |
| 1   | J     | 598 | MLY  | 1       | 0            |
| 1   | J     | 600 | MLY  | 1       | 0            |
| 1   | J     | 617 | MLY  | 1       | 0            |
| 1   | J     | 63  | MLY  | 4       | 0            |
| 1   | J     | 659 | MLY  | 2       | 0            |
| 1   | J     | 764 | MLY  | 26      | 0            |
| 1   | J     | 768 | MLY  | 41      | 0            |
| 1   | J     | 782 | MLY  | 1       | 0            |
| 1   | J     | 827 | MLY  | 1       | 0            |
| 1   | J     | 837 | MLY  | 1       | 0            |
| 1   | J     | 839 | MLY  | 5       | 0            |
| 1   | J     | 84  | MLY  | 25      | 0            |
| 1   | J     | 87  | MLY  | 3       | 0            |

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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.