



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 09:39 PM EDT

PDB ID : 1M57 / pdb\_00001m57  
Title : Structure of cytochrome c oxidase from Rhodobacter sphaeroides (EQ(I-286 mutant))  
Authors : Svensson-Ek, M.; Abramson, J.; Larsson, G.; Tornroth, S.; Brezezinski, P.; Iwata, S.  
Deposited on : 2002-07-08  
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | NOT EXECUTED                                                     |
| EDS                            | : | NOT EXECUTED                                                     |
| Buster-report                  | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.50                                                             |

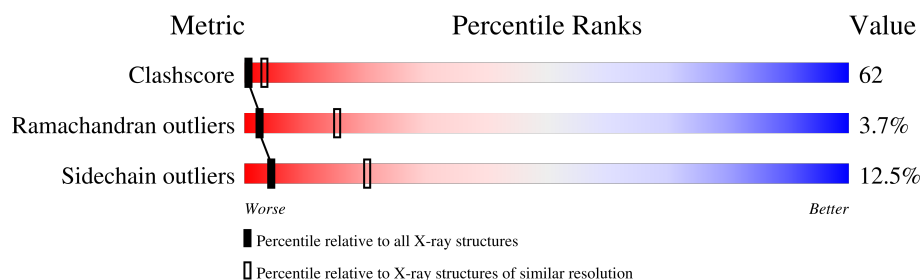
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| Clashscore            | 190562                      | 2977 (3.00-3.00)                                      |
| Ramachandran outliers | 187476                      | 2877 (3.00-3.00)                                      |
| Sidechain outliers    | 187428                      | 2880 (3.00-3.00)                                      |

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

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|-------------------|
| 1   | A     | 566    | 12% 47% 32% 6% .  |
| 1   | G     | 566    | 11% 43% 36% 7% .  |
| 2   | B     | 264    | 23% 47% 23% 6% .  |
| 2   | H     | 264    | 20% 48% 26% 5% .  |
| 3   | C     | 266    | 24% 52% 20% .     |
| 3   | I     | 266    | 26% 46% 24% .     |
| 4   | D     | 51     | 22% 39% 22% 18%   |
| 4   | J     | 51     | 20% 43% 16% . 18% |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 8   | HEA  | G     | 1001 | -         | -        | X       | -                |
| 9   | 3PE  | C     | 2010 | -         | -        | X       | -                |
| 9   | 3PE  | C     | 2013 | -         | -        | X       | -                |
| 9   | 3PE  | G     | 3012 | -         | -        | X       | -                |
| 9   | 3PE  | I     | 3010 | -         | -        | X       | -                |
| 9   | 3PE  | I     | 3013 | -         | -        | X       | -                |

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 18934 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called CYTOCHROME C OXIDASE.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 547      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4322  | 2892 | 685 | 714 | 31 |         |         |       |
| 1   | G     | 547      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4322  | 2892 | 685 | 714 | 31 |         |         |       |

There are 16 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 286     | GLN      | GLU    | engineered mutation | UNP P33517 |
| A     | 436     | ILE      | SER    | SEE REMARK 999      | UNP P33517 |
| A     | 437     | TYR      | THR    | SEE REMARK 999      | UNP P33517 |
| A     | 438     | PHE      | SER    | SEE REMARK 999      | UNP P33517 |
| A     | 439     | TRP      | GLY    | SEE REMARK 999      | UNP P33517 |
| A     | 518     | THR      | SER    | SEE REMARK 999      | UNP P33517 |
| A     | 520     | THR      | SER    | SEE REMARK 999      | UNP P33517 |
| A     | 521     | ARG      | -      | SEE REMARK 999      | UNP P33517 |
| G     | 286     | GLN      | GLU    | engineered mutation | UNP P33517 |
| G     | 436     | ILE      | SER    | SEE REMARK 999      | UNP P33517 |
| G     | 437     | TYR      | THR    | SEE REMARK 999      | UNP P33517 |
| G     | 438     | PHE      | SER    | SEE REMARK 999      | UNP P33517 |
| G     | 439     | TRP      | GLY    | SEE REMARK 999      | UNP P33517 |
| G     | 518     | THR      | SER    | SEE REMARK 999      | UNP P33517 |
| G     | 520     | THR      | SER    | SEE REMARK 999      | UNP P33517 |
| G     | 521     | ARG      | -      | SEE REMARK 999      | UNP P33517 |

- Molecule 2 is a protein called CYTOCHROME C OXIDASE.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | B     | 260      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2046  | 1334 | 332 | 374 | 6 |         |         |       |
| 2   | H     | 260      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2046  | 1334 | 332 | 374 | 6 |         |         |       |

- Molecule 3 is a protein called CYTOCHROME C OXIDASE.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 3   | C     | 265      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2139  | 1448 | 342 | 337 | 12 |         |         |       |
| 3   | I     | 265      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2139  | 1448 | 342 | 337 | 12 |         |         |       |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| C     | 30      | PHE      | ASN    | SEE REMARK 999 | UNP P84153 |
| C     | 92      | MET      | ILE    | SEE REMARK 999 | UNP P84153 |
| C     | 244     | ILE      | MET    | SEE REMARK 999 | UNP P84153 |
| I     | 30      | PHE      | ASN    | SEE REMARK 999 | UNP P84153 |
| I     | 92      | MET      | ILE    | SEE REMARK 999 | UNP P84153 |
| I     | 244     | ILE      | MET    | SEE REMARK 999 | UNP P84153 |

- Molecule 4 is a protein called CYTOCHROME C OXIDASE.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 4   | D     | 42       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 311   | 203 | 52 | 54 | 2 |         |         |       |
| 4   | J     | 42       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 311   | 203 | 52 | 54 | 2 |         |         |       |

- Molecule 5 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 5   | A     | 1        | Total | Cu | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 5   | B     | 2        | Total | Cu | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 5   | G     | 1        | Total | Cu | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 5   | H     | 2        | Total | Cu | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 6   | A     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

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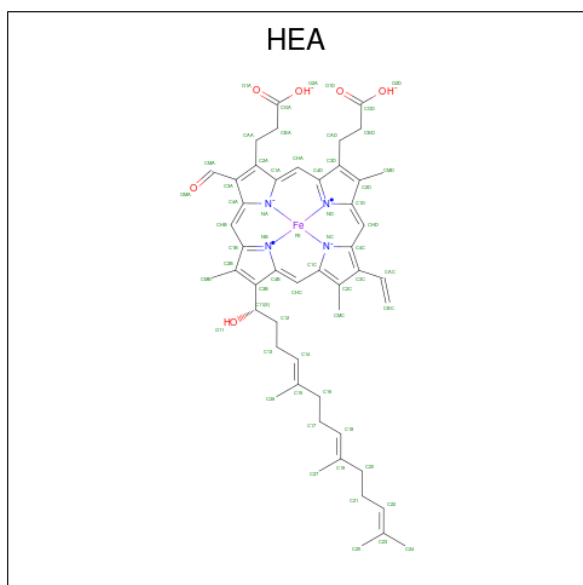
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| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 6   | G     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

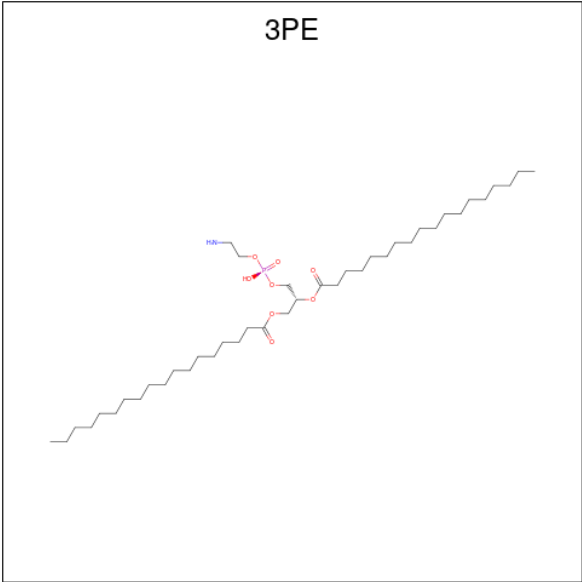
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 7   | A     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 7   | G     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 8 is HEME-A (CCD ID: HEA) (formula: C<sub>49</sub>H<sub>56</sub>FeN<sub>4</sub>O<sub>6</sub>).



| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 8   | A     | 1        | Total<br>60 | C<br>49 | Fe<br>1 | N<br>4 | O<br>6 | 0       | 0       |
| 8   | A     | 1        | Total<br>60 | C<br>49 | Fe<br>1 | N<br>4 | O<br>6 | 0       | 0       |
| 8   | G     | 1        | Total<br>60 | C<br>49 | Fe<br>1 | N<br>4 | O<br>6 | 0       | 0       |
| 8   | G     | 1        | Total<br>60 | C<br>49 | Fe<br>1 | N<br>4 | O<br>6 | 0       | 0       |

- Molecule 9 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C<sub>41</sub>H<sub>82</sub>NO<sub>8</sub>P).



| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 9   | A     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |         |
| 9   | A     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |         |
| 9   | C     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |         |
| 9   | C     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |         |
| 9   | C     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |         |
| 9   | D     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |         |
| 9   | G     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |         |
| 9   | G     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |         |
| 9   | I     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |         |
| 9   | I     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |         |
| 9   | I     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |         |
| 9   | J     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |         |

- Molecule 10 is water.

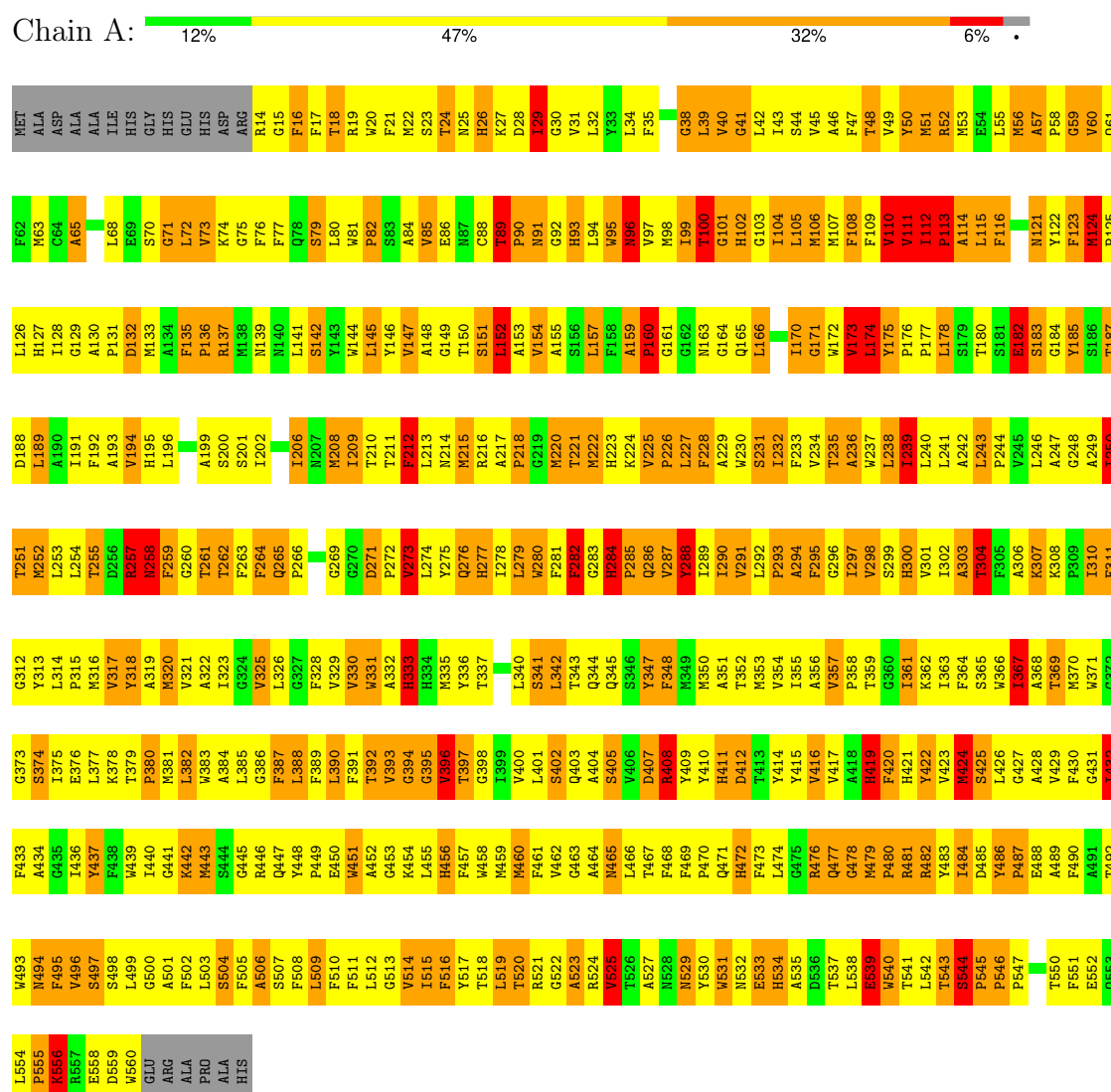
| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 10  | A     | 97       | Total<br>97  | O<br>97  | 0       | 0       |
| 10  | B     | 70       | Total<br>70  | O<br>70  | 0       | 0       |
| 10  | C     | 38       | Total<br>38  | O<br>38  | 0       | 0       |
| 10  | D     | 13       | Total<br>13  | O<br>13  | 0       | 0       |
| 10  | G     | 107      | Total<br>107 | O<br>107 | 0       | 0       |
| 10  | H     | 64       | Total<br>64  | O<br>64  | 0       | 0       |
| 10  | I     | 37       | Total<br>37  | O<br>37  | 0       | 0       |
| 10  | J     | 10       | Total<br>10  | O<br>10  | 0       | 0       |

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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.

Note EDS was not executed.

#### • Molecule 1: CYTOCHROME C OXIDASE



#### • Molecule 1: CYTOCHROME C OXIDASE



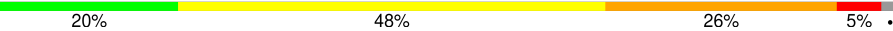
|     |      |      |      |      |      |      |      |      |      |
|-----|------|------|------|------|------|------|------|------|------|
| MET | Q61  | F123 | T187 | G248 | K308 | M370 | G431 | T492 | L554 |
| ALA | P62  | M124 | D188 | A249 | P309 | G373 | F432 | W493 | P555 |
| ASP | M63  | P125 | L189 | I250 | F311 | G374 | F433 | W494 | K556 |
| ALA | C64  | L126 | A190 | T251 | G312 | S374 | A434 | F495 | K557 |
| ALA | A65  | H127 | I191 | M252 | G312 | I375 | G435 | W496 | E558 |
| ILE | E66  | F128 | F192 | L253 | Y313 | E376 | I436 | S497 | D559 |
| HIS | H67  | G129 | A193 | L254 | L314 | L377 | Y437 | S498 | W560 |
| GLY | L68  | A130 | H195 | T255 | P315 | K378 | F438 | L499 | GLU  |
| HIS | P69  | P131 | H195 | D256 | M316 | T379 | G441 | G500 | ARG  |
| GLU | S70  | D132 | G198 | N257 | V317 | P380 | A442 | A501 | ALA  |
| HIS | G71  | M133 | A199 | N258 | Y318 | M381 | P443 | F502 | PRO  |
| ASP | L72  | D134 | A199 | F259 | A319 | L382 | M443 | P503 | ALA  |
| ARG | W73  | F135 | S200 | G260 | M320 | H383 | S444 | S504 | HIS  |
| R14 | K74  | P136 | S201 | T261 | V321 | A384 | G445 | F505 |      |
| G15 | G75  | L137 | S202 | T262 | A322 | L385 | R446 | A506 |      |
| F16 | F76  | M138 | L203 | F263 | I323 | G386 | Q447 | S507 |      |
| F17 | F77  | M139 | G204 | F264 | G324 | F387 | Y448 | F508 |      |
| T18 | Q78  | A84  | A205 | Q265 | V325 | L388 | P449 | F509 |      |
| R19 | S79  | L141 | T206 | P266 | L326 | F389 | E450 | F510 |      |
| W20 | L80  | S142 | W207 | S267 | G327 | L390 | W451 | F511 |      |
| F21 | W81  | Y143 | P208 | G268 | F328 | F391 | A452 | L512 |      |
| M22 | P82  | M144 | T209 | G269 | V329 | T392 | G453 | G513 |      |
| S23 | S83  | L145 | T210 | G270 | V330 | V393 | K454 | V514 |      |
| T24 | A84  | Y146 | T211 | D271 | W331 | G394 | L455 | I515 |      |
| N25 | W85  | Y147 | E212 | P272 | A332 | G395 | H456 | F516 |      |
| H26 | E86  | A148 | L213 | V273 | H333 | V396 | F457 | Y517 |      |
| K27 | N87  |      | M214 | L274 | H334 | T397 | W458 | L518 |      |
| D28 | C88  | L152 | R216 | Q276 | M335 | G398 | M459 | L519 |      |
| G30 | T89  | L152 | R216 | Q276 | M335 | G398 | M459 | L519 |      |
| V31 | N91  | A155 | P218 | H277 | T337 | V400 | W460 | T520 |      |
| L32 | G92  | L156 | Q219 | L278 | L401 | V462 | G463 | G522 |      |
| L33 | H93  | L157 | M220 | L279 | S411 | G464 | A623 | A523 |      |
| F35 | L94  | F158 | T221 | W280 | L342 | Q403 | G524 | G525 |      |
| T36 | N95  | A159 | M222 | F281 | T343 | A404 | L465 | V525 |      |
| G37 | N96  | P160 | H223 | G283 | Q345 | V406 | T467 | N529 |      |
| G38 | N97  |      | K224 | H284 | S346 | D407 | F468 | Y530 |      |
| L39 | N98  | N163 | V225 | P285 | Y347 | R408 | F469 | M531 |      |
| V40 | I99  | G164 | P226 | Q286 | F348 | Y409 | F470 | M532 |      |
| G41 | T100 | Q165 | L227 | V287 | M349 | Y410 | Q471 | E533 |      |
| L42 | G101 |      | F228 | G287 | H411 | H412 | H473 | H534 |      |
| G43 | H102 | S168 | A229 | Y288 | A351 | D412 | F474 | A535 |      |
| S44 | G103 | G169 | W230 | L290 | T352 | T413 | L474 | D536 |      |
| V45 | L104 | I170 | S231 | Y291 | M353 | Y414 | G475 | T537 |      |
| A46 | M106 | G171 | L232 | L292 | V364 | Y415 | R476 | L538 |      |
| F47 | M107 | W172 | F233 | P293 | I355 | V416 | Q477 | E539 |      |
| V48 | F108 | V173 | V234 | A294 | A366 | G478 | M479 | W540 |      |
| T49 | L174 | L174 | T235 | F295 | V357 | A418 | P480 | T541 |      |
| V49 | Y175 | A236 | A236 | G296 | P358 | H419 | P481 | L542 |      |
| Y50 | V110 | W237 | P176 | I297 | T359 | F420 | R481 | T543 |      |
| M51 | V111 | P177 | L238 | V298 | G360 | H421 | R482 | S544 |      |
| R52 | I112 | L178 | T239 | S299 | I361 | Y422 | Y483 | P545 |      |
| M53 | P113 | S179 | L240 | H300 | K362 | Y423 | I484 | P546 |      |
| E54 | L114 | T180 | L241 | V301 | I363 | M424 | D485 | P547 |      |
| L55 | L115 | S181 | A242 | I302 | S364 | S425 | Y486 | E548 |      |
| M56 | F116 | E182 | L243 | A303 | S365 | L426 | Y487 | H549 |      |
| A57 | G120 | S183 | P244 | T304 | W366 | G427 | E488 | T550 |      |
| P88 | M121 | G184 | V245 | F305 | I367 | A428 | A489 | F551 |      |
| G59 | G120 | A185 | L246 | A306 | I367 | F429 | F490 | E552 |      |
| V60 | Y122 | S186 | A247 | K307 | T369 | F430 | A491 | Q553 |      |

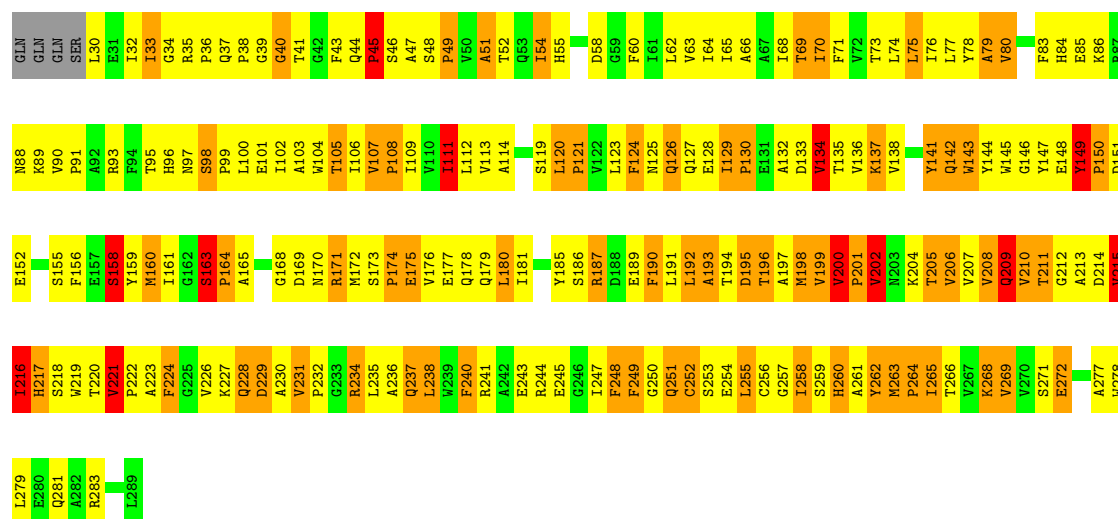
• Molecule 2: CYTOCHROME C OXIDASE

Chain B:  23% 47% 23% 6%

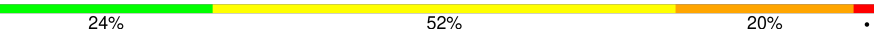
|      |      |      |      |      |
|------|------|------|------|------|
| GLN  | R87  | D151 | H217 | Y278 |
| GLN  | R88  | E152 | S218 | L279 |
| GLN  | R89  |      | W219 | E280 |
| SER  | V90  | F156 | T220 | Q281 |
| L30  | P91  | S157 | V221 | A282 |
| E31  | A92  | S158 | P222 | R283 |
| D59  | R93  | Y159 | A223 |      |
| W560 |      | M160 | F224 | T286 |
| GLU  | N97  | I161 | G225 |      |
| ARG  | S98  | G162 | W226 | L289 |
| ALA  | P99  | S163 | K227 |      |
| PRO  | L100 | P164 | Q228 |      |
| ALA  | E101 | A165 | D229 |      |
| HIS  | I102 | T166 | A230 |      |
|      | A103 | G167 | V231 |      |
|      | G40  | T104 | P232 |      |
|      | T41  | G168 | R233 |      |
|      | G42  | D169 | G234 |      |
|      | T106 | N170 | R234 |      |
|      | F43  | L176 | L235 |      |
|      | Q44  | R171 | L235 |      |
|      | P45  | M172 | A236 |      |
|      | I109 | S173 | Q237 |      |
|      | S48  | P174 | L238 |      |
|      | P49  | E175 | W239 |      |
|      | V110 | T111 | G240 |      |
|      | L112 | V112 | R241 |      |
|      | L113 | E177 | A242 |      |
|      | A51  | Q178 | E243 |      |
|      | T52  | L115 | R244 |      |
|      | Q53  | G116 | E245 |      |
|      | H55  | A117 | G246 |      |
|      | W56  | F118 | L247 |      |
|      | L61  | S119 | R187 |      |
|      | L62  | L120 | D188 |      |
|      | V63  | G59  | E189 |      |
|      | I64  | F60  | F190 |      |
|      | L65  | L123 | I61  |      |
|      | L66  | F124 | L191 |      |
|      | A67  | N125 | A193 |      |
|      | T69  | Q126 | T194 |      |
|      | L70  | Q127 | L195 |      |
|      | F71  | E128 | T196 |      |
|      | V72  | I129 | A197 |      |
|      | T73  | A132 | M198 |      |
|      | L74  | D133 | V199 |      |
|      | T541 | V134 | W200 |      |
|      | L75  | T135 | P201 |      |
|      | L76  | V136 | W202 |      |
|      | L77  | W137 | N203 |      |
|      | L78  | R138 | K204 |      |
|      | L79  | V138 | A137 |      |
|      | L80  | V139 | T205 |      |
|      | L81  | V140 | W206 |      |
|      | L82  | V141 | W207 |      |
|      | L83  | Q142 | V208 |      |
|      | L84  | V143 | Q209 |      |
|      | L85  | Y144 | W210 |      |
|      | L86  | V145 | V211 |      |
|      | L87  | G146 | T211 |      |
|      | L88  | Y147 | G212 |      |
|      | L89  | E148 | A213 |      |
|      | L90  | F149 | D214 |      |
|      | L91  | E150 | V215 |      |
|      | L92  | P150 | I216 |      |

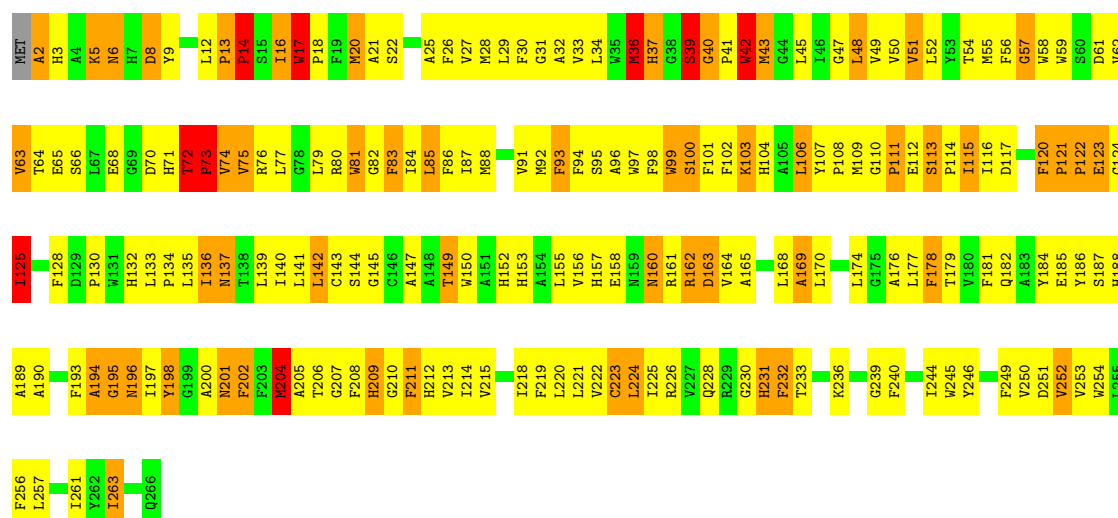
• Molecule 2: CYTOCHROME C OXIDASE

Chain H: 

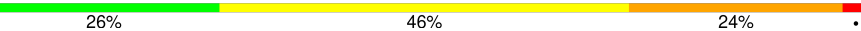


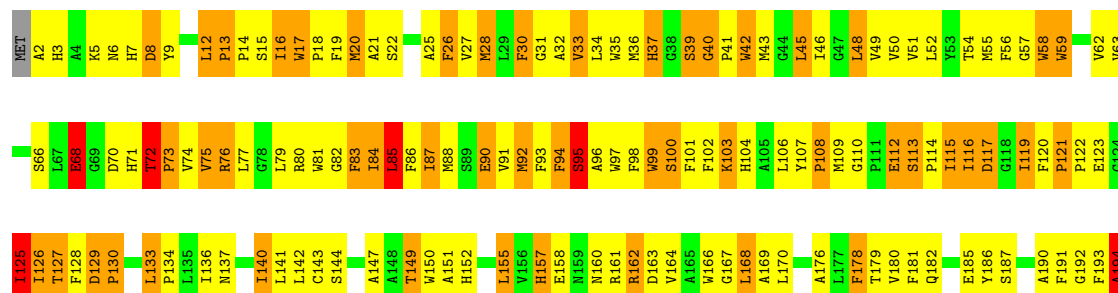
### • Molecule 3: CYTOCHROME C OXIDASE

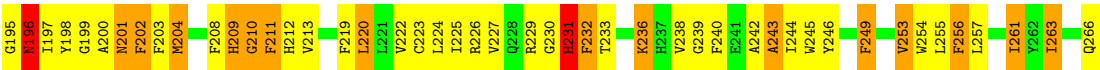
Chain C: 



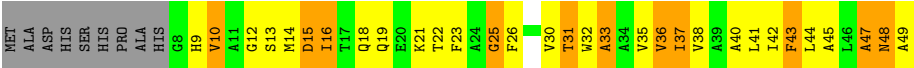
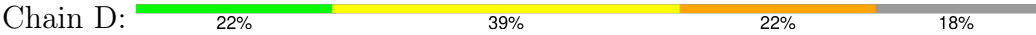
### • Molecule 3: CYTOCHROME C OXIDASE

Chain I: 

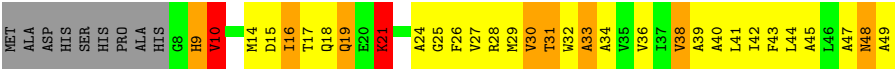
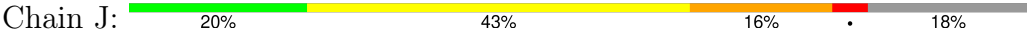




• Molecule 4: CYTOCHROME C OXIDASE



• Molecule 4: CYTOCHROME C OXIDASE



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

| Property                                                 | Value                                                      | Source    |
|----------------------------------------------------------|------------------------------------------------------------|-----------|
| Space group                                              | H 3                                                        | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 340.72 Å   340.72 Å   89.76 Å<br>90.00°   90.00°   120.00° | Depositor |
| Resolution (Å)                                           | 4.00 – 3.00                                                | Depositor |
| % Data completeness<br>(in resolution range)             | (Not available) (4.00-3.00)                                | Depositor |
| $R_{merge}$                                              | (Not available)                                            | Depositor |
| $R_{sym}$                                                | (Not available)                                            | Depositor |
| Refinement program                                       | REFMAC                                                     | Depositor |
| R, $R_{free}$                                            | 0.293 , 0.329                                              | Depositor |
| Estimated twinning fraction                              | No twinning to report.                                     | Xtriage   |
| Total number of atoms                                    | 18934                                                      | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 26.0                                                       | wwPDB-VP  |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEA, MG, CA, CU, 3PE

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

| Mol | Chain | Bond lengths |                | Bond angles |                   |
|-----|-------|--------------|----------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5           |
| 1   | A     | 0.90         | 2/4482 (0.0%)  | 2.58        | 345/6114 (5.6%)   |
| 1   | G     | 0.94         | 4/4482 (0.1%)  | 2.62        | 381/6114 (6.2%)   |
| 2   | B     | 0.75         | 0/2105         | 2.46        | 149/2879 (5.2%)   |
| 2   | H     | 0.83         | 0/2105         | 2.52        | 159/2879 (5.5%)   |
| 3   | C     | 0.68         | 0/2232         | 2.10        | 107/3054 (3.5%)   |
| 3   | I     | 0.71         | 0/2232         | 2.11        | 104/3054 (3.4%)   |
| 4   | D     | 0.70         | 0/316          | 2.15        | 15/428 (3.5%)     |
| 4   | J     | 0.70         | 0/316          | 2.21        | 13/428 (3.0%)     |
| All | All   | 0.83         | 6/18270 (0.0%) | 2.45        | 1273/24950 (5.1%) |

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     | 0                   | 19                  |
| 1   | G     | 0                   | 16                  |
| 2   | B     | 0                   | 6                   |
| 2   | H     | 0                   | 3                   |
| 3   | C     | 0                   | 5                   |
| 3   | I     | 0                   | 7                   |
| 4   | D     | 0                   | 1                   |
| All | All   | 0                   | 57                  |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | G     | 112 | ILE  | N-CA  | 8.07  | 1.56        | 1.46     |
| 1   | A     | 111 | VAL  | C-N   | -6.89 | 1.25        | 1.33     |
| 1   | G     | 543 | THR  | C-N   | -6.24 | 1.24        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | G     | 171 | GLY  | C-N     | 5.64  | 1.41        | 1.33     |
| 1   | G     | 277 | HIS  | CE1-NE2 | 5.25  | 1.37        | 1.32     |
| 1   | A     | 543 | THR  | C-N     | -5.16 | 1.26        | 1.33     |

All (1273) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1   | A     | 543 | THR  | CA-C-N    | 26.72  | 169.80      | 121.70   |
| 1   | A     | 543 | THR  | C-N-CA    | 26.72  | 169.80      | 121.70   |
| 1   | G     | 543 | THR  | CA-C-N    | 22.95  | 163.02      | 121.70   |
| 1   | G     | 543 | THR  | C-N-CA    | 22.95  | 163.02      | 121.70   |
| 1   | G     | 170 | ILE  | CB-CA-C   | -16.65 | 96.23       | 111.05   |
| 2   | B     | 129 | ILE  | N-CA-C    | 16.25  | 122.60      | 108.63   |
| 2   | H     | 252 | CYS  | N-CA-CB   | 14.60  | 131.87      | 109.83   |
| 1   | G     | 534 | HIS  | CA-CB-CG  | -14.58 | 99.22       | 113.80   |
| 1   | A     | 271 | ASP  | CA-CB-CG  | 14.36  | 126.96      | 112.60   |
| 1   | A     | 284 | HIS  | CA-CB-CG  | -14.34 | 99.47       | 113.80   |
| 1   | G     | 545 | PRO  | N-CA-CB   | 14.13  | 116.79      | 103.08   |
| 1   | G     | 172 | TRP  | CA-CB-CG  | 14.08  | 140.35      | 113.60   |
| 1   | A     | 172 | TRP  | CA-CB-CG  | 13.72  | 139.67      | 113.60   |
| 1   | G     | 175 | TYR  | CA-CB-CG  | 13.35  | 137.92      | 113.90   |
| 4   | J     | 48  | ASN  | CA-CB-CG  | -12.80 | 99.80       | 112.60   |
| 1   | G     | 544 | SER  | CA-C-O    | -12.72 | 99.18       | 120.80   |
| 1   | A     | 534 | HIS  | CA-CB-CG  | -12.59 | 101.21      | 113.80   |
| 1   | G     | 333 | HIS  | CA-CB-CG  | 12.45  | 126.25      | 113.80   |
| 1   | G     | 420 | PHE  | CA-CB-CG  | 12.45  | 126.25      | 113.80   |
| 1   | G     | 52  | ARG  | NE-CZ-NH2 | -12.37 | 108.07      | 119.20   |
| 1   | A     | 106 | MET  | CA-CB-CG  | -12.29 | 89.52       | 114.10   |
| 1   | G     | 111 | VAL  | CA-C-N    | -12.25 | 99.47       | 122.13   |
| 1   | G     | 111 | VAL  | C-N-CA    | -12.25 | 99.47       | 122.13   |
| 2   | B     | 216 | ILE  | CA-C-O    | -12.18 | 107.50      | 120.53   |
| 2   | H     | 216 | ILE  | CA-C-O    | -12.17 | 107.51      | 120.53   |
| 1   | A     | 420 | PHE  | CA-CB-CG  | 11.96  | 125.77      | 113.80   |
| 1   | G     | 284 | HIS  | CA-CB-CG  | -11.84 | 101.96      | 113.80   |
| 1   | A     | 544 | SER  | CA-C-O    | -11.77 | 100.79      | 120.80   |
| 2   | B     | 89  | LYS  | CA-C-N    | -11.44 | 113.37      | 123.33   |
| 2   | B     | 89  | LYS  | C-N-CA    | -11.44 | 113.37      | 123.33   |
| 2   | B     | 240 | PHE  | CA-CB-CG  | 11.26  | 125.06      | 113.80   |
| 1   | G     | 106 | MET  | CA-CB-CG  | -11.20 | 91.70       | 114.10   |
| 1   | A     | 173 | VAL  | CA-C-O    | 11.16  | 131.03      | 119.20   |
| 3   | C     | 128 | PHE  | CA-CB-CG  | 11.14  | 124.94      | 113.80   |
| 1   | G     | 412 | ASP  | CA-CB-CG  | -11.13 | 101.47      | 112.60   |

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| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | A     | 545 | PRO  | N-CA-CB    | 11.11  | 113.85      | 103.08   |
| 1   | G     | 543 | THR  | N-CA-C     | -11.07 | 96.79       | 110.41   |
| 1   | G     | 26  | HIS  | CA-CB-CG   | -11.06 | 102.74      | 113.80   |
| 1   | A     | 26  | HIS  | CA-CB-CG   | -11.04 | 102.76      | 113.80   |
| 1   | A     | 194 | VAL  | CA-C-O     | -10.96 | 110.01      | 121.41   |
| 1   | A     | 351 | ALA  | CA-C-O     | -10.95 | 108.81      | 120.63   |
| 1   | A     | 449 | PRO  | N-CA-CB    | 10.94  | 110.56      | 103.23   |
| 1   | G     | 213 | LEU  | CA-C-O     | 10.90  | 132.36      | 119.60   |
| 1   | A     | 175 | TYR  | CA-C-O     | -10.77 | 109.54      | 120.64   |
| 1   | G     | 170 | ILE  | N-CA-CB    | -10.72 | 102.85      | 111.64   |
| 1   | G     | 271 | ASP  | CA-CB-CG   | 10.70  | 123.30      | 112.60   |
| 3   | C     | 8   | ASP  | CA-CB-CG   | 10.62  | 123.22      | 112.60   |
| 1   | A     | 325 | VAL  | CA-C-O     | -10.53 | 110.03      | 121.29   |
| 1   | G     | 486 | TYR  | CA-C-O     | 10.49  | 129.99      | 120.34   |
| 1   | A     | 333 | HIS  | CA-CB-CG   | 10.41  | 124.21      | 113.80   |
| 1   | G     | 170 | ILE  | O-C-N      | 10.38  | 129.97      | 121.98   |
| 2   | H     | 137 | LYS  | N-CA-CB    | 10.37  | 127.68      | 110.77   |
| 1   | G     | 172 | TRP  | N-CA-CB    | 10.36  | 126.67      | 109.78   |
| 1   | G     | 223 | HIS  | CA-CB-CG   | -10.24 | 103.56      | 113.80   |
| 1   | A     | 300 | HIS  | CA-CB-CG   | -10.21 | 103.59      | 113.80   |
| 3   | I     | 94  | PHE  | CA-CB-CG   | -10.19 | 103.61      | 113.80   |
| 2   | B     | 60  | PHE  | CA-CB-CG   | 10.18  | 123.98      | 113.80   |
| 1   | A     | 159 | ALA  | CA-C-O     | 10.16  | 131.63      | 120.97   |
| 1   | A     | 544 | SER  | CA-C-N     | 10.15  | 130.84      | 120.38   |
| 1   | A     | 544 | SER  | C-N-CA     | 10.15  | 130.84      | 120.38   |
| 1   | G     | 552 | GLU  | N-CA-C     | -10.15 | 99.77       | 111.03   |
| 1   | A     | 111 | VAL  | CA-C-O     | -10.14 | 108.11      | 120.78   |
| 2   | B     | 171 | ARG  | CD-NE-CZ   | 10.13  | 138.59      | 124.40   |
| 2   | H     | 240 | PHE  | CA-CB-CG   | 10.10  | 123.90      | 113.80   |
| 1   | A     | 111 | VAL  | O-C-N      | -10.10 | 109.95      | 122.57   |
| 3   | C     | 113 | SER  | CA-C-O     | 10.07  | 129.88      | 119.80   |
| 1   | A     | 109 | PHE  | CA-CB-CG   | -9.90  | 103.90      | 113.80   |
| 1   | G     | 110 | VAL  | CA-CB-CG2  | 9.85   | 127.15      | 110.40   |
| 1   | A     | 552 | GLU  | N-CA-C     | -9.79  | 99.64       | 111.69   |
| 1   | G     | 442 | LYS  | CA-C-O     | -9.76  | 110.09      | 120.63   |
| 2   | B     | 152 | GLU  | CB-CG-CD   | 9.74   | 129.15      | 112.60   |
| 1   | G     | 170 | ILE  | N-CA-C     | 9.69   | 119.27      | 111.62   |
| 3   | I     | 115 | ILE  | N-CA-C     | -9.62  | 100.97      | 110.30   |
| 3   | I     | 119 | ILE  | CB-CA-C    | -9.60  | 96.42       | 110.63   |
| 1   | G     | 236 | ALA  | CA-C-O     | -9.60  | 110.27      | 120.63   |
| 2   | B     | 169 | ASP  | CA-CB-CG   | 9.56   | 122.16      | 112.60   |
| 1   | G     | 91  | ASN  | OD1-CG-ND2 | -9.48  | 113.12      | 122.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | H     | 163 | SER  | CA-C-N     | 9.46  | 129.09      | 119.82   |
| 2   | H     | 163 | SER  | C-N-CA     | 9.46  | 129.09      | 119.82   |
| 2   | H     | 152 | GLU  | CB-CG-CD   | 9.44  | 128.65      | 112.60   |
| 2   | B     | 143 | TRP  | CB-CA-C    | 9.43  | 129.19      | 110.42   |
| 1   | G     | 165 | GLN  | OE1-CD-NE2 | -9.34 | 113.26      | 122.60   |
| 1   | A     | 313 | TYR  | CA-C-O     | -9.31 | 110.94      | 120.90   |
| 1   | A     | 173 | VAL  | O-C-N      | -9.25 | 112.95      | 122.20   |
| 2   | H     | 164 | PRO  | CA-C-N     | 9.23  | 133.85      | 120.38   |
| 2   | H     | 164 | PRO  | C-N-CA     | 9.23  | 133.85      | 120.38   |
| 1   | G     | 419 | HIS  | CA-C-N     | -9.22 | 108.09      | 120.63   |
| 1   | G     | 419 | HIS  | C-N-CA     | -9.22 | 108.09      | 120.63   |
| 2   | H     | 169 | ASP  | CA-CB-CG   | 9.21  | 121.81      | 112.60   |
| 2   | B     | 231 | VAL  | CA-C-O     | 9.19  | 124.72      | 119.94   |
| 1   | G     | 95  | TRP  | CA-C-O     | -9.18 | 110.64      | 120.92   |
| 2   | H     | 215 | VAL  | CA-C-N     | -9.13 | 111.25      | 123.12   |
| 2   | H     | 215 | VAL  | C-N-CA     | -9.13 | 111.25      | 123.12   |
| 2   | B     | 249 | PHE  | N-CA-C     | 9.10  | 123.25      | 108.41   |
| 1   | G     | 252 | MET  | CA-C-O     | -9.07 | 110.04      | 120.20   |
| 3   | I     | 113 | SER  | CA-C-O     | 9.07  | 127.10      | 119.66   |
| 2   | B     | 252 | CYS  | N-CA-CB    | 9.03  | 123.51      | 109.69   |
| 4   | D     | 30  | VAL  | N-CA-CB    | -9.03 | 101.14      | 110.62   |
| 3   | I     | 196 | ASN  | CA-CB-CG   | -8.97 | 103.63      | 112.60   |
| 1   | G     | 545 | PRO  | CA-N-CD    | -8.96 | 99.45       | 112.00   |
| 3   | I     | 40  | GLY  | CA-C-N     | 8.93  | 129.50      | 119.32   |
| 3   | I     | 40  | GLY  | C-N-CA     | 8.93  | 129.50      | 119.32   |
| 1   | A     | 105 | LEU  | CA-C-O     | 8.91  | 130.35      | 121.00   |
| 1   | A     | 282 | PHE  | CA-CB-CG   | -8.89 | 104.91      | 113.80   |
| 1   | G     | 288 | TYR  | CA-CB-CG   | -8.89 | 97.91       | 113.90   |
| 1   | A     | 194 | VAL  | O-C-N      | 8.87  | 131.54      | 121.96   |
| 1   | A     | 109 | PHE  | CA-C-O     | 8.86  | 129.25      | 119.24   |
| 1   | A     | 545 | PRO  | CA-N-CD    | -8.82 | 99.64       | 112.00   |
| 2   | B     | 107 | VAL  | CA-CB-CG1  | 8.80  | 125.36      | 110.40   |
| 1   | A     | 170 | ILE  | CB-CA-C    | -8.79 | 96.88       | 111.29   |
| 1   | A     | 14  | ARG  | NE-CZ-NH2  | 8.74  | 127.06      | 119.20   |
| 1   | A     | 285 | PRO  | O-C-N      | -8.72 | 110.87      | 122.64   |
| 1   | A     | 280 | TRP  | CA-C-O     | -8.66 | 110.02      | 119.97   |
| 1   | A     | 541 | THR  | CA-CB-OG1  | -8.66 | 96.61       | 109.60   |
| 1   | G     | 300 | HIS  | CA-CB-CG   | -8.65 | 105.14      | 113.80   |
| 2   | H     | 262 | TYR  | CA-C-N     | -8.65 | 113.34      | 122.85   |
| 2   | H     | 262 | TYR  | C-N-CA     | -8.65 | 113.34      | 122.85   |
| 1   | A     | 175 | TYR  | CA-CB-CG   | 8.64  | 129.45      | 113.90   |
| 1   | A     | 290 | ILE  | CA-C-O     | -8.64 | 112.29      | 121.27   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | H     | 231 | VAL  | CA-C-O    | 8.62  | 124.42      | 119.94   |
| 3   | C     | 94  | PHE  | CA-CB-CG  | -8.57 | 105.23      | 113.80   |
| 2   | B     | 145 | TRP  | CA-C-O    | -8.56 | 110.77      | 121.55   |
| 3   | I     | 37  | HIS  | CA-CB-CG  | -8.56 | 105.24      | 113.80   |
| 2   | B     | 269 | VAL  | CB-CA-C   | 8.55  | 121.97      | 110.42   |
| 2   | H     | 171 | ARG  | CD-NE-CZ  | 8.55  | 136.37      | 124.40   |
| 2   | H     | 143 | TRP  | CB-CA-C   | 8.54  | 123.25      | 111.63   |
| 1   | A     | 449 | PRO  | CB-CA-C   | -8.54 | 103.63      | 111.40   |
| 1   | G     | 257 | ARG  | CA-C-N    | -8.54 | 108.11      | 122.11   |
| 1   | G     | 257 | ARG  | C-N-CA    | -8.54 | 108.11      | 122.11   |
| 1   | G     | 374 | SER  | CA-C-O    | -8.52 | 111.12      | 120.92   |
| 1   | A     | 110 | VAL  | CA-C-O    | 8.50  | 131.40      | 120.78   |
| 2   | B     | 171 | ARG  | NE-CZ-NH1 | 8.50  | 130.00      | 121.50   |
| 1   | G     | 99  | ILE  | CB-CA-C   | -8.48 | 97.38       | 111.29   |
| 2   | B     | 258 | ILE  | N-CA-C    | 8.42  | 118.50      | 110.42   |
| 3   | I     | 202 | PHE  | CA-CB-CG  | -8.39 | 105.41      | 113.80   |
| 1   | A     | 387 | PHE  | CA-CB-CG  | -8.38 | 105.42      | 113.80   |
| 1   | G     | 236 | ALA  | N-CA-CB   | 8.38  | 122.62      | 110.06   |
| 3   | I     | 117 | ASP  | CA-CB-CG  | -8.37 | 104.23      | 112.60   |
| 1   | A     | 282 | PHE  | CA-C-O    | 8.32  | 127.88      | 118.97   |
| 1   | G     | 317 | VAL  | CA-C-O    | -8.31 | 112.40      | 121.29   |
| 1   | A     | 328 | PHE  | CA-C-O    | -8.30 | 109.69      | 119.15   |
| 3   | I     | 191 | PHE  | CA-CB-CG  | -8.28 | 105.52      | 113.80   |
| 1   | G     | 387 | PHE  | CA-CB-CG  | -8.27 | 105.53      | 113.80   |
| 3   | I     | 8   | ASP  | CA-CB-CG  | 8.26  | 120.86      | 112.60   |
| 1   | A     | 206 | ILE  | CA-C-O    | 8.25  | 129.92      | 121.17   |
| 1   | A     | 226 | PRO  | CA-C-O    | -8.25 | 112.19      | 121.43   |
| 2   | H     | 89  | LYS  | CA-C-N    | -8.24 | 116.16      | 123.33   |
| 2   | H     | 89  | LYS  | C-N-CA    | -8.24 | 116.16      | 123.33   |
| 1   | A     | 411 | HIS  | CA-CB-CG  | -8.24 | 105.56      | 113.80   |
| 1   | A     | 286 | GLN  | CA-C-O    | -8.24 | 111.38      | 121.02   |
| 3   | I     | 158 | GLU  | CA-C-O    | 8.24  | 127.94      | 118.55   |
| 1   | G     | 331 | TRP  | N-CA-C    | 8.23  | 122.75      | 112.87   |
| 1   | G     | 360 | GLY  | CA-C-O    | 8.23  | 129.22      | 120.75   |
| 1   | A     | 259 | PHE  | CA-CB-CG  | -8.21 | 105.59      | 113.80   |
| 1   | G     | 348 | PHE  | N-CA-C    | 8.21  | 121.15      | 111.71   |
| 2   | H     | 35  | ARG  | O-C-N     | -8.21 | 115.42      | 121.83   |
| 4   | J     | 10  | VAL  | CA-C-O    | 8.21  | 131.04      | 120.78   |
| 3   | C     | 83  | PHE  | CA-CB-CG  | -8.18 | 105.62      | 113.80   |
| 1   | A     | 364 | PHE  | CA-CB-CG  | -8.16 | 105.64      | 113.80   |
| 1   | A     | 380 | PRO  | CB-CA-C   | 8.12  | 124.96      | 111.56   |
| 2   | B     | 82  | ARG  | CD-NE-CZ  | 8.12  | 135.76      | 124.40   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 225 | VAL  | CA-C-N     | 8.09  | 128.15      | 119.89   |
| 1   | A     | 225 | VAL  | C-N-CA     | 8.09  | 128.15      | 119.89   |
| 1   | G     | 474 | LEU  | CA-C-O     | 8.06  | 129.23      | 120.20   |
| 1   | G     | 276 | GLN  | OE1-CD-NE2 | 8.03  | 130.63      | 122.60   |
| 1   | G     | 407 | ASP  | CA-CB-CG   | -8.02 | 104.58      | 112.60   |
| 1   | A     | 227 | LEU  | CA-C-O     | 8.01  | 129.41      | 121.00   |
| 2   | H     | 192 | LEU  | N-CA-C     | 8.00  | 123.34      | 113.50   |
| 1   | G     | 287 | VAL  | CA-C-N     | -8.00 | 107.36      | 120.72   |
| 1   | G     | 287 | VAL  | C-N-CA     | -8.00 | 107.36      | 120.72   |
| 1   | A     | 96  | ASN  | OD1-CG-ND2 | 8.00  | 130.60      | 122.60   |
| 1   | G     | 419 | HIS  | O-C-N      | 7.99  | 130.59      | 122.12   |
| 3   | I     | 94  | PHE  | CA-C-O     | -7.98 | 111.09      | 120.10   |
| 1   | A     | 442 | LYS  | CA-C-O     | -7.95 | 112.39      | 120.90   |
| 2   | B     | 135 | THR  | CB-CA-C    | -7.94 | 100.78      | 110.94   |
| 1   | A     | 297 | ILE  | CA-C-O     | -7.92 | 112.77      | 121.17   |
| 1   | A     | 91  | ASN  | OD1-CG-ND2 | -7.92 | 114.68      | 122.60   |
| 1   | A     | 59  | GLY  | CA-C-N     | -7.91 | 112.35      | 123.11   |
| 1   | A     | 59  | GLY  | C-N-CA     | -7.91 | 112.35      | 123.11   |
| 1   | A     | 173 | VAL  | N-CA-CB    | -7.90 | 100.06      | 112.07   |
| 3   | C     | 14  | PRO  | N-CA-CB    | 7.90  | 111.54      | 103.25   |
| 1   | G     | 265 | GLN  | OE1-CD-NE2 | 7.88  | 130.48      | 122.60   |
| 2   | B     | 35  | ARG  | NH1-CZ-NH2 | 7.87  | 129.54      | 119.30   |
| 1   | G     | 478 | GLY  | N-CA-C     | 7.87  | 125.77      | 115.47   |
| 1   | A     | 265 | GLN  | CA-C-O     | 7.86  | 129.88      | 121.00   |
| 1   | G     | 50  | TYR  | O-C-N      | 7.84  | 130.46      | 122.08   |
| 2   | H     | 231 | VAL  | CB-CA-C    | -7.81 | 102.27      | 110.16   |
| 1   | A     | 214 | ASN  | CA-C-O     | -7.81 | 111.11      | 120.56   |
| 1   | A     | 331 | TRP  | CA-C-O     | -7.81 | 110.40      | 119.61   |
| 1   | G     | 159 | ALA  | CA-C-N     | 7.81  | 129.60      | 119.84   |
| 1   | G     | 159 | ALA  | C-N-CA     | 7.81  | 129.60      | 119.84   |
| 1   | A     | 132 | ASP  | O-C-N      | -7.80 | 115.07      | 123.26   |
| 2   | H     | 160 | MET  | CA-C-O     | -7.80 | 112.97      | 121.94   |
| 2   | H     | 214 | ASP  | N-CA-CB    | -7.80 | 97.31       | 110.49   |
| 1   | G     | 234 | VAL  | CA-CB-CG1  | 7.79  | 123.64      | 110.40   |
| 1   | G     | 52  | ARG  | NH1-CZ-NH2 | 7.77  | 129.40      | 119.30   |
| 2   | H     | 214 | ASP  | O-C-N      | -7.76 | 112.27      | 122.59   |
| 1   | G     | 472 | HIS  | CA-CB-CG   | 7.76  | 121.56      | 113.80   |
| 1   | G     | 146 | TYR  | CA-C-O     | -7.75 | 112.26      | 120.63   |
| 1   | A     | 280 | TRP  | CA-CB-CG   | -7.73 | 98.91       | 113.60   |
| 2   | H     | 214 | ASP  | CA-CB-CG   | 7.70  | 120.30      | 112.60   |
| 1   | A     | 65  | ALA  | CA-C-O     | 7.69  | 128.86      | 119.79   |
| 2   | H     | 269 | VAL  | CB-CA-C    | 7.68  | 119.87      | 110.73   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 255 | THR  | CA-CB-OG1  | -7.66 | 98.11       | 109.60   |
| 1   | A     | 288 | TYR  | CA-CB-CG   | -7.66 | 100.12      | 113.90   |
| 1   | A     | 494 | ASN  | CA-CB-CG   | -7.65 | 104.95      | 112.60   |
| 2   | B     | 252 | CYS  | CB-CA-C    | -7.65 | 97.97       | 109.90   |
| 1   | A     | 229 | ALA  | N-CA-CB    | 7.65  | 122.13      | 110.28   |
| 1   | G     | 265 | GLN  | CA-C-O     | 7.64  | 129.64      | 121.00   |
| 1   | G     | 555 | PRO  | N-CA-CB    | 7.63  | 111.26      | 103.25   |
| 1   | A     | 112 | ILE  | CA-C-O     | -7.62 | 109.73      | 119.95   |
| 1   | A     | 132 | ASP  | CA-C-O     | 7.61  | 129.45      | 121.38   |
| 1   | A     | 159 | ALA  | O-C-N      | -7.61 | 112.00      | 121.21   |
| 1   | A     | 24  | THR  | N-CA-CB    | 7.59  | 121.35      | 110.88   |
| 1   | A     | 174 | LEU  | CA-C-O     | -7.59 | 112.55      | 122.03   |
| 3   | C     | 50  | VAL  | N-CA-C     | 7.58  | 118.35      | 110.62   |
| 1   | G     | 214 | ASN  | CA-C-O     | -7.58 | 111.39      | 120.56   |
| 2   | H     | 75  | LEU  | N-CA-CB    | 7.58  | 120.96      | 109.98   |
| 2   | H     | 93  | ARG  | CD-NE-CZ   | 7.58  | 135.00      | 124.40   |
| 3   | I     | 3   | HIS  | CA-CB-CG   | -7.57 | 106.23      | 113.80   |
| 2   | H     | 224 | PHE  | CA-CB-CG   | -7.56 | 106.24      | 113.80   |
| 1   | A     | 328 | PHE  | CA-CB-CG   | -7.55 | 106.25      | 113.80   |
| 1   | A     | 281 | PHE  | CA-CB-CG   | 7.55  | 121.35      | 113.80   |
| 1   | G     | 77  | PHE  | CA-CB-CG   | -7.55 | 106.25      | 113.80   |
| 2   | H     | 234 | ARG  | NE-CZ-NH2  | 7.54  | 125.99      | 119.20   |
| 2   | H     | 260 | HIS  | CB-CG-CD2  | 7.54  | 141.00      | 131.20   |
| 1   | G     | 18  | THR  | O-C-N      | 7.54  | 129.87      | 122.03   |
| 1   | G     | 305 | PHE  | CA-CB-CG   | -7.54 | 106.26      | 113.80   |
| 1   | A     | 288 | TYR  | N-CA-CB    | 7.53  | 124.02      | 110.32   |
| 2   | B     | 215 | VAL  | CA-C-N     | -7.52 | 113.34      | 123.12   |
| 2   | B     | 215 | VAL  | C-N-CA     | -7.52 | 113.34      | 123.12   |
| 1   | A     | 486 | TYR  | CA-C-O     | 7.52  | 127.25      | 120.71   |
| 3   | C     | 137 | ASN  | CA-CB-CG   | -7.50 | 105.10      | 112.60   |
| 1   | A     | 209 | ILE  | CA-C-O     | -7.50 | 113.22      | 121.17   |
| 4   | J     | 48  | ASN  | OD1-CG-ND2 | 7.49  | 130.09      | 122.60   |
| 3   | C     | 17  | TRP  | CB-CA-C    | 7.48  | 124.90      | 110.17   |
| 1   | A     | 101 | GLY  | CA-C-O     | 7.46  | 129.06      | 121.00   |
| 3   | C     | 37  | HIS  | CA-CB-CG   | -7.45 | 106.35      | 113.80   |
| 3   | I     | 125 | ILE  | CA-C-N     | -7.43 | 113.17      | 123.13   |
| 3   | I     | 125 | ILE  | C-N-CA     | -7.43 | 113.17      | 123.13   |
| 1   | A     | 487 | PRO  | CA-C-O     | 7.43  | 131.24      | 121.95   |
| 1   | G     | 291 | VAL  | O-C-N      | 7.43  | 130.74      | 122.12   |
| 1   | G     | 191 | ILE  | N-CA-CB    | 7.43  | 119.24      | 110.55   |
| 1   | A     | 187 | THR  | CA-C-O     | -7.42 | 111.71      | 120.10   |
| 1   | G     | 408 | ARG  | CG-CD-NE   | -7.42 | 95.67       | 112.00   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 48  | THR  | CA-CB-OG1  | 7.41  | 120.72      | 109.60   |
| 1   | G     | 544 | SER  | CA-C-N     | 7.41  | 128.01      | 120.38   |
| 1   | G     | 544 | SER  | C-N-CA     | 7.41  | 128.01      | 120.38   |
| 1   | G     | 383 | TRP  | CA-C-O     | 7.39  | 128.58      | 120.82   |
| 2   | H     | 60  | PHE  | CA-CB-CG   | 7.39  | 121.19      | 113.80   |
| 1   | G     | 476 | ARG  | NE-CZ-NH2  | 7.39  | 125.85      | 119.20   |
| 1   | G     | 357 | VAL  | CA-C-N     | 7.37  | 126.64      | 118.97   |
| 1   | G     | 357 | VAL  | C-N-CA     | 7.37  | 126.64      | 118.97   |
| 1   | G     | 93  | HIS  | CA-CB-CG   | -7.36 | 106.44      | 113.80   |
| 1   | A     | 250 | ILE  | CB-CG1-CD1 | 7.35  | 129.24      | 113.80   |
| 1   | G     | 484 | ILE  | CA-C-O     | 7.35  | 128.36      | 119.54   |
| 2   | B     | 217 | HIS  | CA-C-O     | -7.35 | 111.68      | 121.46   |
| 2   | B     | 129 | ILE  | CB-CA-C    | -7.34 | 104.11      | 110.94   |
| 1   | A     | 479 | MET  | CA-C-N     | 7.34  | 129.01      | 119.84   |
| 1   | A     | 479 | MET  | C-N-CA     | 7.34  | 129.01      | 119.84   |
| 2   | B     | 43  | PHE  | CA-CB-CG   | 7.33  | 121.13      | 113.80   |
| 1   | G     | 174 | LEU  | O-C-N      | -7.33 | 114.19      | 122.91   |
| 1   | G     | 532 | ASN  | CA-CB-CG   | -7.31 | 105.29      | 112.60   |
| 1   | G     | 490 | PHE  | CA-C-O     | -7.31 | 110.43      | 119.28   |
| 1   | A     | 331 | TRP  | N-CA-C     | 7.29  | 121.82      | 112.34   |
| 1   | G     | 65  | ALA  | CA-C-O     | 7.29  | 128.39      | 119.79   |
| 2   | H     | 39  | GLY  | CA-C-N     | 7.27  | 127.73      | 120.31   |
| 2   | H     | 39  | GLY  | C-N-CA     | 7.27  | 127.73      | 120.31   |
| 2   | H     | 234 | ARG  | NE-CZ-NH1  | -7.27 | 114.23      | 121.50   |
| 2   | B     | 208 | VAL  | N-CA-C     | 7.26  | 118.33      | 107.51   |
| 3   | C     | 198 | TYR  | CA-C-O     | -7.22 | 113.17      | 120.90   |
| 1   | A     | 465 | ASN  | CA-CB-CG   | -7.22 | 105.38      | 112.60   |
| 1   | A     | 124 | MET  | CA-C-N     | 7.22  | 128.87      | 119.84   |
| 1   | A     | 124 | MET  | C-N-CA     | 7.22  | 128.87      | 119.84   |
| 1   | G     | 100 | THR  | CA-CB-OG1  | -7.22 | 98.78       | 109.60   |
| 1   | A     | 136 | PRO  | CA-C-N     | -7.20 | 111.07      | 120.44   |
| 1   | A     | 136 | PRO  | C-N-CA     | -7.20 | 111.07      | 120.44   |
| 3   | I     | 127 | THR  | N-CA-CB    | 7.20  | 120.56      | 109.97   |
| 3   | I     | 92  | MET  | O-C-N      | -7.20 | 114.65      | 122.07   |
| 2   | B     | 258 | ILE  | CB-CA-C    | -7.20 | 102.76      | 111.97   |
| 1   | A     | 223 | HIS  | CA-CB-CG   | -7.19 | 106.61      | 113.80   |
| 1   | G     | 484 | ILE  | CB-CA-C    | -7.19 | 99.29       | 111.37   |
| 1   | A     | 419 | HIS  | CA-C-O     | -7.17 | 112.95      | 120.55   |
| 2   | H     | 252 | CYS  | O-C-N      | 7.16  | 131.68      | 122.87   |
| 1   | G     | 140 | ASN  | CA-CB-CG   | -7.16 | 105.44      | 112.60   |
| 1   | G     | 304 | THR  | CA-CB-OG1  | -7.16 | 98.86       | 109.60   |
| 3   | I     | 108 | PRO  | CA-C-O     | 7.16  | 130.40      | 121.67   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A     | 72  | LEU  | CA-C-O      | 7.14  | 127.99      | 120.42   |
| 3   | C     | 74  | VAL  | N-CA-CB     | 7.14  | 119.71      | 110.57   |
| 1   | A     | 284 | HIS  | ND1-CE1-NE2 | -7.13 | 101.27      | 108.40   |
| 2   | H     | 104 | TRP  | CA-C-O      | 7.13  | 128.06      | 119.43   |
| 1   | A     | 121 | ASN  | OD1-CG-ND2  | -7.13 | 115.47      | 122.60   |
| 1   | G     | 95  | TRP  | CA-C-N      | -7.13 | 111.17      | 120.44   |
| 1   | G     | 95  | TRP  | C-N-CA      | -7.13 | 111.17      | 120.44   |
| 3   | I     | 121 | PRO  | N-CA-CB     | 7.12  | 110.43      | 102.60   |
| 1   | A     | 545 | PRO  | N-CD-CG     | 7.12  | 113.88      | 103.20   |
| 1   | A     | 51  | MET  | N-CA-CB     | 7.11  | 120.30      | 109.91   |
| 1   | A     | 374 | SER  | CA-C-N      | -7.11 | 113.92      | 123.10   |
| 1   | A     | 374 | SER  | C-N-CA      | -7.11 | 113.92      | 123.10   |
| 2   | H     | 201 | PRO  | CB-CA-C     | -7.10 | 103.82      | 111.56   |
| 1   | G     | 33  | TYR  | N-CA-C      | 7.10  | 119.92      | 111.33   |
| 1   | G     | 541 | THR  | CA-CB-OG1   | -7.10 | 98.95       | 109.60   |
| 3   | C     | 209 | HIS  | O-C-N       | 7.09  | 130.24      | 122.15   |
| 1   | G     | 419 | HIS  | CB-CA-C     | -7.09 | 99.02       | 110.79   |
| 1   | A     | 552 | GLU  | CA-C-O      | 7.09  | 128.11      | 120.24   |
| 4   | D     | 47  | ALA  | N-CA-C      | 7.08  | 119.08      | 111.36   |
| 1   | A     | 123 | PHE  | N-CA-C      | 7.07  | 120.02      | 111.40   |
| 1   | G     | 401 | LEU  | CA-C-O      | -7.07 | 113.06      | 120.55   |
| 3   | I     | 90  | GLU  | CA-C-O      | -7.06 | 113.41      | 120.82   |
| 2   | H     | 141 | TYR  | O-C-N       | 7.05  | 131.21      | 123.10   |
| 3   | I     | 70  | ASP  | CA-CB-CG    | 7.05  | 119.65      | 112.60   |
| 1   | A     | 502 | PHE  | CA-CB-CG    | 7.04  | 120.84      | 113.80   |
| 1   | A     | 555 | PRO  | N-CA-CB     | 7.04  | 110.64      | 103.25   |
| 2   | H     | 252 | CYS  | CB-CA-C     | -7.03 | 98.05       | 109.72   |
| 1   | G     | 348 | PHE  | CA-CB-CG    | -7.02 | 106.78      | 113.80   |
| 3   | C     | 142 | LEU  | O-C-N       | 7.02  | 130.69      | 122.20   |
| 1   | A     | 260 | GLY  | CA-C-N      | -7.02 | 109.94      | 122.15   |
| 1   | A     | 260 | GLY  | C-N-CA      | -7.02 | 109.94      | 122.15   |
| 1   | A     | 24  | THR  | N-CA-C      | -7.01 | 104.37      | 114.12   |
| 1   | G     | 96  | ASN  | OD1-CG-ND2  | 7.01  | 129.61      | 122.60   |
| 3   | C     | 115 | ILE  | N-CA-C      | -7.01 | 103.94      | 110.53   |
| 2   | H     | 54  | ILE  | CA-C-O      | -7.01 | 113.74      | 121.17   |
| 1   | A     | 60  | VAL  | CB-CA-C     | -7.01 | 101.45      | 111.19   |
| 1   | G     | 56  | MET  | CA-C-O      | -7.01 | 113.46      | 120.82   |
| 1   | G     | 258 | ASN  | CA-CB-CG    | -7.01 | 105.59      | 112.60   |
| 3   | C     | 117 | ASP  | CA-CB-CG    | -7.01 | 105.59      | 112.60   |
| 1   | G     | 383 | TRP  | CB-CG-CD2   | 7.00  | 136.60      | 126.80   |
| 2   | B     | 260 | HIS  | CA-C-O      | 6.99  | 127.95      | 119.49   |
| 1   | G     | 545 | PRO  | N-CA-C      | -6.99 | 102.17      | 110.70   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 3   | I     | 30  | PHE  | CA-C-N     | 6.99  | 127.73      | 119.98   |
| 3   | I     | 30  | PHE  | C-N-CA     | 6.99  | 127.73      | 119.98   |
| 4   | J     | 18  | GLN  | OE1-CD-NE2 | -6.98 | 115.62      | 122.60   |
| 2   | B     | 215 | VAL  | CB-CA-C    | -6.97 | 99.86       | 111.29   |
| 2   | H     | 258 | ILE  | N-CA-C     | 6.96  | 117.10      | 110.42   |
| 2   | B     | 164 | PRO  | CA-C-O     | 6.96  | 129.13      | 119.18   |
| 2   | B     | 210 | VAL  | N-CA-C     | 6.96  | 119.45      | 108.87   |
| 3   | I     | 249 | PHE  | CA-C-O     | -6.96 | 113.51      | 120.82   |
| 3   | C     | 74  | VAL  | CB-CA-C    | -6.96 | 102.91      | 112.02   |
| 1   | G     | 169 | GLY  | CA-C-N     | -6.95 | 115.79      | 123.16   |
| 1   | G     | 169 | GLY  | C-N-CA     | -6.95 | 115.79      | 123.16   |
| 2   | B     | 234 | ARG  | O-C-N      | 6.95  | 131.17      | 123.52   |
| 1   | G     | 24  | THR  | N-CA-CB    | 6.95  | 120.14      | 110.90   |
| 2   | H     | 58  | ASP  | CA-CB-CG   | -6.95 | 105.65      | 112.60   |
| 2   | B     | 166 | THR  | CA-CB-OG1  | -6.94 | 99.19       | 109.60   |
| 1   | A     | 226 | PRO  | CA-C-N     | -6.94 | 111.49      | 120.65   |
| 1   | A     | 226 | PRO  | C-N-CA     | -6.94 | 111.49      | 120.65   |
| 1   | G     | 477 | GLN  | CA-C-N     | 6.92  | 135.49      | 121.78   |
| 1   | G     | 477 | GLN  | C-N-CA     | 6.92  | 135.49      | 121.78   |
| 1   | G     | 392 | THR  | O-C-N      | 6.92  | 129.57      | 122.09   |
| 2   | B     | 178 | GLN  | OE1-CD-NE2 | -6.92 | 115.68      | 122.60   |
| 1   | G     | 483 | TYR  | CA-C-O     | -6.92 | 113.52      | 121.47   |
| 3   | I     | 116 | ILE  | CB-CA-C    | -6.92 | 100.39      | 110.63   |
| 1   | G     | 28  | ASP  | CA-C-O     | 6.92  | 128.44      | 120.00   |
| 1   | G     | 270 | GLY  | O-C-N      | 6.89  | 130.39      | 122.60   |
| 1   | G     | 520 | THR  | N-CA-CB    | -6.89 | 98.84       | 110.49   |
| 3   | C     | 190 | ALA  | CA-C-O     | 6.89  | 127.38      | 119.18   |
| 1   | A     | 106 | MET  | N-CA-CB    | -6.88 | 100.04      | 110.01   |
| 1   | G     | 342 | LEU  | N-CA-C     | -6.88 | 103.71      | 111.07   |
| 1   | A     | 160 | PRO  | CA-C-N     | -6.87 | 115.22      | 122.30   |
| 1   | A     | 160 | PRO  | C-N-CA     | -6.87 | 115.22      | 122.30   |
| 1   | A     | 516 | PHE  | CA-C-O     | 6.87  | 129.06      | 121.02   |
| 1   | A     | 348 | PHE  | CA-CB-CG   | -6.87 | 106.94      | 113.80   |
| 1   | A     | 303 | ALA  | CB-CA-C    | -6.86 | 99.41       | 110.79   |
| 3   | C     | 195 | GLY  | N-CA-C     | 6.86  | 129.43      | 113.18   |
| 1   | G     | 297 | ILE  | N-CA-CB    | 6.85  | 117.81      | 110.62   |
| 1   | G     | 328 | PHE  | CA-CB-CG   | -6.85 | 106.95      | 113.80   |
| 2   | H     | 229 | ASP  | CA-CB-CG   | 6.85  | 119.45      | 112.60   |
| 1   | G     | 228 | PHE  | CA-CB-CG   | -6.85 | 106.95      | 113.80   |
| 2   | H     | 141 | TYR  | CA-C-N     | -6.84 | 110.38      | 121.26   |
| 2   | H     | 141 | TYR  | C-N-CA     | -6.84 | 110.38      | 121.26   |
| 1   | A     | 428 | ALA  | CA-C-O     | 6.84  | 128.58      | 120.92   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | G     | 297 | ILE  | CA-C-O     | -6.84 | 114.30      | 121.41   |
| 2   | B     | 35  | ARG  | NE-CZ-NH2  | -6.83 | 113.05      | 119.20   |
| 3   | C     | 163 | ASP  | CA-CB-CG   | -6.83 | 105.77      | 112.60   |
| 2   | B     | 241 | ARG  | CA-C-O     | -6.83 | 113.01      | 120.24   |
| 2   | B     | 54  | ILE  | CA-C-O     | -6.82 | 113.94      | 121.17   |
| 3   | C     | 211 | PHE  | CA-CB-CG   | -6.82 | 106.98      | 113.80   |
| 1   | A     | 481 | ARG  | CD-NE-CZ   | 6.82  | 133.94      | 124.40   |
| 1   | G     | 422 | TYR  | N-CA-CB    | 6.81  | 119.89      | 110.01   |
| 2   | B     | 91  | PRO  | CA-C-O     | -6.80 | 112.51      | 122.31   |
| 2   | B     | 142 | GLN  | N-CA-CB    | 6.80  | 119.66      | 109.19   |
| 1   | A     | 351 | ALA  | N-CA-CB    | 6.79  | 120.25      | 110.06   |
| 3   | C     | 42  | TRP  | CA-CB-CG   | -6.78 | 100.71      | 113.60   |
| 2   | H     | 170 | ASN  | CA-CB-CG   | 6.78  | 119.38      | 112.60   |
| 3   | I     | 112 | GLU  | CA-C-O     | 6.78  | 127.94      | 119.95   |
| 1   | G     | 291 | VAL  | CA-C-O     | -6.77 | 111.37      | 119.36   |
| 1   | A     | 532 | ASN  | OD1-CG-ND2 | 6.75  | 129.35      | 122.60   |
| 2   | H     | 196 | THR  | CA-C-O     | 6.75  | 127.52      | 120.30   |
| 1   | A     | 276 | GLN  | OE1-CD-NE2 | -6.75 | 115.85      | 122.60   |
| 1   | G     | 419 | HIS  | CA-C-O     | -6.74 | 113.40      | 120.55   |
| 1   | G     | 520 | THR  | CA-CB-CG2  | 6.74  | 121.96      | 110.50   |
| 2   | H     | 90  | VAL  | N-CA-C     | 6.74  | 115.64      | 107.61   |
| 1   | A     | 273 | VAL  | CA-C-O     | -6.74 | 113.57      | 121.05   |
| 1   | A     | 318 | TYR  | CB-CA-C    | 6.74  | 122.14      | 110.68   |
| 1   | G     | 225 | VAL  | CA-C-N     | 6.74  | 126.78      | 119.90   |
| 1   | G     | 225 | VAL  | C-N-CA     | 6.74  | 126.78      | 119.90   |
| 1   | G     | 532 | ASN  | OD1-CG-ND2 | 6.73  | 129.33      | 122.60   |
| 2   | B     | 142 | GLN  | OE1-CD-NE2 | 6.73  | 129.33      | 122.60   |
| 2   | H     | 108 | PRO  | N-CA-CB    | 6.72  | 110.31      | 103.25   |
| 4   | D     | 25  | GLY  | CA-C-O     | 6.71  | 128.24      | 121.00   |
| 1   | G     | 175 | TYR  | O-C-N      | -6.71 | 114.02      | 121.53   |
| 1   | A     | 545 | PRO  | CA-C-N     | 6.70  | 127.28      | 120.38   |
| 1   | A     | 545 | PRO  | C-N-CA     | 6.70  | 127.28      | 120.38   |
| 1   | G     | 270 | GLY  | CA-C-O     | -6.70 | 114.17      | 122.82   |
| 1   | G     | 449 | PRO  | N-CA-CB    | 6.70  | 108.66      | 103.30   |
| 2   | H     | 178 | GLN  | OE1-CD-NE2 | -6.70 | 115.90      | 122.60   |
| 1   | A     | 136 | PRO  | N-CA-CB    | 6.70  | 110.40      | 103.23   |
| 2   | B     | 54  | ILE  | O-C-N      | 6.70  | 128.47      | 121.91   |
| 3   | C     | 165 | ALA  | CA-C-O     | -6.69 | 113.46      | 120.55   |
| 1   | G     | 489 | ALA  | CA-C-O     | -6.69 | 112.71      | 120.20   |
| 1   | A     | 236 | ALA  | CA-C-O     | -6.69 | 113.43      | 120.92   |
| 3   | C     | 142 | LEU  | CA-C-O     | -6.68 | 113.20      | 121.02   |
| 2   | H     | 200 | VAL  | CA-C-N     | 6.68  | 128.44      | 120.23   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | H     | 200 | VAL  | C-N-CA     | 6.68  | 128.44      | 120.23   |
| 2   | H     | 171 | ARG  | NE-CZ-NH1  | 6.67  | 128.17      | 121.50   |
| 1   | A     | 100 | THR  | N-CA-C     | 6.67  | 120.52      | 112.38   |
| 1   | A     | 442 | LYS  | O-C-N      | 6.67  | 129.03      | 122.09   |
| 1   | G     | 425 | SER  | O-C-N      | 6.67  | 129.75      | 122.15   |
| 3   | C     | 194 | ALA  | CA-C-N     | 6.66  | 134.46      | 121.41   |
| 3   | C     | 194 | ALA  | C-N-CA     | 6.66  | 134.46      | 121.41   |
| 1   | G     | 247 | ALA  | O-C-N      | 6.66  | 128.93      | 122.07   |
| 1   | A     | 556 | LYS  | CA-C-O     | 6.65  | 128.51      | 121.19   |
| 2   | B     | 256 | CYS  | N-CA-CB    | -6.64 | 101.03      | 111.39   |
| 1   | A     | 166 | LEU  | N-CA-C     | -6.63 | 100.64      | 110.46   |
| 2   | B     | 75  | LEU  | N-CA-C     | -6.63 | 103.67      | 111.03   |
| 1   | G     | 458 | TRP  | CB-CA-C    | 6.63  | 121.29      | 110.88   |
| 2   | B     | 206 | VAL  | CA-C-N     | -6.61 | 114.43      | 122.90   |
| 2   | B     | 206 | VAL  | C-N-CA     | -6.61 | 114.43      | 122.90   |
| 3   | C     | 8   | ASP  | N-CA-C     | 6.61  | 121.20      | 113.20   |
| 3   | I     | 102 | PHE  | CA-CB-CG   | -6.61 | 107.19      | 113.80   |
| 1   | A     | 238 | LEU  | O-C-N      | 6.61  | 129.15      | 122.08   |
| 1   | A     | 460 | MET  | O-C-N      | 6.60  | 129.12      | 122.12   |
| 2   | B     | 42  | GLY  | O-C-N      | -6.60 | 114.12      | 122.70   |
| 1   | G     | 280 | TRP  | CA-CB-CG   | -6.60 | 101.06      | 113.60   |
| 3   | I     | 162 | ARG  | N-CA-C     | -6.60 | 103.78      | 110.97   |
| 2   | H     | 107 | VAL  | CA-CB-CG1  | 6.59  | 121.61      | 110.40   |
| 2   | H     | 149 | TYR  | CA-C-O     | 6.59  | 128.52      | 120.54   |
| 3   | C     | 223 | CYS  | CA-CB-SG   | -6.59 | 99.25       | 114.40   |
| 1   | A     | 56  | MET  | O-C-N      | 6.58  | 128.93      | 122.09   |
| 1   | G     | 445 | GLY  | CA-C-O     | -6.58 | 110.89      | 119.44   |
| 3   | I     | 17  | TRP  | CA-C-N     | 6.58  | 126.82      | 119.32   |
| 3   | I     | 17  | TRP  | C-N-CA     | 6.58  | 126.82      | 119.32   |
| 1   | A     | 480 | PRO  | CB-CA-C    | -6.58 | 100.71      | 111.56   |
| 1   | G     | 135 | PHE  | CA-CB-CG   | 6.58  | 120.38      | 113.80   |
| 1   | G     | 529 | ASN  | CA-C-O     | -6.57 | 113.28      | 120.24   |
| 1   | A     | 422 | TYR  | CA-C-O     | -6.56 | 113.93      | 120.82   |
| 1   | A     | 269 | GLY  | CA-C-O     | 6.56  | 127.19      | 119.19   |
| 2   | B     | 201 | PRO  | CB-CA-C    | -6.56 | 103.52      | 111.46   |
| 2   | H     | 95  | THR  | CB-CA-C    | -6.55 | 98.52       | 109.27   |
| 3   | I     | 211 | PHE  | CA-CB-CG   | -6.55 | 107.25      | 113.80   |
| 1   | A     | 60  | VAL  | CA-C-O     | -6.54 | 113.01      | 120.66   |
| 2   | B     | 205 | THR  | CB-CA-C    | -6.54 | 99.85       | 110.77   |
| 1   | G     | 445 | GLY  | N-CA-C     | -6.54 | 105.01      | 115.08   |
| 1   | G     | 403 | GLN  | OE1-CD-NE2 | -6.53 | 116.07      | 122.60   |
| 1   | A     | 182 | GLU  | CB-CG-CD   | -6.53 | 101.51      | 112.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 476 | ARG  | NE-CZ-NH2  | 6.52  | 125.07      | 119.20   |
| 1   | G     | 220 | MET  | N-CA-CB    | 6.52  | 119.70      | 110.24   |
| 3   | I     | 49  | VAL  | CA-C-O     | -6.52 | 114.25      | 121.17   |
| 3   | I     | 12  | LEU  | N-CA-C     | 6.52  | 119.98      | 110.14   |
| 1   | G     | 358 | PRO  | CA-C-N     | -6.51 | 111.04      | 120.29   |
| 1   | G     | 358 | PRO  | C-N-CA     | -6.51 | 111.04      | 120.29   |
| 2   | H     | 48  | SER  | N-CA-CB    | -6.51 | 105.15      | 111.27   |
| 2   | H     | 91  | PRO  | CB-CA-C    | -6.51 | 102.72      | 111.12   |
| 1   | G     | 407 | ASP  | CA-C-O     | -6.50 | 113.99      | 120.82   |
| 1   | G     | 247 | ALA  | CA-C-O     | -6.50 | 113.99      | 120.82   |
| 2   | H     | 251 | GLN  | CA-C-O     | -6.50 | 113.76      | 121.11   |
| 1   | G     | 482 | ARG  | CD-NE-CZ   | 6.50  | 133.50      | 124.40   |
| 3   | I     | 70  | ASP  | N-CA-C     | -6.50 | 105.17      | 113.23   |
| 1   | A     | 77  | PHE  | CA-CB-CG   | -6.50 | 107.30      | 113.80   |
| 2   | H     | 193 | ALA  | CA-C-O     | 6.49  | 129.15      | 121.36   |
| 1   | A     | 215 | MET  | N-CA-C     | 6.48  | 120.87      | 113.15   |
| 1   | A     | 95  | TRP  | CA-C-O     | -6.48 | 113.66      | 120.92   |
| 1   | A     | 407 | ASP  | CA-CB-CG   | -6.48 | 106.12      | 112.60   |
| 3   | C     | 160 | ASN  | OD1-CG-ND2 | -6.48 | 116.12      | 122.60   |
| 3   | I     | 42  | TRP  | CA-CB-CG   | -6.48 | 101.29      | 113.60   |
| 1   | A     | 110 | VAL  | O-C-N      | -6.47 | 114.48      | 122.57   |
| 2   | H     | 35  | ARG  | CA-C-N     | 6.47  | 126.42      | 119.76   |
| 2   | H     | 35  | ARG  | C-N-CA     | 6.47  | 126.42      | 119.76   |
| 3   | I     | 17  | TRP  | CB-CA-C    | 6.47  | 122.91      | 110.17   |
| 3   | C     | 98  | PHE  | CA-C-O     | -6.47 | 113.69      | 120.55   |
| 1   | G     | 155 | ALA  | O-C-N      | -6.46 | 115.37      | 122.09   |
| 1   | G     | 359 | THR  | CA-CB-OG1  | -6.46 | 99.91       | 109.60   |
| 2   | H     | 178 | GLN  | CB-CG-CD   | 6.46  | 123.58      | 112.60   |
| 1   | G     | 464 | ALA  | CA-C-N     | -6.45 | 112.06      | 120.44   |
| 1   | G     | 464 | ALA  | C-N-CA     | -6.45 | 112.06      | 120.44   |
| 1   | G     | 469 | PHE  | CA-C-N     | 6.45  | 127.90      | 119.84   |
| 1   | G     | 469 | PHE  | C-N-CA     | 6.45  | 127.90      | 119.84   |
| 3   | C     | 153 | HIS  | CA-C-O     | -6.44 | 114.01      | 120.90   |
| 1   | A     | 367 | ILE  | CA-C-O     | -6.43 | 114.36      | 121.05   |
| 1   | G     | 392 | THR  | CA-C-O     | -6.43 | 114.08      | 120.70   |
| 3   | I     | 40  | GLY  | N-CA-C     | 6.42  | 125.44      | 112.34   |
| 2   | H     | 234 | ARG  | N-CA-C     | 6.42  | 119.72      | 108.75   |
| 3   | C     | 51  | VAL  | O-C-N      | 6.41  | 128.19      | 121.91   |
| 2   | B     | 129 | ILE  | CA-C-O     | 6.41  | 124.73      | 119.47   |
| 1   | G     | 200 | SER  | CA-C-O     | -6.41 | 113.52      | 121.02   |
| 1   | A     | 159 | ALA  | CB-CA-C    | 6.41  | 118.76      | 109.09   |
| 1   | A     | 361 | ILE  | N-CA-C     | -6.41 | 103.63      | 110.36   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | G     | 358 | PRO  | N-CA-CB    | 6.41  | 110.08      | 103.23   |
| 3   | C     | 194 | ALA  | O-C-N      | -6.40 | 113.78      | 122.36   |
| 1   | A     | 113 | PRO  | CA-C-O     | -6.39 | 108.97      | 120.60   |
| 3   | I     | 129 | ASP  | CA-C-O     | 6.39  | 124.38      | 119.46   |
| 1   | G     | 254 | LEU  | N-CA-CB    | -6.39 | 100.81      | 110.07   |
| 2   | B     | 39  | GLY  | CA-C-O     | 6.38  | 127.41      | 119.25   |
| 3   | C     | 40  | GLY  | CA-C-N     | 6.38  | 125.87      | 119.24   |
| 3   | C     | 40  | GLY  | C-N-CA     | 6.38  | 125.87      | 119.24   |
| 1   | A     | 461 | PHE  | CA-CB-CG   | 6.37  | 120.17      | 113.80   |
| 2   | H     | 201 | PRO  | N-CA-C     | 6.37  | 120.50      | 110.50   |
| 1   | G     | 383 | TRP  | CB-CG-CD1  | -6.36 | 117.36      | 126.90   |
| 3   | I     | 72  | THR  | CB-CA-C    | -6.36 | 99.14       | 109.56   |
| 1   | G     | 107 | MET  | CA-C-N     | -6.35 | 112.27      | 122.24   |
| 1   | G     | 107 | MET  | C-N-CA     | -6.35 | 112.27      | 122.24   |
| 1   | G     | 16  | PHE  | CA-C-N     | 6.35  | 128.79      | 120.28   |
| 1   | G     | 16  | PHE  | C-N-CA     | 6.35  | 128.79      | 120.28   |
| 1   | G     | 215 | MET  | N-CA-C     | 6.35  | 120.04      | 112.93   |
| 2   | B     | 268 | LYS  | CA-C-N     | -6.35 | 113.97      | 122.98   |
| 2   | B     | 268 | LYS  | C-N-CA     | -6.35 | 113.97      | 122.98   |
| 2   | H     | 209 | GLN  | CA-C-N     | -6.34 | 113.84      | 122.91   |
| 2   | H     | 209 | GLN  | C-N-CA     | -6.34 | 113.84      | 122.91   |
| 1   | A     | 151 | SER  | O-C-N      | 6.34  | 128.60      | 122.07   |
| 3   | I     | 232 | PHE  | N-CA-C     | 6.34  | 119.83      | 109.24   |
| 1   | A     | 35  | PHE  | CA-C-O     | 6.33  | 127.27      | 120.55   |
| 1   | A     | 428 | ALA  | CB-CA-C    | -6.33 | 100.22      | 110.74   |
| 2   | B     | 171 | ARG  | NH1-CZ-NH2 | -6.33 | 111.07      | 119.30   |
| 2   | H     | 160 | MET  | CB-CA-C    | -6.32 | 97.31       | 110.40   |
| 4   | D     | 10  | VAL  | CA-C-O     | 6.32  | 128.68      | 120.78   |
| 2   | B     | 141 | TYR  | CA-C-N     | -6.32 | 111.04      | 121.97   |
| 2   | B     | 141 | TYR  | C-N-CA     | -6.32 | 111.04      | 121.97   |
| 1   | G     | 373 | GLY  | CA-C-O     | -6.32 | 114.50      | 121.77   |
| 2   | B     | 160 | MET  | CA-C-O     | -6.31 | 114.79      | 121.99   |
| 1   | G     | 532 | ASN  | CB-CG-ND2  | -6.31 | 106.93      | 116.40   |
| 2   | H     | 149 | TYR  | CA-C-N     | 6.31  | 126.51      | 119.32   |
| 2   | H     | 149 | TYR  | C-N-CA     | 6.31  | 126.51      | 119.32   |
| 1   | G     | 416 | VAL  | O-C-N      | 6.31  | 130.46      | 121.82   |
| 1   | A     | 408 | ARG  | NE-CZ-NH1  | -6.30 | 115.20      | 121.50   |
| 1   | G     | 208 | MET  | CA-CB-CG   | -6.30 | 101.50      | 114.10   |
| 2   | H     | 249 | PHE  | N-CA-C     | 6.29  | 118.65      | 108.34   |
| 2   | B     | 129 | ILE  | N-CA-CB    | -6.29 | 103.50      | 110.23   |
| 3   | I     | 128 | PHE  | CA-CB-CG   | 6.29  | 120.08      | 113.80   |
| 1   | G     | 152 | LEU  | N-CA-C     | -6.28 | 103.35      | 111.02   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | A     | 218 | PRO  | N-CA-CB  | 6.28  | 108.78      | 103.25   |
| 3   | C     | 208 | PHE  | CA-CB-CG | -6.28 | 107.52      | 113.80   |
| 2   | B     | 164 | PRO  | CA-C-N   | 6.27  | 130.64      | 120.60   |
| 2   | B     | 164 | PRO  | C-N-CA   | 6.27  | 130.64      | 120.60   |
| 3   | C     | 83  | PHE  | O-C-N    | 6.27  | 128.77      | 122.12   |
| 1   | A     | 422 | TYR  | N-CA-CB  | 6.27  | 119.10      | 110.01   |
| 2   | B     | 215 | VAL  | CA-C-O   | -6.27 | 112.94      | 120.78   |
| 1   | G     | 109 | PHE  | CA-CB-CG | -6.27 | 107.53      | 113.80   |
| 1   | A     | 392 | THR  | N-CA-C   | -6.26 | 103.76      | 111.40   |
| 1   | A     | 61  | GLN  | N-CA-CB  | 6.26  | 119.61      | 110.47   |
| 3   | C     | 120 | PHE  | O-C-N    | 6.26  | 127.18      | 121.80   |
| 1   | G     | 442 | LYS  | O-C-N    | 6.26  | 128.75      | 122.12   |
| 1   | A     | 106 | MET  | N-CA-C   | 6.25  | 117.76      | 111.07   |
| 2   | B     | 200 | VAL  | CA-C-N   | 6.25  | 126.46      | 119.90   |
| 2   | B     | 200 | VAL  | C-N-CA   | 6.25  | 126.46      | 119.90   |
| 2   | B     | 39  | GLY  | CA-C-N   | 6.25  | 126.28      | 120.34   |
| 2   | B     | 39  | GLY  | C-N-CA   | 6.25  | 126.28      | 120.34   |
| 1   | A     | 520 | THR  | N-CA-CB  | -6.25 | 99.94       | 110.49   |
| 1   | A     | 212 | PHE  | CA-CB-CG | 6.24  | 120.04      | 113.80   |
| 3   | I     | 209 | HIS  | CA-CB-CG | -6.24 | 107.56      | 113.80   |
| 1   | G     | 301 | VAL  | CA-C-O   | -6.24 | 114.46      | 120.95   |
| 1   | A     | 311 | PHE  | O-C-N    | -6.24 | 115.20      | 122.87   |
| 1   | G     | 523 | ALA  | CA-C-O   | -6.24 | 114.06      | 120.80   |
| 2   | B     | 107 | VAL  | N-CA-CB  | 6.23  | 119.93      | 111.21   |
| 2   | H     | 259 | SER  | CB-CA-C  | 6.22  | 120.69      | 111.17   |
| 3   | I     | 256 | PHE  | N-CA-C   | -6.22 | 104.42      | 111.14   |
| 2   | B     | 67  | ALA  | CA-C-O   | -6.22 | 114.29      | 120.82   |
| 2   | H     | 134 | VAL  | CA-C-O   | -6.22 | 115.21      | 121.49   |
| 1   | G     | 539 | GLU  | CB-CA-C  | 6.21  | 120.75      | 110.81   |
| 4   | D     | 48  | ASN  | CA-CB-CG | -6.21 | 106.39      | 112.60   |
| 1   | G     | 381 | MET  | N-CA-C   | 6.21  | 118.56      | 111.11   |
| 2   | H     | 95  | THR  | O-C-N    | 6.20  | 128.57      | 122.19   |
| 1   | A     | 50  | TYR  | O-C-N    | 6.19  | 129.23      | 122.11   |
| 1   | A     | 41  | GLY  | CA-C-N   | -6.19 | 112.19      | 120.79   |
| 1   | A     | 41  | GLY  | C-N-CA   | -6.19 | 112.19      | 120.79   |
| 3   | I     | 19  | PHE  | O-C-N    | 6.19  | 129.21      | 122.15   |
| 3   | C     | 43  | MET  | CA-C-O   | 6.18  | 127.10      | 120.55   |
| 1   | G     | 448 | TYR  | CA-CB-CG | -6.18 | 102.77      | 113.90   |
| 2   | H     | 133 | ASP  | N-CA-C   | -6.18 | 106.06      | 113.97   |
| 1   | G     | 173 | VAL  | CA-C-N   | -6.18 | 113.73      | 122.63   |
| 1   | G     | 173 | VAL  | C-N-CA   | -6.18 | 113.73      | 122.63   |
| 3   | I     | 28  | MET  | CA-C-O   | -6.18 | 113.79      | 121.02   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | B     | 66  | ALA  | N-CA-C    | -6.17 | 104.47      | 111.14   |
| 2   | H     | 195 | ASP  | CA-CB-CG  | 6.17  | 118.77      | 112.60   |
| 1   | A     | 437 | TYR  | CA-C-N    | 6.16  | 129.38      | 120.38   |
| 1   | A     | 437 | TYR  | C-N-CA    | 6.16  | 129.38      | 120.38   |
| 1   | G     | 545 | PRO  | N-CD-CG   | 6.16  | 112.44      | 103.20   |
| 3   | I     | 99  | TRP  | N-CA-C    | -6.16 | 103.51      | 111.02   |
| 4   | J     | 27  | VAL  | CA-C-O    | -6.16 | 115.00      | 121.41   |
| 1   | A     | 113 | PRO  | CA-C-N    | -6.16 | 111.66      | 120.89   |
| 1   | A     | 113 | PRO  | C-N-CA    | -6.16 | 111.66      | 120.89   |
| 1   | G     | 542 | LEU  | N-CA-CB   | -6.16 | 101.06      | 110.42   |
| 4   | D     | 9   | HIS  | CA-CB-CG  | 6.15  | 119.95      | 113.80   |
| 2   | B     | 254 | GLU  | O-C-N     | -6.15 | 114.41      | 122.59   |
| 2   | H     | 265 | ILE  | CA-C-O    | -6.15 | 113.79      | 120.67   |
| 1   | G     | 297 | ILE  | N-CA-C    | -6.14 | 103.84      | 110.23   |
| 1   | G     | 355 | ILE  | N-CA-C    | 6.14  | 119.65      | 111.17   |
| 2   | B     | 93  | ARG  | CD-NE-CZ  | 6.14  | 133.00      | 124.40   |
| 2   | H     | 252 | CYS  | CA-C-N    | -6.14 | 112.62      | 122.62   |
| 2   | H     | 252 | CYS  | C-N-CA    | -6.14 | 112.62      | 122.62   |
| 3   | C     | 263 | ILE  | CA-C-O    | -6.13 | 114.73      | 121.29   |
| 3   | C     | 104 | HIS  | CA-C-O    | 6.13  | 127.02      | 119.97   |
| 2   | B     | 48  | SER  | CB-CA-C   | -6.12 | 101.64      | 110.03   |
| 3   | I     | 94  | PHE  | O-C-N     | 6.12  | 129.39      | 122.22   |
| 1   | G     | 87  | ASN  | CA-C-N    | -6.12 | 114.62      | 122.77   |
| 1   | G     | 87  | ASN  | C-N-CA    | -6.12 | 114.62      | 122.77   |
| 1   | G     | 308 | LYS  | CA-C-N    | 6.12  | 127.50      | 119.84   |
| 1   | G     | 308 | LYS  | C-N-CA    | 6.12  | 127.50      | 119.84   |
| 2   | B     | 256 | CYS  | O-C-N     | 6.12  | 130.40      | 122.20   |
| 1   | A     | 214 | ASN  | O-C-N     | 6.12  | 129.35      | 122.32   |
| 2   | B     | 208 | VAL  | CB-CA-C   | -6.11 | 102.76      | 111.31   |
| 2   | B     | 249 | PHE  | CA-C-N    | -6.11 | 117.97      | 122.18   |
| 2   | B     | 249 | PHE  | C-N-CA    | -6.11 | 117.97      | 122.18   |
| 2   | H     | 206 | VAL  | CA-C-O    | -6.10 | 114.04      | 120.57   |
| 2   | B     | 272 | GLU  | CA-C-O    | -6.10 | 113.96      | 120.42   |
| 1   | A     | 142 | SER  | CA-CB-OG  | 6.09  | 123.28      | 111.10   |
| 1   | G     | 539 | GLU  | O-C-N     | -6.09 | 115.75      | 122.09   |
| 2   | H     | 80  | VAL  | N-CA-CB   | 6.09  | 118.08      | 110.47   |
| 3   | C     | 204 | MET  | CA-CB-CG  | 6.09  | 126.27      | 114.10   |
| 2   | B     | 277 | ALA  | N-CA-C    | -6.08 | 104.73      | 111.36   |
| 1   | G     | 457 | PHE  | CA-CB-CG  | -6.08 | 107.72      | 113.80   |
| 1   | G     | 481 | ARG  | CD-NE-CZ  | 6.08  | 132.91      | 124.40   |
| 1   | G     | 537 | THR  | CA-CB-OG1 | -6.08 | 100.48      | 109.60   |
| 1   | G     | 234 | VAL  | O-C-N     | 6.08  | 127.86      | 121.91   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 171 | GLY  | O-C-N      | -6.07 | 114.81      | 122.70   |
| 1   | A     | 279 | LEU  | CD1-CG-CD2 | 6.07  | 124.14      | 110.80   |
| 1   | G     | 553 | GLN  | OE1-CD-NE2 | -6.06 | 116.54      | 122.60   |
| 2   | H     | 187 | ARG  | CA-C-N     | 6.06  | 131.75      | 121.14   |
| 2   | H     | 187 | ARG  | C-N-CA     | 6.06  | 131.75      | 121.14   |
| 2   | H     | 248 | PHE  | CA-CB-CG   | -6.06 | 107.74      | 113.80   |
| 1   | A     | 419 | HIS  | N-CA-CB    | 6.06  | 119.03      | 110.12   |
| 1   | G     | 335 | MET  | CB-CG-SD   | 6.05  | 130.86      | 112.70   |
| 1   | G     | 271 | ASP  | CA-C-N     | 6.05  | 126.49      | 119.47   |
| 1   | G     | 271 | ASP  | C-N-CA     | 6.05  | 126.49      | 119.47   |
| 1   | G     | 106 | MET  | CG-SD-CE   | -6.05 | 87.60       | 100.90   |
| 2   | H     | 217 | HIS  | CA-C-O     | -6.04 | 114.28      | 121.60   |
| 1   | A     | 451 | TRP  | CA-C-O     | 6.04  | 127.13      | 120.90   |
| 2   | H     | 95  | THR  | CA-C-N     | -6.04 | 111.98      | 122.37   |
| 2   | H     | 95  | THR  | C-N-CA     | -6.04 | 111.98      | 122.37   |
| 1   | A     | 357 | VAL  | CA-C-N     | 6.04  | 125.52      | 119.24   |
| 1   | A     | 357 | VAL  | C-N-CA     | 6.04  | 125.52      | 119.24   |
| 1   | A     | 28  | ASP  | CA-C-O     | 6.03  | 127.36      | 120.00   |
| 1   | A     | 301 | VAL  | CA-C-N     | -6.03 | 111.86      | 120.42   |
| 1   | A     | 301 | VAL  | C-N-CA     | -6.03 | 111.86      | 120.42   |
| 1   | A     | 328 | PHE  | O-C-N      | 6.03  | 130.32      | 122.42   |
| 2   | H     | 69  | THR  | CB-CA-C    | -6.03 | 101.34      | 110.92   |
| 1   | G     | 213 | LEU  | O-C-N      | -6.02 | 113.81      | 122.36   |
| 1   | A     | 185 | TYR  | CA-CB-CG   | 6.02  | 124.74      | 113.90   |
| 1   | A     | 228 | PHE  | CA-C-O     | -6.02 | 111.90      | 120.51   |
| 2   | B     | 109 | ILE  | CA-CB-CG1  | -6.02 | 100.17      | 110.40   |
| 2   | H     | 208 | VAL  | CA-C-N     | -6.02 | 114.56      | 123.11   |
| 2   | H     | 208 | VAL  | C-N-CA     | -6.02 | 114.56      | 123.11   |
| 1   | G     | 335 | MET  | CA-CB-CG   | 6.01  | 126.13      | 114.10   |
| 2   | B     | 243 | GLU  | N-CA-C     | -6.01 | 105.98      | 113.38   |
| 1   | G     | 258 | ASN  | CB-CG-ND2  | -6.00 | 107.39      | 116.40   |
| 1   | A     | 100 | THR  | CA-CB-OG1  | -6.00 | 100.60      | 109.60   |
| 2   | B     | 222 | PRO  | CA-C-O     | -6.00 | 109.68      | 120.60   |
| 1   | G     | 206 | ILE  | N-CA-CB    | -6.00 | 103.53      | 110.55   |
| 1   | A     | 546 | PRO  | N-CA-C     | 6.00  | 118.02      | 110.70   |
| 2   | H     | 175 | GLU  | CA-C-O     | 6.00  | 128.04      | 121.02   |
| 1   | A     | 135 | PHE  | CA-C-N     | 6.00  | 125.20      | 118.97   |
| 1   | A     | 135 | PHE  | C-N-CA     | 6.00  | 125.20      | 118.97   |
| 1   | A     | 277 | HIS  | N-CA-CB    | 6.00  | 118.71      | 110.01   |
| 2   | H     | 107 | VAL  | CA-C-N     | 5.99  | 127.33      | 119.84   |
| 2   | H     | 107 | VAL  | C-N-CA     | 5.99  | 127.33      | 119.84   |
| 2   | B     | 206 | VAL  | N-CA-C     | 5.99  | 116.48      | 107.80   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | G     | 54  | GLU  | CB-CG-CD   | -5.99 | 102.42      | 112.60   |
| 1   | G     | 446 | ARG  | NE-CZ-NH2  | 5.98  | 124.58      | 119.20   |
| 3   | I     | 87  | ILE  | CA-C-O     | 5.98  | 126.71      | 120.25   |
| 1   | A     | 38  | GLY  | CA-C-O     | 5.98  | 130.97      | 120.57   |
| 1   | G     | 438 | PHE  | N-CA-C     | 5.98  | 118.58      | 111.71   |
| 2   | H     | 91  | PRO  | CA-C-O     | -5.98 | 114.48      | 121.95   |
| 1   | A     | 424 | MET  | CA-CB-CG   | -5.98 | 102.15      | 114.10   |
| 2   | B     | 216 | ILE  | CB-CA-C    | -5.98 | 102.23      | 110.96   |
| 1   | A     | 40  | VAL  | CA-C-O     | -5.97 | 115.20      | 121.41   |
| 1   | G     | 35  | PHE  | CA-C-O     | 5.97  | 127.29      | 120.90   |
| 1   | G     | 178 | LEU  | CA-C-O     | 5.96  | 127.28      | 120.90   |
| 1   | G     | 302 | ILE  | N-CA-C     | 5.96  | 116.14      | 110.42   |
| 1   | G     | 163 | ASN  | CA-C-O     | 5.95  | 126.96      | 120.12   |
| 1   | G     | 347 | TYR  | N-CA-CB    | 5.95  | 118.87      | 109.82   |
| 2   | B     | 32  | ILE  | N-CA-CB    | 5.95  | 118.44      | 111.66   |
| 2   | B     | 195 | ASP  | CA-CB-CG   | 5.95  | 118.55      | 112.60   |
| 1   | A     | 303 | ALA  | N-CA-C     | 5.94  | 117.75      | 111.28   |
| 1   | G     | 82  | PRO  | CA-C-O     | 5.94  | 131.41      | 120.60   |
| 1   | G     | 277 | HIS  | CA-CB-CG   | -5.94 | 107.86      | 113.80   |
| 1   | G     | 172 | TRP  | CA-C-N     | 5.94  | 130.89      | 121.09   |
| 1   | G     | 172 | TRP  | C-N-CA     | 5.94  | 130.89      | 121.09   |
| 3   | C     | 102 | PHE  | CA-CB-CG   | -5.94 | 107.86      | 113.80   |
| 1   | A     | 121 | ASN  | CA-C-O     | 5.93  | 127.57      | 120.92   |
| 2   | B     | 170 | ASN  | CA-CB-CG   | 5.93  | 118.53      | 112.60   |
| 2   | B     | 264 | PRO  | N-CA-CB    | 5.93  | 109.48      | 103.25   |
| 1   | A     | 189 | LEU  | CB-CA-C    | 5.93  | 120.09      | 110.96   |
| 1   | A     | 468 | PHE  | CA-C-N     | -5.92 | 112.33      | 120.26   |
| 1   | A     | 468 | PHE  | C-N-CA     | -5.92 | 112.33      | 120.26   |
| 1   | A     | 484 | ILE  | CB-CA-C    | -5.91 | 100.24      | 110.94   |
| 1   | A     | 342 | LEU  | N-CA-C     | -5.90 | 104.76      | 111.07   |
| 2   | H     | 125 | ASN  | CA-CB-CG   | 5.89  | 118.50      | 112.60   |
| 2   | H     | 252 | CYS  | CA-C-O     | -5.89 | 114.71      | 121.19   |
| 1   | A     | 532 | ASN  | CB-CG-ND2  | -5.89 | 107.56      | 116.40   |
| 2   | B     | 137 | LYS  | CA-CB-CG   | -5.89 | 102.32      | 114.10   |
| 2   | H     | 69  | THR  | N-CA-CB    | 5.89  | 118.77      | 109.82   |
| 2   | B     | 214 | ASP  | CA-CB-CG   | 5.88  | 118.48      | 112.60   |
| 1   | G     | 226 | PRO  | CA-C-O     | -5.88 | 114.72      | 121.36   |
| 1   | G     | 287 | VAL  | CA-C-O     | -5.88 | 114.28      | 120.57   |
| 1   | A     | 363 | ILE  | CB-CA-C    | -5.88 | 104.20      | 112.14   |
| 1   | G     | 143 | TYR  | CA-C-O     | -5.88 | 113.62      | 120.20   |
| 1   | G     | 14  | ARG  | N-CA-CB    | -5.87 | 100.52      | 110.50   |
| 3   | C     | 201 | ASN  | OD1-CG-ND2 | -5.86 | 116.74      | 122.60   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 3   | C     | 93  | PHE  | CA-CB-CG  | 5.86  | 119.66      | 113.80   |
| 1   | G     | 282 | PHE  | CA-C-O    | 5.86  | 125.24      | 118.97   |
| 2   | B     | 286 | THR  | CA-C-O    | 5.85  | 126.99      | 120.43   |
| 1   | G     | 468 | PHE  | CA-C-O    | -5.85 | 112.80      | 119.41   |
| 3   | I     | 129 | ASP  | CA-C-N    | 5.85  | 125.54      | 119.05   |
| 3   | I     | 129 | ASP  | C-N-CA    | 5.85  | 125.54      | 119.05   |
| 1   | A     | 482 | ARG  | CD-NE-CZ  | 5.84  | 132.58      | 124.40   |
| 4   | J     | 28  | ARG  | NE-CZ-NH2 | 5.84  | 124.46      | 119.20   |
| 4   | J     | 47  | ALA  | N-CA-C    | 5.84  | 118.59      | 111.82   |
| 4   | J     | 38  | VAL  | O-C-N     | 5.84  | 127.63      | 121.91   |
| 1   | G     | 89  | THR  | CA-C-N    | 5.83  | 127.13      | 119.84   |
| 1   | G     | 89  | THR  | C-N-CA    | 5.83  | 127.13      | 119.84   |
| 1   | G     | 419 | HIS  | N-CA-CB   | 5.83  | 118.69      | 110.12   |
| 2   | B     | 202 | VAL  | CA-CB-CG2 | 5.83  | 120.31      | 110.40   |
| 2   | B     | 248 | PHE  | CA-CB-CG  | -5.83 | 107.97      | 113.80   |
| 3   | C     | 3   | HIS  | CA-CB-CG  | -5.83 | 107.97      | 113.80   |
| 3   | I     | 84  | ILE  | CA-C-O    | 5.83  | 126.95      | 120.71   |
| 1   | A     | 142 | SER  | CA-C-O    | 5.83  | 127.12      | 121.00   |
| 1   | G     | 175 | TYR  | CA-C-O    | 5.82  | 127.40      | 120.88   |
| 1   | G     | 542 | LEU  | N-CA-C    | 5.82  | 119.03      | 110.59   |
| 1   | A     | 333 | HIS  | CA-C-O    | -5.82 | 113.53      | 120.10   |
| 3   | C     | 201 | ASN  | CB-CG-OD1 | 5.82  | 132.43      | 120.80   |
| 1   | G     | 260 | GLY  | CA-C-N    | -5.82 | 111.56      | 122.73   |
| 1   | G     | 260 | GLY  | C-N-CA    | -5.82 | 111.56      | 122.73   |
| 4   | D     | 37  | ILE  | CA-C-O    | 5.82  | 127.51      | 121.29   |
| 1   | G     | 358 | PRO  | CA-C-O    | -5.82 | 111.60      | 120.03   |
| 1   | A     | 531 | TRP  | CA-C-O    | -5.81 | 112.20      | 120.51   |
| 1   | G     | 501 | ALA  | CA-C-O    | -5.81 | 114.68      | 120.90   |
| 4   | D     | 43  | PHE  | CA-C-O    | 5.80  | 128.81      | 120.51   |
| 1   | G     | 168 | SER  | N-CA-C    | 5.80  | 117.75      | 108.41   |
| 1   | G     | 416 | VAL  | CA-C-O    | -5.80 | 113.98      | 120.25   |
| 2   | H     | 202 | VAL  | O-C-N     | -5.80 | 116.64      | 122.62   |
| 1   | A     | 502 | PHE  | CB-CA-C   | 5.80  | 119.99      | 110.88   |
| 3   | I     | 208 | PHE  | CA-CB-CG  | -5.80 | 108.00      | 113.80   |
| 2   | H     | 90  | VAL  | CA-C-N    | 5.79  | 126.12      | 119.92   |
| 2   | H     | 90  | VAL  | C-N-CA    | 5.79  | 126.12      | 119.92   |
| 1   | A     | 159 | ALA  | CA-C-N    | 5.79  | 127.07      | 119.84   |
| 1   | A     | 159 | ALA  | C-N-CA    | 5.79  | 127.07      | 119.84   |
| 1   | G     | 302 | ILE  | CA-C-O    | 5.79  | 127.30      | 121.17   |
| 1   | A     | 193 | ALA  | O-C-N     | 5.78  | 128.03      | 122.07   |
| 2   | B     | 201 | PRO  | N-CA-C    | 5.78  | 119.53      | 110.80   |
| 2   | B     | 205 | THR  | CA-CB-OG1 | 5.78  | 118.27      | 109.60   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | G     | 135 | PHE  | O-C-N       | 5.78  | 126.70      | 121.04   |
| 1   | A     | 261 | THR  | CA-C-N      | -5.78 | 113.28      | 121.83   |
| 1   | A     | 261 | THR  | C-N-CA      | -5.78 | 113.28      | 121.83   |
| 3   | I     | 193 | PHE  | CA-C-O      | -5.78 | 114.73      | 120.80   |
| 1   | A     | 280 | TRP  | CE2-CD2-CE3 | -5.77 | 113.03      | 118.80   |
| 3   | C     | 98  | PHE  | O-C-N       | 5.76  | 128.23      | 122.12   |
| 1   | G     | 466 | LEU  | CA-C-N      | -5.76 | 113.04      | 120.65   |
| 1   | G     | 466 | LEU  | C-N-CA      | -5.76 | 113.04      | 120.65   |
| 1   | A     | 106 | MET  | CA-C-O      | -5.76 | 114.77      | 120.82   |
| 3   | I     | 160 | ASN  | CA-C-O      | -5.76 | 113.81      | 120.49   |
| 1   | A     | 236 | ALA  | N-CA-CB     | 5.76  | 119.16      | 109.78   |
| 1   | G     | 471 | GLN  | CA-CB-CG    | -5.75 | 102.59      | 114.10   |
| 1   | G     | 234 | VAL  | N-CA-C      | -5.75 | 104.90      | 110.42   |
| 3   | I     | 178 | PHE  | O-C-N       | 5.75  | 128.23      | 122.08   |
| 1   | G     | 368 | ALA  | N-CA-CB     | 5.75  | 119.94      | 110.39   |
| 1   | A     | 419 | HIS  | CB-CG-CD2   | 5.75  | 138.67      | 131.20   |
| 1   | G     | 544 | SER  | O-C-N       | -5.75 | 113.81      | 123.00   |
| 1   | G     | 417 | VAL  | N-CA-CB     | 5.75  | 116.65      | 110.62   |
| 1   | G     | 436 | ILE  | N-CA-C      | 5.75  | 116.39      | 110.36   |
| 1   | A     | 481 | ARG  | CA-CB-CG    | 5.74  | 125.59      | 114.10   |
| 3   | C     | 5   | LYS  | CA-CB-CG    | 5.74  | 125.59      | 114.10   |
| 2   | B     | 105 | THR  | CB-CA-C     | 5.74  | 118.33      | 109.03   |
| 1   | A     | 416 | VAL  | CB-CA-C     | -5.74 | 102.81      | 112.16   |
| 2   | B     | 256 | CYS  | CA-C-O      | -5.73 | 113.60      | 120.65   |
| 3   | C     | 6   | ASN  | CA-CB-CG    | 5.73  | 118.33      | 112.60   |
| 1   | G     | 303 | ALA  | CA-C-O      | -5.73 | 114.80      | 120.82   |
| 1   | A     | 172 | TRP  | N-CA-CB     | 5.73  | 119.19      | 110.14   |
| 1   | A     | 298 | VAL  | N-CA-C      | 5.73  | 116.19      | 110.23   |
| 1   | G     | 316 | MET  | CA-C-O      | -5.73 | 114.81      | 120.82   |
| 2   | B     | 166 | THR  | CB-CA-C     | -5.73 | 101.60      | 111.45   |
| 1   | G     | 421 | HIS  | CA-C-O      | -5.73 | 112.32      | 120.51   |
| 2   | B     | 88  | ASN  | OD1-CG-ND2  | -5.72 | 116.88      | 122.60   |
| 3   | I     | 40  | GLY  | O-C-N       | -5.72 | 116.05      | 121.77   |
| 1   | A     | 333 | HIS  | N-CA-CB     | 5.72  | 119.03      | 110.22   |
| 2   | H     | 125 | ASN  | N-CA-C      | -5.72 | 104.95      | 111.07   |
| 3   | I     | 68  | GLU  | N-CA-C      | -5.72 | 106.34      | 113.15   |
| 1   | A     | 333 | HIS  | N-CA-C      | -5.72 | 105.14      | 111.71   |
| 1   | A     | 361 | ILE  | CA-C-N      | -5.72 | 112.62      | 120.28   |
| 1   | A     | 361 | ILE  | C-N-CA      | -5.72 | 112.62      | 120.28   |
| 1   | G     | 59  | GLY  | CA-C-N      | -5.72 | 115.33      | 123.10   |
| 1   | G     | 59  | GLY  | C-N-CA      | -5.72 | 115.33      | 123.10   |
| 1   | G     | 323 | ILE  | CA-C-N      | 5.72  | 126.43      | 120.03   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | G     | 323 | ILE  | C-N-CA     | 5.72  | 126.43      | 120.03   |
| 1   | A     | 247 | ALA  | O-C-N      | 5.71  | 128.03      | 122.09   |
| 3   | C     | 125 | ILE  | CA-C-N     | -5.71 | 115.33      | 123.10   |
| 3   | C     | 125 | ILE  | C-N-CA     | -5.71 | 115.33      | 123.10   |
| 1   | A     | 304 | THR  | CA-CB-OG1  | -5.71 | 101.03      | 109.60   |
| 1   | A     | 509 | LEU  | O-C-N      | -5.71 | 116.15      | 122.09   |
| 3   | C     | 121 | PRO  | CA-C-N     | 5.71  | 125.72      | 119.90   |
| 3   | C     | 121 | PRO  | C-N-CA     | 5.71  | 125.72      | 119.90   |
| 1   | G     | 364 | PHE  | CA-CB-CG   | -5.71 | 108.09      | 113.80   |
| 1   | G     | 433 | PHE  | CA-CB-CG   | -5.71 | 108.09      | 113.80   |
| 1   | G     | 468 | PHE  | O-C-N      | 5.71  | 130.46      | 122.36   |
| 2   | H     | 35  | ARG  | CB-CA-C    | 5.71  | 117.68      | 109.92   |
| 1   | A     | 383 | TRP  | CA-C-O     | 5.70  | 127.34      | 121.07   |
| 2   | B     | 206 | VAL  | CB-CA-C    | -5.70 | 102.64      | 110.96   |
| 2   | H     | 124 | PHE  | O-C-N      | 5.70  | 128.16      | 122.12   |
| 1   | A     | 487 | PRO  | N-CA-CB    | 5.70  | 108.75      | 103.39   |
| 3   | C     | 36  | MET  | N-CA-C     | -5.70 | 105.91      | 112.92   |
| 1   | A     | 449 | PRO  | O-C-N      | 5.70  | 128.45      | 122.93   |
| 2   | B     | 200 | VAL  | CA-C-O     | 5.69  | 127.57      | 119.95   |
| 3   | C     | 37  | HIS  | N-CA-C     | 5.69  | 118.16      | 110.88   |
| 2   | B     | 149 | TYR  | CA-CB-CG   | 5.69  | 124.14      | 113.90   |
| 2   | B     | 133 | ASP  | CA-C-O     | 5.68  | 125.30      | 119.05   |
| 1   | G     | 48  | THR  | CA-C-O     | -5.68 | 114.53      | 120.55   |
| 1   | G     | 323 | ILE  | CB-CG1-CD1 | 5.68  | 125.74      | 113.80   |
| 3   | I     | 12  | LEU  | CB-CA-C    | -5.68 | 100.35      | 108.88   |
| 1   | A     | 24  | THR  | CA-CB-OG1  | 5.68  | 118.12      | 109.60   |
| 3   | C     | 204 | MET  | CG-SD-CE   | 5.68  | 113.40      | 100.90   |
| 2   | H     | 158 | SER  | CA-C-O     | 5.68  | 127.58      | 121.16   |
| 2   | H     | 196 | THR  | N-CA-C     | 5.68  | 117.67      | 108.41   |
| 2   | B     | 187 | ARG  | CD-NE-CZ   | 5.68  | 132.35      | 124.40   |
| 3   | C     | 252 | VAL  | CB-CA-C    | -5.68 | 104.70      | 111.97   |
| 1   | A     | 257 | ARG  | CA-C-N     | -5.68 | 113.31      | 122.23   |
| 1   | A     | 257 | ARG  | C-N-CA     | -5.68 | 113.31      | 122.23   |
| 1   | G     | 112 | ILE  | CB-CG1-CD1 | -5.67 | 101.89      | 113.80   |
| 3   | C     | 2   | ALA  | CA-C-O     | 5.66  | 130.43      | 120.80   |
| 2   | B     | 235 | LEU  | CA-C-O     | -5.66 | 114.72      | 120.84   |
| 2   | H     | 181 | ILE  | O-C-N      | 5.66  | 127.60      | 121.94   |
| 1   | A     | 60  | VAL  | O-C-N      | 5.66  | 130.29      | 122.88   |
| 1   | G     | 56  | MET  | N-CA-C     | -5.66 | 105.02      | 111.07   |
| 1   | G     | 256 | ASP  | O-C-N      | 5.65  | 128.11      | 122.12   |
| 3   | C     | 39  | SER  | CA-C-N     | 5.64  | 130.73      | 121.87   |
| 3   | C     | 39  | SER  | C-N-CA     | 5.64  | 130.73      | 121.87   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | H     | 205 | THR  | CA-CB-OG1   | 5.64  | 118.06      | 109.60   |
| 3   | C     | 209 | HIS  | CA-C-O      | -5.64 | 114.44      | 120.42   |
| 1   | A     | 419 | HIS  | CB-CA-C     | -5.64 | 101.43      | 110.79   |
| 3   | I     | 220 | LEU  | CA-C-O      | -5.63 | 114.88      | 120.90   |
| 1   | G     | 43  | ILE  | CB-CG1-CD1  | -5.63 | 101.98      | 113.80   |
| 1   | A     | 317 | VAL  | N-CA-CB     | 5.62  | 116.53      | 110.62   |
| 1   | G     | 203 | LEU  | N-CA-C      | -5.62 | 105.07      | 111.14   |
| 1   | A     | 320 | MET  | CA-C-N      | -5.62 | 112.77      | 120.46   |
| 1   | A     | 320 | MET  | C-N-CA      | -5.62 | 112.77      | 120.46   |
| 1   | A     | 308 | LYS  | CA-C-N      | 5.61  | 126.85      | 119.84   |
| 1   | A     | 308 | LYS  | C-N-CA      | 5.61  | 126.85      | 119.84   |
| 1   | A     | 279 | LEU  | CA-C-N      | -5.61 | 111.78      | 120.31   |
| 1   | A     | 279 | LEU  | C-N-CA      | -5.61 | 111.78      | 120.31   |
| 2   | B     | 251 | GLN  | CA-C-N      | 5.61  | 128.72      | 120.82   |
| 2   | B     | 251 | GLN  | C-N-CA      | 5.61  | 128.72      | 120.82   |
| 3   | C     | 174 | LEU  | N-CA-CB     | 5.60  | 118.93      | 110.30   |
| 1   | A     | 172 | TRP  | CA-C-O      | 5.60  | 126.47      | 120.20   |
| 2   | B     | 231 | VAL  | CB-CA-C     | -5.60 | 104.51      | 110.16   |
| 3   | C     | 232 | PHE  | N-CA-C      | 5.60  | 118.22      | 108.76   |
| 2   | B     | 93  | ARG  | NE-CZ-NH1   | 5.59  | 127.09      | 121.50   |
| 3   | C     | 72  | THR  | CB-CA-C     | -5.59 | 100.68      | 109.52   |
| 3   | I     | 92  | MET  | CA-C-O      | 5.59  | 126.69      | 120.82   |
| 4   | J     | 19  | GLN  | OE1-CD-NE2  | -5.58 | 117.02      | 122.60   |
| 2   | H     | 95  | THR  | N-CA-CB     | 5.58  | 118.34      | 110.98   |
| 1   | A     | 284 | HIS  | CE1-NE2-CD2 | 5.58  | 114.58      | 109.00   |
| 1   | A     | 347 | TYR  | N-CA-CB     | 5.58  | 118.25      | 109.94   |
| 1   | A     | 504 | SER  | CA-C-O      | -5.58 | 114.93      | 121.07   |
| 1   | A     | 175 | TYR  | CA-C-N      | 5.57  | 126.12      | 120.38   |
| 1   | A     | 175 | TYR  | C-N-CA      | 5.57  | 126.12      | 120.38   |
| 1   | G     | 357 | VAL  | CB-CA-C     | 5.57  | 121.50      | 111.36   |
| 1   | A     | 465 | ASN  | OD1-CG-ND2  | 5.57  | 128.17      | 122.60   |
| 3   | C     | 196 | ASN  | CA-C-O      | 5.57  | 126.77      | 119.98   |
| 1   | G     | 311 | PHE  | CA-C-O      | -5.57 | 115.03      | 121.15   |
| 2   | H     | 207 | VAL  | N-CA-C      | 5.57  | 115.87      | 107.80   |
| 1   | A     | 303 | ALA  | CA-C-N      | -5.56 | 112.87      | 120.44   |
| 1   | A     | 303 | ALA  | C-N-CA      | -5.56 | 112.87      | 120.44   |
| 1   | A     | 416 | VAL  | CA-C-O      | -5.56 | 114.24      | 120.25   |
| 1   | G     | 212 | PHE  | CA-CB-CG    | 5.56  | 119.36      | 113.80   |
| 1   | A     | 472 | HIS  | CA-CB-CG    | 5.56  | 119.36      | 113.80   |
| 3   | C     | 123 | GLU  | CA-C-O      | -5.55 | 114.91      | 120.96   |
| 2   | B     | 250 | GLY  | N-CA-C      | 5.55  | 120.91      | 111.19   |
| 2   | H     | 51  | ALA  | O-C-N       | 5.55  | 127.86      | 122.09   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | H     | 66  | ALA  | N-CA-C     | -5.55 | 105.13      | 111.07   |
| 1   | A     | 16  | PHE  | CA-CB-CG   | -5.55 | 108.25      | 113.80   |
| 3   | C     | 158 | GLU  | N-CA-C     | -5.55 | 107.15      | 114.31   |
| 2   | B     | 281 | GLN  | CA-C-O     | 5.55  | 126.20      | 119.38   |
| 1   | A     | 265 | GLN  | O-C-N      | -5.55 | 116.83      | 121.27   |
| 1   | A     | 437 | TYR  | O-C-N      | -5.54 | 116.15      | 122.08   |
| 2   | H     | 149 | TYR  | CA-CB-CG   | 5.54  | 123.88      | 113.90   |
| 2   | B     | 209 | GLN  | OE1-CD-NE2 | -5.54 | 117.06      | 122.60   |
| 1   | A     | 407 | ASP  | CA-C-O     | -5.54 | 114.97      | 120.90   |
| 1   | G     | 399 | ILE  | O-C-N      | 5.54  | 127.66      | 121.90   |
| 3   | I     | 233 | THR  | CA-C-N     | 5.53  | 125.36      | 119.28   |
| 3   | I     | 233 | THR  | C-N-CA     | 5.53  | 125.36      | 119.28   |
| 2   | B     | 157 | GLU  | CG-CD-OE2  | -5.53 | 105.68      | 118.40   |
| 3   | C     | 83  | PHE  | CA-C-O     | -5.52 | 114.67      | 120.63   |
| 4   | D     | 36  | VAL  | O-C-N      | -5.52 | 116.52      | 121.87   |
| 1   | A     | 160 | PRO  | N-CA-CB    | -5.52 | 97.46       | 103.25   |
| 1   | G     | 354 | VAL  | CA-C-O     | -5.52 | 114.51      | 120.47   |
| 3   | I     | 90  | GLU  | O-C-N      | 5.52  | 127.75      | 122.07   |
| 3   | I     | 59  | TRP  | N-CA-C     | 5.51  | 118.05      | 111.71   |
| 1   | G     | 251 | THR  | N-CA-C     | -5.51 | 104.97      | 110.97   |
| 3   | C     | 219 | PHE  | O-C-N      | 5.51  | 128.86      | 122.20   |
| 2   | H     | 74  | LEU  | CA-C-N     | -5.51 | 113.14      | 120.63   |
| 2   | H     | 74  | LEU  | C-N-CA     | -5.51 | 113.14      | 120.63   |
| 1   | A     | 531 | TRP  | O-C-N      | 5.50  | 129.91      | 122.59   |
| 1   | A     | 142 | SER  | N-CA-CB    | 5.50  | 117.94      | 109.91   |
| 2   | B     | 163 | SER  | CA-C-N     | 5.50  | 125.17      | 119.56   |
| 2   | B     | 163 | SER  | C-N-CA     | 5.50  | 125.17      | 119.56   |
| 3   | C     | 233 | THR  | CA-C-N     | 5.50  | 125.33      | 119.28   |
| 3   | C     | 233 | THR  | C-N-CA     | 5.50  | 125.33      | 119.28   |
| 3   | I     | 110 | GLY  | CA-C-N     | 5.50  | 126.71      | 119.84   |
| 3   | I     | 110 | GLY  | C-N-CA     | 5.50  | 126.71      | 119.84   |
| 2   | B     | 255 | LEU  | CA-C-N     | -5.49 | 113.84      | 122.79   |
| 2   | B     | 255 | LEU  | C-N-CA     | -5.49 | 113.84      | 122.79   |
| 2   | H     | 214 | ASP  | CA-C-N     | 5.49  | 131.85      | 121.97   |
| 2   | H     | 214 | ASP  | C-N-CA     | 5.49  | 131.85      | 121.97   |
| 1   | G     | 48  | THR  | N-CA-CB    | 5.49  | 118.19      | 110.12   |
| 4   | J     | 30  | VAL  | N-CA-CB    | -5.49 | 104.86      | 110.62   |
| 1   | A     | 464 | ALA  | N-CA-C     | -5.49 | 105.46      | 111.82   |
| 1   | G     | 363 | ILE  | O-C-N      | 5.49  | 127.29      | 121.91   |
| 1   | G     | 254 | LEU  | CA-C-O     | 5.49  | 126.35      | 120.70   |
| 1   | A     | 82  | PRO  | N-CA-CB    | 5.48  | 109.01      | 103.25   |
| 1   | G     | 47  | PHE  | CA-CB-CG   | 5.48  | 119.28      | 113.80   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | G     | 92  | GLY  | CA-C-O      | 5.48  | 126.04      | 120.45   |
| 2   | H     | 263 | MET  | O-C-N       | 5.48  | 125.67      | 121.23   |
| 3   | I     | 59  | TRP  | CA-C-N      | 5.48  | 127.57      | 120.44   |
| 3   | I     | 59  | TRP  | C-N-CA      | 5.48  | 127.57      | 120.44   |
| 1   | G     | 510 | PHE  | O-C-N       | 5.48  | 127.79      | 122.09   |
| 3   | I     | 83  | PHE  | CA-CB-CG    | -5.48 | 108.32      | 113.80   |
| 2   | H     | 205 | THR  | CB-CA-C     | -5.48 | 101.78      | 110.81   |
| 1   | G     | 14  | ARG  | NE-CZ-NH2   | 5.47  | 124.13      | 119.20   |
| 1   | G     | 172 | TRP  | CD2-CE2-CZ2 | 5.47  | 127.87      | 122.40   |
| 1   | A     | 23  | SER  | N-CA-C      | 5.47  | 118.28      | 110.24   |
| 3   | I     | 127 | THR  | CB-CA-C     | -5.47 | 100.29      | 109.65   |
| 1   | G     | 337 | THR  | OG1-CB-CG2  | 5.47  | 120.24      | 109.30   |
| 1   | A     | 232 | ILE  | CA-CB-CG1   | -5.47 | 101.11      | 110.40   |
| 1   | A     | 294 | ALA  | CB-CA-C     | -5.46 | 102.07      | 110.81   |
| 1   | G     | 32  | LEU  | CB-CA-C     | 5.46  | 119.55      | 110.81   |
| 2   | B     | 88  | ASN  | CB-CG-ND2   | 5.46  | 124.59      | 116.40   |
| 1   | G     | 486 | TYR  | N-CA-C      | 5.46  | 114.58      | 108.25   |
| 3   | C     | 106 | LEU  | CA-C-N      | -5.46 | 116.30      | 123.34   |
| 3   | C     | 106 | LEU  | C-N-CA      | -5.46 | 116.30      | 123.34   |
| 1   | A     | 502 | PHE  | O-C-N       | -5.46 | 116.45      | 122.07   |
| 3   | C     | 188 | HIS  | N-CA-CB     | -5.46 | 102.06      | 110.25   |
| 1   | G     | 52  | ARG  | CB-CA-C     | 5.46  | 119.80      | 110.74   |
| 1   | G     | 56  | MET  | O-C-N       | 5.45  | 127.69      | 122.07   |
| 1   | G     | 104 | ILE  | CA-C-O      | -5.45 | 115.60      | 121.27   |
| 2   | B     | 135 | THR  | N-CA-C      | 5.45  | 116.97      | 107.49   |
| 1   | A     | 114 | ALA  | O-C-N       | -5.45 | 115.69      | 122.11   |
| 1   | G     | 50  | TYR  | CA-C-O      | -5.45 | 115.08      | 121.07   |
| 1   | G     | 376 | GLU  | CA-C-O      | -5.45 | 114.41      | 121.11   |
| 2   | H     | 150 | PRO  | N-CA-CB     | 5.44  | 109.47      | 103.26   |
| 3   | I     | 168 | LEU  | N-CA-C      | 5.44  | 116.89      | 111.07   |
| 3   | I     | 126 | ILE  | CA-C-N      | 5.44  | 128.59      | 120.87   |
| 3   | I     | 126 | ILE  | C-N-CA      | 5.44  | 128.59      | 120.87   |
| 3   | C     | 120 | PHE  | CA-C-O      | -5.43 | 114.32      | 120.46   |
| 3   | C     | 169 | ALA  | N-CA-CB     | 5.43  | 117.84      | 109.91   |
| 1   | G     | 412 | ASP  | OD1-CG-OD2  | 5.43  | 135.94      | 122.90   |
| 2   | H     | 88  | ASN  | N-CA-CB     | 5.43  | 119.65      | 110.79   |
| 1   | G     | 48  | THR  | CA-CB-OG1   | 5.43  | 117.74      | 109.60   |
| 4   | D     | 23  | PHE  | CA-CB-CG    | 5.42  | 119.22      | 113.80   |
| 1   | G     | 504 | SER  | CA-C-O      | -5.42 | 115.10      | 121.07   |
| 3   | I     | 117 | ASP  | N-CA-C      | 5.42  | 117.87      | 110.55   |
| 3   | C     | 184 | TYR  | N-CA-C      | -5.42 | 104.41      | 111.02   |
| 1   | G     | 301 | VAL  | CA-CB-CG2   | -5.42 | 101.18      | 110.40   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | H     | 281 | GLN  | CA-C-O      | 5.42  | 126.20      | 119.97   |
| 2   | B     | 249 | PHE  | CB-CA-C     | -5.42 | 101.17      | 110.16   |
| 3   | C     | 263 | ILE  | CB-CA-C     | -5.42 | 105.04      | 111.81   |
| 1   | G     | 546 | PRO  | N-CA-CB     | 5.42  | 108.33      | 103.08   |
| 3   | C     | 122 | PRO  | N-CA-CB     | 5.41  | 108.01      | 103.25   |
| 2   | B     | 224 | PHE  | CA-CB-CG    | -5.41 | 108.39      | 113.80   |
| 1   | G     | 445 | GLY  | O-C-N       | 5.41  | 129.03      | 122.32   |
| 2   | H     | 75  | LEU  | N-CA-C      | -5.41 | 105.02      | 111.03   |
| 2   | H     | 79  | ALA  | CA-C-O      | -5.41 | 115.11      | 120.90   |
| 1   | A     | 261 | THR  | N-CA-C      | -5.41 | 101.63      | 109.31   |
| 1   | G     | 504 | SER  | CA-C-N      | 5.40  | 127.78      | 120.38   |
| 1   | G     | 504 | SER  | C-N-CA      | 5.40  | 127.78      | 120.38   |
| 1   | A     | 29  | ILE  | N-CA-C      | -5.40 | 105.11      | 110.62   |
| 1   | G     | 40  | VAL  | CA-C-O      | -5.40 | 114.03      | 120.78   |
| 3   | I     | 210 | GLY  | N-CA-C      | -5.40 | 106.25      | 112.73   |
| 3   | C     | 196 | ASN  | CA-CB-CG    | -5.40 | 107.20      | 112.60   |
| 3   | C     | 202 | PHE  | O-C-N       | 5.40  | 127.84      | 122.12   |
| 1   | A     | 99  | ILE  | CA-C-O      | -5.39 | 114.04      | 120.78   |
| 1   | A     | 115 | LEU  | N-CA-C      | 5.39  | 119.35      | 112.34   |
| 2   | H     | 217 | HIS  | ND1-CE1-NE2 | -5.39 | 103.00      | 108.40   |
| 3   | I     | 116 | ILE  | N-CA-C      | 5.39  | 115.66      | 108.11   |
| 3   | C     | 17  | TRP  | CA-C-N      | 5.39  | 126.58      | 119.84   |
| 3   | C     | 17  | TRP  | C-N-CA      | 5.39  | 126.58      | 119.84   |
| 1   | A     | 262 | THR  | CA-C-N      | -5.39 | 113.54      | 120.65   |
| 1   | A     | 262 | THR  | C-N-CA      | -5.39 | 113.54      | 120.65   |
| 1   | A     | 255 | THR  | CA-C-O      | -5.39 | 113.77      | 119.97   |
| 3   | C     | 96  | ALA  | CB-CA-C     | -5.39 | 102.66      | 110.96   |
| 1   | A     | 19  | ARG  | CA-CB-CG    | -5.39 | 103.33      | 114.10   |
| 1   | G     | 229 | ALA  | CA-C-O      | -5.39 | 113.43      | 119.79   |
| 1   | G     | 390 | LEU  | CA-C-O      | -5.39 | 115.14      | 120.90   |
| 1   | G     | 121 | ASN  | CA-C-N      | 5.38  | 127.75      | 120.65   |
| 1   | G     | 121 | ASN  | C-N-CA      | 5.38  | 127.75      | 120.65   |
| 1   | A     | 456 | HIS  | CA-CB-CG    | 5.38  | 119.18      | 113.80   |
| 2   | B     | 251 | GLN  | CG-CD-NE2   | 5.38  | 124.47      | 116.40   |
| 1   | G     | 385 | LEU  | CB-CA-C     | 5.38  | 119.40      | 110.90   |
| 3   | I     | 2   | ALA  | CA-C-O      | 5.37  | 129.94      | 120.80   |
| 1   | A     | 509 | LEU  | CB-CA-C     | 5.37  | 119.40      | 110.81   |
| 1   | G     | 413 | THR  | N-CA-C      | -5.37 | 102.51      | 110.46   |
| 2   | H     | 128 | GLU  | CA-C-O      | 5.37  | 126.21      | 120.46   |
| 1   | A     | 104 | ILE  | CA-C-O      | -5.37 | 115.69      | 121.27   |
| 2   | B     | 259 | SER  | O-C-N       | -5.37 | 115.45      | 122.59   |
| 1   | G     | 279 | LEU  | CA-CB-CG    | -5.37 | 97.51       | 116.30   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A     | 96  | ASN  | CA-CB-CG    | -5.36 | 107.24      | 112.60   |
| 3   | C     | 169 | ALA  | N-CA-C      | -5.36 | 105.13      | 110.97   |
| 1   | G     | 257 | ARG  | NE-CZ-NH2   | 5.35  | 124.02      | 119.20   |
| 2   | H     | 129 | ILE  | CA-C-N      | 5.35  | 126.53      | 119.84   |
| 2   | H     | 129 | ILE  | C-N-CA      | 5.35  | 126.53      | 119.84   |
| 1   | G     | 345 | GLN  | OE1-CD-NE2  | -5.35 | 117.25      | 122.60   |
| 3   | I     | 263 | ILE  | N-CA-C      | 5.35  | 115.49      | 110.30   |
| 2   | H     | 46  | SER  | CA-C-O      | 5.35  | 126.30      | 120.58   |
| 1   | G     | 213 | LEU  | N-CA-CB     | -5.34 | 102.31      | 110.33   |
| 1   | A     | 57  | ALA  | O-C-N       | 5.34  | 125.71      | 121.55   |
| 1   | G     | 403 | GLN  | CA-C-O      | 5.34  | 127.16      | 121.02   |
| 1   | G     | 381 | MET  | CB-CA-C     | -5.33 | 102.27      | 110.81   |
| 1   | G     | 101 | GLY  | O-C-N       | 5.33  | 127.30      | 122.18   |
| 2   | H     | 200 | VAL  | N-CA-C      | 5.33  | 120.40      | 108.88   |
| 2   | H     | 248 | PHE  | CA-C-O      | -5.33 | 114.99      | 121.28   |
| 1   | G     | 351 | ALA  | CB-CA-C     | -5.32 | 101.63      | 110.68   |
| 1   | A     | 89  | THR  | CA-C-N      | 5.32  | 126.49      | 119.84   |
| 1   | A     | 89  | THR  | C-N-CA      | 5.32  | 126.49      | 119.84   |
| 3   | I     | 158 | GLU  | O-C-N       | -5.32 | 116.46      | 122.10   |
| 1   | G     | 538 | LEU  | CA-C-N      | -5.32 | 113.36      | 120.54   |
| 1   | G     | 538 | LEU  | C-N-CA      | -5.32 | 113.36      | 120.54   |
| 3   | I     | 51  | VAL  | CB-CA-C     | -5.32 | 105.16      | 111.97   |
| 3   | C     | 68  | GLU  | CA-CB-CG    | 5.32  | 124.73      | 114.10   |
| 4   | D     | 18  | GLN  | N-CA-C      | 5.32  | 117.08      | 111.28   |
| 1   | G     | 127 | HIS  | CA-C-N      | -5.32 | 112.95      | 121.35   |
| 1   | G     | 127 | HIS  | C-N-CA      | -5.32 | 112.95      | 121.35   |
| 1   | G     | 172 | TRP  | NE1-CE2-CZ2 | -5.32 | 122.12      | 130.10   |
| 1   | G     | 258 | ASN  | OD1-CG-ND2  | 5.32  | 127.92      | 122.60   |
| 3   | I     | 201 | ASN  | CA-CB-CG    | -5.32 | 107.28      | 112.60   |
| 1   | G     | 303 | ALA  | CA-C-N      | -5.32 | 113.21      | 120.44   |
| 1   | G     | 303 | ALA  | C-N-CA      | -5.32 | 113.21      | 120.44   |
| 1   | G     | 428 | ALA  | CB-CA-C     | -5.31 | 101.92      | 110.74   |
| 1   | G     | 45  | VAL  | O-C-N       | -5.31 | 115.93      | 122.57   |
| 1   | A     | 123 | PHE  | CA-C-O      | -5.31 | 114.87      | 120.55   |
| 1   | A     | 527 | ALA  | N-CA-C      | 5.31  | 117.99      | 110.50   |
| 4   | D     | 36  | VAL  | CA-C-O      | 5.31  | 126.47      | 120.95   |
| 2   | B     | 149 | TYR  | CA-C-N      | 5.30  | 126.47      | 119.84   |
| 2   | B     | 149 | TYR  | C-N-CA      | 5.30  | 126.47      | 119.84   |
| 1   | G     | 277 | HIS  | ND1-CG-CD2  | 5.30  | 111.40      | 106.10   |
| 3   | I     | 19  | PHE  | CB-CA-C     | -5.30 | 101.84      | 110.85   |
| 1   | A     | 253 | LEU  | N-CA-CB     | 5.30  | 118.49      | 110.28   |
| 1   | G     | 479 | MET  | CA-C-N      | 5.30  | 126.46      | 119.84   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | G     | 479 | MET  | C-N-CA    | 5.30  | 126.46      | 119.84   |
| 2   | B     | 216 | ILE  | N-CA-C    | 5.29  | 115.48      | 107.80   |
| 1   | A     | 116 | PHE  | N-CA-C    | -5.29 | 106.88      | 113.55   |
| 1   | A     | 159 | ALA  | N-CA-C    | 5.29  | 117.33      | 110.40   |
| 1   | G     | 23  | SER  | N-CA-C    | 5.29  | 118.15      | 110.42   |
| 2   | H     | 49  | PRO  | N-CA-CB   | 5.29  | 108.81      | 103.25   |
| 2   | B     | 107 | VAL  | CA-C-N    | 5.29  | 126.45      | 119.84   |
| 2   | B     | 107 | VAL  | C-N-CA    | 5.29  | 126.45      | 119.84   |
| 3   | I     | 236 | LYS  | CA-C-O    | -5.29 | 115.04      | 120.54   |
| 4   | J     | 9   | HIS  | CB-CA-C   | -5.29 | 101.22      | 109.84   |
| 1   | G     | 205 | ALA  | CB-CA-C   | -5.29 | 101.96      | 110.74   |
| 1   | G     | 160 | PRO  | CA-CB-CG  | -5.29 | 94.45       | 104.50   |
| 2   | H     | 213 | ALA  | CB-CA-C   | -5.29 | 102.98      | 111.39   |
| 3   | C     | 36  | MET  | N-CA-CB   | 5.29  | 118.28      | 110.56   |
| 1   | A     | 182 | GLU  | CA-CB-CG  | -5.28 | 103.53      | 114.10   |
| 1   | G     | 430 | PHE  | CB-CA-C   | 5.28  | 119.32      | 110.92   |
| 2   | H     | 209 | GLN  | CA-C-O    | 5.28  | 126.11      | 120.46   |
| 1   | A     | 540 | TRP  | N-CA-C    | 5.28  | 118.82      | 112.38   |
| 2   | B     | 84  | HIS  | CA-CB-CG  | -5.28 | 108.52      | 113.80   |
| 1   | G     | 308 | LYS  | CA-C-O    | 5.28  | 127.39      | 120.16   |
| 1   | G     | 441 | GLY  | O-C-N     | 5.28  | 129.56      | 122.70   |
| 2   | B     | 251 | GLN  | CG-CD-OE1 | -5.27 | 110.26      | 120.80   |
| 1   | G     | 323 | ILE  | CA-C-O    | 5.27  | 126.93      | 121.29   |
| 1   | A     | 258 | ASN  | CA-CB-CG  | -5.27 | 107.33      | 112.60   |
| 1   | A     | 295 | PHE  | CA-C-O    | -5.27 | 115.26      | 120.90   |
| 1   | G     | 226 | PRO  | CA-C-N    | -5.26 | 113.60      | 120.44   |
| 1   | G     | 226 | PRO  | C-N-CA    | -5.26 | 113.60      | 120.44   |
| 1   | G     | 442 | LYS  | N-CA-CB   | 5.26  | 117.95      | 110.06   |
| 2   | B     | 75  | LEU  | N-CA-CB   | 5.26  | 117.61      | 109.98   |
| 1   | G     | 112 | ILE  | O-C-N     | 5.26  | 127.10      | 121.10   |
| 1   | A     | 471 | GLN  | CA-CB-CG  | -5.26 | 103.59      | 114.10   |
| 2   | H     | 111 | ILE  | CA-C-O    | 5.26  | 126.74      | 121.27   |
| 1   | A     | 516 | PHE  | O-C-N     | -5.25 | 115.84      | 122.20   |
| 1   | A     | 164 | GLY  | CA-C-O    | 5.25  | 124.61      | 119.04   |
| 1   | G     | 90  | PRO  | N-CA-CB   | 5.25  | 108.77      | 103.25   |
| 1   | G     | 108 | PHE  | CA-C-N    | -5.25 | 114.05      | 122.08   |
| 1   | G     | 108 | PHE  | C-N-CA    | -5.25 | 114.05      | 122.08   |
| 1   | G     | 239 | ILE  | CA-CB-CG1 | -5.25 | 101.48      | 110.40   |
| 2   | B     | 261 | ALA  | N-CA-C    | -5.24 | 106.47      | 112.92   |
| 1   | A     | 537 | THR  | N-CA-CB   | -5.24 | 103.16      | 110.29   |
| 1   | G     | 460 | MET  | N-CA-C    | 5.24  | 116.99      | 111.28   |
| 1   | G     | 19  | ARG  | CA-C-O    | -5.24 | 115.50      | 121.00   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | G     | 363 | ILE  | N-CA-CB     | 5.23  | 116.67      | 110.55   |
| 2   | B     | 251 | GLN  | N-CA-C      | 5.23  | 118.27      | 109.95   |
| 2   | H     | 210 | VAL  | CA-C-O      | -5.23 | 114.77      | 120.84   |
| 3   | I     | 151 | ALA  | CA-C-O      | 5.23  | 126.82      | 121.07   |
| 1   | G     | 467 | THR  | CA-C-O      | -5.23 | 115.51      | 121.00   |
| 2   | B     | 58  | ASP  | CA-C-O      | -5.23 | 115.31      | 120.90   |
| 1   | G     | 126 | LEU  | N-CA-CB     | 5.23  | 117.73      | 109.94   |
| 3   | I     | 119 | ILE  | N-CA-C      | 5.23  | 115.43      | 108.11   |
| 3   | I     | 130 | PRO  | CB-CA-C     | -5.22 | 104.00      | 112.62   |
| 3   | C     | 50  | VAL  | CA-C-O      | 5.22  | 126.38      | 120.95   |
| 1   | A     | 280 | TRP  | CB-CA-C     | -5.22 | 100.65      | 110.67   |
| 3   | I     | 98  | PHE  | CB-CA-C     | -5.22 | 101.81      | 110.68   |
| 3   | I     | 232 | PHE  | O-C-N       | -5.22 | 116.90      | 123.27   |
| 2   | H     | 179 | GLN  | CA-C-O      | 5.22  | 126.30      | 120.82   |
| 3   | C     | 13  | PRO  | CA-C-N      | 5.22  | 126.36      | 119.84   |
| 3   | C     | 13  | PRO  | C-N-CA      | 5.22  | 126.36      | 119.84   |
| 1   | A     | 396 | VAL  | CB-CA-C     | -5.21 | 102.74      | 111.29   |
| 2   | H     | 221 | VAL  | CA-C-O      | 5.21  | 126.94      | 119.95   |
| 1   | G     | 380 | PRO  | CB-CA-C     | 5.21  | 120.16      | 111.56   |
| 2   | H     | 126 | GLN  | CB-CG-CD    | -5.21 | 103.74      | 112.60   |
| 1   | A     | 506 | ALA  | O-C-N       | 5.21  | 127.66      | 122.08   |
| 2   | B     | 91  | PRO  | CB-CA-C     | -5.21 | 103.38      | 111.40   |
| 1   | A     | 48  | THR  | N-CA-CB     | 5.21  | 117.78      | 110.12   |
| 1   | A     | 425 | SER  | CA-CB-OG    | -5.21 | 100.68      | 111.10   |
| 4   | D     | 47  | ALA  | CB-CA-C     | -5.21 | 102.00      | 110.85   |
| 2   | B     | 31  | GLU  | CA-C-O      | -5.21 | 114.01      | 120.57   |
| 1   | G     | 300 | HIS  | ND1-CE1-NE2 | 5.21  | 113.61      | 108.40   |
| 1   | G     | 465 | ASN  | CA-CB-CG    | -5.21 | 107.39      | 112.60   |
| 3   | I     | 231 | HIS  | CA-C-O      | -5.21 | 113.26      | 119.35   |
| 3   | I     | 50  | VAL  | N-CA-C      | 5.21  | 115.98      | 110.72   |
| 2   | B     | 142 | GLN  | O-C-N       | -5.20 | 116.44      | 122.89   |
| 1   | G     | 102 | HIS  | CA-CB-CG    | 5.20  | 119.00      | 113.80   |
| 1   | G     | 347 | TYR  | CA-C-O      | -5.20 | 115.35      | 121.07   |
| 1   | G     | 223 | HIS  | N-CA-C      | 5.20  | 120.54      | 113.37   |
| 1   | A     | 525 | VAL  | CA-C-N      | -5.20 | 114.08      | 122.24   |
| 1   | A     | 525 | VAL  | C-N-CA      | -5.20 | 114.08      | 122.24   |
| 2   | H     | 214 | ASP  | CA-C-O      | 5.20  | 127.94      | 120.51   |
| 2   | B     | 100 | LEU  | N-CA-C      | 5.19  | 116.94      | 111.28   |
| 2   | H     | 205 | THR  | CA-C-N      | -5.19 | 116.39      | 122.93   |
| 2   | H     | 205 | THR  | C-N-CA      | -5.19 | 116.39      | 122.93   |
| 2   | B     | 251 | GLN  | N-CA-CB     | -5.19 | 102.55      | 110.85   |
| 1   | A     | 73  | VAL  | CA-C-N      | 5.19  | 131.45      | 121.54   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A     | 73  | VAL  | C-N-CA      | 5.19  | 131.45      | 121.54   |
| 1   | A     | 287 | VAL  | CB-CA-C     | -5.19 | 105.14      | 112.14   |
| 1   | A     | 194 | VAL  | CA-C-N      | -5.18 | 113.58      | 120.79   |
| 1   | A     | 194 | VAL  | C-N-CA      | -5.18 | 113.58      | 120.79   |
| 1   | A     | 220 | MET  | N-CA-CB     | 5.18  | 118.23      | 109.94   |
| 1   | G     | 95  | TRP  | O-C-N       | 5.18  | 128.07      | 122.11   |
| 1   | G     | 172 | TRP  | CH2-CZ2-CE2 | -5.18 | 110.76      | 117.50   |
| 1   | A     | 384 | ALA  | O-C-N       | 5.18  | 127.61      | 122.12   |
| 3   | C     | 40  | GLY  | N-CA-C      | 5.18  | 122.90      | 112.34   |
| 1   | G     | 21  | PHE  | CA-CB-CG    | -5.18 | 108.62      | 113.80   |
| 1   | G     | 128 | ILE  | CA-C-O      | -5.18 | 113.25      | 119.36   |
| 1   | G     | 545 | PRO  | CA-C-N      | 5.18  | 125.71      | 120.38   |
| 1   | G     | 545 | PRO  | C-N-CA      | 5.18  | 125.71      | 120.38   |
| 1   | A     | 152 | LEU  | O-C-N       | -5.17 | 116.54      | 122.08   |
| 1   | A     | 160 | PRO  | CA-CB-CG    | -5.17 | 94.67       | 104.50   |
| 3   | C     | 99  | TRP  | CA-C-O      | -5.17 | 115.39      | 120.82   |
| 1   | G     | 189 | LEU  | O-C-N       | -5.17 | 116.54      | 122.08   |
| 1   | G     | 532 | ASN  | CA-C-N      | 5.17  | 127.47      | 120.38   |
| 1   | G     | 532 | ASN  | C-N-CA      | 5.17  | 127.47      | 120.38   |
| 1   | A     | 89  | THR  | N-CA-CB     | -5.17 | 102.35      | 110.11   |
| 1   | G     | 191 | ILE  | CB-CA-C     | -5.17 | 105.35      | 111.97   |
| 3   | I     | 13  | PRO  | CB-CA-C     | 5.17  | 117.22      | 110.92   |
| 3   | I     | 140 | ILE  | CB-CA-C     | -5.17 | 104.15      | 112.16   |
| 1   | A     | 374 | SER  | N-CA-C      | -5.17 | 101.29      | 109.76   |
| 2   | B     | 192 | LEU  | N-CA-C      | 5.16  | 119.71      | 113.41   |
| 1   | A     | 116 | PHE  | CA-C-O      | -5.16 | 113.74      | 119.67   |
| 1   | A     | 523 | ALA  | CA-C-N      | -5.15 | 113.64      | 120.90   |
| 1   | A     | 523 | ALA  | C-N-CA      | -5.15 | 113.64      | 120.90   |
| 2   | H     | 95  | THR  | CA-C-O      | -5.15 | 112.77      | 118.69   |
| 1   | G     | 14  | ARG  | NE-CZ-NH1   | -5.15 | 116.35      | 121.50   |
| 1   | A     | 214 | ASN  | CB-CA-C     | -5.14 | 101.42      | 111.03   |
| 1   | G     | 189 | LEU  | CB-CA-C     | 5.14  | 119.09      | 110.92   |
| 3   | I     | 263 | ILE  | CA-C-O      | -5.14 | 115.79      | 121.29   |
| 3   | C     | 121 | PRO  | N-CA-CB     | 5.14  | 108.25      | 102.60   |
| 2   | H     | 214 | ASP  | CB-CG-OD1   | 5.14  | 130.22      | 118.40   |
| 1   | A     | 154 | VAL  | N-CA-CB     | -5.14 | 102.87      | 110.58   |
| 2   | H     | 258 | ILE  | CB-CA-C     | -5.14 | 105.39      | 111.97   |
| 3   | C     | 95  | SER  | CA-C-N      | -5.13 | 113.88      | 120.65   |
| 3   | C     | 95  | SER  | C-N-CA      | -5.13 | 113.88      | 120.65   |
| 3   | I     | 95  | SER  | CA-C-O      | -5.13 | 114.45      | 120.20   |
| 1   | G     | 186 | SER  | CA-C-O      | -5.13 | 115.61      | 121.00   |
| 1   | G     | 222 | MET  | CB-CA-C     | 5.13  | 119.02      | 110.81   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | G     | 111 | VAL  | CA-CB-CG1  | 5.12  | 119.11      | 110.40   |
| 2   | H     | 174 | PRO  | N-CA-C     | -5.12 | 101.92      | 112.47   |
| 4   | J     | 48  | ASN  | CB-CG-ND2  | -5.12 | 108.72      | 116.40   |
| 3   | C     | 139 | LEU  | CA-C-N     | 5.12  | 127.48      | 120.46   |
| 3   | C     | 139 | LEU  | C-N-CA     | 5.12  | 127.48      | 120.46   |
| 4   | J     | 21  | LYS  | O-C-N      | 5.12  | 127.36      | 122.03   |
| 2   | B     | 108 | PRO  | N-CA-CB    | 5.12  | 108.62      | 103.25   |
| 3   | I     | 229 | ARG  | NE-CZ-NH2  | -5.12 | 114.59      | 119.20   |
| 1   | G     | 362 | LYS  | CA-C-O     | -5.12 | 115.13      | 120.55   |
| 1   | A     | 28  | ASP  | CA-CB-CG   | -5.11 | 107.49      | 112.60   |
| 1   | A     | 144 | TRP  | CA-CB-CG   | -5.11 | 103.89      | 113.60   |
| 1   | G     | 193 | ALA  | N-CA-C     | -5.11 | 105.41      | 111.69   |
| 1   | G     | 495 | PHE  | CA-CB-CG   | -5.11 | 108.69      | 113.80   |
| 3   | I     | 8   | ASP  | OD1-CG-OD2 | -5.11 | 110.64      | 122.90   |
| 2   | B     | 118 | PHE  | CA-CB-CG   | -5.11 | 108.69      | 113.80   |
| 2   | B     | 62  | LEU  | N-CA-C     | 5.11  | 116.84      | 111.28   |
| 1   | A     | 478 | GLY  | CA-C-N     | -5.10 | 112.53      | 121.35   |
| 1   | A     | 478 | GLY  | C-N-CA     | -5.10 | 112.53      | 121.35   |
| 3   | C     | 137 | ASN  | N-CA-C     | 5.10  | 117.58      | 111.71   |
| 3   | C     | 202 | PHE  | CA-C-O     | -5.10 | 115.12      | 120.63   |
| 1   | A     | 291 | VAL  | CA-C-O     | -5.10 | 113.71      | 119.42   |
| 1   | A     | 497 | SER  | CA-C-N     | -5.09 | 113.18      | 120.82   |
| 1   | A     | 497 | SER  | C-N-CA     | -5.09 | 113.18      | 120.82   |
| 1   | G     | 287 | VAL  | CA-CB-CG2  | -5.09 | 101.74      | 110.40   |
| 1   | G     | 481 | ARG  | NE-CZ-NH2  | 5.09  | 123.78      | 119.20   |
| 2   | H     | 196 | THR  | OG1-CB-CG2 | 5.09  | 119.48      | 109.30   |
| 1   | G     | 173 | VAL  | N-CA-C     | 5.09  | 119.99      | 113.07   |
| 1   | A     | 502 | PHE  | N-CA-CB    | -5.09 | 102.64      | 110.01   |
| 4   | D     | 15  | ASP  | CA-CB-CG   | -5.09 | 107.51      | 112.60   |
| 3   | C     | 207 | GLY  | O-C-N      | -5.08 | 117.30      | 122.18   |
| 2   | B     | 208 | VAL  | CA-C-N     | -5.08 | 115.79      | 122.85   |
| 2   | B     | 208 | VAL  | C-N-CA     | -5.08 | 115.79      | 122.85   |
| 2   | H     | 211 | THR  | N-CA-CB    | 5.08  | 119.59      | 111.56   |
| 3   | I     | 178 | PHE  | CA-C-O     | -5.08 | 115.48      | 121.07   |
| 1   | A     | 421 | HIS  | CA-C-O     | -5.08 | 114.52      | 120.20   |
| 1   | G     | 194 | VAL  | CB-CA-C    | -5.08 | 105.29      | 112.14   |
| 2   | H     | 216 | ILE  | CA-C-N     | -5.08 | 113.78      | 123.32   |
| 2   | H     | 216 | ILE  | C-N-CA     | -5.08 | 113.78      | 123.32   |
| 1   | G     | 412 | ASP  | CB-CG-OD1  | -5.07 | 106.73      | 118.40   |
| 1   | G     | 79  | SER  | CA-CB-OG   | 5.07  | 121.24      | 111.10   |
| 1   | A     | 374 | SER  | CA-C-O     | -5.07 | 115.17      | 120.80   |
| 1   | G     | 423 | VAL  | CA-C-N     | -5.07 | 113.34      | 122.46   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | G     | 423 | VAL  | C-N-CA     | -5.07 | 113.34      | 122.46   |
| 3   | C     | 224 | LEU  | N-CA-C     | -5.07 | 105.03      | 111.11   |
| 1   | G     | 101 | GLY  | N-CA-C     | -5.06 | 106.63      | 112.50   |
| 2   | H     | 190 | PHE  | CA-C-O     | 5.06  | 127.75      | 120.51   |
| 3   | C     | 81  | TRP  | N-CA-CB    | -5.06 | 102.13      | 109.82   |
| 1   | G     | 289 | ILE  | N-CA-CB    | -5.06 | 104.09      | 110.57   |
| 1   | G     | 62  | PHE  | N-CA-C     | 5.06  | 119.44      | 113.12   |
| 3   | I     | 157 | HIS  | N-CA-CB    | -5.06 | 103.64      | 110.67   |
| 2   | B     | 48  | SER  | N-CA-CB    | -5.06 | 106.52      | 111.27   |
| 1   | G     | 151 | SER  | O-C-N      | 5.06  | 127.29      | 122.03   |
| 1   | A     | 543 | THR  | N-CA-C     | -5.06 | 103.47      | 110.35   |
| 1   | A     | 540 | TRP  | O-C-N      | -5.05 | 115.82      | 122.39   |
| 1   | G     | 442 | LYS  | CA-C-N     | -5.05 | 114.56      | 122.65   |
| 1   | G     | 442 | LYS  | C-N-CA     | -5.05 | 114.56      | 122.65   |
| 1   | G     | 498 | SER  | CA-C-O     | -5.05 | 115.26      | 120.92   |
| 1   | G     | 469 | PHE  | CA-C-O     | -5.05 | 113.24      | 120.16   |
| 1   | A     | 159 | ALA  | N-CA-CB    | -5.05 | 102.71      | 109.88   |
| 1   | A     | 288 | TYR  | N-CA-C     | -5.05 | 106.81      | 112.87   |
| 1   | A     | 172 | TRP  | CB-CG-CD2  | 5.05  | 133.87      | 126.80   |
| 1   | G     | 331 | TRP  | CA-C-O     | -5.05 | 112.74      | 119.10   |
| 2   | H     | 37  | GLN  | OE1-CD-NE2 | 5.05  | 127.65      | 122.60   |
| 3   | I     | 261 | ILE  | CB-CA-C    | 5.05  | 117.35      | 111.55   |
| 1   | G     | 286 | GLN  | N-CA-C     | 5.04  | 119.64      | 111.37   |
| 1   | A     | 96  | ASN  | O-C-N      | -5.04 | 116.78      | 122.03   |
| 3   | I     | 5   | LYS  | CA-CB-CG   | 5.04  | 124.19      | 114.10   |
| 2   | B     | 260 | HIS  | O-C-N      | -5.04 | 115.84      | 122.39   |
| 1   | G     | 204 | GLY  | CA-C-N     | 5.04  | 128.38      | 120.82   |
| 1   | G     | 204 | GLY  | C-N-CA     | 5.04  | 128.38      | 120.82   |
| 1   | G     | 333 | HIS  | N-CA-C     | -5.04 | 105.92      | 111.71   |
| 1   | A     | 93  | HIS  | CA-C-O     | -5.04 | 113.31      | 120.51   |
| 2   | B     | 133 | ASP  | N-CA-C     | -5.04 | 107.17      | 113.72   |
| 1   | G     | 108 | PHE  | CA-CB-CG   | 5.04  | 118.83      | 113.80   |
| 1   | G     | 106 | MET  | N-CA-C     | 5.03  | 117.16      | 111.02   |
| 2   | B     | 143 | TRP  | N-CA-CB    | -5.03 | 101.99      | 110.49   |
| 3   | C     | 239 | GLY  | N-CA-C     | -5.03 | 106.67      | 112.50   |
| 2   | H     | 100 | LEU  | N-CA-C     | 5.03  | 116.76      | 111.28   |
| 1   | A     | 533 | GLU  | N-CA-C     | 5.03  | 117.41      | 111.33   |
| 1   | G     | 81  | TRP  | CA-C-O     | 5.03  | 127.05      | 120.16   |
| 3   | I     | 194 | ALA  | O-C-N      | -5.03 | 115.90      | 122.59   |
| 1   | G     | 114 | ALA  | O-C-N      | -5.02 | 116.18      | 122.11   |
| 1   | G     | 211 | THR  | CA-C-O     | -5.02 | 113.33      | 120.51   |
| 1   | G     | 256 | ASP  | N-CA-C     | -5.02 | 105.81      | 111.28   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | A     | 14  | ARG  | CD-NE-CZ | 5.02  | 131.43      | 124.40   |
| 1   | A     | 79  | SER  | CA-C-O   | 5.02  | 125.57      | 119.05   |
| 2   | B     | 220 | THR  | CB-CA-C  | -5.02 | 101.64      | 109.72   |
| 2   | H     | 268 | LYS  | CB-CA-C  | 5.02  | 118.09      | 109.51   |
| 2   | H     | 70  | ILE  | N-CA-C   | -5.02 | 105.01      | 110.23   |
| 1   | A     | 462 | VAL  | N-CA-CB  | -5.01 | 105.36      | 110.62   |
| 3   | C     | 73  | PRO  | CA-C-O   | -5.01 | 111.48      | 120.60   |
| 1   | A     | 539 | GLU  | CA-C-O   | 5.01  | 125.73      | 120.42   |
| 1   | A     | 293 | PRO  | N-CA-CB  | 5.01  | 108.51      | 103.25   |
| 3   | C     | 206 | THR  | N-CA-CB  | 5.01  | 118.83      | 110.32   |
| 1   | A     | 481 | ARG  | N-CA-CB  | 5.01  | 118.37      | 110.56   |
| 2   | H     | 130 | PRO  | CA-C-O   | 5.01  | 129.71      | 120.60   |
| 1   | G     | 319 | ALA  | N-CA-C   | -5.00 | 105.10      | 111.11   |
| 3   | I     | 58  | TRP  | CA-C-O   | -5.00 | 115.16      | 121.02   |
| 1   | A     | 257 | ARG  | CB-CA-C  | -5.00 | 99.53       | 109.99   |
| 3   | C     | 178 | PHE  | CA-CB-CG | 5.00  | 118.80      | 113.80   |
| 2   | H     | 40  | GLY  | CA-C-O   | 5.00  | 126.08      | 121.58   |
| 2   | H     | 129 | ILE  | N-CA-C   | 5.00  | 119.69      | 108.88   |
| 4   | D     | 22  | THR  | O-C-N    | -5.00 | 116.73      | 122.08   |
| 1   | G     | 368 | ALA  | CB-CA-C  | -5.00 | 99.86       | 110.31   |

There are no chirality outliers.

All (57) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 1   | A     | 108 | PHE  | Mainchain         |
| 1   | A     | 112 | ILE  | Mainchain         |
| 1   | A     | 114 | ALA  | Mainchain         |
| 1   | A     | 124 | MET  | Mainchain         |
| 1   | A     | 145 | LEU  | Mainchain         |
| 1   | A     | 152 | LEU  | Mainchain         |
| 1   | A     | 157 | LEU  | Mainchain         |
| 1   | A     | 222 | MET  | Mainchain         |
| 1   | A     | 257 | ARG  | Mainchain         |
| 1   | A     | 258 | ASN  | Mainchain         |
| 1   | A     | 261 | THR  | Mainchain         |
| 1   | A     | 283 | GLY  | Mainchain         |
| 1   | A     | 288 | TYR  | Mainchain         |
| 1   | A     | 29  | ILE  | Mainchain         |
| 1   | A     | 333 | HIS  | Mainchain         |
| 1   | A     | 340 | LEU  | Mainchain         |
| 1   | A     | 544 | SER  | Mainchain,Peptide |

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| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 1   | A     | 96  | ASN  | Mainchain         |
| 2   | B     | 136 | VAL  | Mainchain         |
| 2   | B     | 142 | GLN  | Mainchain         |
| 2   | B     | 160 | MET  | Mainchain         |
| 2   | B     | 222 | PRO  | Mainchain         |
| 2   | B     | 253 | SER  | Mainchain         |
| 2   | B     | 259 | SER  | Mainchain         |
| 3   | C     | 162 | ARG  | Mainchain         |
| 3   | C     | 17  | TRP  | Mainchain         |
| 3   | C     | 194 | ALA  | Mainchain         |
| 3   | C     | 36  | MET  | Mainchain         |
| 3   | C     | 57  | GLY  | Mainchain         |
| 4   | D     | 47  | ALA  | Mainchain         |
| 1   | G     | 171 | GLY  | Mainchain         |
| 1   | G     | 285 | PRO  | Mainchain         |
| 1   | G     | 287 | VAL  | Mainchain         |
| 1   | G     | 301 | VAL  | Mainchain         |
| 1   | G     | 303 | ALA  | Mainchain         |
| 1   | G     | 326 | LEU  | Mainchain         |
| 1   | G     | 368 | ALA  | Mainchain         |
| 1   | G     | 380 | PRO  | Mainchain         |
| 1   | G     | 385 | LEU  | Mainchain         |
| 1   | G     | 444 | SER  | Mainchain         |
| 1   | G     | 473 | PHE  | Mainchain         |
| 1   | G     | 481 | ARG  | Mainchain         |
| 1   | G     | 488 | GLU  | Mainchain         |
| 1   | G     | 544 | SER  | Mainchain,Peptide |
| 1   | G     | 66  | GLU  | Mainchain         |
| 2   | H     | 105 | THR  | Mainchain         |
| 2   | H     | 142 | GLN  | Mainchain         |
| 2   | H     | 202 | VAL  | Mainchain         |
| 3   | I     | 117 | ASP  | Mainchain         |
| 3   | I     | 26  | PHE  | Mainchain         |
| 3   | I     | 33  | VAL  | Mainchain         |
| 3   | I     | 35  | TRP  | Mainchain         |
| 3   | I     | 76  | ARG  | Mainchain         |
| 3   | I     | 85  | LEU  | Mainchain         |
| 3   | I     | 94  | PHE  | Mainchain         |

## 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     | 4322  | 0        | 4240     | 650     | 0            |
| 1   | G     | 4322  | 0        | 4240     | 657     | 0            |
| 2   | B     | 2046  | 0        | 2011     | 232     | 0            |
| 2   | H     | 2046  | 0        | 2011     | 247     | 0            |
| 3   | C     | 2139  | 0        | 2056     | 242     | 0            |
| 3   | I     | 2139  | 0        | 2056     | 233     | 0            |
| 4   | D     | 311   | 0        | 319      | 34      | 0            |
| 4   | J     | 311   | 0        | 319      | 42      | 0            |
| 5   | A     | 1     | 0        | 0        | 0       | 0            |
| 5   | B     | 2     | 0        | 0        | 0       | 0            |
| 5   | G     | 1     | 0        | 0        | 0       | 0            |
| 5   | H     | 2     | 0        | 0        | 0       | 0            |
| 6   | A     | 1     | 0        | 0        | 0       | 0            |
| 6   | G     | 1     | 0        | 0        | 0       | 0            |
| 7   | A     | 1     | 0        | 0        | 0       | 0            |
| 7   | G     | 1     | 0        | 0        | 0       | 0            |
| 8   | A     | 120   | 0        | 108      | 37      | 0            |
| 8   | G     | 120   | 0        | 108      | 38      | 0            |
| 9   | A     | 102   | 0        | 164      | 38      | 0            |
| 9   | C     | 153   | 0        | 246      | 56      | 0            |
| 9   | D     | 51    | 0        | 82       | 17      | 0            |
| 9   | G     | 102   | 0        | 164      | 42      | 0            |
| 9   | I     | 153   | 0        | 246      | 59      | 0            |
| 9   | J     | 51    | 0        | 82       | 12      | 0            |
| 10  | A     | 97    | 0        | 0        | 27      | 0            |
| 10  | B     | 70    | 0        | 0        | 20      | 0            |
| 10  | C     | 38    | 0        | 0        | 8       | 0            |
| 10  | D     | 13    | 0        | 0        | 0       | 0            |
| 10  | G     | 107   | 0        | 0        | 30      | 0            |
| 10  | H     | 64    | 0        | 0        | 18      | 0            |
| 10  | I     | 37    | 0        | 0        | 7       | 0            |
| 10  | J     | 10    | 0        | 0        | 1       | 0            |
| All | All   | 18934 | 0        | 18452    | 2278    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 62.

All (2278) 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:379:THR:HB    | 1:G:380:PRO:HD3   | 1.18                     | 1.17              |
| 1:A:106:MET:HG2   | 8:A:1001:HEA:HAC  | 1.17                     | 1.16              |
| 9:C:2010:3PE:H3E2 | 9:C:2010:3PE:H3I2 | 1.22                     | 1.13              |
| 9:I:3010:3PE:H3E2 | 9:I:3010:3PE:C3I  | 1.78                     | 1.13              |
| 1:A:279:LEU:HD23  | 1:A:279:LEU:C     | 1.73                     | 1.12              |
| 1:A:106:MET:HG2   | 8:A:1001:HEA:CAC  | 1.79                     | 1.10              |
| 1:G:414:TYR:HA    | 1:G:417:VAL:HG23  | 1.31                     | 1.10              |
| 1:A:177:PRO:HG2   | 2:B:215:VAL:HA    | 1.34                     | 1.09              |
| 1:G:401:LEU:HD13  | 1:G:416:VAL:HG22  | 1.31                     | 1.09              |
| 1:G:106:MET:HG2   | 8:G:1001:HEA:CAC  | 1.81                     | 1.08              |
| 9:I:3010:3PE:C3E  | 9:I:3010:3PE:H3I2 | 1.80                     | 1.08              |
| 1:G:106:MET:HG2   | 8:G:1001:HEA:HAC  | 1.23                     | 1.08              |
| 1:G:127:HIS:HB3   | 1:G:226:PRO:HG3   | 1.29                     | 1.08              |
| 1:G:279:LEU:HD23  | 1:G:279:LEU:C     | 1.81                     | 1.05              |
| 1:A:379:THR:HB    | 1:A:380:PRO:HD3   | 1.35                     | 1.04              |
| 3:I:8:ASP:HB3     | 3:I:72:THR:HG21   | 1.40                     | 1.04              |
| 3:I:8:ASP:H       | 4:J:14:MET:HE3    | 1.23                     | 1.02              |
| 1:G:243:LEU:N     | 1:G:244:PRO:HD2   | 1.74                     | 1.02              |
| 9:A:2009:3PE:H392 | 9:A:2009:3PE:H291 | 1.42                     | 1.01              |
| 9:I:3010:3PE:H3E2 | 9:I:3010:3PE:H3I2 | 1.07                     | 1.01              |
| 1:A:284:HIS:NE2   | 1:A:288:TYR:HE2   | 1.58                     | 1.00              |
| 2:B:98:SER:HB2    | 2:B:99:PRO:HD3    | 1.41                     | 1.00              |
| 3:C:21:ALA:HB2    | 3:C:54:THR:HG21   | 1.42                     | 1.00              |
| 1:G:381:MET:HE3   | 1:G:385:LEU:HD21  | 1.42                     | 0.99              |
| 1:G:222:MET:HG3   | 9:G:3012:3PE:H111 | 1.41                     | 0.99              |
| 1:A:381:MET:HE3   | 1:A:385:LEU:HD21  | 1.45                     | 0.99              |
| 1:G:249:ALA:HB2   | 1:G:278:ILE:HG22  | 1.46                     | 0.98              |
| 1:A:401:LEU:HD13  | 1:A:416:VAL:HG22  | 1.45                     | 0.97              |
| 3:C:8:ASP:HB3     | 3:C:72:THR:HG21   | 1.47                     | 0.97              |
| 1:A:25:ASN:HD21   | 1:A:27:LYS:HZ3    | 1.05                     | 0.97              |
| 2:H:62:LEU:HD12   | 2:H:65:ILE:HD11   | 1.46                     | 0.96              |
| 2:B:107:VAL:HG13  | 2:B:108:PRO:HD3   | 1.46                     | 0.96              |
| 9:C:2010:3PE:H3I2 | 9:C:2010:3PE:C3E  | 1.94                     | 0.96              |
| 9:A:2012:3PE:H2F1 | 9:D:2011:3PE:H2I2 | 1.44                     | 0.96              |
| 1:A:243:LEU:H     | 1:A:244:PRO:HD2   | 1.32                     | 0.95              |
| 1:G:345:GLN:HE22  | 1:G:408:ARG:HH22  | 1.07                     | 0.95              |
| 2:H:98:SER:HB2    | 2:H:99:PRO:HD3    | 1.48                     | 0.95              |
| 3:C:122:PRO:HG2   | 3:C:125:ILE:HG13  | 1.46                     | 0.95              |
| 1:A:243:LEU:N     | 1:A:244:PRO:HD2   | 1.82                     | 0.94              |
| 1:G:342:LEU:HD13  | 2:H:127:GLN:HB2   | 1.49                     | 0.94              |
| 2:H:30:LEU:HD22   | 2:H:247:ILE:HD11  | 1.50                     | 0.94              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:520:THR:HG22  | 1:A:521:ARG:HG2   | 1.48                     | 0.93              |
| 1:G:520:THR:HG22  | 1:G:521:ARG:HG2   | 1.51                     | 0.93              |
| 1:A:342:LEU:HD13  | 2:B:127:GLN:HB2   | 1.51                     | 0.93              |
| 1:A:25:ASN:HD21   | 1:A:27:LYS:NZ     | 1.67                     | 0.93              |
| 3:I:21:ALA:HB2    | 3:I:54:THR:HG21   | 1.50                     | 0.93              |
| 1:G:136:PRO:HG2   | 3:I:12:LEU:HD12   | 1.51                     | 0.92              |
| 1:G:63:MET:HG2    | 1:G:94:LEU:HD23   | 1.48                     | 0.92              |
| 1:G:432:ILE:HG21  | 8:G:1001:HEA:H252 | 1.52                     | 0.92              |
| 1:G:284:HIS:HB3   | 1:G:285:PRO:HD3   | 1.48                     | 0.92              |
| 1:G:396:VAL:HG11  | 2:H:65:ILE:HD13   | 1.51                     | 0.92              |
| 1:G:63:MET:HE1    | 1:G:95:TRP:HE3    | 1.35                     | 0.91              |
| 1:G:106:MET:HE3   | 1:G:110:VAL:HB    | 1.52                     | 0.91              |
| 3:I:253:VAL:HA    | 9:I:3010:3PE:H3H1 | 1.50                     | 0.91              |
| 9:C:2010:3PE:H3E2 | 9:C:2010:3PE:C3I  | 1.99                     | 0.91              |
| 2:B:30:LEU:HD22   | 2:B:247:ILE:HD11  | 1.52                     | 0.90              |
| 9:I:3013:3PE:H261 | 9:I:3013:3PE:H3A2 | 1.54                     | 0.89              |
| 2:B:62:LEU:HD12   | 2:B:65:ILE:HD11   | 1.55                     | 0.89              |
| 9:G:3012:3PE:H2H1 | 9:I:3010:3PE:H2I3 | 1.53                     | 0.89              |
| 1:A:345:GLN:NE2   | 1:A:408:ARG:HH22  | 1.70                     | 0.89              |
| 1:G:445:GLY:HA2   | 1:G:525:VAL:HG12  | 1.55                     | 0.88              |
| 1:A:284:HIS:HB3   | 1:A:285:PRO:HD3   | 1.53                     | 0.88              |
| 1:G:25:ASN:HD21   | 1:G:27:LYS:NZ     | 1.69                     | 0.88              |
| 1:A:135:PHE:HE1   | 3:C:79:LEU:HD23   | 1.38                     | 0.87              |
| 1:A:284:HIS:HE2   | 1:A:288:TYR:HE2   | 1.15                     | 0.87              |
| 2:B:238:LEU:C     | 2:B:238:LEU:HD12  | 2.01                     | 0.86              |
| 1:A:345:GLN:HE22  | 1:A:408:ARG:HH22  | 0.92                     | 0.86              |
| 2:B:111:ILE:HG22  | 2:B:112:LEU:HD23  | 1.56                     | 0.86              |
| 1:G:284:HIS:NE2   | 1:G:288:TYR:HE2   | 1.74                     | 0.86              |
| 3:C:254:TRP:HA    | 3:C:257:LEU:HD12  | 1.57                     | 0.85              |
| 9:C:2013:3PE:O14  | 9:C:2013:3PE:H121 | 1.75                     | 0.85              |
| 8:A:1002:HEA:CMC  | 8:A:1002:HEA:HBC1 | 2.07                     | 0.85              |
| 1:A:170:ILE:HG21  | 1:A:174:LEU:HA    | 1.59                     | 0.85              |
| 9:I:3013:3PE:H3F2 | 9:I:3013:3PE:H2B2 | 1.57                     | 0.84              |
| 1:A:243:LEU:HD21  | 10:A:2034:HOH:O   | 1.74                     | 0.84              |
| 3:I:161:ARG:HH12  | 3:I:230:GLY:HA2   | 1.42                     | 0.84              |
| 1:G:55:LEU:HD11   | 10:G:3022:HOH:O   | 1.76                     | 0.84              |
| 9:I:3010:3PE:C3I  | 9:I:3010:3PE:C3E  | 2.40                     | 0.84              |
| 9:I:3013:3PE:H2D2 | 9:I:3013:3PE:C3G  | 2.06                     | 0.84              |
| 1:A:100:THR:HG23  | 1:A:104:ILE:HD12  | 1.59                     | 0.84              |
| 3:I:103:LYS:HD3   | 3:I:103:LYS:C     | 2.02                     | 0.84              |
| 1:G:20:TRP:CE3    | 1:G:32:LEU:HD21   | 2.13                     | 0.83              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:G:3009:3PE:H392 | 9:G:3009:3PE:H291 | 1.58                     | 0.83              |
| 1:A:414:TYR:HA    | 1:A:417:VAL:HG23  | 1.58                     | 0.83              |
| 1:G:127:HIS:HB3   | 1:G:226:PRO:CG    | 2.08                     | 0.83              |
| 1:G:177:PRO:HG2   | 2:H:215:VAL:HA    | 1.60                     | 0.83              |
| 9:I:3013:3PE:O14  | 9:I:3013:3PE:H121 | 1.78                     | 0.83              |
| 3:I:59:TRP:HA     | 3:I:62:VAL:HG23   | 1.60                     | 0.83              |
| 1:A:26:HIS:C      | 1:A:26:HIS:CD2    | 2.55                     | 0.83              |
| 1:G:170:ILE:HD11  | 1:G:187:THR:OG1   | 1.77                     | 0.83              |
| 1:G:379:THR:HB    | 1:G:380:PRO:CD    | 2.05                     | 0.83              |
| 1:G:302:ILE:HG22  | 1:G:369:THR:HG21  | 1.59                     | 0.82              |
| 8:G:1002:HEA:O11  | 8:G:1002:HEA:HHC  | 1.79                     | 0.82              |
| 2:H:145:TRP:NE1   | 2:H:263:MET:HE2   | 1.94                     | 0.82              |
| 9:A:2009:3PE:H291 | 9:A:2009:3PE:C39  | 2.10                     | 0.82              |
| 1:G:379:THR:CB    | 1:G:380:PRO:HD3   | 2.03                     | 0.82              |
| 3:I:161:ARG:NH2   | 3:I:232:PHE:H     | 1.77                     | 0.82              |
| 1:A:63:MET:HE1    | 1:A:95:TRP:HE3    | 1.44                     | 0.81              |
| 1:G:212:PHE:HE1   | 1:G:222:MET:HE3   | 1.44                     | 0.81              |
| 1:G:387:PHE:CD1   | 1:G:387:PHE:C     | 2.57                     | 0.81              |
| 1:A:529:ASN:C     | 1:A:529:ASN:OD1   | 2.24                     | 0.81              |
| 1:G:25:ASN:HD21   | 1:G:27:LYS:HZ3    | 1.24                     | 0.81              |
| 9:I:3013:3PE:H3H2 | 9:I:3013:3PE:H2E1 | 1.61                     | 0.81              |
| 1:G:243:LEU:H     | 1:G:244:PRO:HD2   | 1.38                     | 0.81              |
| 1:G:547:PRO:HD2   | 1:G:550:THR:HG22  | 1.62                     | 0.80              |
| 1:A:127:HIS:HB3   | 1:A:226:PRO:HG3   | 1.63                     | 0.80              |
| 3:C:253:VAL:HA    | 9:C:2010:3PE:H3H1 | 1.62                     | 0.80              |
| 1:G:180:THR:HA    | 1:G:257:ARG:HD2   | 1.63                     | 0.80              |
| 1:G:505:PHE:O     | 1:G:509:LEU:HG    | 1.80                     | 0.80              |
| 2:H:107:VAL:HG13  | 2:H:108:PRO:HD3   | 1.62                     | 0.80              |
| 3:C:59:TRP:HA     | 3:C:62:VAL:HG23   | 1.64                     | 0.80              |
| 4:D:14:MET:HG2    | 4:D:15:ASP:N      | 1.96                     | 0.80              |
| 2:B:158:SER:HA    | 2:B:196:THR:HB    | 1.63                     | 0.79              |
| 1:G:160:PRO:HG2   | 1:G:185:TYR:CE1   | 2.17                     | 0.79              |
| 1:G:455:LEU:HG    | 1:G:459:MET:HE2   | 1.62                     | 0.79              |
| 2:B:141:TYR:O     | 2:B:142:GLN:C     | 2.23                     | 0.79              |
| 1:A:106:MET:CG    | 8:A:1001:HEA:HAC  | 2.08                     | 0.79              |
| 1:G:115:LEU:HD22  | 1:G:293:PRO:HB2   | 1.63                     | 0.79              |
| 9:C:2010:3PE:C3E  | 9:C:2010:3PE:C3I  | 2.55                     | 0.78              |
| 1:A:237:TRP:CZ3   | 3:C:88:MET:HE1    | 2.18                     | 0.78              |
| 1:A:379:THR:HB    | 1:A:380:PRO:CD    | 2.12                     | 0.78              |
| 1:G:345:GLN:NE2   | 1:G:408:ARG:HH22  | 1.80                     | 0.78              |
| 1:A:91:ASN:ND2    | 1:A:165:GLN:HE22  | 1.81                     | 0.78              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:199:VAL:HG21  | 2:H:278:TRP:CE3   | 2.18                     | 0.78              |
| 2:H:200:VAL:O     | 2:H:269:VAL:HA    | 1.84                     | 0.78              |
| 1:A:222:MET:HG3   | 9:A:2012:3PE:H111 | 1.65                     | 0.78              |
| 1:A:403:GLN:O     | 1:A:404:ALA:C     | 2.27                     | 0.78              |
| 3:I:8:ASP:CB      | 3:I:72:THR:HG21   | 2.13                     | 0.78              |
| 2:H:163:SER:HB2   | 2:H:165:ALA:HB3   | 1.65                     | 0.77              |
| 4:J:45:ALA:HA     | 9:J:3011:3PE:H321 | 1.66                     | 0.77              |
| 1:A:533:GLU:OE1   | 10:A:2107:HOH:O   | 2.03                     | 0.77              |
| 1:A:237:TRP:HZ3   | 3:C:88:MET:HE1    | 1.50                     | 0.77              |
| 3:I:62:VAL:HG11   | 9:I:3008:3PE:H31  | 1.67                     | 0.77              |
| 1:A:345:GLN:HE22  | 1:A:408:ARG:NH2   | 1.76                     | 0.77              |
| 3:C:9:TYR:HB3     | 10:C:2017:HOH:O   | 1.85                     | 0.77              |
| 3:I:137:ASN:HA    | 3:I:140:ILE:HD12  | 1.67                     | 0.77              |
| 1:G:63:MET:CG     | 1:G:94:LEU:HD23   | 2.15                     | 0.76              |
| 8:G:1002:HEA:CMC  | 8:G:1002:HEA:HBC1 | 2.15                     | 0.76              |
| 1:A:74:LYS:H      | 1:A:74:LYS:HD2    | 1.50                     | 0.76              |
| 1:A:350:MET:HA    | 1:A:353:MET:HE2   | 1.66                     | 0.76              |
| 3:C:161:ARG:HH12  | 3:C:230:GLY:HA2   | 1.48                     | 0.76              |
| 1:G:350:MET:HA    | 1:G:353:MET:HE2   | 1.67                     | 0.76              |
| 3:I:62:VAL:CG1    | 9:I:3008:3PE:H31  | 2.16                     | 0.76              |
| 8:A:1002:HEA:HMC1 | 8:A:1002:HEA:CBC  | 2.15                     | 0.76              |
| 1:A:285:PRO:O     | 1:A:286:GLN:C     | 2.25                     | 0.76              |
| 1:G:203:LEU:O     | 1:G:204:GLY:C     | 2.29                     | 0.76              |
| 1:A:367:ILE:HD13  | 2:B:75:LEU:HD22   | 1.66                     | 0.76              |
| 9:A:2009:3PE:H261 | 3:C:55:MET:HG2    | 1.68                     | 0.76              |
| 2:B:145:TRP:HB2   | 10:B:1049:HOH:O   | 1.85                     | 0.76              |
| 1:A:505:PHE:O     | 1:A:509:LEU:HG    | 1.86                     | 0.76              |
| 1:A:473:PHE:CD1   | 2:B:41:THR:HB     | 2.20                     | 0.75              |
| 1:G:174:LEU:HD13  | 1:G:191:ILE:HD13  | 1.69                     | 0.75              |
| 1:G:50:TYR:O      | 1:G:53:MET:HB2    | 1.86                     | 0.75              |
| 1:G:401:LEU:CD1   | 1:G:416:VAL:HG22  | 2.14                     | 0.75              |
| 3:C:13:PRO:HD3    | 10:C:2018:HOH:O   | 1.86                     | 0.75              |
| 3:C:162:ARG:HG3   | 3:C:163:ASP:H     | 1.51                     | 0.75              |
| 2:H:76:ILE:O      | 2:H:80:VAL:HG23   | 1.87                     | 0.75              |
| 3:C:8:ASP:CB      | 3:C:72:THR:HG21   | 2.16                     | 0.75              |
| 3:I:31:GLY:HA2    | 3:I:43:MET:SD     | 2.27                     | 0.75              |
| 1:A:445:GLY:HA2   | 1:A:525:VAL:HG12  | 1.68                     | 0.74              |
| 1:G:26:HIS:C      | 1:G:26:HIS:CD2    | 2.65                     | 0.74              |
| 2:H:111:ILE:HG22  | 2:H:112:LEU:HD23  | 1.68                     | 0.74              |
| 3:I:8:ASP:H       | 4:J:14:MET:CE     | 1.99                     | 0.74              |
| 1:G:345:GLN:HE22  | 1:G:408:ARG:NH2   | 1.85                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:226:VAL:HA    | 10:H:1157:HOH:O   | 1.86                     | 0.74              |
| 1:A:379:THR:HA    | 1:A:382:LEU:HD12  | 1.66                     | 0.74              |
| 9:C:2010:3PE:H342 | 9:D:2011:3PE:H342 | 1.67                     | 0.74              |
| 3:I:133:LEU:H     | 3:I:134:PRO:CD    | 2.00                     | 0.74              |
| 1:A:417:VAL:HA    | 1:A:420:PHE:CE1   | 2.22                     | 0.74              |
| 9:I:3013:3PE:H2D2 | 9:I:3013:3PE:H3G1 | 1.70                     | 0.74              |
| 1:G:231:SER:N     | 1:G:320:MET:HE1   | 2.02                     | 0.74              |
| 1:A:299:SER:O     | 1:A:300:HIS:C     | 2.29                     | 0.74              |
| 1:G:63:MET:HE1    | 1:G:95:TRP:CE3    | 2.19                     | 0.74              |
| 8:G:1002:HEA:HBC1 | 8:G:1002:HEA:HMC1 | 1.70                     | 0.74              |
| 2:H:172:MET:HE1   | 2:H:190:PHE:HB2   | 1.70                     | 0.74              |
| 1:G:331:TRP:CD1   | 1:G:331:TRP:C     | 2.65                     | 0.74              |
| 1:G:429:VAL:HG13  | 8:G:1001:HEA:H273 | 1.69                     | 0.74              |
| 2:H:132:ALA:HB1   | 2:H:134:VAL:O     | 1.87                     | 0.74              |
| 1:A:112:ILE:H     | 1:A:113:PRO:CD    | 2.00                     | 0.74              |
| 1:G:106:MET:HE3   | 1:G:110:VAL:CB    | 2.17                     | 0.73              |
| 1:A:284:HIS:NE2   | 1:A:288:TYR:CE2   | 2.50                     | 0.73              |
| 3:I:123:GLU:HB2   | 10:I:3032:HOH:O   | 1.85                     | 0.73              |
| 3:C:8:ASP:H       | 4:D:14:MET:HE3    | 1.51                     | 0.73              |
| 1:G:367:ILE:HD13  | 2:H:75:LEU:HB2    | 1.70                     | 0.73              |
| 3:C:101:PHE:CE1   | 3:C:261:ILE:HG12  | 2.23                     | 0.73              |
| 1:G:378:LYS:HE2   | 10:G:3035:HOH:O   | 1.88                     | 0.73              |
| 1:A:93:HIS:HA     | 10:A:2026:HOH:O   | 1.86                     | 0.73              |
| 1:A:425:SER:HA    | 1:A:429:VAL:HG21  | 1.70                     | 0.73              |
| 1:A:240:LEU:HD21  | 3:C:85:LEU:HB3    | 1.69                     | 0.73              |
| 1:G:91:ASN:CG     | 1:G:165:GLN:HE22  | 1.97                     | 0.73              |
| 1:G:455:LEU:HD23  | 1:G:510:PHE:CE2   | 2.22                     | 0.73              |
| 3:C:122:PRO:HG2   | 3:C:125:ILE:CG1   | 2.18                     | 0.73              |
| 1:G:376:GLU:HG2   | 1:G:378:LYS:HG2   | 1.70                     | 0.73              |
| 1:A:63:MET:HG2    | 1:A:94:LEU:HD23   | 1.69                     | 0.73              |
| 1:G:403:GLN:O     | 1:G:404:ALA:C     | 2.30                     | 0.73              |
| 1:G:18:THR:HA     | 1:G:22:MET:HE3    | 1.69                     | 0.73              |
| 1:G:91:ASN:ND2    | 1:G:165:GLN:HE22  | 1.86                     | 0.73              |
| 1:G:395:GLY:O     | 1:G:396:VAL:C     | 2.32                     | 0.73              |
| 1:A:165:GLN:HB3   | 10:A:2044:HOH:O   | 1.88                     | 0.72              |
| 1:A:378:LYS:HE2   | 10:A:2031:HOH:O   | 1.89                     | 0.72              |
| 1:G:414:TYR:HA    | 1:G:417:VAL:CG2   | 2.15                     | 0.72              |
| 9:A:2012:3PE:H2F1 | 9:D:2011:3PE:C2I  | 2.19                     | 0.72              |
| 1:A:376:GLU:HG2   | 1:A:378:LYS:HG2   | 1.71                     | 0.72              |
| 2:B:76:ILE:O      | 2:B:80:VAL:HG23   | 1.89                     | 0.72              |
| 1:A:432:ILE:HG21  | 8:A:1001:HEA:H252 | 1.71                     | 0.72              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:284:HIS:O     | 1:G:287:VAL:HG22  | 1.89                     | 0.72              |
| 1:G:485:ASP:OD1   | 1:G:486:TYR:N     | 2.22                     | 0.72              |
| 9:C:2013:3PE:H261 | 9:C:2013:3PE:H3A2 | 1.70                     | 0.72              |
| 1:G:170:ILE:HG21  | 1:G:174:LEU:HA    | 1.72                     | 0.72              |
| 1:A:393:VAL:O     | 1:A:394:GLY:C     | 2.33                     | 0.72              |
| 1:G:332:ALA:HB3   | 1:G:348:PHE:CD2   | 2.25                     | 0.72              |
| 1:A:480:PRO:HG2   | 1:A:483:TYR:CE2   | 2.25                     | 0.72              |
| 1:G:243:LEU:N     | 1:G:244:PRO:CD    | 2.52                     | 0.72              |
| 1:G:386:GLY:O     | 1:G:390:LEU:HG    | 1.90                     | 0.72              |
| 3:C:62:VAL:HG11   | 9:C:2008:3PE:H31  | 1.72                     | 0.71              |
| 2:H:192:LEU:HB3   | 2:H:249:PHE:CD2   | 2.24                     | 0.71              |
| 1:A:387:PHE:CD1   | 1:A:387:PHE:C     | 2.67                     | 0.71              |
| 1:G:95:TRP:CZ2    | 1:G:99:ILE:HD11   | 2.25                     | 0.71              |
| 1:G:246:LEU:HD22  | 1:G:282:PHE:CZ    | 2.24                     | 0.71              |
| 1:G:432:ILE:HG22  | 1:G:436:ILE:HD11  | 1.71                     | 0.71              |
| 9:G:3009:3PE:H242 | 9:G:3009:3PE:H371 | 1.71                     | 0.71              |
| 1:A:20:TRP:CE3    | 1:A:32:LEU:HD21   | 2.26                     | 0.71              |
| 1:A:396:VAL:HG11  | 2:B:65:ILE:HD13   | 1.71                     | 0.71              |
| 1:A:485:ASP:OD1   | 1:A:486:TYR:N     | 2.23                     | 0.71              |
| 1:G:486:TYR:CD2   | 1:G:490:PHE:HB2   | 2.26                     | 0.71              |
| 8:G:1002:HEA:HHA  | 10:G:3052:HOH:O   | 1.90                     | 0.71              |
| 1:A:170:ILE:CG2   | 1:A:174:LEU:HA    | 2.20                     | 0.71              |
| 3:C:226:ARG:HH21  | 3:C:231:HIS:HB3   | 1.55                     | 0.71              |
| 1:G:489:ALA:CB    | 2:H:36:PRO:HB2    | 2.21                     | 0.71              |
| 8:G:1002:HEA:H131 | 10:G:3026:HOH:O   | 1.90                     | 0.71              |
| 1:A:112:ILE:H     | 1:A:113:PRO:HD2   | 1.55                     | 0.71              |
| 1:A:497:SER:O     | 1:A:498:SER:C     | 2.31                     | 0.71              |
| 8:A:1002:HEA:H131 | 10:A:2022:HOH:O   | 1.90                     | 0.71              |
| 3:C:162:ARG:HG3   | 3:C:163:ASP:N     | 2.03                     | 0.71              |
| 1:G:332:ALA:HB3   | 1:G:348:PHE:CG    | 2.25                     | 0.71              |
| 3:C:249:PHE:O     | 3:C:253:VAL:HG23  | 1.89                     | 0.71              |
| 2:H:173:SER:O     | 2:H:174:PRO:C     | 2.33                     | 0.71              |
| 1:G:24:THR:HG21   | 3:I:13:PRO:O      | 1.91                     | 0.70              |
| 1:G:111:VAL:CG1   | 1:G:290:ILE:HG23  | 2.21                     | 0.70              |
| 1:A:422:TYR:CD2   | 1:A:426:LEU:HD12  | 2.26                     | 0.70              |
| 1:G:433:PHE:HA    | 1:G:436:ILE:HD12  | 1.72                     | 0.70              |
| 2:H:208:VAL:HB    | 2:H:238:LEU:HG    | 1.73                     | 0.70              |
| 2:H:211:THR:HG22  | 2:H:212:GLY:H     | 1.57                     | 0.70              |
| 1:A:277:HIS:CD2   | 1:A:335:MET:HE1   | 2.25                     | 0.70              |
| 2:H:211:THR:HG22  | 2:H:212:GLY:N     | 2.07                     | 0.70              |
| 1:G:135:PHE:HE1   | 3:I:79:LEU:HD23   | 1.56                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:133:LEU:H     | 3:I:134:PRO:HD2   | 1.56                     | 0.70              |
| 3:C:111:PRO:HA    | 4:J:10:VAL:HB     | 1.73                     | 0.70              |
| 3:I:240:PHE:CE1   | 3:I:244:ILE:HD11  | 2.27                     | 0.70              |
| 1:A:289:ILE:O     | 1:A:293:PRO:HD2   | 1.90                     | 0.70              |
| 1:G:212:PHE:CE1   | 1:G:222:MET:HE3   | 2.26                     | 0.70              |
| 2:H:191:LEU:O     | 2:H:264:PRO:HG3   | 1.91                     | 0.70              |
| 1:A:342:LEU:HD21  | 2:B:124:PHE:CD1   | 2.27                     | 0.70              |
| 1:G:262:THR:HG22  | 10:I:3029:HOH:O   | 1.91                     | 0.70              |
| 2:H:105:THR:O     | 2:H:109:ILE:HD12  | 1.91                     | 0.70              |
| 1:A:99:ILE:HD12   | 8:A:1001:HEA:HBA2 | 1.73                     | 0.69              |
| 9:G:3012:3PE:H2F1 | 9:J:3011:3PE:H2I2 | 1.74                     | 0.69              |
| 2:H:201:PRO:HB2   | 2:H:204:LYS:HG3   | 1.75                     | 0.69              |
| 3:I:137:ASN:HD21  | 3:I:181:PHE:HB3   | 1.57                     | 0.69              |
| 1:A:217:ALA:HB1   | 10:A:2082:HOH:O   | 1.90                     | 0.69              |
| 2:H:217:HIS:HB3   | 2:H:252:CYS:SG    | 2.32                     | 0.69              |
| 2:H:234:ARG:NH1   | 3:I:114:PRO:HG3   | 2.08                     | 0.69              |
| 1:A:116:PHE:CZ    | 1:A:208:MET:HE3   | 2.28                     | 0.69              |
| 3:C:240:PHE:CE1   | 3:C:244:ILE:HD11  | 2.28                     | 0.69              |
| 1:G:394:GLY:HA3   | 1:G:423:VAL:CG1   | 2.22                     | 0.69              |
| 3:I:83:PHE:HE1    | 9:I:3008:3PE:H262 | 1.58                     | 0.69              |
| 1:A:176:PRO:O     | 2:B:216:ILE:HD11  | 1.91                     | 0.69              |
| 1:G:367:ILE:HD13  | 2:H:75:LEU:HD22   | 1.72                     | 0.69              |
| 1:A:22:MET:HG2    | 3:C:16:ILE:HA     | 1.75                     | 0.69              |
| 1:A:115:LEU:HD22  | 1:A:293:PRO:HB2   | 1.75                     | 0.69              |
| 1:A:174:LEU:HD13  | 1:A:191:ILE:CD1   | 2.23                     | 0.69              |
| 1:A:243:LEU:N     | 1:A:244:PRO:CD    | 2.55                     | 0.69              |
| 1:A:486:TYR:CD2   | 1:A:490:PHE:HB2   | 2.27                     | 0.69              |
| 8:A:1002:HEA:HBC1 | 8:A:1002:HEA:HMC1 | 1.72                     | 0.69              |
| 2:B:132:ALA:HB1   | 2:B:134:VAL:O     | 1.93                     | 0.69              |
| 1:G:136:PRO:CG    | 3:I:12:LEU:HD12   | 2.23                     | 0.69              |
| 1:G:173:VAL:HG12  | 1:G:279:LEU:HD13  | 1.75                     | 0.69              |
| 2:H:199:VAL:HG11  | 2:H:278:TRP:CE2   | 2.28                     | 0.69              |
| 3:I:194:ALA:O     | 3:I:196:ASN:N     | 2.26                     | 0.69              |
| 2:B:158:SER:HB2   | 2:B:196:THR:O     | 1.93                     | 0.69              |
| 2:H:136:VAL:HG11  | 2:H:198:MET:HE3   | 1.74                     | 0.69              |
| 1:A:99:ILE:CD1    | 8:A:1001:HEA:HBA2 | 2.24                     | 0.68              |
| 2:B:136:VAL:HG11  | 2:B:198:MET:HE3   | 1.74                     | 0.68              |
| 1:G:50:TYR:OH     | 1:G:79:SER:HB3    | 1.93                     | 0.68              |
| 3:I:162:ARG:HG3   | 3:I:163:ASP:N     | 2.08                     | 0.68              |
| 1:A:115:LEU:CD1   | 1:A:432:ILE:HG12  | 2.23                     | 0.68              |
| 1:A:509:LEU:HA    | 1:A:512:LEU:HD12  | 1.75                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:201:PRO:HB2   | 2:H:204:LYS:CG    | 2.23                     | 0.68              |
| 2:H:238:LEU:C     | 2:H:238:LEU:HD12  | 2.18                     | 0.68              |
| 2:B:260:HIS:N     | 10:B:1034:HOH:O   | 2.26                     | 0.68              |
| 4:D:40:ALA:O      | 4:D:41:LEU:C      | 2.35                     | 0.68              |
| 3:I:104:HIS:HB2   | 10:I:3021:HOH:O   | 1.92                     | 0.68              |
| 1:A:367:ILE:CD1   | 2:B:75:LEU:HB2    | 2.23                     | 0.68              |
| 1:A:538:LEU:HD21  | 1:A:560:TRP:CE3   | 2.28                     | 0.68              |
| 2:B:176:VAL:HG12  | 2:B:180:LEU:HD11  | 1.75                     | 0.68              |
| 9:C:2013:3PE:H3F2 | 9:C:2013:3PE:H2B2 | 1.74                     | 0.68              |
| 1:G:299:SER:HB3   | 1:G:310:ILE:HD13  | 1.76                     | 0.68              |
| 2:H:199:VAL:O     | 2:H:200:VAL:HG23  | 1.92                     | 0.68              |
| 1:A:127:HIS:HB3   | 1:A:226:PRO:CG    | 2.22                     | 0.68              |
| 2:B:254:GLU:H     | 2:B:260:HIS:HE1   | 1.41                     | 0.68              |
| 1:G:99:ILE:HD12   | 8:G:1001:HEA:HBA2 | 1.75                     | 0.68              |
| 2:H:143:TRP:HZ2   | 2:H:257:GLY:HA3   | 1.58                     | 0.68              |
| 1:G:65:ALA:O      | 1:G:68:LEU:HG     | 1.92                     | 0.68              |
| 1:A:255:THR:HG21  | 3:C:204:MET:HE2   | 1.75                     | 0.68              |
| 1:A:277:HIS:CG    | 1:A:335:MET:HE1   | 2.29                     | 0.68              |
| 3:C:101:PHE:CZ    | 3:C:261:ILE:HG12  | 2.28                     | 0.68              |
| 1:G:393:VAL:O     | 1:G:394:GLY:C     | 2.34                     | 0.68              |
| 1:A:442:LYS:HD3   | 1:A:540:TRP:CZ3   | 2.28                     | 0.68              |
| 2:B:200:VAL:O     | 2:B:269:VAL:HA    | 1.93                     | 0.68              |
| 2:B:84:HIS:HD2    | 2:B:86:LYS:H      | 1.41                     | 0.68              |
| 3:C:62:VAL:CG1    | 9:C:2008:3PE:H31  | 2.24                     | 0.68              |
| 4:D:44:LEU:HD23   | 9:D:2011:3PE:H322 | 1.75                     | 0.68              |
| 1:G:74:LYS:H      | 1:G:74:LYS:HD2    | 1.58                     | 0.68              |
| 1:G:426:LEU:HD21  | 1:G:464:ALA:HB1   | 1.76                     | 0.68              |
| 3:C:210:GLY:O     | 3:C:211:PHE:C     | 2.35                     | 0.68              |
| 1:G:506:ALA:HA    | 1:G:509:LEU:HD12  | 1.76                     | 0.68              |
| 2:H:158:SER:HB2   | 2:H:196:THR:O     | 1.94                     | 0.67              |
| 2:B:199:VAL:HG11  | 2:B:278:TRP:CE2   | 2.29                     | 0.67              |
| 1:G:176:PRO:HA    | 1:G:177:PRO:C     | 2.19                     | 0.67              |
| 1:A:202:ILE:HD11  | 1:A:244:PRO:HD3   | 1.76                     | 0.67              |
| 1:A:373:GLY:O     | 2:B:83:PHE:HB3    | 1.94                     | 0.67              |
| 1:A:489:ALA:CB    | 2:B:36:PRO:HB2    | 2.24                     | 0.67              |
| 1:A:161:GLY:H     | 1:A:166:LEU:HA    | 1.60                     | 0.67              |
| 1:A:424:MET:HB3   | 8:A:1001:HEA:HBC1 | 1.75                     | 0.67              |
| 1:A:543:THR:HG23  | 1:A:546:PRO:HA    | 1.77                     | 0.67              |
| 3:C:130:PRO:HA    | 3:C:134:PRO:HG2   | 1.77                     | 0.67              |
| 3:C:152:HIS:HA    | 3:C:240:PHE:CE1   | 2.29                     | 0.67              |
| 1:A:170:ILE:HD11  | 1:A:187:THR:OG1   | 1.95                     | 0.67              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:G:165:GLN:HB3   | 10:G:3049:HOH:O  | 1.93                     | 0.67              |
| 1:A:63:MET:CG     | 1:A:94:LEU:HD23  | 2.25                     | 0.67              |
| 1:A:160:PRO:HG2   | 1:A:185:TYR:CE1  | 2.30                     | 0.67              |
| 1:A:212:PHE:HE1   | 1:A:222:MET:HE3  | 1.60                     | 0.67              |
| 3:C:56:PHE:O      | 3:C:57:GLY:C     | 2.35                     | 0.67              |
| 2:H:220:THR:O     | 2:H:250:GLY:HA3  | 1.95                     | 0.67              |
| 1:A:63:MET:HE1    | 1:A:95:TRP:CE3   | 2.28                     | 0.67              |
| 1:A:132:ASP:OD1   | 1:A:133:MET:N    | 2.28                     | 0.67              |
| 1:A:374:SER:HB2   | 2:B:85:GLU:HA    | 1.76                     | 0.67              |
| 1:G:180:THR:HA    | 1:G:257:ARG:CD   | 2.24                     | 0.67              |
| 1:G:211:THR:HG22  | 1:G:212:PHE:N    | 2.10                     | 0.67              |
| 1:A:175:TYR:HB2   | 10:A:2056:HOH:O  | 1.95                     | 0.67              |
| 1:A:414:TYR:HA    | 1:A:417:VAL:CG2  | 2.24                     | 0.67              |
| 9:G:3009:3PE:H291 | 9:G:3009:3PE:C39 | 2.25                     | 0.67              |
| 2:H:136:VAL:HG21  | 2:H:198:MET:HE2  | 1.77                     | 0.67              |
| 3:I:161:ARG:NH1   | 3:I:230:GLY:HA2  | 2.10                     | 0.67              |
| 1:A:249:ALA:HB2   | 1:A:278:ILE:HG22 | 1.77                     | 0.66              |
| 1:G:473:PHE:CD1   | 2:H:41:THR:HB    | 2.30                     | 0.66              |
| 1:A:246:LEU:HD22  | 1:A:282:PHE:CE2  | 2.30                     | 0.66              |
| 2:B:156:PHE:HD2   | 2:B:196:THR:HG21 | 1.60                     | 0.66              |
| 1:A:44:SER:O      | 1:A:45:VAL:C     | 2.37                     | 0.66              |
| 1:A:106:MET:HE3   | 1:A:110:VAL:HB   | 1.76                     | 0.66              |
| 1:G:325:VAL:O     | 1:G:326:LEU:C    | 2.37                     | 0.66              |
| 1:A:279:LEU:C     | 1:A:279:LEU:CD2  | 2.53                     | 0.66              |
| 1:A:407:ASP:O     | 1:A:408:ARG:C    | 2.39                     | 0.66              |
| 2:B:192:LEU:HB3   | 2:B:249:PHE:CD2  | 2.31                     | 0.66              |
| 1:G:51:MET:O      | 1:G:52:ARG:C     | 2.39                     | 0.66              |
| 2:B:32:ILE:HD13   | 2:B:189:GLU:OE2  | 1.95                     | 0.66              |
| 1:G:367:ILE:CD1   | 2:H:75:LEU:HB2   | 2.25                     | 0.66              |
| 1:A:177:PRO:HD2   | 2:B:216:ILE:HG12 | 1.77                     | 0.66              |
| 1:G:213:LEU:HB3   | 3:I:81:TRP:CH2   | 2.31                     | 0.66              |
| 1:G:560:TRP:C     | 1:G:560:TRP:CD1  | 2.73                     | 0.66              |
| 2:H:160:MET:HE1   | 2:H:262:TYR:HB3  | 1.76                     | 0.66              |
| 3:I:186:TYR:O     | 3:I:187:SER:C    | 2.39                     | 0.66              |
| 9:I:3013:3PE:H3G1 | 9:I:3013:3PE:C2D | 2.26                     | 0.66              |
| 8:A:1002:HEA:O11  | 8:A:1002:HEA:HHC | 1.96                     | 0.66              |
| 3:C:124:GLY:HA2   | 1:G:557:ARG:HH12 | 1.60                     | 0.66              |
| 3:I:253:VAL:HG13  | 9:I:3010:3PE:C3I | 2.26                     | 0.66              |
| 1:A:388:LEU:HD12  | 2:B:76:ILE:HD11  | 1.76                     | 0.66              |
| 2:B:173:SER:O     | 2:B:174:PRO:C    | 2.39                     | 0.66              |
| 1:A:112:ILE:N     | 1:A:113:PRO:CD   | 2.53                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:367:ILE:HD13  | 2:B:75:LEU:HB2    | 1.78                     | 0.65              |
| 2:H:224:PHE:HB2   | 2:H:226:VAL:HG22  | 1.77                     | 0.65              |
| 3:I:21:ALA:HB2    | 3:I:54:THR:CG2    | 2.25                     | 0.65              |
| 1:A:115:LEU:HD12  | 1:A:432:ILE:HD11  | 1.77                     | 0.65              |
| 9:C:2010:3PE:H231 | 9:C:2010:3PE:H332 | 1.79                     | 0.65              |
| 2:H:245:GLU:HA    | 2:H:269:VAL:HG13  | 1.79                     | 0.65              |
| 2:H:158:SER:HA    | 2:H:196:THR:HB    | 1.78                     | 0.65              |
| 1:A:65:ALA:HB3    | 1:A:89:THR:HB     | 1.78                     | 0.65              |
| 1:A:174:LEU:HD13  | 1:A:191:ILE:HD13  | 1.79                     | 0.65              |
| 1:G:128:ILE:HD12  | 1:G:216:ARG:HA    | 1.76                     | 0.65              |
| 1:G:249:ALA:HB2   | 1:G:278:ILE:CG2   | 2.23                     | 0.65              |
| 1:G:380:PRO:HG3   | 1:G:437:TYR:HB3   | 1.78                     | 0.65              |
| 1:G:433:PHE:O     | 1:G:436:ILE:N     | 2.29                     | 0.65              |
| 1:G:529:ASN:OD1   | 1:G:531:TRP:N     | 2.30                     | 0.65              |
| 3:I:101:PHE:CZ    | 3:I:261:ILE:HG12  | 2.31                     | 0.65              |
| 1:A:433:PHE:HA    | 1:A:436:ILE:HD12  | 1.77                     | 0.65              |
| 1:A:493:TRP:HA    | 1:A:493:TRP:CE3   | 2.29                     | 0.65              |
| 9:C:2010:3PE:H231 | 9:C:2010:3PE:C33  | 2.26                     | 0.65              |
| 1:A:455:LEU:HG    | 1:A:459:MET:HE2   | 1.78                     | 0.65              |
| 2:B:120:LEU:O     | 2:B:123:LEU:N     | 2.29                     | 0.65              |
| 1:G:451:TRP:O     | 1:G:452:ALA:C     | 2.40                     | 0.65              |
| 1:A:202:ILE:HD11  | 1:A:243:LEU:HB2   | 1.78                     | 0.65              |
| 1:A:332:ALA:HB3   | 1:A:348:PHE:CG    | 2.31                     | 0.65              |
| 1:A:357:VAL:HB    | 1:A:358:PRO:HD3   | 1.79                     | 0.65              |
| 3:I:120:PHE:HA    | 3:I:121:PRO:C     | 2.22                     | 0.65              |
| 1:G:221:THR:HA    | 9:G:3012:3PE:H121 | 1.79                     | 0.65              |
| 1:G:307:LYS:HA    | 1:G:534:HIS:CB    | 2.27                     | 0.65              |
| 1:A:135:PHE:CE1   | 3:C:79:LEU:HD23   | 2.27                     | 0.65              |
| 1:G:367:ILE:HG21  | 2:H:75:LEU:HD22   | 1.77                     | 0.65              |
| 1:A:211:THR:HG22  | 1:A:212:PHE:N     | 2.12                     | 0.64              |
| 1:G:46:ALA:O      | 1:G:49:VAL:HG12   | 1.97                     | 0.64              |
| 1:G:357:VAL:HB    | 1:G:358:PRO:HD3   | 1.79                     | 0.64              |
| 1:G:509:LEU:HA    | 1:G:512:LEU:HD12  | 1.79                     | 0.64              |
| 3:I:133:LEU:N     | 3:I:134:PRO:CD    | 2.59                     | 0.64              |
| 2:B:59:GLY:HA2    | 10:B:1017:HOH:O   | 1.98                     | 0.64              |
| 4:D:45:ALA:HA     | 9:D:2011:3PE:H321 | 1.79                     | 0.64              |
| 1:G:40:VAL:O      | 1:G:41:GLY:C      | 2.40                     | 0.64              |
| 1:G:246:LEU:HD22  | 1:G:282:PHE:CE2   | 2.32                     | 0.64              |
| 3:I:176:ALA:O     | 3:I:179:THR:HB    | 1.97                     | 0.64              |
| 1:A:483:TYR:OH    | 2:B:251:GLN:HB3   | 1.97                     | 0.64              |
| 1:G:48:THR:HA     | 1:G:51:MET:SD     | 2.38                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:493:TRP:CE3   | 1:G:493:TRP:HA    | 2.30                     | 0.64              |
| 1:G:520:THR:CG2   | 1:G:521:ARG:HG2   | 2.26                     | 0.64              |
| 3:C:133:LEU:H     | 3:C:134:PRO:HD2   | 1.61                     | 0.64              |
| 1:G:467:THR:HG21  | 8:G:1001:HEA:HMB2 | 1.79                     | 0.64              |
| 1:G:481:ARG:NH1   | 10:G:3018:HOH:O   | 2.26                     | 0.64              |
| 2:B:98:SER:HB2    | 2:B:99:PRO:CD     | 2.21                     | 0.64              |
| 1:G:284:HIS:HE2   | 1:G:288:TYR:HE2   | 1.44                     | 0.64              |
| 3:I:103:LYS:HE2   | 3:I:107:TYR:HB2   | 1.79                     | 0.64              |
| 2:B:105:THR:O     | 2:B:109:ILE:HD12  | 1.97                     | 0.64              |
| 3:C:123:GLU:HB2   | 10:C:2031:HOH:O   | 1.96                     | 0.64              |
| 1:G:300:HIS:HB3   | 10:G:3023:HOH:O   | 1.97                     | 0.64              |
| 3:C:82:GLY:HA2    | 3:C:85:LEU:HD12   | 1.80                     | 0.64              |
| 3:I:212:HIS:O     | 3:I:213:VAL:C     | 2.39                     | 0.64              |
| 1:A:25:ASN:ND2    | 1:A:27:LYS:NZ     | 2.45                     | 0.64              |
| 1:A:511:PHE:CZ    | 1:A:515:ILE:HD11  | 2.33                     | 0.64              |
| 1:G:127:HIS:NE2   | 1:G:539:GLU:OE1   | 2.31                     | 0.64              |
| 1:G:284:HIS:H     | 1:G:285:PRO:CD    | 2.11                     | 0.64              |
| 1:A:235:THR:OG1   | 1:A:293:PRO:HD3   | 1.97                     | 0.64              |
| 1:A:456:HIS:CE1   | 1:A:511:PHE:HB2   | 2.33                     | 0.64              |
| 1:G:91:ASN:HD21   | 1:G:165:GLN:CD    | 2.06                     | 0.64              |
| 9:I:3013:3PE:H2D2 | 9:I:3013:3PE:H3H2 | 1.80                     | 0.63              |
| 1:A:286:GLN:HA    | 1:A:289:ILE:HD12  | 1.80                     | 0.63              |
| 1:G:176:PRO:HD2   | 10:G:3016:HOH:O   | 1.98                     | 0.63              |
| 4:J:15:ASP:OD1    | 4:J:16:ILE:N      | 2.30                     | 0.63              |
| 1:A:98:MET:O      | 1:A:99:ILE:C      | 2.42                     | 0.63              |
| 1:A:287:VAL:HG23  | 1:A:288:TYR:N     | 2.14                     | 0.63              |
| 1:G:237:TRP:CZ3   | 3:I:88:MET:HE1    | 2.32                     | 0.63              |
| 1:G:284:HIS:CB    | 1:G:285:PRO:HD3   | 2.21                     | 0.63              |
| 2:H:200:VAL:HG12  | 2:H:269:VAL:HG23  | 1.80                     | 0.63              |
| 2:B:199:VAL:HG21  | 2:B:278:TRP:CE3   | 2.33                     | 0.63              |
| 4:J:15:ASP:OD1    | 4:J:15:ASP:C      | 2.41                     | 0.63              |
| 1:A:126:LEU:O     | 1:A:129:GLY:N     | 2.31                     | 0.63              |
| 3:C:59:TRP:HA     | 3:C:62:VAL:CG2    | 2.28                     | 0.63              |
| 3:C:152:HIS:HA    | 3:C:240:PHE:HE1   | 1.63                     | 0.63              |
| 1:G:86:GLU:O      | 2:H:171:ARG:NH1   | 2.31                     | 0.63              |
| 1:G:407:ASP:O     | 1:G:408:ARG:C     | 2.41                     | 0.63              |
| 2:B:201:PRO:HB2   | 2:B:204:LYS:HG3   | 1.80                     | 0.63              |
| 1:G:237:TRP:HZ3   | 3:I:88:MET:HE1    | 1.62                     | 0.63              |
| 1:G:287:VAL:HA    | 1:G:290:ILE:HD12  | 1.81                     | 0.63              |
| 3:I:68:GLU:HB2    | 10:I:3014:HOH:O   | 1.99                     | 0.63              |
| 3:I:92:MET:O      | 3:I:93:PHE:C      | 2.36                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:433:PHE:HE2   | 1:A:460:MET:HE3   | 1.64                     | 0.63              |
| 1:A:290:ILE:HA    | 10:A:2024:HOH:O   | 1.99                     | 0.63              |
| 1:G:95:TRP:HB2    | 1:G:484:ILE:HG13  | 1.81                     | 0.63              |
| 1:G:381:MET:CE    | 1:G:385:LEU:HD21  | 2.24                     | 0.62              |
| 3:I:34:LEU:HB3    | 3:I:39:SER:OG     | 1.98                     | 0.62              |
| 1:A:27:LYS:O      | 1:A:31:VAL:HG23   | 1.99                     | 0.62              |
| 1:A:287:VAL:HB    | 8:A:1002:HEA:CBC  | 2.29                     | 0.62              |
| 1:A:529:ASN:OD1   | 1:A:531:TRP:N     | 2.32                     | 0.62              |
| 1:G:116:PHE:CD1   | 1:G:235:THR:HG21  | 2.33                     | 0.62              |
| 1:G:274:LEU:O     | 1:G:277:HIS:N     | 2.32                     | 0.62              |
| 1:G:279:LEU:C     | 1:G:279:LEU:CD2   | 2.55                     | 0.62              |
| 2:H:32:ILE:HD13   | 2:H:189:GLU:OE2   | 1.99                     | 0.62              |
| 1:A:38:GLY:O      | 1:A:39:LEU:C      | 2.41                     | 0.62              |
| 1:A:495:PHE:O     | 1:A:496:VAL:C     | 2.42                     | 0.62              |
| 9:A:2012:3PE:H2H1 | 9:C:2010:3PE:H2I3 | 1.81                     | 0.62              |
| 1:G:65:ALA:HB3    | 1:G:89:THR:HB     | 1.81                     | 0.62              |
| 1:G:277:HIS:CD2   | 1:G:335:MET:HE1   | 2.35                     | 0.62              |
| 1:A:439:TRP:O     | 1:A:443:MET:HG3   | 1.99                     | 0.62              |
| 2:B:278:TRP:HZ2   | 10:B:1028:HOH:O   | 1.81                     | 0.62              |
| 1:G:141:LEU:HB2   | 3:I:18:PRO:HB3    | 1.80                     | 0.62              |
| 1:G:152:LEU:HD23  | 3:I:26:PHE:CE2    | 2.34                     | 0.62              |
| 1:G:390:LEU:N     | 1:G:390:LEU:HD23  | 2.14                     | 0.62              |
| 2:H:252:CYS:HB2   | 2:H:263:MET:SD    | 2.40                     | 0.62              |
| 9:I:3013:3PE:H3H2 | 9:I:3013:3PE:C2E  | 2.28                     | 0.62              |
| 1:A:95:TRP:HB2    | 1:A:484:ILE:HG13  | 1.82                     | 0.62              |
| 2:B:141:TYR:HE1   | 2:B:146:GLY:HA3   | 1.64                     | 0.62              |
| 2:H:220:THR:HB    | 2:H:227:LYS:HG3   | 1.82                     | 0.62              |
| 3:I:59:TRP:HA     | 3:I:62:VAL:CG2    | 2.30                     | 0.62              |
| 1:A:115:LEU:HD11  | 1:A:432:ILE:HG12  | 1.80                     | 0.62              |
| 1:A:314:LEU:HB3   | 1:A:315:PRO:HD3   | 1.82                     | 0.62              |
| 1:A:455:LEU:HD23  | 1:A:510:PHE:CE2   | 2.33                     | 0.62              |
| 1:G:284:HIS:N     | 1:G:285:PRO:CD    | 2.63                     | 0.62              |
| 1:G:401:LEU:HD13  | 1:G:416:VAL:CG2   | 2.19                     | 0.62              |
| 1:A:221:THR:HG23  | 1:A:224:LYS:HD2   | 1.81                     | 0.62              |
| 1:G:307:LYS:HD3   | 1:G:374:SER:OG    | 2.00                     | 0.62              |
| 9:I:3013:3PE:H2D2 | 9:I:3013:3PE:C3H  | 2.29                     | 0.62              |
| 2:B:245:GLU:HA    | 2:B:269:VAL:HG13  | 1.81                     | 0.62              |
| 3:C:150:TRP:NE1   | 3:C:163:ASP:OD1   | 2.31                     | 0.62              |
| 3:C:161:ARG:NH2   | 3:C:232:PHE:H     | 1.98                     | 0.62              |
| 1:G:474:LEU:HD13  | 10:G:3047:HOH:O   | 1.98                     | 0.62              |
| 1:A:279:LEU:HD23  | 1:A:279:LEU:O     | 1.99                     | 0.61              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:376:GLU:O    | 1:A:378:LYS:N     | 2.32                     | 0.61              |
| 2:B:211:THR:HG22 | 2:B:212:GLY:N     | 2.15                     | 0.61              |
| 2:H:176:VAL:HG12 | 2:H:180:LEU:HD11  | 1.82                     | 0.61              |
| 1:G:220:MET:HE2  | 1:G:225:VAL:HA    | 1.82                     | 0.61              |
| 1:G:307:LYS:HA   | 1:G:534:HIS:CG    | 2.34                     | 0.61              |
| 1:G:342:LEU:HD21 | 2:H:124:PHE:CD1   | 2.35                     | 0.61              |
| 2:H:271:SER:HA   | 10:H:1091:HOH:O   | 2.00                     | 0.61              |
| 1:A:65:ALA:O     | 1:A:68:LEU:HG     | 1.99                     | 0.61              |
| 3:C:152:HIS:CG   | 3:C:244:ILE:HD13  | 2.35                     | 0.61              |
| 1:G:212:PHE:C    | 1:G:212:PHE:CD1   | 2.78                     | 0.61              |
| 2:H:197:ALA:HB2  | 2:H:268:LYS:HZ3   | 1.64                     | 0.61              |
| 3:I:80:ARG:HH12  | 9:I:3013:3PE:H111 | 1.65                     | 0.61              |
| 1:A:18:THR:HA    | 1:A:22:MET:HE3    | 1.81                     | 0.61              |
| 1:A:48:THR:HA    | 1:A:51:MET:SD     | 2.40                     | 0.61              |
| 1:A:147:VAL:O    | 1:A:148:ALA:C     | 2.43                     | 0.61              |
| 1:A:170:ILE:HG22 | 1:A:171:GLY:N     | 2.15                     | 0.61              |
| 1:A:379:THR:O    | 1:A:380:PRO:C     | 2.42                     | 0.61              |
| 1:G:404:ALA:O    | 1:G:407:ASP:N     | 2.34                     | 0.61              |
| 2:H:145:TRP:CE2  | 2:H:263:MET:HE2   | 2.36                     | 0.61              |
| 2:H:164:PRO:HB3  | 10:H:1122:HOH:O   | 2.00                     | 0.61              |
| 1:A:70:SER:HB2   | 1:A:74:LYS:HB2    | 1.82                     | 0.61              |
| 1:A:81:TRP:CD2   | 1:A:82:PRO:HD2    | 2.36                     | 0.61              |
| 2:B:107:VAL:CG1  | 2:B:108:PRO:HD3   | 2.25                     | 0.61              |
| 2:B:151:ASP:HB2  | 10:B:1025:HOH:O   | 1.99                     | 0.61              |
| 3:C:133:LEU:N    | 3:C:134:PRO:CD    | 2.64                     | 0.61              |
| 1:G:99:ILE:CD1   | 8:G:1001:HEA:HBA2 | 2.30                     | 0.61              |
| 1:G:130:ALA:HB1  | 1:G:131:PRO:HD2   | 1.80                     | 0.61              |
| 1:G:170:ILE:O    | 2:H:255:LEU:HD23  | 2.01                     | 0.61              |
| 1:G:222:MET:HG3  | 9:G:3012:3PE:C11  | 2.26                     | 0.61              |
| 3:I:9:TYR:HB3    | 10:I:3018:HOH:O   | 1.99                     | 0.61              |
| 1:A:520:THR:CG2  | 1:A:521:ARG:HG2   | 2.29                     | 0.61              |
| 1:G:463:GLY:N    | 1:G:503:LEU:HD23  | 2.16                     | 0.61              |
| 2:H:248:PHE:HE2  | 2:H:269:VAL:CG1   | 2.14                     | 0.61              |
| 3:I:253:VAL:CA   | 9:I:3010:3PE:H3H1 | 2.27                     | 0.61              |
| 1:A:40:VAL:O     | 1:A:41:GLY:C      | 2.43                     | 0.61              |
| 1:A:332:ALA:HB3  | 1:A:348:PHE:CD2   | 2.35                     | 0.61              |
| 1:G:265:GLN:H    | 1:G:270:GLY:HA3   | 1.65                     | 0.61              |
| 1:A:92:GLY:HA2   | 1:A:484:ILE:HD12  | 1.83                     | 0.61              |
| 1:A:128:ILE:HD12 | 1:A:216:ARG:HA    | 1.82                     | 0.61              |
| 1:A:397:THR:O    | 1:A:400:VAL:N     | 2.34                     | 0.61              |
| 3:I:73:PRO:HB2   | 4:J:16:ILE:HD11   | 1.82                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:99:TRP:O      | 3:I:100:SER:C     | 2.44                     | 0.61              |
| 4:J:16:ILE:HG22   | 4:J:19:GLN:HB2    | 1.81                     | 0.61              |
| 1:G:264:PHE:HB3   | 1:G:272:PRO:HA    | 1.83                     | 0.61              |
| 1:G:417:VAL:HA    | 1:G:420:PHE:CE1   | 2.36                     | 0.61              |
| 1:G:543:THR:HG23  | 1:G:546:PRO:HA    | 1.83                     | 0.61              |
| 2:H:43:PHE:CD2    | 2:H:55:HIS:CD2    | 2.89                     | 0.61              |
| 2:H:250:GLY:O     | 2:H:265:ILE:N     | 2.33                     | 0.61              |
| 1:A:447:GLN:HG3   | 1:A:448:TYR:N     | 2.15                     | 0.60              |
| 1:A:543:THR:CG2   | 1:A:547:PRO:HD3   | 2.31                     | 0.60              |
| 2:B:234:ARG:NH1   | 3:C:114:PRO:HG3   | 2.16                     | 0.60              |
| 1:G:176:PRO:HB2   | 1:G:177:PRO:HA    | 1.82                     | 0.60              |
| 1:G:302:ILE:HG22  | 1:G:369:THR:CG2   | 2.30                     | 0.60              |
| 3:I:162:ARG:HG3   | 3:I:163:ASP:H     | 1.65                     | 0.60              |
| 1:A:284:HIS:H     | 1:A:285:PRO:HD2   | 1.66                     | 0.60              |
| 3:C:133:LEU:N     | 3:C:134:PRO:HD2   | 2.15                     | 0.60              |
| 1:G:202:ILE:HD11  | 1:G:243:LEU:HB2   | 1.81                     | 0.60              |
| 3:I:21:ALA:CB     | 3:I:54:THR:HG21   | 2.26                     | 0.60              |
| 1:G:28:ASP:O      | 1:G:32:LEU:HG     | 2.02                     | 0.60              |
| 2:H:98:SER:HB2    | 2:H:99:PRO:CD     | 2.28                     | 0.60              |
| 3:I:152:HIS:HA    | 3:I:240:PHE:CE1   | 2.35                     | 0.60              |
| 4:J:14:MET:HG2    | 4:J:15:ASP:N      | 2.17                     | 0.60              |
| 1:A:65:ALA:H      | 1:A:89:THR:HB     | 1.67                     | 0.60              |
| 1:A:298:VAL:O     | 1:A:299:SER:C     | 2.44                     | 0.60              |
| 1:A:432:ILE:O     | 1:A:436:ILE:HG13  | 2.01                     | 0.60              |
| 2:B:199:VAL:O     | 2:B:200:VAL:HG23  | 2.00                     | 0.60              |
| 1:G:323:ILE:HD11  | 1:G:359:THR:OG1   | 2.01                     | 0.60              |
| 2:H:103:ALA:O     | 2:H:107:VAL:HG12  | 2.00                     | 0.60              |
| 3:I:239:GLY:H     | 9:I:3008:3PE:H11  | 1.66                     | 0.60              |
| 1:A:29:ILE:HD13   | 1:A:139:ASN:ND2   | 2.15                     | 0.60              |
| 1:G:538:LEU:HD21  | 1:G:560:TRP:CE3   | 2.37                     | 0.60              |
| 1:A:192:PHE:CZ    | 1:A:254:LEU:HD21  | 2.37                     | 0.60              |
| 1:A:213:LEU:HB3   | 3:C:81:TRP:CH2    | 2.36                     | 0.60              |
| 1:A:390:LEU:HD12  | 1:A:426:LEU:HB3   | 1.84                     | 0.60              |
| 9:A:2012:3PE:H2I3 | 9:C:2010:3PE:H2H1 | 1.83                     | 0.60              |
| 2:B:228:GLN:NE2   | 2:B:229:ASP:H     | 1.99                     | 0.60              |
| 2:H:228:GLN:HB2   | 10:H:1069:HOH:O   | 2.02                     | 0.60              |
| 1:A:50:TYR:OH     | 1:A:79:SER:HB3    | 2.02                     | 0.60              |
| 1:A:357:VAL:HG21  | 2:B:109:ILE:HD11  | 1.83                     | 0.60              |
| 1:A:390:LEU:HD23  | 1:A:390:LEU:N     | 2.16                     | 0.60              |
| 1:A:503:LEU:O     | 1:A:506:ALA:HB3   | 2.01                     | 0.60              |
| 1:A:367:ILE:HG21  | 2:B:75:LEU:HD22   | 1.83                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:431:GLY:O     | 1:A:432:ILE:C     | 2.43                     | 0.60              |
| 2:B:235:LEU:HD21  | 4:J:9:HIS:HB2     | 1.84                     | 0.60              |
| 9:C:2013:3PE:H2I3 | 4:D:35:VAL:HG21   | 1.84                     | 0.60              |
| 1:G:394:GLY:HA3   | 1:G:423:VAL:HG12  | 1.82                     | 0.60              |
| 1:G:433:PHE:O     | 1:G:434:ALA:C     | 2.45                     | 0.60              |
| 2:H:145:TRP:CD1   | 2:H:263:MET:HE2   | 2.37                     | 0.60              |
| 3:I:77:LEU:HA     | 3:I:80:ARG:HD3    | 1.83                     | 0.60              |
| 3:I:81:TRP:O      | 3:I:82:GLY:C      | 2.45                     | 0.60              |
| 1:G:442:LYS:HD3   | 1:G:540:TRP:CZ3   | 2.36                     | 0.60              |
| 1:A:52:ARG:HD3    | 1:A:498:SER:HA    | 1.84                     | 0.60              |
| 1:A:60:VAL:HG21   | 1:A:90:PRO:HB3    | 1.84                     | 0.60              |
| 1:A:390:LEU:HA    | 1:A:393:VAL:HG23  | 1.83                     | 0.60              |
| 1:A:466:LEU:O     | 1:A:470:PRO:HD2   | 2.02                     | 0.60              |
| 3:C:76:ARG:O      | 3:C:80:ARG:HG3    | 2.01                     | 0.60              |
| 1:G:294:ALA:O     | 1:G:295:PHE:C     | 2.44                     | 0.60              |
| 1:G:420:PHE:O     | 1:G:421:HIS:C     | 2.43                     | 0.60              |
| 8:G:1002:HEA:HMC1 | 8:G:1002:HEA:CBC  | 2.32                     | 0.60              |
| 4:J:49:ALA:O      | 9:J:3011:3PE:H122 | 2.02                     | 0.60              |
| 2:B:78:TYR:CD1    | 2:B:78:TYR:C      | 2.80                     | 0.59              |
| 1:G:486:TYR:HB2   | 1:G:487:PRO:HD2   | 1.83                     | 0.59              |
| 1:A:381:MET:O     | 1:A:382:LEU:C     | 2.43                     | 0.59              |
| 3:C:133:LEU:H     | 3:C:134:PRO:CD    | 2.15                     | 0.59              |
| 3:C:253:VAL:HG22  | 9:C:2010:3PE:H3I1 | 1.83                     | 0.59              |
| 1:G:432:ILE:CG2   | 8:G:1001:HEA:H252 | 2.31                     | 0.59              |
| 2:H:197:ALA:HB2   | 2:H:268:LYS:NZ    | 2.17                     | 0.59              |
| 3:C:209:HIS:NE2   | 3:C:254:TRP:HB2   | 2.18                     | 0.59              |
| 1:A:489:ALA:HB3   | 2:B:36:PRO:HB2    | 1.82                     | 0.59              |
| 1:A:396:VAL:O     | 1:A:397:THR:C     | 2.45                     | 0.59              |
| 1:A:494:ASN:O     | 1:A:495:PHE:C     | 2.45                     | 0.59              |
| 2:B:175:GLU:O     | 2:B:178:GLN:HG2   | 2.03                     | 0.59              |
| 3:C:149:THR:O     | 3:C:152:HIS:HB3   | 2.03                     | 0.59              |
| 1:G:357:VAL:CB    | 1:G:358:PRO:HD3   | 2.32                     | 0.59              |
| 1:G:491:ALA:HB1   | 10:G:3036:HOH:O   | 2.02                     | 0.59              |
| 2:H:160:MET:CE    | 2:H:262:TYR:HB3   | 2.32                     | 0.59              |
| 3:I:155:LEU:HB2   | 3:I:164:VAL:HG21  | 1.84                     | 0.59              |
| 1:A:38:GLY:HA2    | 8:A:1001:HEA:H22  | 1.84                     | 0.59              |
| 9:C:2010:3PE:H2I1 | 9:C:2013:3PE:H2B2 | 1.84                     | 0.59              |
| 1:A:65:ALA:CB     | 1:A:89:THR:HB     | 2.32                     | 0.59              |
| 1:A:107:MET:HE1   | 1:A:424:MET:SD    | 2.43                     | 0.59              |
| 1:A:299:SER:HB3   | 1:A:310:ILE:HD13  | 1.83                     | 0.59              |
| 1:A:486:TYR:HB2   | 1:A:487:PRO:HD2   | 1.84                     | 0.59              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:200:VAL:HG12 | 2:B:269:VAL:HG23  | 1.83                     | 0.59              |
| 2:B:228:GLN:HB2  | 10:B:1014:HOH:O   | 2.02                     | 0.59              |
| 1:G:210:THR:O    | 1:G:211:THR:C     | 2.46                     | 0.59              |
| 1:A:380:PRO:HG3  | 1:A:437:TYR:HB3   | 1.83                     | 0.59              |
| 1:G:268:GLY:O    | 3:I:197:ILE:HG23  | 2.02                     | 0.59              |
| 1:A:96:ASN:O     | 1:A:97:VAL:C      | 2.46                     | 0.59              |
| 2:B:65:ILE:C     | 2:B:65:ILE:HD12   | 2.28                     | 0.59              |
| 2:B:208:VAL:HB   | 2:B:238:LEU:HG    | 1.84                     | 0.59              |
| 1:G:40:VAL:HG12  | 1:G:110:VAL:HG22  | 1.85                     | 0.59              |
| 1:A:17:PHE:O     | 1:A:21:PHE:HB2    | 2.03                     | 0.59              |
| 1:A:188:ASP:CG   | 1:A:257:ARG:HH12  | 2.11                     | 0.59              |
| 1:G:178:LEU:HD12 | 1:G:178:LEU:O     | 2.02                     | 0.59              |
| 4:J:40:ALA:O     | 4:J:41:LEU:C      | 2.44                     | 0.59              |
| 1:A:262:THR:HG22 | 10:C:2028:HOH:O   | 2.02                     | 0.58              |
| 4:D:15:ASP:C     | 4:D:15:ASP:OD1    | 2.46                     | 0.58              |
| 1:G:106:MET:SD   | 8:G:1001:HEA:HMC1 | 2.42                     | 0.58              |
| 1:G:486:TYR:HD2  | 1:G:490:PHE:HB2   | 1.67                     | 0.58              |
| 2:H:279:LEU:O    | 2:H:283:ARG:HG2   | 2.03                     | 0.58              |
| 1:A:212:PHE:CE1  | 1:A:222:MET:HE3   | 2.37                     | 0.58              |
| 1:A:239:ILE:O    | 1:A:240:LEU:C     | 2.43                     | 0.58              |
| 3:C:186:TYR:O    | 3:C:187:SER:C     | 2.45                     | 0.58              |
| 1:G:63:MET:SD    | 1:G:94:LEU:HD23   | 2.43                     | 0.58              |
| 1:G:93:HIS:HA    | 10:G:3030:HOH:O   | 2.02                     | 0.58              |
| 1:G:318:TYR:O    | 1:G:319:ALA:C     | 2.46                     | 0.58              |
| 3:I:74:VAL:HG12  | 4:J:16:ILE:HG23   | 1.85                     | 0.58              |
| 1:A:287:VAL:HG11 | 8:A:1002:HEA:CHD  | 2.33                     | 0.58              |
| 1:A:452:ALA:O    | 1:A:453:GLY:C     | 2.46                     | 0.58              |
| 2:B:51:ALA:HA    | 2:B:54:ILE:HD12   | 1.85                     | 0.58              |
| 1:G:277:HIS:CG   | 1:G:335:MET:HE1   | 2.38                     | 0.58              |
| 3:I:85:LEU:O     | 3:I:88:MET:N      | 2.36                     | 0.58              |
| 1:A:41:GLY:O     | 1:A:42:LEU:C      | 2.44                     | 0.58              |
| 1:A:70:SER:HB2   | 1:A:74:LYS:CB     | 2.32                     | 0.58              |
| 1:A:227:LEU:O    | 1:A:230:TRP:N     | 2.36                     | 0.58              |
| 1:G:125:PRO:HG3  | 1:G:133:MET:SD    | 2.43                     | 0.58              |
| 1:G:396:VAL:O    | 1:G:397:THR:C     | 2.46                     | 0.58              |
| 1:A:441:GLY:O    | 1:A:442:LYS:C     | 2.46                     | 0.58              |
| 2:B:200:VAL:HG22 | 2:B:201:PRO:HD2   | 1.85                     | 0.58              |
| 3:C:120:PHE:CD1  | 3:C:120:PHE:C     | 2.82                     | 0.58              |
| 1:G:91:ASN:ND2   | 1:G:165:GLN:NE2   | 2.51                     | 0.58              |
| 1:G:112:ILE:N    | 1:G:113:PRO:CD    | 2.66                     | 0.58              |
| 1:A:227:LEU:O    | 1:A:228:PHE:C     | 2.47                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:342:LEU:HD13  | 2:B:127:GLN:CB    | 2.30                     | 0.58              |
| 1:G:102:HIS:O     | 1:G:103:GLY:C     | 2.47                     | 0.58              |
| 2:H:78:TYR:C      | 2:H:78:TYR:CD1    | 2.82                     | 0.58              |
| 1:G:252:MET:HE2   | 1:G:264:PHE:CZ    | 2.39                     | 0.58              |
| 1:A:95:TRP:CZ2    | 1:A:99:ILE:HD11   | 2.38                     | 0.58              |
| 2:B:252:CYS:HB2   | 2:B:263:MET:CG    | 2.34                     | 0.58              |
| 1:G:456:HIS:CE1   | 1:G:511:PHE:HB2   | 2.38                     | 0.58              |
| 1:G:474:LEU:HD21  | 1:G:494:ASN:HD22  | 1.68                     | 0.58              |
| 1:G:314:LEU:O     | 1:G:315:PRO:C     | 2.47                     | 0.58              |
| 1:G:336:TYR:HD2   | 1:G:407:ASP:OD2   | 1.87                     | 0.58              |
| 1:G:379:THR:CB    | 1:G:380:PRO:CD    | 2.76                     | 0.58              |
| 1:G:456:HIS:HA    | 1:G:459:MET:HE3   | 1.85                     | 0.58              |
| 3:I:127:THR:OG1   | 3:I:266:GLN:HG3   | 2.04                     | 0.58              |
| 3:I:147:ALA:CB    | 3:I:170:LEU:HD23  | 2.33                     | 0.58              |
| 1:A:108:PHE:CE2   | 1:A:194:VAL:HG13  | 2.39                     | 0.58              |
| 1:A:160:PRO:O     | 1:A:184:GLY:HA3   | 2.03                     | 0.58              |
| 1:A:330:VAL:HG11  | 1:A:352:THR:HA    | 1.86                     | 0.58              |
| 1:A:493:TRP:O     | 1:A:494:ASN:C     | 2.47                     | 0.58              |
| 3:I:130:PRO:O     | 3:I:134:PRO:HB2   | 2.03                     | 0.58              |
| 1:A:24:THR:HG23   | 3:C:14:PRO:HA     | 1.85                     | 0.57              |
| 1:A:264:PHE:HB3   | 1:A:272:PRO:HA    | 1.86                     | 0.57              |
| 1:A:451:TRP:O     | 1:A:452:ALA:C     | 2.47                     | 0.57              |
| 1:G:185:TYR:HB3   | 3:I:37:HIS:CD2    | 2.39                     | 0.57              |
| 1:G:259:PHE:O     | 1:G:260:GLY:C     | 2.48                     | 0.57              |
| 1:G:273:VAL:O     | 1:G:274:LEU:C     | 2.45                     | 0.57              |
| 1:G:284:HIS:H     | 1:G:285:PRO:HD2   | 1.69                     | 0.57              |
| 1:G:482:ARG:HD2   | 10:G:3111:HOH:O   | 2.03                     | 0.57              |
| 1:A:22:MET:HG2    | 3:C:16:ILE:CA     | 2.34                     | 0.57              |
| 1:A:212:PHE:CD1   | 1:A:213:LEU:HD23  | 2.39                     | 0.57              |
| 3:C:42:TRP:CD1    | 3:C:42:TRP:H      | 2.16                     | 0.57              |
| 1:G:27:LYS:O      | 1:G:31:VAL:HG23   | 2.04                     | 0.57              |
| 1:G:131:PRO:HG2   | 3:I:9:TYR:HD2     | 1.69                     | 0.57              |
| 1:G:295:PHE:O     | 1:G:298:VAL:HB    | 2.04                     | 0.57              |
| 1:G:389:PHE:O     | 1:G:392:THR:N     | 2.38                     | 0.57              |
| 8:A:1002:HEA:HBC1 | 8:A:1002:HEA:HMC2 | 1.86                     | 0.57              |
| 2:B:43:PHE:CD2    | 2:B:55:HIS:CD2    | 2.92                     | 0.57              |
| 1:G:253:LEU:HD21  | 1:G:275:TYR:CE1   | 2.39                     | 0.57              |
| 9:G:3009:3PE:H381 | 9:G:3009:3PE:H251 | 1.86                     | 0.57              |
| 3:I:141:LEU:O     | 3:I:142:LEU:C     | 2.47                     | 0.57              |
| 3:I:240:PHE:CD1   | 3:I:244:ILE:HD11  | 2.38                     | 0.57              |
| 3:I:249:PHE:O     | 3:I:253:VAL:HG23  | 2.05                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:41:GLY:O      | 1:A:45:VAL:N      | 2.35                     | 0.57              |
| 1:A:128:ILE:HD12  | 1:A:216:ARG:CA    | 2.35                     | 0.57              |
| 1:A:237:TRP:O     | 1:A:238:LEU:C     | 2.47                     | 0.57              |
| 1:A:315:PRO:O     | 1:A:316:MET:C     | 2.45                     | 0.57              |
| 1:G:350:MET:O     | 1:G:353:MET:HB2   | 2.05                     | 0.57              |
| 1:G:432:ILE:O     | 1:G:436:ILE:HG13  | 2.04                     | 0.57              |
| 3:I:56:PHE:O      | 3:I:57:GLY:C      | 2.45                     | 0.57              |
| 3:I:161:ARG:HH21  | 3:I:232:PHE:H     | 1.52                     | 0.57              |
| 1:A:246:LEU:HD22  | 1:A:282:PHE:CZ    | 2.39                     | 0.57              |
| 4:D:43:PHE:O      | 4:D:44:LEU:C      | 2.47                     | 0.57              |
| 2:H:120:LEU:O     | 2:H:123:LEU:N     | 2.35                     | 0.57              |
| 1:A:357:VAL:CB    | 1:A:358:PRO:HD3   | 2.35                     | 0.57              |
| 1:A:378:LYS:O     | 1:A:379:THR:C     | 2.45                     | 0.57              |
| 1:G:217:ALA:HB1   | 10:G:3090:HOH:O   | 2.04                     | 0.57              |
| 1:G:430:PHE:O     | 1:G:431:GLY:C     | 2.47                     | 0.57              |
| 2:H:86:LYS:HE3    | 10:H:1179:HOH:O   | 2.03                     | 0.57              |
| 2:H:278:TRP:HZ2   | 10:H:1115:HOH:O   | 1.87                     | 0.57              |
| 3:I:141:LEU:HD11  | 3:I:178:PHE:CE2   | 2.40                     | 0.57              |
| 1:A:551:PHE:CE1   | 1:A:555:PRO:HG3   | 2.40                     | 0.57              |
| 3:C:17:TRP:O      | 3:C:20:MET:HB3    | 2.04                     | 0.57              |
| 3:C:220:LEU:O     | 3:C:221:LEU:C     | 2.48                     | 0.57              |
| 1:G:307:LYS:HB3   | 1:G:534:HIS:CD2   | 2.40                     | 0.57              |
| 1:G:547:PRO:O     | 1:G:548:GLU:C     | 2.44                     | 0.57              |
| 3:I:92:MET:O      | 3:I:95:SER:N      | 2.38                     | 0.57              |
| 1:A:508:PHE:CD1   | 1:A:512:LEU:HD11  | 2.39                     | 0.57              |
| 1:G:364:PHE:O     | 1:G:365:SER:C     | 2.46                     | 0.57              |
| 1:G:378:LYS:O     | 1:G:379:THR:C     | 2.48                     | 0.57              |
| 1:A:99:ILE:O      | 1:A:102:HIS:HB3   | 2.05                     | 0.57              |
| 1:A:469:PHE:O     | 1:A:470:PRO:C     | 2.46                     | 0.57              |
| 2:B:145:TRP:NE1   | 2:B:263:MET:HE2   | 2.19                     | 0.57              |
| 1:G:249:ALA:O     | 1:G:252:MET:HG3   | 2.05                     | 0.57              |
| 1:G:341:SER:OG    | 1:G:344:GLN:HG3   | 2.05                     | 0.57              |
| 1:A:111:VAL:HG13  | 1:A:111:VAL:O     | 2.04                     | 0.57              |
| 1:A:425:SER:HA    | 1:A:429:VAL:CG2   | 2.35                     | 0.57              |
| 9:C:2013:3PE:H2G2 | 4:D:35:VAL:CG2    | 2.35                     | 0.57              |
| 2:H:120:LEU:CB    | 2:H:121:PRO:CD    | 2.83                     | 0.57              |
| 2:H:147:TYR:HE1   | 10:H:1159:HOH:O   | 1.87                     | 0.57              |
| 1:A:222:MET:H     | 9:A:2012:3PE:H111 | 1.70                     | 0.56              |
| 1:A:228:PHE:CE1   | 1:A:297:ILE:HG13  | 2.40                     | 0.56              |
| 1:A:284:HIS:H     | 1:A:285:PRO:CD    | 2.18                     | 0.56              |
| 1:A:394:GLY:O     | 1:A:395:GLY:C     | 2.46                     | 0.56              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:C:72:THR:O     | 3:C:73:PRO:C      | 2.48                     | 0.56              |
| 1:G:198:GLY:HA2  | 1:G:243:LEU:HD13  | 1.87                     | 0.56              |
| 1:G:212:PHE:CD1  | 1:G:213:LEU:HD23  | 2.40                     | 0.56              |
| 1:G:402:SER:OG   | 1:G:403:GLN:NE2   | 2.34                     | 0.56              |
| 1:G:450:GLU:O    | 1:G:454:LYS:HG3   | 2.04                     | 0.56              |
| 3:I:130:PRO:HB3  | 3:I:263:ILE:HD13  | 1.87                     | 0.56              |
| 9:I:3010:3PE:C33 | 9:I:3010:3PE:H231 | 2.35                     | 0.56              |
| 1:A:452:ALA:HB1  | 1:A:514:VAL:HG21  | 1.87                     | 0.56              |
| 1:G:107:MET:HE1  | 1:G:424:MET:SD    | 2.45                     | 0.56              |
| 1:G:188:ASP:CG   | 1:G:257:ARG:HH12  | 2.13                     | 0.56              |
| 2:H:176:VAL:O    | 2:H:177:GLU:C     | 2.48                     | 0.56              |
| 3:I:72:THR:O     | 3:I:75:VAL:HG23   | 2.06                     | 0.56              |
| 1:A:26:HIS:HB3   | 1:A:132:ASP:OD1   | 2.05                     | 0.56              |
| 1:A:91:ASN:CG    | 1:A:165:GLN:HE22  | 2.12                     | 0.56              |
| 1:A:292:LEU:O    | 1:A:293:PRO:C     | 2.46                     | 0.56              |
| 4:D:37:ILE:O     | 4:D:38:VAL:C      | 2.46                     | 0.56              |
| 1:G:34:LEU:HD23  | 1:G:114:ALA:HB1   | 1.86                     | 0.56              |
| 1:G:145:LEU:HD23 | 3:I:22:SER:OG     | 2.05                     | 0.56              |
| 1:G:222:MET:H    | 9:G:3012:3PE:H111 | 1.69                     | 0.56              |
| 1:G:463:GLY:CA   | 1:G:503:LEU:HD23  | 2.35                     | 0.56              |
| 1:G:480:PRO:HG2  | 1:G:483:TYR:CE2   | 2.40                     | 0.56              |
| 3:I:99:TRP:CD1   | 9:I:3010:3PE:H352 | 2.41                     | 0.56              |
| 4:J:44:LEU:O     | 4:J:45:ALA:C      | 2.49                     | 0.56              |
| 1:A:40:VAL:CG1   | 1:A:105:LEU:HD22  | 2.36                     | 0.56              |
| 3:C:70:ASP:O     | 3:C:75:VAL:HG21   | 2.06                     | 0.56              |
| 1:G:404:ALA:O    | 1:G:405:SER:C     | 2.48                     | 0.56              |
| 3:I:81:TRP:O     | 3:I:84:ILE:N      | 2.34                     | 0.56              |
| 3:I:245:TRP:HE1  | 9:I:3013:3PE:H322 | 1.71                     | 0.56              |
| 1:A:176:PRO:HD2  | 10:A:2013:HOH:O   | 2.06                     | 0.56              |
| 1:A:396:VAL:HG13 | 2:B:65:ILE:HG21   | 1.87                     | 0.56              |
| 4:D:16:ILE:HA    | 4:D:19:GLN:OE1    | 2.05                     | 0.56              |
| 1:G:239:ILE:HD11 | 1:G:289:ILE:HG21  | 1.88                     | 0.56              |
| 1:G:251:THR:O    | 1:G:254:LEU:N     | 2.37                     | 0.56              |
| 1:G:503:LEU:O    | 1:G:506:ALA:HB3   | 2.06                     | 0.56              |
| 3:I:101:PHE:CE1  | 3:I:261:ILE:HG12  | 2.40                     | 0.56              |
| 3:I:125:ILE:CD1  | 3:I:198:TYR:HB3   | 2.36                     | 0.56              |
| 3:I:202:PHE:CD1  | 3:I:202:PHE:C     | 2.83                     | 0.56              |
| 1:A:336:TYR:HD2  | 1:A:407:ASP:OD2   | 1.89                     | 0.56              |
| 2:B:84:HIS:C     | 2:B:84:HIS:CD2    | 2.83                     | 0.56              |
| 2:B:259:SER:HB3  | 2:B:262:TYR:HB2   | 1.86                     | 0.56              |
| 3:C:84:ILE:HG23  | 9:C:2013:3PE:H272 | 1.88                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:170:ILE:O     | 2:B:255:LEU:HD23  | 2.05                     | 0.56              |
| 1:A:319:ALA:O     | 1:A:322:ALA:HB3   | 2.04                     | 0.56              |
| 1:A:511:PHE:CE1   | 1:A:515:ILE:HD11  | 2.41                     | 0.56              |
| 2:B:224:PHE:HB2   | 2:B:226:VAL:HG22  | 1.86                     | 0.56              |
| 3:C:226:ARG:NH2   | 3:C:231:HIS:HB3   | 2.21                     | 0.56              |
| 1:G:137:ARG:HH21  | 9:G:3009:3PE:C11  | 2.19                     | 0.56              |
| 1:G:287:VAL:HG23  | 1:G:288:TYR:N     | 2.20                     | 0.56              |
| 1:A:394:GLY:HA3   | 1:A:423:VAL:HG13  | 1.88                     | 0.56              |
| 1:G:314:LEU:HB3   | 1:G:315:PRO:HD3   | 1.88                     | 0.56              |
| 9:G:3012:3PE:H261 | 4:J:29:MET:SD     | 2.46                     | 0.56              |
| 2:H:196:THR:O     | 2:H:196:THR:HG22  | 2.06                     | 0.56              |
| 2:H:221:VAL:HB    | 2:H:224:PHE:HD2   | 1.71                     | 0.56              |
| 1:A:176:PRO:HB2   | 1:A:177:PRO:HA    | 1.86                     | 0.56              |
| 2:B:263:MET:HG3   | 2:B:263:MET:O     | 2.04                     | 0.56              |
| 3:C:86:PHE:CZ     | 9:C:2008:3PE:H2A1 | 2.41                     | 0.56              |
| 1:G:381:MET:O     | 1:G:382:LEU:C     | 2.48                     | 0.56              |
| 2:H:106:ILE:O     | 2:H:107:VAL:C     | 2.48                     | 0.56              |
| 1:A:27:LYS:HG2    | 1:A:122:TYR:CE1   | 2.40                     | 0.56              |
| 1:A:481:ARG:NH1   | 10:A:2015:HOH:O   | 2.23                     | 0.56              |
| 1:A:520:THR:HG22  | 1:A:521:ARG:N     | 2.20                     | 0.56              |
| 1:G:91:ASN:HD21   | 1:G:165:GLN:NE2   | 2.04                     | 0.56              |
| 1:G:423:VAL:HG21  | 8:G:1002:HEA:C3C  | 2.35                     | 0.56              |
| 1:A:46:ALA:O      | 1:A:49:VAL:HG12   | 2.05                     | 0.55              |
| 1:A:220:MET:HE2   | 1:A:225:VAL:HA    | 1.87                     | 0.55              |
| 1:A:390:LEU:CD1   | 1:A:426:LEU:HB3   | 2.36                     | 0.55              |
| 2:B:33:ILE:HD11   | 10:B:1042:HOH:O   | 2.06                     | 0.55              |
| 2:B:145:TRP:CE2   | 2:B:263:MET:HE2   | 2.41                     | 0.55              |
| 1:G:101:GLY:HA2   | 10:G:3027:HOH:O   | 2.05                     | 0.55              |
| 1:G:233:PHE:O     | 1:G:234:VAL:C     | 2.47                     | 0.55              |
| 2:H:255:LEU:N     | 10:H:1052:HOH:O   | 2.39                     | 0.55              |
| 1:A:284:HIS:HB3   | 1:A:285:PRO:CD    | 2.32                     | 0.55              |
| 1:A:402:SER:OG    | 1:A:403:GLN:NE2   | 2.38                     | 0.55              |
| 1:G:18:THR:HA     | 1:G:22:MET:CE     | 2.35                     | 0.55              |
| 1:G:375:ILE:CG2   | 1:G:377:LEU:HD23  | 2.37                     | 0.55              |
| 2:H:194:THR:HG22  | 2:H:266:THR:HB    | 1.88                     | 0.55              |
| 1:A:106:MET:HG2   | 8:A:1001:HEA:C3C  | 2.33                     | 0.55              |
| 2:B:271:SER:HA    | 10:B:1024:HOH:O   | 2.05                     | 0.55              |
| 3:C:222:VAL:HG11  | 9:C:2008:3PE:H351 | 1.87                     | 0.55              |
| 1:G:557:ARG:NH1   | 10:G:3015:HOH:O   | 2.39                     | 0.55              |
| 2:H:45:PRO:HB3    | 2:H:244:ARG:NH2   | 2.21                     | 0.55              |
| 2:H:217:HIS:CE1   | 2:H:256:CYS:HB2   | 2.41                     | 0.55              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:J:45:ALA:CA    | 9:J:3011:3PE:H321 | 2.34                     | 0.55              |
| 1:A:173:VAL:HG12 | 1:A:279:LEU:HD13  | 1.87                     | 0.55              |
| 1:A:411:HIS:CD2  | 1:A:412:ASP:HB2   | 2.42                     | 0.55              |
| 3:C:31:GLY:HA2   | 3:C:43:MET:SD     | 2.46                     | 0.55              |
| 1:G:24:THR:HG23  | 3:I:14:PRO:HA     | 1.88                     | 0.55              |
| 1:G:38:GLY:HA2   | 8:G:1001:HEA:H22  | 1.88                     | 0.55              |
| 1:A:75:GLY:O     | 1:A:76:PHE:C      | 2.50                     | 0.55              |
| 1:A:137:ARG:HB2  | 9:A:2009:3PE:O14  | 2.06                     | 0.55              |
| 3:C:124:GLY:CA   | 1:G:557:ARG:HH12  | 2.19                     | 0.55              |
| 2:H:220:THR:HB   | 2:H:227:LYS:CG    | 2.37                     | 0.55              |
| 1:A:91:ASN:HD21  | 1:A:165:GLN:NE2   | 2.05                     | 0.55              |
| 1:A:228:PHE:CD1  | 1:A:297:ILE:HG13  | 2.42                     | 0.55              |
| 1:A:237:TRP:CZ2  | 9:A:2012:3PE:H282 | 2.42                     | 0.55              |
| 1:A:284:HIS:O    | 1:A:287:VAL:HG22  | 2.07                     | 0.55              |
| 1:A:539:GLU:HG2  | 1:A:540:TRP:H     | 1.72                     | 0.55              |
| 3:C:34:LEU:HB3   | 3:C:39:SER:OG     | 2.07                     | 0.55              |
| 1:G:29:ILE:HD13  | 1:G:139:ASN:ND2   | 2.22                     | 0.55              |
| 1:G:175:TYR:HB3  | 10:G:3016:HOH:O   | 2.07                     | 0.55              |
| 1:G:269:GLY:O    | 3:I:109:MET:HG3   | 2.07                     | 0.55              |
| 1:G:289:ILE:O    | 1:G:293:PRO:HD2   | 2.07                     | 0.55              |
| 1:G:450:GLU:OE2  | 1:G:454:LYS:HE3   | 2.07                     | 0.55              |
| 1:A:76:PHE:O     | 1:A:79:SER:HB2    | 2.07                     | 0.55              |
| 1:A:123:PHE:O    | 1:A:124:MET:C     | 2.49                     | 0.55              |
| 1:G:192:PHE:CZ   | 1:G:254:LEU:HD21  | 2.41                     | 0.55              |
| 1:G:402:SER:HA   | 8:G:1002:HEA:OMA  | 2.07                     | 0.55              |
| 1:A:116:PHE:CD1  | 1:A:235:THR:HG21  | 2.42                     | 0.55              |
| 1:A:248:GLY:O    | 1:A:249:ALA:C     | 2.50                     | 0.55              |
| 1:A:473:PHE:HB3  | 2:B:41:THR:HA     | 1.88                     | 0.55              |
| 3:C:52:LEU:HD22  | 9:C:2008:3PE:H3C2 | 1.89                     | 0.55              |
| 1:G:111:VAL:HG11 | 1:G:290:ILE:HG23  | 1.88                     | 0.55              |
| 1:G:255:THR:HG21 | 3:I:204:MET:HE2   | 1.89                     | 0.55              |
| 1:A:386:GLY:O    | 1:A:390:LEU:HG    | 2.07                     | 0.55              |
| 1:A:474:LEU:HD13 | 10:A:2042:HOH:O   | 2.06                     | 0.55              |
| 1:G:235:THR:OG1  | 1:G:293:PRO:HD3   | 2.06                     | 0.55              |
| 2:H:33:ILE:HG22  | 2:H:34:GLY:N      | 2.21                     | 0.55              |
| 1:A:52:ARG:CD    | 1:A:498:SER:HA    | 2.37                     | 0.55              |
| 1:A:159:ALA:HB1  | 1:A:160:PRO:HD2   | 1.89                     | 0.55              |
| 1:A:354:VAL:O    | 1:A:355:ILE:C     | 2.49                     | 0.55              |
| 8:A:1002:HEA:C22 | 2:B:68:ILE:HD13   | 2.37                     | 0.55              |
| 4:D:25:GLY:O     | 4:D:26:PHE:C      | 2.48                     | 0.55              |
| 2:H:120:LEU:O    | 2:H:121:PRO:C     | 2.49                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:176:VAL:O     | 2:H:180:LEU:HG    | 2.07                     | 0.55              |
| 2:H:195:ASP:OD1   | 2:H:196:THR:N     | 2.40                     | 0.55              |
| 1:A:42:LEU:O      | 1:A:43:ILE:C      | 2.49                     | 0.54              |
| 1:A:52:ARG:O      | 1:A:53:MET:C      | 2.49                     | 0.54              |
| 1:A:274:LEU:HD21  | 3:C:100:SER:HA    | 1.89                     | 0.54              |
| 1:A:329:VAL:HG23  | 1:A:329:VAL:O     | 2.05                     | 0.54              |
| 1:G:15:GLY:O      | 1:G:18:THR:HB     | 2.07                     | 0.54              |
| 2:H:210:VAL:N     | 2:H:236:ALA:O     | 2.34                     | 0.54              |
| 1:G:284:HIS:HB3   | 1:G:285:PRO:CD    | 2.30                     | 0.54              |
| 1:G:411:HIS:CD2   | 1:G:412:ASP:HB2   | 2.43                     | 0.54              |
| 1:G:529:ASN:OD1   | 1:G:529:ASN:C     | 2.50                     | 0.54              |
| 1:A:295:PHE:CD2   | 1:A:362:LYS:HE2   | 2.43                     | 0.54              |
| 1:A:304:THR:OG1   | 1:A:535:ALA:HA    | 2.08                     | 0.54              |
| 1:G:123:PHE:O     | 1:G:124:MET:C     | 2.47                     | 0.54              |
| 1:G:147:VAL:O     | 1:G:148:ALA:C     | 2.49                     | 0.54              |
| 1:G:231:SER:CA    | 1:G:320:MET:HE1   | 2.36                     | 0.54              |
| 9:G:3009:3PE:H2C2 | 9:G:3009:3PE:H3B2 | 1.89                     | 0.54              |
| 3:I:152:HIS:HA    | 3:I:240:PHE:HE1   | 1.70                     | 0.54              |
| 3:I:256:PHE:O     | 3:I:257:LEU:C     | 2.51                     | 0.54              |
| 1:A:292:LEU:HB2   | 1:A:293:PRO:HD3   | 1.90                     | 0.54              |
| 1:A:318:TYR:O     | 1:A:319:ALA:C     | 2.49                     | 0.54              |
| 3:C:161:ARG:NH1   | 3:C:230:GLY:HA2   | 2.18                     | 0.54              |
| 1:G:394:GLY:HA3   | 1:G:423:VAL:HG13  | 1.89                     | 0.54              |
| 1:G:459:MET:O     | 1:G:462:VAL:HB    | 2.07                     | 0.54              |
| 2:H:73:THR:HG22   | 2:H:77:LEU:HG     | 1.89                     | 0.54              |
| 1:A:148:ALA:O     | 1:A:149:GLY:C     | 2.50                     | 0.54              |
| 1:A:356:ALA:O     | 1:A:357:VAL:C     | 2.47                     | 0.54              |
| 3:C:137:ASN:HA    | 3:C:140:ILE:HD12  | 1.89                     | 0.54              |
| 1:G:221:THR:O     | 1:G:222:MET:C     | 2.48                     | 0.54              |
| 9:I:3010:3PE:H342 | 9:J:3011:3PE:H342 | 1.88                     | 0.54              |
| 1:A:331:TRP:CD1   | 1:A:331:TRP:C     | 2.84                     | 0.54              |
| 1:A:390:LEU:HD23  | 1:A:390:LEU:H     | 1.72                     | 0.54              |
| 1:G:70:SER:HB2    | 1:G:74:LYS:HB2    | 1.90                     | 0.54              |
| 2:H:161:ILE:HG13  | 2:H:193:ALA:O     | 2.08                     | 0.54              |
| 1:A:401:LEU:CD1   | 1:A:416:VAL:HG22  | 2.29                     | 0.54              |
| 1:A:407:ASP:OD1   | 1:A:411:HIS:HB2   | 2.07                     | 0.54              |
| 3:C:110:GLY:HA2   | 10:J:1118:HOH:O   | 2.07                     | 0.54              |
| 1:G:137:ARG:HH21  | 9:G:3009:3PE:H112 | 1.72                     | 0.54              |
| 2:H:173:SER:HG    | 2:H:175:GLU:HB2   | 1.72                     | 0.54              |
| 1:A:124:MET:SD    | 1:A:125:PRO:HD3   | 2.47                     | 0.54              |
| 1:A:424:MET:SD    | 8:A:1002:HEA:HAC  | 2.47                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:130:PRO:O     | 3:C:134:PRO:HB2   | 2.08                     | 0.54              |
| 1:G:25:ASN:ND2    | 1:G:27:LYS:NZ     | 2.50                     | 0.54              |
| 1:G:176:PRO:HA    | 1:G:178:LEU:N     | 2.23                     | 0.54              |
| 1:G:276:GLN:HB2   | 1:G:335:MET:HE3   | 1.89                     | 0.54              |
| 1:G:431:GLY:O     | 1:G:432:ILE:C     | 2.50                     | 0.54              |
| 2:H:62:LEU:CD1    | 2:H:65:ILE:HD11   | 2.28                     | 0.54              |
| 3:I:226:ARG:HH21  | 3:I:231:HIS:HB3   | 1.72                     | 0.54              |
| 1:A:126:LEU:O     | 1:A:127:HIS:C     | 2.51                     | 0.54              |
| 1:A:370:MET:O     | 1:A:371:TRP:C     | 2.49                     | 0.54              |
| 3:C:100:SER:O     | 3:C:101:PHE:C     | 2.50                     | 0.54              |
| 1:G:231:SER:O     | 1:G:232:ILE:C     | 2.49                     | 0.54              |
| 3:I:31:GLY:CA     | 3:I:43:MET:SD     | 2.96                     | 0.54              |
| 1:A:49:VAL:O      | 1:A:50:TYR:C      | 2.51                     | 0.54              |
| 1:A:91:ASN:ND2    | 1:A:165:GLN:NE2   | 2.51                     | 0.54              |
| 1:A:178:LEU:O     | 1:A:178:LEU:HD12  | 2.07                     | 0.54              |
| 8:A:1001:HEA:H122 | 8:A:1001:HEA:HMB3 | 1.89                     | 0.54              |
| 2:B:201:PRO:HB2   | 2:B:204:LYS:CG    | 2.38                     | 0.54              |
| 2:B:228:GLN:HG3   | 2:B:229:ASP:N     | 2.19                     | 0.54              |
| 1:G:127:HIS:CE1   | 1:G:300:HIS:CE1   | 2.96                     | 0.54              |
| 1:G:176:PRO:O     | 2:H:216:ILE:HD11  | 2.08                     | 0.54              |
| 1:G:191:ILE:HD12  | 1:G:250:ILE:HB    | 1.90                     | 0.54              |
| 1:G:263:PHE:HE1   | 3:I:201:ASN:ND2   | 2.06                     | 0.54              |
| 1:A:27:LYS:HG2    | 1:A:122:TYR:CD1   | 2.43                     | 0.53              |
| 1:A:212:PHE:CD1   | 1:A:212:PHE:C     | 2.85                     | 0.53              |
| 3:C:152:HIS:CA    | 3:C:240:PHE:HE1   | 2.21                     | 0.53              |
| 1:G:178:LEU:HD12  | 1:G:178:LEU:C     | 2.33                     | 0.53              |
| 1:G:473:PHE:HB3   | 2:H:41:THR:HA     | 1.90                     | 0.53              |
| 2:H:211:THR:CG2   | 2:H:212:GLY:H     | 2.20                     | 0.53              |
| 3:I:7:HIS:HA      | 4:J:14:MET:HE2    | 1.90                     | 0.53              |
| 3:I:222:VAL:HA    | 3:I:225:ILE:HD12  | 1.89                     | 0.53              |
| 1:A:91:ASN:O      | 1:A:92:GLY:C      | 2.51                     | 0.53              |
| 1:A:115:LEU:HD12  | 1:A:432:ILE:CD1   | 2.38                     | 0.53              |
| 1:A:163:ASN:CG    | 2:B:258:ILE:HD11  | 2.33                     | 0.53              |
| 1:A:300:HIS:O     | 1:A:303:ALA:HB3   | 2.08                     | 0.53              |
| 1:A:312:GLY:O     | 1:A:316:MET:HG2   | 2.08                     | 0.53              |
| 1:A:329:VAL:HG12  | 9:D:2011:3PE:H2B2 | 1.88                     | 0.53              |
| 2:B:142:GLN:O     | 2:B:143:TRP:HB2   | 2.08                     | 0.53              |
| 2:H:143:TRP:CZ2   | 2:H:257:GLY:HA3   | 2.40                     | 0.53              |
| 3:I:125:ILE:HD12  | 3:I:198:TYR:HB3   | 1.89                     | 0.53              |
| 3:I:161:ARG:HH22  | 3:I:232:PHE:H     | 1.55                     | 0.53              |
| 1:A:486:TYR:HD2   | 1:A:490:PHE:HB2   | 1.71                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:152:HIS:O     | 3:C:156:VAL:HG23  | 2.07                     | 0.53              |
| 3:I:108:PRO:HA    | 10:I:3016:HOH:O   | 2.07                     | 0.53              |
| 1:A:279:LEU:HD23  | 1:A:280:TRP:N     | 2.20                     | 0.53              |
| 2:B:70:ILE:O      | 2:B:71:PHE:C      | 2.50                     | 0.53              |
| 2:B:248:PHE:HE2   | 2:B:269:VAL:CG1   | 2.20                     | 0.53              |
| 1:G:235:THR:HG22  | 1:G:236:ALA:N     | 2.19                     | 0.53              |
| 2:H:71:PHE:O      | 2:H:75:LEU:HD12   | 2.07                     | 0.53              |
| 3:I:256:PHE:CZ    | 9:J:3011:3PE:H391 | 2.43                     | 0.53              |
| 8:A:1002:HEA:H202 | 8:A:1002:HEA:H253 | 1.91                     | 0.53              |
| 2:B:106:ILE:O     | 2:B:107:VAL:C     | 2.51                     | 0.53              |
| 2:B:143:TRP:N     | 2:B:143:TRP:CD1   | 2.75                     | 0.53              |
| 1:G:489:ALA:HB3   | 2:H:36:PRO:HB2    | 1.90                     | 0.53              |
| 3:I:192:GLY:O     | 3:I:199:GLY:HA3   | 2.07                     | 0.53              |
| 3:I:242:ALA:O     | 3:I:243:ALA:C     | 2.52                     | 0.53              |
| 4:J:36:VAL:O      | 4:J:39:ALA:HB3    | 2.08                     | 0.53              |
| 1:A:152:LEU:HD23  | 3:C:26:PHE:CE2    | 2.44                     | 0.53              |
| 1:A:437:TYR:O     | 1:A:440:ILE:HG22  | 2.08                     | 0.53              |
| 9:A:2012:3PE:H361 | 9:A:2012:3PE:H291 | 1.90                     | 0.53              |
| 9:A:2012:3PE:H2D1 | 9:D:2011:3PE:H2I1 | 1.90                     | 0.53              |
| 3:C:74:VAL:HG23   | 3:C:75:VAL:N      | 2.24                     | 0.53              |
| 1:G:538:LEU:HD21  | 1:G:560:TRP:HE3   | 1.73                     | 0.53              |
| 9:G:3009:3PE:H251 | 9:G:3009:3PE:C38  | 2.38                     | 0.53              |
| 3:C:66:SER:HB2    | 3:C:71:HIS:CE1    | 2.42                     | 0.53              |
| 3:C:150:TRP:CD1   | 3:C:150:TRP:C     | 2.87                     | 0.53              |
| 1:G:425:SER:HA    | 1:G:429:VAL:HG21  | 1.91                     | 0.53              |
| 2:H:148:GLU:HG2   | 2:H:155:SER:OG    | 2.09                     | 0.53              |
| 2:H:200:VAL:O     | 2:H:269:VAL:HG23  | 2.09                     | 0.53              |
| 3:I:30:PHE:CD2    | 3:I:43:MET:HE1    | 2.44                     | 0.53              |
| 3:I:59:TRP:CE3    | 9:I:3008:3PE:H361 | 2.43                     | 0.53              |
| 1:A:401:LEU:HD21  | 1:A:415:TYR:CD1   | 2.43                     | 0.53              |
| 1:A:482:ARG:N     | 8:A:1001:HEA:O2A  | 2.41                     | 0.53              |
| 2:B:176:VAL:O     | 2:B:180:LEU:HG    | 2.09                     | 0.53              |
| 3:C:8:ASP:OD2     | 4:D:14:MET:HB3    | 2.09                     | 0.53              |
| 1:G:260:GLY:O     | 3:I:194:ALA:HA    | 2.08                     | 0.53              |
| 1:G:286:GLN:HA    | 1:G:289:ILE:HD12  | 1.91                     | 0.53              |
| 1:G:376:GLU:O     | 1:G:378:LYS:N     | 2.42                     | 0.53              |
| 1:G:462:VAL:HG12  | 1:G:503:LEU:CD2   | 2.39                     | 0.53              |
| 1:A:404:ALA:O     | 1:A:407:ASP:N     | 2.41                     | 0.53              |
| 1:A:509:LEU:O     | 1:A:510:PHE:C     | 2.50                     | 0.53              |
| 2:B:33:ILE:HG22   | 2:B:34:GLY:N      | 2.23                     | 0.53              |
| 2:B:57:LEU:HG     | 2:B:61:ILE:HD12   | 1.90                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:221:VAL:HB    | 2:B:224:PHE:HD2   | 1.74                     | 0.53              |
| 1:G:38:GLY:O      | 1:G:39:LEU:C      | 2.50                     | 0.53              |
| 1:G:160:PRO:O     | 1:G:184:GLY:HA3   | 2.09                     | 0.53              |
| 1:G:313:TYR:O     | 1:G:314:LEU:C     | 2.52                     | 0.53              |
| 2:H:263:MET:HG3   | 2:H:263:MET:O     | 2.09                     | 0.53              |
| 10:A:2079:HOH:O   | 2:B:44:GLN:HG2    | 2.09                     | 0.53              |
| 3:I:45:LEU:O      | 3:I:46:ILE:C      | 2.51                     | 0.53              |
| 3:I:182:GLN:O     | 3:I:185:GLU:HB2   | 2.09                     | 0.53              |
| 1:A:325:VAL:HG22  | 9:A:2012:3PE:H3B2 | 1.91                     | 0.52              |
| 1:A:392:THR:O     | 1:A:393:VAL:C     | 2.51                     | 0.52              |
| 1:A:411:HIS:HD1   | 8:A:1002:HEA:CGA  | 2.21                     | 0.52              |
| 1:A:424:MET:HE1   | 8:A:1002:HEA:HMD3 | 1.91                     | 0.52              |
| 2:B:234:ARG:HG2   | 3:C:114:PRO:HD3   | 1.92                     | 0.52              |
| 1:G:22:MET:HG2    | 3:I:16:ILE:HA     | 1.91                     | 0.52              |
| 1:G:127:HIS:HE1   | 1:G:300:HIS:CE1   | 2.27                     | 0.52              |
| 1:G:139:ASN:O     | 1:G:140:ASN:C     | 2.51                     | 0.52              |
| 1:G:181:SER:O     | 1:G:182:GLU:C     | 2.50                     | 0.52              |
| 1:G:254:LEU:O     | 1:G:258:ASN:N     | 2.38                     | 0.52              |
| 2:H:137:LYS:HG2   | 2:H:138:VAL:N     | 2.19                     | 0.52              |
| 2:B:141:TYR:O     | 2:B:143:TRP:N     | 2.42                     | 0.52              |
| 1:G:191:ILE:HG23  | 1:G:250:ILE:HG13  | 1.91                     | 0.52              |
| 1:G:422:TYR:OH    | 1:G:469:PHE:HB2   | 2.08                     | 0.52              |
| 2:H:156:PHE:HD1   | 2:H:196:THR:HG21  | 1.72                     | 0.52              |
| 2:H:215:VAL:O     | 2:H:232:PRO:HD3   | 2.10                     | 0.52              |
| 3:I:133:LEU:N     | 3:I:134:PRO:HD2   | 2.21                     | 0.52              |
| 3:I:143:CYS:O     | 3:I:144:SER:C     | 2.53                     | 0.52              |
| 9:A:2012:3PE:H3E1 | 9:D:2011:3PE:H2I3 | 1.91                     | 0.52              |
| 3:C:30:PHE:CD2    | 3:C:43:MET:HE1    | 2.44                     | 0.52              |
| 1:G:385:LEU:O     | 1:G:388:LEU:HB2   | 2.08                     | 0.52              |
| 1:G:493:TRP:HA    | 1:G:493:TRP:HE3   | 1.73                     | 0.52              |
| 3:I:85:LEU:HD23   | 3:I:88:MET:HE2    | 1.90                     | 0.52              |
| 1:A:287:VAL:HB    | 8:A:1002:HEA:CAC  | 2.40                     | 0.52              |
| 1:A:534:HIS:HA    | 10:A:2043:HOH:O   | 2.08                     | 0.52              |
| 1:A:550:THR:O     | 1:A:551:PHE:HB2   | 2.09                     | 0.52              |
| 9:A:2009:3PE:C26  | 3:C:55:MET:HG2    | 2.38                     | 0.52              |
| 2:B:177:GLU:HA    | 2:B:180:LEU:HD12  | 1.91                     | 0.52              |
| 3:C:120:PHE:HA    | 3:C:121:PRO:C     | 2.35                     | 0.52              |
| 3:C:133:LEU:HD23  | 3:C:185:GLU:HG3   | 1.92                     | 0.52              |
| 1:G:558:GLU:O     | 1:G:560:TRP:N     | 2.42                     | 0.52              |
| 2:H:211:THR:CG2   | 2:H:212:GLY:N     | 2.73                     | 0.52              |
| 2:H:226:VAL:HG12  | 10:H:1157:HOH:O   | 2.08                     | 0.52              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:I:62:VAL:HG12  | 9:I:3008:3PE:H31  | 1.92                     | 0.52              |
| 3:I:72:THR:HG22  | 3:I:74:VAL:H      | 1.73                     | 0.52              |
| 3:I:253:VAL:HG13 | 9:I:3010:3PE:H3I1 | 1.92                     | 0.52              |
| 4:J:38:VAL:HG12  | 4:J:42:ILE:HD12   | 1.91                     | 0.52              |
| 1:A:202:ILE:CD1  | 1:A:244:PRO:HD3   | 2.38                     | 0.52              |
| 1:A:215:MET:HE3  | 10:A:2033:HOH:O   | 2.09                     | 0.52              |
| 1:A:493:TRP:HA   | 1:A:493:TRP:HE3   | 1.74                     | 0.52              |
| 2:B:158:SER:CA   | 2:B:196:THR:HB    | 2.35                     | 0.52              |
| 2:B:254:GLU:O    | 2:B:255:LEU:C     | 2.53                     | 0.52              |
| 1:G:380:PRO:HG3  | 1:G:437:TYR:CB    | 2.39                     | 0.52              |
| 1:G:506:ALA:O    | 1:G:509:LEU:N     | 2.42                     | 0.52              |
| 2:H:201:PRO:CB   | 2:H:204:LYS:HG3   | 2.39                     | 0.52              |
| 3:I:106:LEU:O    | 3:I:108:PRO:HD3   | 2.10                     | 0.52              |
| 3:I:150:TRP:NE1  | 3:I:163:ASP:OD1   | 2.31                     | 0.52              |
| 3:I:155:LEU:O    | 3:I:155:LEU:HG    | 2.08                     | 0.52              |
| 3:I:196:ASN:HD21 | 3:I:199:GLY:HA3   | 1.75                     | 0.52              |
| 3:I:245:TRP:NE1  | 9:I:3013:3PE:H322 | 2.24                     | 0.52              |
| 1:A:213:LEU:CB   | 3:C:81:TRP:CH2    | 2.93                     | 0.52              |
| 1:A:234:VAL:O    | 1:A:235:THR:C     | 2.52                     | 0.52              |
| 1:A:262:THR:OG1  | 1:A:265:GLN:HB2   | 2.10                     | 0.52              |
| 3:C:72:THR:HG22  | 3:C:74:VAL:H      | 1.75                     | 0.52              |
| 1:G:230:TRP:O    | 1:G:231:SER:C     | 2.52                     | 0.52              |
| 1:G:293:PRO:O    | 1:G:294:ALA:C     | 2.53                     | 0.52              |
| 1:G:330:VAL:HG11 | 1:G:352:THR:HA    | 1.90                     | 0.52              |
| 1:G:459:MET:HE1  | 1:G:510:PHE:CD2   | 2.43                     | 0.52              |
| 1:G:477:GLN:NE2  | 1:G:477:GLN:HA    | 2.25                     | 0.52              |
| 2:H:84:HIS:HD2   | 2:H:86:LYS:H      | 1.57                     | 0.52              |
| 2:H:234:ARG:HG2  | 3:I:114:PRO:HD3   | 1.91                     | 0.52              |
| 1:A:91:ASN:HD21  | 1:A:165:GLN:CD    | 2.17                     | 0.52              |
| 1:A:251:THR:HG22 | 3:C:97:TRP:HH2    | 1.75                     | 0.52              |
| 3:C:212:HIS:O    | 3:C:213:VAL:C     | 2.53                     | 0.52              |
| 1:G:230:TRP:O    | 1:G:233:PHE:HB3   | 2.09                     | 0.52              |
| 1:A:302:ILE:HG22 | 1:A:369:THR:HG21  | 1.91                     | 0.52              |
| 3:C:55:MET:O     | 3:C:56:PHE:C      | 2.51                     | 0.52              |
| 1:G:198:GLY:HA2  | 1:G:243:LEU:CD1   | 2.39                     | 0.52              |
| 1:G:253:LEU:HD21 | 1:G:275:TYR:CD1   | 2.45                     | 0.52              |
| 3:I:72:THR:O     | 3:I:73:PRO:C      | 2.53                     | 0.52              |
| 3:I:196:ASN:CG   | 3:I:196:ASN:O     | 2.53                     | 0.52              |
| 2:B:112:LEU:O    | 2:B:113:VAL:C     | 2.51                     | 0.52              |
| 4:D:44:LEU:O     | 4:D:45:ALA:C      | 2.53                     | 0.52              |
| 1:G:171:GLY:O    | 1:G:172:TRP:C     | 2.53                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:221:THR:HG23  | 1:G:224:LYS:HD2   | 1.92                     | 0.52              |
| 1:G:237:TRP:CG    | 9:G:3012:3PE:H382 | 2.45                     | 0.52              |
| 2:H:173:SER:OG    | 2:H:175:GLU:HB2   | 2.10                     | 0.52              |
| 3:I:254:TRP:HA    | 3:I:257:LEU:HD12  | 1.92                     | 0.52              |
| 9:I:3013:3PE:H3H2 | 9:I:3013:3PE:C2D  | 2.40                     | 0.52              |
| 1:A:221:THR:H     | 1:A:224:LYS:HB2   | 1.75                     | 0.52              |
| 2:B:71:PHE:CE1    | 2:B:75:LEU:HD11   | 2.45                     | 0.52              |
| 2:B:147:TYR:HE1   | 10:B:1049:HOH:O   | 1.93                     | 0.52              |
| 3:C:253:VAL:CA    | 9:C:2010:3PE:H3H1 | 2.36                     | 0.52              |
| 1:G:220:MET:HE2   | 1:G:224:LYS:O     | 2.09                     | 0.52              |
| 2:H:144:TYR:HB2   | 2:H:158:SER:O     | 2.09                     | 0.52              |
| 1:A:202:ILE:O     | 1:A:206:ILE:HG13  | 2.10                     | 0.51              |
| 1:A:294:ALA:O     | 1:A:295:PHE:C     | 2.53                     | 0.51              |
| 1:A:316:MET:O     | 1:A:317:VAL:C     | 2.53                     | 0.51              |
| 1:G:212:PHE:HD1   | 1:G:213:LEU:HD23  | 1.74                     | 0.51              |
| 1:G:356:ALA:O     | 1:G:357:VAL:C     | 2.52                     | 0.51              |
| 1:A:196:LEU:O     | 1:A:199:ALA:HB3   | 2.11                     | 0.51              |
| 8:A:1001:HEA:HMB3 | 8:A:1001:HEA:C12  | 2.40                     | 0.51              |
| 1:G:237:TRP:CH2   | 9:G:3012:3PE:H282 | 2.44                     | 0.51              |
| 1:G:373:GLY:O     | 2:H:83:PHE:HB3    | 2.10                     | 0.51              |
| 9:G:3009:3PE:H221 | 3:I:58:TRP:CE2    | 2.46                     | 0.51              |
| 10:G:3087:HOH:O   | 2:H:44:GLN:HG2    | 2.11                     | 0.51              |
| 2:H:45:PRO:HB3    | 2:H:244:ARG:HH21  | 1.75                     | 0.51              |
| 2:H:219:TRP:CD1   | 2:H:265:ILE:HD13  | 2.45                     | 0.51              |
| 1:A:63:MET:SD     | 1:A:94:LEU:HD23   | 2.50                     | 0.51              |
| 1:A:273:VAL:O     | 1:A:274:LEU:C     | 2.51                     | 0.51              |
| 1:A:367:ILE:HD11  | 2:B:75:LEU:HB2    | 1.91                     | 0.51              |
| 1:G:63:MET:CE     | 1:G:95:TRP:HB2    | 2.40                     | 0.51              |
| 1:G:132:ASP:OD1   | 1:G:133:MET:N     | 2.44                     | 0.51              |
| 1:G:291:VAL:O     | 1:G:294:ALA:HB3   | 2.11                     | 0.51              |
| 2:H:221:VAL:O     | 2:H:222:PRO:C     | 2.52                     | 0.51              |
| 2:H:236:ALA:HB2   | 10:H:1128:HOH:O   | 2.09                     | 0.51              |
| 1:G:84:ALA:O      | 1:G:85:VAL:C      | 2.53                     | 0.51              |
| 1:G:188:ASP:O     | 1:G:189:LEU:C     | 2.54                     | 0.51              |
| 1:G:234:VAL:HG12  | 1:G:292:LEU:HD11  | 1.93                     | 0.51              |
| 1:G:291:VAL:O     | 1:G:291:VAL:HG22  | 2.10                     | 0.51              |
| 2:H:40:GLY:HA2    | 10:H:1216:HOH:O   | 2.09                     | 0.51              |
| 1:A:154:VAL:HA    | 1:A:157:LEU:HD12  | 1.93                     | 0.51              |
| 1:A:291:VAL:O     | 1:A:292:LEU:C     | 2.54                     | 0.51              |
| 1:G:127:HIS:CE1   | 1:G:300:HIS:HE1   | 2.29                     | 0.51              |
| 1:G:306:ALA:O     | 1:G:307:LYS:C     | 2.53                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:125:ILE:HD12  | 3:I:198:TYR:CB    | 2.40                     | 0.51              |
| 1:A:222:MET:HG3   | 9:A:2012:3PE:C11  | 2.39                     | 0.51              |
| 1:A:231:SER:N     | 1:A:320:MET:HE1   | 2.26                     | 0.51              |
| 1:A:307:LYS:HA    | 1:A:534:HIS:CG    | 2.45                     | 0.51              |
| 3:C:74:VAL:HG23   | 3:C:75:VAL:H      | 1.76                     | 0.51              |
| 3:C:99:TRP:CZ2    | 9:C:2010:3PE:H222 | 2.44                     | 0.51              |
| 1:G:128:ILE:HD12  | 1:G:216:ARG:CA    | 2.40                     | 0.51              |
| 1:G:128:ILE:HB    | 1:G:216:ARG:HG2   | 1.92                     | 0.51              |
| 1:G:296:GLY:O     | 1:G:297:ILE:C     | 2.54                     | 0.51              |
| 2:H:231:VAL:O     | 2:H:232:PRO:C     | 2.53                     | 0.51              |
| 3:I:71:HIS:O      | 3:I:76:ARG:HG3    | 2.11                     | 0.51              |
| 1:A:122:TYR:CD1   | 1:A:122:TYR:C     | 2.89                     | 0.51              |
| 1:A:263:PHE:HE1   | 3:C:201:ASN:ND2   | 2.09                     | 0.51              |
| 1:A:390:LEU:HA    | 1:A:393:VAL:CG2   | 2.41                     | 0.51              |
| 1:G:367:ILE:HA    | 1:G:370:MET:CE    | 2.41                     | 0.51              |
| 2:H:143:TRP:NE1   | 2:H:256:CYS:O     | 2.42                     | 0.51              |
| 3:I:120:PHE:C     | 3:I:120:PHE:CD1   | 2.89                     | 0.51              |
| 1:A:74:LYS:HD2    | 1:A:74:LYS:N      | 2.22                     | 0.51              |
| 1:A:136:PRO:HG2   | 3:C:12:LEU:HD12   | 1.93                     | 0.51              |
| 1:A:409:TYR:C     | 1:A:409:TYR:CD1   | 2.88                     | 0.51              |
| 1:A:508:PHE:CE1   | 1:A:512:LEU:HD21  | 2.46                     | 0.51              |
| 2:B:172:MET:HE1   | 2:B:190:PHE:HB2   | 1.93                     | 0.51              |
| 1:G:189:LEU:HD23  | 3:I:33:VAL:HG21   | 1.93                     | 0.51              |
| 3:I:119:ILE:HG22  | 3:I:120:PHE:N     | 2.26                     | 0.51              |
| 9:I:3013:3PE:H2D2 | 9:I:3013:3PE:C3F  | 2.39                     | 0.51              |
| 1:A:307:LYS:HA    | 1:A:534:HIS:CB    | 2.41                     | 0.51              |
| 3:C:256:PHE:CZ    | 9:D:2011:3PE:H391 | 2.46                     | 0.51              |
| 1:G:284:HIS:NE2   | 1:G:288:TYR:CE2   | 2.66                     | 0.51              |
| 1:G:425:SER:HA    | 1:G:429:VAL:CG2   | 2.40                     | 0.51              |
| 1:G:535:ALA:HB1   | 1:G:540:TRP:CD1   | 2.46                     | 0.51              |
| 2:H:84:HIS:CD2    | 2:H:85:GLU:HG2    | 2.46                     | 0.51              |
| 2:H:200:VAL:HG22  | 2:H:201:PRO:HD2   | 1.93                     | 0.51              |
| 1:A:478:GLY:O     | 1:A:480:PRO:HD3   | 2.11                     | 0.51              |
| 2:B:238:LEU:C     | 2:B:238:LEU:CD1   | 2.74                     | 0.51              |
| 1:G:41:GLY:O      | 1:G:45:VAL:HG23   | 2.11                     | 0.51              |
| 1:G:177:PRO:HD3   | 1:G:272:PRO:HG3   | 1.93                     | 0.51              |
| 1:G:325:VAL:HG22  | 9:G:3012:3PE:H3D1 | 1.92                     | 0.51              |
| 1:G:494:ASN:O     | 1:G:495:PHE:C     | 2.53                     | 0.51              |
| 9:G:3012:3PE:H2G2 | 9:I:3010:3PE:H2E2 | 1.93                     | 0.51              |
| 3:I:147:ALA:HB1   | 3:I:170:LEU:HD23  | 1.91                     | 0.51              |
| 1:A:127:HIS:NE2   | 1:A:539:GLU:OE1   | 2.44                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:307:LYS:HB3   | 1:A:534:HIS:CD2   | 2.46                     | 0.50              |
| 2:B:254:GLU:H     | 2:B:260:HIS:CE1   | 2.26                     | 0.50              |
| 9:C:2013:3PE:H3F2 | 9:C:2013:3PE:H2D2 | 1.93                     | 0.50              |
| 1:G:416:VAL:HG21  | 8:G:1002:HEA:CBA  | 2.40                     | 0.50              |
| 1:G:442:LYS:NZ    | 1:G:542:LEU:O     | 2.31                     | 0.50              |
| 3:I:209:HIS:NE2   | 3:I:254:TRP:HB2   | 2.26                     | 0.50              |
| 1:A:112:ILE:HB    | 1:A:113:PRO:HD3   | 1.92                     | 0.50              |
| 1:A:124:MET:N     | 1:A:125:PRO:HD2   | 2.25                     | 0.50              |
| 1:A:154:VAL:HA    | 1:A:157:LEU:CD1   | 2.42                     | 0.50              |
| 1:A:395:GLY:O     | 1:A:396:VAL:C     | 2.52                     | 0.50              |
| 2:B:86:LYS:HA     | 2:B:89:LYS:HE2    | 1.93                     | 0.50              |
| 1:G:99:ILE:HD12   | 8:G:1001:HEA:CBA  | 2.40                     | 0.50              |
| 1:G:234:VAL:O     | 1:G:235:THR:C     | 2.54                     | 0.50              |
| 2:H:101:GLU:O     | 2:H:102:ILE:C     | 2.54                     | 0.50              |
| 9:I:3013:3PE:H3F2 | 9:I:3013:3PE:H2D2 | 1.93                     | 0.50              |
| 4:J:33:ALA:O      | 4:J:36:VAL:N      | 2.44                     | 0.50              |
| 1:A:433:PHE:O     | 1:A:434:ALA:C     | 2.54                     | 0.50              |
| 1:A:433:PHE:CD1   | 1:A:436:ILE:HD12  | 2.46                     | 0.50              |
| 2:B:62:LEU:O      | 2:B:66:ALA:N      | 2.44                     | 0.50              |
| 2:B:169:ASP:O     | 2:B:170:ASN:HB2   | 2.10                     | 0.50              |
| 3:C:122:PRO:O     | 3:C:125:ILE:HB    | 2.12                     | 0.50              |
| 1:G:180:THR:HG22  | 1:G:257:ARG:HG3   | 1.93                     | 0.50              |
| 1:G:482:ARG:N     | 8:G:1001:HEA:O2A  | 2.45                     | 0.50              |
| 2:H:164:PRO:HA    | 2:H:168:GLY:O     | 2.10                     | 0.50              |
| 3:I:107:TYR:OH    | 4:J:49:ALA:HA     | 2.11                     | 0.50              |
| 1:A:189:LEU:HD21  | 3:C:30:PHE:CD1    | 2.46                     | 0.50              |
| 1:A:442:LYS:HE2   | 1:A:539:GLU:O     | 2.12                     | 0.50              |
| 2:B:50:VAL:HG12   | 2:B:54:ILE:HD11   | 1.93                     | 0.50              |
| 9:C:2013:3PE:H2D2 | 9:C:2013:3PE:H3H2 | 1.92                     | 0.50              |
| 2:H:136:VAL:HG11  | 2:H:198:MET:CE    | 2.41                     | 0.50              |
| 1:A:99:ILE:HD12   | 8:A:1001:HEA:CBA  | 2.39                     | 0.50              |
| 1:A:180:THR:HA    | 1:A:257:ARG:HD2   | 1.94                     | 0.50              |
| 2:B:108:PRO:O     | 2:B:111:ILE:HB    | 2.12                     | 0.50              |
| 3:C:54:THR:O      | 3:C:55:MET:C      | 2.54                     | 0.50              |
| 2:H:161:ILE:HD11  | 2:H:193:ALA:HB1   | 1.93                     | 0.50              |
| 1:A:22:MET:SD     | 3:C:16:ILE:HB     | 2.51                     | 0.50              |
| 1:A:136:PRO:HA    | 10:A:2049:HOH:O   | 2.12                     | 0.50              |
| 1:A:325:VAL:HG22  | 9:A:2012:3PE:H3D1 | 1.94                     | 0.50              |
| 1:G:238:LEU:O     | 1:G:239:ILE:C     | 2.53                     | 0.50              |
| 1:G:244:PRO:O     | 1:G:245:VAL:C     | 2.50                     | 0.50              |
| 1:G:396:VAL:HG13  | 2:H:65:ILE:HG21   | 1.94                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:250:GLY:O     | 2:H:265:ILE:HB    | 2.12                     | 0.50              |
| 3:I:152:HIS:CG    | 3:I:244:ILE:HD13  | 2.47                     | 0.50              |
| 1:A:47:PHE:HB3    | 1:A:98:MET:HE3    | 1.94                     | 0.50              |
| 1:A:517:TYR:O     | 1:A:521:ARG:N     | 2.40                     | 0.50              |
| 2:B:120:LEU:HB2   | 2:B:121:PRO:CD    | 2.42                     | 0.50              |
| 3:C:72:THR:HG23   | 4:D:12:GLY:HA2    | 1.94                     | 0.50              |
| 1:G:311:PHE:CZ    | 2:H:96:HIS:HA     | 2.47                     | 0.50              |
| 1:G:424:MET:HB3   | 8:G:1001:HEA:HBC1 | 1.93                     | 0.50              |
| 1:G:534:HIS:HA    | 10:G:3048:HOH:O   | 2.10                     | 0.50              |
| 9:G:3012:3PE:H3E1 | 9:J:3011:3PE:H2I3 | 1.94                     | 0.50              |
| 3:I:254:TRP:O     | 3:I:257:LEU:HB2   | 2.11                     | 0.50              |
| 1:A:51:MET:O      | 1:A:52:ARG:C      | 2.54                     | 0.50              |
| 1:A:282:PHE:C     | 1:A:282:PHE:CD2   | 2.82                     | 0.50              |
| 2:B:156:PHE:CD2   | 2:B:196:THR:HG21  | 2.42                     | 0.50              |
| 1:G:124:MET:N     | 1:G:125:PRO:HD2   | 2.27                     | 0.50              |
| 1:G:134:ALA:H     | 1:G:211:THR:HG1   | 1.57                     | 0.50              |
| 1:G:240:LEU:HD21  | 3:I:85:LEU:HB3    | 1.94                     | 0.50              |
| 2:H:197:ALA:HB1   | 2:H:268:LYS:HG3   | 1.92                     | 0.50              |
| 1:A:24:THR:HG21   | 3:C:13:PRO:O      | 2.12                     | 0.50              |
| 1:A:275:TYR:O     | 1:A:276:GLN:C     | 2.54                     | 0.50              |
| 9:A:2009:3PE:H2G1 | 9:A:2009:3PE:H3F2 | 1.93                     | 0.50              |
| 2:B:279:LEU:O     | 2:B:283:ARG:HG2   | 2.11                     | 0.50              |
| 1:G:121:ASN:O     | 1:G:125:PRO:HG2   | 2.12                     | 0.50              |
| 2:H:84:HIS:CD2    | 2:H:84:HIS:C      | 2.90                     | 0.50              |
| 2:H:209:GLN:CG    | 2:H:235:LEU:HD22  | 2.42                     | 0.50              |
| 2:H:217:HIS:O     | 2:H:230:ALA:N     | 2.42                     | 0.50              |
| 1:A:425:SER:OG    | 1:A:426:LEU:HD23  | 2.11                     | 0.49              |
| 3:C:92:MET:O      | 3:C:93:PHE:C      | 2.55                     | 0.49              |
| 3:C:132:HIS:O     | 3:C:136:ILE:HG12  | 2.12                     | 0.49              |
| 4:D:32:TRP:O      | 4:D:33:ALA:C      | 2.54                     | 0.49              |
| 1:G:52:ARG:HD3    | 1:G:498:SER:HA    | 1.93                     | 0.49              |
| 1:G:291:VAL:HG22  | 1:G:295:PHE:CE1   | 2.47                     | 0.49              |
| 2:H:159:TYR:O     | 2:H:194:THR:OG1   | 2.23                     | 0.49              |
| 2:B:209:GLN:CG    | 2:B:235:LEU:HD22  | 2.42                     | 0.49              |
| 1:G:256:ASP:OD1   | 1:G:261:THR:OG1   | 2.20                     | 0.49              |
| 2:H:192:LEU:HD13  | 2:H:249:PHE:CD2   | 2.47                     | 0.49              |
| 1:A:18:THR:HA     | 1:A:22:MET:CE     | 2.42                     | 0.49              |
| 3:C:32:ALA:O      | 3:C:36:MET:HG3    | 2.12                     | 0.49              |
| 9:C:2010:3PE:H231 | 9:C:2010:3PE:H331 | 1.94                     | 0.49              |
| 1:G:244:PRO:O     | 1:G:247:ALA:N     | 2.45                     | 0.49              |
| 3:I:130:PRO:HA    | 3:I:134:PRO:HG2   | 1.93                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:137:ARG:HH21  | 9:A:2009:3PE:H112 | 1.76                     | 0.49              |
| 1:A:212:PHE:HD1   | 1:A:213:LEU:HD23  | 1.77                     | 0.49              |
| 1:A:213:LEU:HB3   | 3:C:81:TRP:HH2    | 1.76                     | 0.49              |
| 1:A:419:HIS:CD2   | 1:A:419:HIS:C     | 2.89                     | 0.49              |
| 2:B:113:VAL:O     | 2:B:116:GLY:N     | 2.46                     | 0.49              |
| 2:B:190:PHE:CD1   | 2:B:190:PHE:C     | 2.89                     | 0.49              |
| 2:B:196:THR:O     | 2:B:196:THR:HG22  | 2.09                     | 0.49              |
| 3:C:245:TRP:NE1   | 9:C:2013:3PE:H322 | 2.28                     | 0.49              |
| 3:C:249:PHE:O     | 3:C:250:VAL:C     | 2.55                     | 0.49              |
| 4:D:37:ILE:HG22   | 4:D:38:VAL:N      | 2.27                     | 0.49              |
| 1:G:138:MET:HE1   | 9:G:3009:3PE:H331 | 1.94                     | 0.49              |
| 1:G:227:LEU:O     | 1:G:230:TRP:N     | 2.44                     | 0.49              |
| 2:H:151:ASP:HB2   | 10:H:1112:HOH:O   | 2.11                     | 0.49              |
| 1:A:106:MET:HE3   | 1:A:110:VAL:CB    | 2.42                     | 0.49              |
| 1:A:178:LEU:HD12  | 1:A:178:LEU:C     | 2.36                     | 0.49              |
| 1:A:325:VAL:HG22  | 9:A:2012:3PE:C3D  | 2.42                     | 0.49              |
| 1:A:446:ARG:NH1   | 1:A:522:GLY:O     | 2.46                     | 0.49              |
| 1:A:523:ALA:O     | 1:A:524:ARG:C     | 2.56                     | 0.49              |
| 2:B:161:ILE:HD11  | 2:B:193:ALA:HB1   | 1.95                     | 0.49              |
| 3:C:103:LYS:C     | 3:C:103:LYS:HD3   | 2.37                     | 0.49              |
| 3:C:115:ILE:H     | 3:C:115:ILE:HD12  | 1.77                     | 0.49              |
| 3:C:147:ALA:HB1   | 3:C:170:LEU:HD23  | 1.93                     | 0.49              |
| 3:C:155:LEU:O     | 3:C:155:LEU:HG    | 2.10                     | 0.49              |
| 4:D:38:VAL:HG12   | 4:D:42:ILE:HD12   | 1.95                     | 0.49              |
| 1:G:95:TRP:CE2    | 1:G:99:ILE:HD11   | 2.47                     | 0.49              |
| 1:G:458:TRP:O     | 1:G:459:MET:C     | 2.56                     | 0.49              |
| 2:H:137:LYS:HB3   | 2:H:148:GLU:HB2   | 1.94                     | 0.49              |
| 2:H:143:TRP:CD1   | 2:H:143:TRP:N     | 2.79                     | 0.49              |
| 2:H:156:PHE:CD1   | 2:H:196:THR:HG21  | 2.46                     | 0.49              |
| 3:I:238:VAL:HG12  | 9:I:3008:3PE:O21  | 2.11                     | 0.49              |
| 1:A:173:VAL:O     | 1:A:174:LEU:HB2   | 2.12                     | 0.49              |
| 1:A:538:LEU:HD21  | 1:A:560:TRP:HE3   | 1.77                     | 0.49              |
| 4:D:44:LEU:HD21   | 9:D:2011:3PE:H31  | 1.94                     | 0.49              |
| 1:G:274:LEU:HD21  | 3:I:100:SER:HA    | 1.93                     | 0.49              |
| 1:G:323:ILE:HG22  | 1:G:324:GLY:N     | 2.28                     | 0.49              |
| 1:G:365:SER:O     | 1:G:366:TRP:C     | 2.53                     | 0.49              |
| 9:G:3009:3PE:H261 | 3:I:55:MET:HG2    | 1.94                     | 0.49              |
| 1:A:145:LEU:O     | 1:A:146:TYR:C     | 2.55                     | 0.49              |
| 8:A:1002:HEA:HAD2 | 10:A:2047:HOH:O   | 2.10                     | 0.49              |
| 3:C:63:VAL:O      | 3:C:64:THR:C      | 2.56                     | 0.49              |
| 1:G:478:GLY:O     | 1:G:479:MET:C     | 2.55                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:H:141:TYR:HE1  | 2:H:146:GLY:HA3   | 1.76                     | 0.49              |
| 1:A:175:TYR:HB3  | 10:A:2013:HOH:O   | 2.11                     | 0.49              |
| 1:A:176:PRO:O    | 10:A:2013:HOH:O   | 2.20                     | 0.49              |
| 1:A:316:MET:SD   | 1:A:365:SER:CB    | 3.01                     | 0.49              |
| 1:A:547:PRO:HD2  | 1:A:550:THR:HG22  | 1.94                     | 0.49              |
| 1:G:104:ILE:O    | 1:G:105:LEU:C     | 2.55                     | 0.49              |
| 2:H:248:PHE:HE2  | 2:H:269:VAL:HG12  | 1.77                     | 0.49              |
| 3:I:74:VAL:O     | 3:I:75:VAL:C      | 2.56                     | 0.49              |
| 1:A:131:PRO:HG2  | 3:C:9:TYR:HD2     | 1.78                     | 0.49              |
| 1:A:231:SER:CA   | 1:A:320:MET:HE1   | 2.42                     | 0.49              |
| 2:B:228:GLN:CG   | 2:B:229:ASP:N     | 2.76                     | 0.49              |
| 1:G:52:ARG:O     | 1:G:53:MET:C      | 2.55                     | 0.49              |
| 1:G:292:LEU:HB2  | 1:G:293:PRO:HD3   | 1.95                     | 0.49              |
| 2:H:136:VAL:HG12 | 2:H:137:LYS:N     | 2.27                     | 0.49              |
| 3:I:52:LEU:HD22  | 9:I:3008:3PE:H3C2 | 1.95                     | 0.49              |
| 3:I:106:LEU:C    | 3:I:108:PRO:HD3   | 2.37                     | 0.49              |
| 3:I:122:PRO:HG2  | 3:I:125:ILE:HD12  | 1.95                     | 0.49              |
| 1:A:26:HIS:HD2   | 1:A:122:TYR:HA    | 1.77                     | 0.49              |
| 1:A:70:SER:C     | 1:A:71:GLY:O      | 2.53                     | 0.49              |
| 1:A:291:VAL:HG22 | 1:A:295:PHE:CE1   | 2.48                     | 0.49              |
| 1:A:145:LEU:HD23 | 3:C:22:SER:OG     | 2.13                     | 0.48              |
| 1:A:185:TYR:HB3  | 3:C:37:HIS:CD2    | 2.48                     | 0.48              |
| 1:A:359:THR:HG22 | 8:A:1002:HEA:H172 | 1.95                     | 0.48              |
| 2:B:224:PHE:HE1  | 2:B:242:ALA:HB2   | 1.77                     | 0.48              |
| 2:B:275:TYR:O    | 2:B:278:TRP:HB3   | 2.12                     | 0.48              |
| 3:C:155:LEU:HB2  | 3:C:164:VAL:HG21  | 1.94                     | 0.48              |
| 3:C:228:GLN:OE1  | 3:C:228:GLN:HA    | 2.12                     | 0.48              |
| 1:G:120:GLY:O    | 1:G:121:ASN:C     | 2.55                     | 0.48              |
| 1:G:496:VAL:O    | 1:G:497:SER:C     | 2.56                     | 0.48              |
| 1:G:509:LEU:O    | 1:G:510:PHE:C     | 2.56                     | 0.48              |
| 2:H:77:LEU:O     | 2:H:78:TYR:C      | 2.56                     | 0.48              |
| 3:I:212:HIS:HD2  | 3:I:246:TYR:OH    | 1.96                     | 0.48              |
| 1:A:128:ILE:HB   | 1:A:216:ARG:HG2   | 1.95                     | 0.48              |
| 1:A:380:PRO:HG3  | 1:A:437:TYR:CB    | 2.43                     | 0.48              |
| 2:B:221:VAL:HG11 | 2:B:224:PHE:CD2   | 2.48                     | 0.48              |
| 2:B:221:VAL:CB   | 2:B:224:PHE:HD2   | 2.26                     | 0.48              |
| 3:C:85:LEU:HD23  | 3:C:88:MET:HE2    | 1.95                     | 0.48              |
| 1:G:75:GLY:O     | 1:G:76:PHE:C      | 2.56                     | 0.48              |
| 1:G:106:MET:CG   | 8:G:1001:HEA:CAC  | 2.73                     | 0.48              |
| 3:I:133:LEU:HD11 | 3:I:181:PHE:CD2   | 2.49                     | 0.48              |
| 1:A:499:LEU:O    | 1:A:500:GLY:C     | 2.56                     | 0.48              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:113:VAL:O     | 2:B:114:ALA:C    | 2.55                     | 0.48              |
| 2:B:142:GLN:O     | 2:B:143:TRP:CB   | 2.61                     | 0.48              |
| 3:C:130:PRO:HD2   | 10:C:2037:HOH:O  | 2.13                     | 0.48              |
| 3:C:214:ILE:O     | 3:C:218:ILE:HG12 | 2.12                     | 0.48              |
| 1:G:41:GLY:N      | 1:G:110:VAL:HG22 | 2.27                     | 0.48              |
| 1:G:487:PRO:HG2   | 1:G:490:PHE:HE2  | 1.79                     | 0.48              |
| 3:I:72:THR:HB     | 3:I:75:VAL:HG23  | 1.95                     | 0.48              |
| 1:A:477:GLN:HA    | 1:A:477:GLN:NE2  | 2.28                     | 0.48              |
| 2:B:220:THR:O     | 2:B:250:GLY:HA3  | 2.13                     | 0.48              |
| 3:C:48:LEU:O      | 3:C:49:VAL:C     | 2.56                     | 0.48              |
| 4:D:15:ASP:OD1    | 4:D:16:ILE:N     | 2.46                     | 0.48              |
| 1:G:329:VAL:HB    | 1:G:347:TYR:OH   | 2.13                     | 0.48              |
| 1:G:487:PRO:HG2   | 1:G:490:PHE:CE2  | 2.48                     | 0.48              |
| 1:G:498:SER:O     | 1:G:499:LEU:C    | 2.56                     | 0.48              |
| 8:G:1002:HEA:O11  | 8:G:1002:HEA:CHC | 2.49                     | 0.48              |
| 2:H:142:GLN:NE2   | 10:H:1015:HOH:O  | 2.36                     | 0.48              |
| 1:A:72:LEU:O      | 1:A:73:VAL:C     | 2.56                     | 0.48              |
| 1:A:217:ALA:O     | 1:A:218:PRO:C    | 2.56                     | 0.48              |
| 2:B:195:ASP:OD1   | 2:B:196:THR:N    | 2.46                     | 0.48              |
| 3:C:123:GLU:HG3   | 1:G:557:ARG:NH2  | 2.29                     | 0.48              |
| 3:C:141:LEU:HD12  | 3:C:254:TRP:CD1  | 2.49                     | 0.48              |
| 1:G:377:LEU:HD21  | 2:H:80:VAL:CG1   | 2.42                     | 0.48              |
| 1:G:408:ARG:HG3   | 2:H:126:GLN:OE1  | 2.13                     | 0.48              |
| 1:G:416:VAL:HG11  | 10:G:3018:HOH:O  | 2.13                     | 0.48              |
| 9:G:3012:3PE:H232 | 4:J:29:MET:HE1   | 1.94                     | 0.48              |
| 2:H:159:TYR:O     | 2:H:194:THR:HA   | 2.14                     | 0.48              |
| 2:H:161:ILE:HD11  | 2:H:193:ALA:CB   | 2.44                     | 0.48              |
| 2:H:194:THR:CG2   | 2:H:266:THR:HB   | 2.44                     | 0.48              |
| 3:I:100:SER:O     | 3:I:101:PHE:C    | 2.57                     | 0.48              |
| 3:I:112:GLU:CB    | 3:I:116:ILE:HB   | 2.44                     | 0.48              |
| 4:J:33:ALA:O      | 4:J:34:ALA:C     | 2.56                     | 0.48              |
| 1:A:314:LEU:O     | 1:A:317:VAL:N    | 2.47                     | 0.48              |
| 1:A:404:ALA:O     | 1:A:405:SER:C    | 2.57                     | 0.48              |
| 2:B:252:CYS:HB2   | 2:B:263:MET:SD   | 2.53                     | 0.48              |
| 3:C:147:ALA:CB    | 3:C:170:LEU:HD23 | 2.42                     | 0.48              |
| 1:G:23:SER:O      | 1:G:140:ASN:HB2  | 2.14                     | 0.48              |
| 3:I:126:ILE:HB    | 3:I:190:ALA:HB1  | 1.94                     | 0.48              |
| 2:B:163:SER:O     | 2:B:166:THR:OG1  | 2.31                     | 0.48              |
| 2:B:226:VAL:HG12  | 10:B:1047:HOH:O  | 2.12                     | 0.48              |
| 1:G:130:ALA:HB1   | 1:G:131:PRO:CD   | 2.44                     | 0.48              |
| 1:G:208:MET:O     | 1:G:209:ILE:C    | 2.57                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:G:287:VAL:HG11 | 8:G:1002:HEA:CHD  | 2.44                     | 0.48              |
| 2:H:108:PRO:O    | 2:H:111:ILE:HB    | 2.13                     | 0.48              |
| 2:H:190:PHE:CD1  | 2:H:190:PHE:C     | 2.90                     | 0.48              |
| 3:I:122:PRO:HG2  | 3:I:125:ILE:CG1   | 2.44                     | 0.48              |
| 1:A:209:ILE:HG21 | 3:C:85:LEU:HD22   | 1.96                     | 0.48              |
| 1:A:398:GLY:O    | 1:A:402:SER:N     | 2.43                     | 0.48              |
| 3:C:141:LEU:O    | 3:C:142:LEU:C     | 2.56                     | 0.48              |
| 1:G:26:HIS:HD2   | 1:G:122:TYR:HA    | 1.79                     | 0.48              |
| 1:G:41:GLY:O     | 1:G:45:VAL:N      | 2.31                     | 0.48              |
| 1:G:292:LEU:CB   | 1:G:293:PRO:HD3   | 2.43                     | 0.48              |
| 1:G:298:VAL:O    | 1:G:299:SER:C     | 2.54                     | 0.48              |
| 1:G:300:HIS:CD2  | 1:G:300:HIS:N     | 2.81                     | 0.48              |
| 1:G:385:LEU:O    | 1:G:386:GLY:C     | 2.57                     | 0.48              |
| 1:G:474:LEU:HD21 | 1:G:494:ASN:ND2   | 2.29                     | 0.48              |
| 2:H:84:HIS:CD2   | 2:H:85:GLU:N      | 2.81                     | 0.48              |
| 2:H:220:THR:OG1  | 2:H:227:LYS:HB2   | 2.13                     | 0.48              |
| 3:I:152:HIS:CD2  | 9:I:3013:3PE:H332 | 2.48                     | 0.48              |
| 1:A:128:ILE:CD1  | 1:A:216:ARG:HA    | 2.44                     | 0.48              |
| 1:A:237:TRP:CG   | 9:A:2012:3PE:H382 | 2.49                     | 0.48              |
| 2:B:200:VAL:O    | 2:B:269:VAL:HG23  | 2.14                     | 0.48              |
| 3:C:111:PRO:HA   | 4:J:10:VAL:CB     | 2.42                     | 0.48              |
| 1:G:279:LEU:HD23 | 1:G:279:LEU:O     | 2.10                     | 0.48              |
| 1:G:463:GLY:H    | 1:G:503:LEU:HD23  | 1.77                     | 0.48              |
| 1:G:489:ALA:O    | 2:H:38:PRO:HA     | 2.14                     | 0.48              |
| 4:J:42:ILE:O     | 4:J:43:PHE:C      | 2.57                     | 0.48              |
| 1:A:213:LEU:HD12 | 3:C:81:TRP:CZ2    | 2.49                     | 0.48              |
| 1:A:284:HIS:O    | 1:A:285:PRO:C     | 2.56                     | 0.48              |
| 1:A:452:ALA:HB1  | 1:A:514:VAL:CG2   | 2.44                     | 0.48              |
| 1:A:497:SER:O    | 1:A:500:GLY:N     | 2.47                     | 0.48              |
| 1:A:539:GLU:HG2  | 1:A:540:TRP:N     | 2.28                     | 0.48              |
| 2:B:258:ILE:HG22 | 2:B:259:SER:N     | 2.26                     | 0.48              |
| 3:C:225:ILE:O    | 3:C:226:ARG:C     | 2.56                     | 0.48              |
| 2:H:201:PRO:HB2  | 2:H:204:LYS:HB2   | 1.96                     | 0.48              |
| 3:I:91:VAL:HG11  | 9:I:3010:3PE:H2H1 | 1.95                     | 0.48              |
| 1:A:31:VAL:O     | 1:A:32:LEU:C      | 2.56                     | 0.47              |
| 2:B:194:THR:HG22 | 2:B:266:THR:HB    | 1.96                     | 0.47              |
| 3:C:28:MET:HG2   | 3:C:29:LEU:HD23   | 1.96                     | 0.47              |
| 1:G:123:PHE:O    | 1:G:126:LEU:N     | 2.47                     | 0.47              |
| 1:G:263:PHE:CZ   | 3:I:200:ALA:HB1   | 2.49                     | 0.47              |
| 1:A:302:ILE:HG22 | 1:A:369:THR:CG2   | 2.45                     | 0.47              |
| 3:C:196:ASN:O    | 3:C:197:ILE:C     | 2.57                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:212:HIS:HD2  | 3:C:246:TYR:OH   | 1.97                     | 0.47              |
| 1:G:52:ARG:CD    | 1:G:498:SER:HA   | 2.44                     | 0.47              |
| 2:H:200:VAL:O    | 2:H:200:VAL:HG12 | 2.10                     | 0.47              |
| 4:J:16:ILE:HA    | 4:J:19:GLN:OE1   | 2.15                     | 0.47              |
| 1:A:176:PRO:CB   | 1:A:177:PRO:HA   | 2.44                     | 0.47              |
| 1:A:248:GLY:O    | 1:A:251:THR:N    | 2.47                     | 0.47              |
| 1:A:402:SER:HA   | 8:A:1002:HEA:OMA | 2.14                     | 0.47              |
| 9:C:2013:3PE:O14 | 9:C:2013:3PE:C12 | 2.53                     | 0.47              |
| 1:G:112:ILE:HB   | 1:G:113:PRO:HD3  | 1.95                     | 0.47              |
| 1:G:177:PRO:O    | 1:G:178:LEU:C    | 2.57                     | 0.47              |
| 3:I:74:VAL:HG23  | 3:I:75:VAL:N     | 2.29                     | 0.47              |
| 4:J:25:GLY:O     | 4:J:26:PHE:C     | 2.57                     | 0.47              |
| 1:A:122:TYR:C    | 1:A:122:TYR:HD1  | 2.22                     | 0.47              |
| 1:A:213:LEU:HD21 | 1:A:233:PHE:CZ   | 2.49                     | 0.47              |
| 1:A:237:TRP:CH2  | 3:C:88:MET:HE1   | 2.49                     | 0.47              |
| 2:B:45:PRO:HB3   | 2:B:244:ARG:NH2  | 2.29                     | 0.47              |
| 2:B:120:LEU:CB   | 2:B:121:PRO:CD   | 2.92                     | 0.47              |
| 2:B:251:GLN:HG3  | 10:B:1016:HOH:O  | 2.13                     | 0.47              |
| 3:C:202:PHE:CD1  | 3:C:202:PHE:C    | 2.92                     | 0.47              |
| 4:D:16:ILE:HG22  | 4:D:19:GLN:HB2   | 1.95                     | 0.47              |
| 1:G:44:SER:O     | 1:G:45:VAL:C     | 2.57                     | 0.47              |
| 1:G:81:TRP:CD2   | 1:G:82:PRO:HD2   | 2.49                     | 0.47              |
| 1:G:232:ILE:HA   | 1:G:232:ILE:HD13 | 1.71                     | 0.47              |
| 1:G:312:GLY:O    | 1:G:313:TYR:C    | 2.56                     | 0.47              |
| 1:G:341:SER:OG   | 1:G:344:GLN:N    | 2.34                     | 0.47              |
| 1:G:433:PHE:HE1  | 1:G:511:PHE:CZ   | 2.32                     | 0.47              |
| 1:G:547:PRO:O    | 1:G:550:THR:HG23 | 2.15                     | 0.47              |
| 1:A:231:SER:OG   | 1:A:293:PRO:HA   | 2.14                     | 0.47              |
| 1:A:292:LEU:HD23 | 1:A:292:LEU:HA   | 1.85                     | 0.47              |
| 1:A:543:THR:HG23 | 1:A:547:PRO:HD3  | 1.96                     | 0.47              |
| 1:G:106:MET:SD   | 8:G:1001:HEA:CMC | 3.03                     | 0.47              |
| 1:G:419:HIS:CD2  | 1:G:419:HIS:C    | 2.87                     | 0.47              |
| 2:H:249:PHE:HE1  | 2:H:266:THR:HG1  | 1.62                     | 0.47              |
| 2:H:254:GLU:H    | 2:H:260:HIS:HE1  | 1.62                     | 0.47              |
| 3:I:26:PHE:O     | 3:I:27:VAL:C     | 2.56                     | 0.47              |
| 3:I:57:GLY:O     | 3:I:58:TRP:C     | 2.58                     | 0.47              |
| 3:I:74:VAL:HG13  | 4:J:16:ILE:HG12  | 1.96                     | 0.47              |
| 1:A:59:GLY:HA2   | 1:A:485:ASP:OD2  | 2.15                     | 0.47              |
| 1:A:112:ILE:CB   | 1:A:113:PRO:HD3  | 2.43                     | 0.47              |
| 1:A:300:HIS:H    | 1:A:300:HIS:CD2  | 2.32                     | 0.47              |
| 3:C:79:LEU:O     | 3:C:80:ARG:C     | 2.57                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:231:SER:OG    | 1:G:232:ILE:N     | 2.48                     | 0.47              |
| 1:G:252:MET:HE2   | 1:G:264:PHE:HZ    | 1.76                     | 0.47              |
| 1:G:444:SER:OG    | 1:G:445:GLY:N     | 2.46                     | 0.47              |
| 1:A:314:LEU:HD12  | 1:A:314:LEU:HA    | 1.83                     | 0.47              |
| 1:A:404:ALA:HB3   | 2:B:123:LEU:HD13  | 1.97                     | 0.47              |
| 1:A:433:PHE:CE2   | 1:A:460:MET:HE3   | 2.47                     | 0.47              |
| 2:B:77:LEU:O      | 2:B:78:TYR:C      | 2.57                     | 0.47              |
| 2:B:84:HIS:CD2    | 2:B:85:GLU:HG2    | 2.50                     | 0.47              |
| 3:C:74:VAL:O      | 3:C:75:VAL:C      | 2.58                     | 0.47              |
| 3:C:245:TRP:HE1   | 9:C:2013:3PE:H322 | 1.79                     | 0.47              |
| 1:G:124:MET:O     | 1:G:125:PRO:C     | 2.58                     | 0.47              |
| 1:G:140:ASN:ND2   | 10:G:3041:HOH:O   | 2.32                     | 0.47              |
| 1:G:155:ALA:HB1   | 10:G:3088:HOH:O   | 2.13                     | 0.47              |
| 1:G:332:ALA:HB3   | 1:G:348:PHE:CD1   | 2.50                     | 0.47              |
| 1:G:387:PHE:HD1   | 1:G:388:LEU:N     | 2.13                     | 0.47              |
| 1:G:479:MET:HG2   | 1:G:480:PRO:O     | 2.15                     | 0.47              |
| 1:G:550:THR:O     | 1:G:551:PHE:HB2   | 2.14                     | 0.47              |
| 1:A:243:LEU:N     | 1:A:243:LEU:HD23  | 2.29                     | 0.47              |
| 1:G:446:ARG:NH1   | 1:G:522:GLY:O     | 2.48                     | 0.47              |
| 2:H:217:HIS:ND1   | 2:H:256:CYS:HB2   | 2.29                     | 0.47              |
| 1:A:124:MET:SD    | 1:A:125:PRO:CD    | 3.03                     | 0.47              |
| 1:A:243:LEU:O     | 1:A:244:PRO:C     | 2.58                     | 0.47              |
| 1:A:307:LYS:O     | 2:B:91:PRO:HB3    | 2.15                     | 0.47              |
| 1:A:337:THR:HG22  | 1:A:408:ARG:HH11  | 1.79                     | 0.47              |
| 9:A:2009:3PE:H291 | 9:A:2009:3PE:C3A  | 2.45                     | 0.47              |
| 3:C:91:VAL:HG11   | 9:C:2010:3PE:H2H1 | 1.97                     | 0.47              |
| 3:C:99:TRP:HZ2    | 9:C:2010:3PE:H222 | 1.80                     | 0.47              |
| 1:G:180:THR:HA    | 1:G:257:ARG:CG    | 2.45                     | 0.47              |
| 9:G:3009:3PE:H221 | 3:I:58:TRP:CZ2    | 2.50                     | 0.47              |
| 9:I:3010:3PE:H231 | 9:I:3010:3PE:H332 | 1.97                     | 0.47              |
| 4:J:15:ASP:OD1    | 4:J:17:THR:N      | 2.37                     | 0.47              |
| 2:B:86:LYS:HD2    | 2:B:89:LYS:NZ     | 2.30                     | 0.47              |
| 2:B:136:VAL:HG12  | 2:B:137:LYS:N     | 2.29                     | 0.47              |
| 2:B:221:VAL:O     | 2:B:222:PRO:C     | 2.56                     | 0.47              |
| 2:B:250:GLY:O     | 2:B:265:ILE:N     | 2.48                     | 0.47              |
| 3:C:72:THR:O      | 3:C:75:VAL:HG23   | 2.15                     | 0.47              |
| 3:C:178:PHE:O     | 3:C:179:THR:C     | 2.58                     | 0.47              |
| 1:G:237:TRP:O     | 1:G:238:LEU:C     | 2.58                     | 0.47              |
| 1:G:274:LEU:HD13  | 3:I:103:LYS:HG3   | 1.97                     | 0.47              |
| 1:G:489:ALA:HA    | 2:H:38:PRO:HG3    | 1.97                     | 0.47              |
| 1:G:517:TYR:O     | 1:G:521:ARG:N     | 2.46                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:42:TRP:CD1    | 3:I:42:TRP:H      | 2.22                     | 0.47              |
| 1:A:306:ALA:O     | 1:A:307:LYS:C     | 2.57                     | 0.46              |
| 9:A:2012:3PE:H3F1 | 9:D:2011:3PE:H2D1 | 1.96                     | 0.46              |
| 2:B:97:ASN:O      | 2:B:101:GLU:HG3   | 2.15                     | 0.46              |
| 1:G:424:MET:HB3   | 8:G:1001:HEA:CBC  | 2.45                     | 0.46              |
| 1:G:517:TYR:O     | 1:G:520:THR:HB    | 2.15                     | 0.46              |
| 2:H:49:PRO:HD3    | 2:H:243:GLU:OE2   | 2.14                     | 0.46              |
| 2:H:107:VAL:N     | 2:H:108:PRO:HD2   | 2.31                     | 0.46              |
| 1:A:249:ALA:HB2   | 1:A:278:ILE:CG2   | 2.44                     | 0.46              |
| 1:A:470:PRO:HA    | 1:A:473:PHE:CD2   | 2.51                     | 0.46              |
| 3:C:226:ARG:NH2   | 9:C:2008:3PE:H121 | 2.31                     | 0.46              |
| 4:D:42:ILE:O      | 4:D:43:PHE:C      | 2.57                     | 0.46              |
| 1:G:282:PHE:CD2   | 1:G:282:PHE:C     | 2.86                     | 0.46              |
| 1:G:508:PHE:CD2   | 1:G:512:LEU:HD11  | 2.50                     | 0.46              |
| 1:G:519:LEU:N     | 1:G:519:LEU:HD23  | 2.30                     | 0.46              |
| 8:G:1002:HEA:OMA  | 8:G:1002:HEA:HHB  | 2.15                     | 0.46              |
| 3:I:103:LYS:HD3   | 3:I:103:LYS:O     | 2.14                     | 0.46              |
| 3:I:115:ILE:HD12  | 3:I:115:ILE:H     | 1.80                     | 0.46              |
| 4:J:32:TRP:O      | 4:J:33:ALA:C      | 2.58                     | 0.46              |
| 1:A:127:HIS:CE1   | 1:A:300:HIS:CE1   | 3.03                     | 0.46              |
| 1:A:136:PRO:CG    | 3:C:12:LEU:HD12   | 2.46                     | 0.46              |
| 1:A:141:LEU:HD12  | 1:A:141:LEU:O     | 2.16                     | 0.46              |
| 1:A:292:LEU:CB    | 1:A:293:PRO:HD3   | 2.44                     | 0.46              |
| 1:A:299:SER:O     | 1:A:302:ILE:N     | 2.48                     | 0.46              |
| 1:A:389:PHE:HB3   | 1:A:390:LEU:HD23  | 1.96                     | 0.46              |
| 1:A:458:TRP:O     | 1:A:459:MET:C     | 2.59                     | 0.46              |
| 3:C:83:PHE:HE1    | 9:C:2008:3PE:H262 | 1.80                     | 0.46              |
| 3:C:240:PHE:CD1   | 3:C:244:ILE:HD11  | 2.50                     | 0.46              |
| 1:G:71:GLY:CA     | 1:G:74:LYS:HD3    | 2.46                     | 0.46              |
| 1:G:248:GLY:O     | 1:G:249:ALA:C     | 2.58                     | 0.46              |
| 1:G:300:HIS:CD2   | 1:G:300:HIS:H     | 2.33                     | 0.46              |
| 1:G:316:MET:O     | 1:G:320:MET:HG3   | 2.15                     | 0.46              |
| 1:G:344:GLN:O     | 1:G:345:GLN:C     | 2.57                     | 0.46              |
| 1:G:375:ILE:CG2   | 1:G:376:GLU:N     | 2.78                     | 0.46              |
| 4:J:9:HIS:O       | 4:J:10:VAL:HG23   | 2.16                     | 0.46              |
| 4:J:21:LYS:O      | 4:J:24:ALA:HB3    | 2.15                     | 0.46              |
| 1:A:496:VAL:O     | 1:A:497:SER:C     | 2.58                     | 0.46              |
| 2:B:119:SER:O     | 2:B:120:LEU:C     | 2.59                     | 0.46              |
| 2:B:120:LEU:O     | 2:B:121:PRO:C     | 2.56                     | 0.46              |
| 4:D:43:PHE:C      | 4:D:43:PHE:CD1    | 2.93                     | 0.46              |
| 1:G:72:LEU:O      | 1:G:76:PHE:HB2    | 2.15                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:451:TRP:CD2   | 1:G:452:ALA:N     | 2.83                     | 0.46              |
| 8:G:1001:HEA:H252 | 8:G:1001:HEA:H212 | 1.77                     | 0.46              |
| 2:H:75:LEU:O      | 2:H:76:ILE:C      | 2.58                     | 0.46              |
| 2:H:136:VAL:CG1   | 2:H:137:LYS:N     | 2.78                     | 0.46              |
| 1:A:225:VAL:HG13  | 1:A:226:PRO:HD2   | 1.97                     | 0.46              |
| 1:A:227:LEU:HD23  | 1:A:227:LEU:HA    | 1.59                     | 0.46              |
| 1:A:288:TYR:O     | 1:A:292:LEU:HG    | 2.15                     | 0.46              |
| 1:A:538:LEU:HG    | 10:A:2076:HOH:O   | 2.15                     | 0.46              |
| 1:A:560:TRP:C     | 1:A:560:TRP:CD1   | 2.94                     | 0.46              |
| 2:B:161:ILE:HD12  | 2:B:180:LEU:HD23  | 1.97                     | 0.46              |
| 2:B:250:GLY:O     | 2:B:265:ILE:HB    | 2.14                     | 0.46              |
| 1:G:91:ASN:OD1    | 1:G:93:HIS:HB3    | 2.15                     | 0.46              |
| 1:G:112:ILE:N     | 1:G:113:PRO:HD2   | 2.30                     | 0.46              |
| 1:A:71:GLY:HA3    | 1:A:74:LYS:HD3    | 1.98                     | 0.46              |
| 1:A:127:HIS:CE1   | 1:A:300:HIS:HE1   | 2.34                     | 0.46              |
| 2:B:73:THR:HG22   | 2:B:77:LEU:HG     | 1.98                     | 0.46              |
| 3:C:109:MET:HG2   | 10:C:2014:HOH:O   | 2.14                     | 0.46              |
| 3:C:161:ARG:HH21  | 3:C:232:PHE:H     | 1.64                     | 0.46              |
| 3:C:226:ARG:HH22  | 9:C:2008:3PE:H121 | 1.80                     | 0.46              |
| 1:G:93:HIS:O      | 1:G:97:VAL:HG23   | 2.16                     | 0.46              |
| 1:G:173:VAL:CG1   | 1:G:279:LEU:HD22  | 2.45                     | 0.46              |
| 3:I:113:SER:HA    | 3:I:114:PRO:HA    | 1.59                     | 0.46              |
| 3:I:122:PRO:HG2   | 3:I:125:ILE:HG13  | 1.97                     | 0.46              |
| 3:I:253:VAL:O     | 3:I:257:LEU:HG    | 2.15                     | 0.46              |
| 1:A:86:GLU:HA     | 1:A:86:GLU:OE1    | 2.15                     | 0.46              |
| 1:A:124:MET:HE3   | 1:A:208:MET:SD    | 2.56                     | 0.46              |
| 1:A:200:SER:O     | 1:A:201:SER:C     | 2.58                     | 0.46              |
| 1:A:300:HIS:CD2   | 1:A:300:HIS:N     | 2.78                     | 0.46              |
| 1:A:432:ILE:HG22  | 1:A:436:ILE:HD11  | 1.97                     | 0.46              |
| 1:A:498:SER:O     | 1:A:499:LEU:C     | 2.58                     | 0.46              |
| 1:A:543:THR:O     | 1:A:546:PRO:HA    | 2.16                     | 0.46              |
| 1:A:543:THR:HG22  | 1:A:547:PRO:HD3   | 1.98                     | 0.46              |
| 3:C:122:PRO:HA    | 10:C:2045:HOH:O   | 2.15                     | 0.46              |
| 3:C:256:PHE:HE1   | 9:D:2011:3PE:H3B1 | 1.81                     | 0.46              |
| 1:G:342:LEU:HD11  | 2:H:124:PHE:HD1   | 1.81                     | 0.46              |
| 1:G:375:ILE:HG22  | 1:G:377:LEU:HD23  | 1.97                     | 0.46              |
| 1:G:390:LEU:HD13  | 1:G:426:LEU:HD13  | 1.98                     | 0.46              |
| 9:G:3009:3PE:H341 | 3:I:86:PHE:CD2    | 2.51                     | 0.46              |
| 2:H:98:SER:CB     | 2:H:99:PRO:HD3    | 2.31                     | 0.46              |
| 1:A:442:LYS:HD3   | 1:A:540:TRP:CE3   | 2.50                     | 0.46              |
| 3:C:141:LEU:HD21  | 3:C:178:PHE:CD2   | 2.51                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:253:VAL:HG13 | 9:C:2010:3PE:C3I | 2.45                     | 0.46              |
| 1:G:20:TRP:HE3   | 1:G:32:LEU:HD21  | 1.74                     | 0.46              |
| 1:G:134:ALA:O    | 1:G:136:PRO:HD3  | 2.16                     | 0.46              |
| 1:G:179:SER:O    | 1:G:257:ARG:HD2  | 2.16                     | 0.46              |
| 1:A:112:ILE:HG12 | 10:A:2024:HOH:O  | 2.16                     | 0.46              |
| 1:A:241:LEU:HD13 | 9:D:2011:3PE:C2H | 2.46                     | 0.46              |
| 2:B:90:VAL:HG13  | 2:B:91:PRO:HD2   | 1.98                     | 0.46              |
| 2:B:220:THR:OG1  | 2:B:221:VAL:N    | 2.46                     | 0.46              |
| 2:B:235:LEU:HD11 | 4:J:9:HIS:N      | 2.31                     | 0.46              |
| 3:C:250:VAL:O    | 3:C:251:ASP:C    | 2.58                     | 0.46              |
| 1:G:292:LEU:HD23 | 1:G:292:LEU:HA   | 1.81                     | 0.46              |
| 2:H:147:TYR:CD2  | 2:H:198:MET:HE3  | 2.51                     | 0.46              |
| 2:H:202:VAL:HG12 | 2:H:269:VAL:HG22 | 1.97                     | 0.46              |
| 2:B:111:ILE:O    | 2:B:114:ALA:HB3  | 2.16                     | 0.46              |
| 3:C:25:ALA:O     | 3:C:26:PHE:C     | 2.57                     | 0.46              |
| 3:C:72:THR:HB    | 3:C:75:VAL:HG23  | 1.97                     | 0.46              |
| 4:D:41:LEU:O     | 4:D:42:ILE:C     | 2.58                     | 0.46              |
| 1:G:49:VAL:O     | 1:G:50:TYR:C     | 2.59                     | 0.46              |
| 1:G:51:MET:HE1   | 8:G:1001:HEA:C3A | 2.45                     | 0.46              |
| 1:G:107:MET:CE   | 1:G:424:MET:SD   | 3.04                     | 0.46              |
| 1:G:124:MET:SD   | 1:G:125:PRO:HD3  | 2.56                     | 0.46              |
| 1:G:189:LEU:CD2  | 3:I:33:VAL:HG21  | 2.46                     | 0.46              |
| 1:G:203:LEU:O    | 1:G:204:GLY:O    | 2.34                     | 0.46              |
| 2:H:171:ARG:HD2  | 10:H:1142:HOH:O  | 2.16                     | 0.46              |
| 3:I:150:TRP:HE1  | 3:I:163:ASP:CG   | 2.23                     | 0.46              |
| 3:I:202:PHE:CD1  | 3:I:202:PHE:O    | 2.69                     | 0.46              |
| 4:J:31:THR:HG22  | 4:J:32:TRP:N     | 2.31                     | 0.46              |
| 1:A:105:LEU:HD23 | 1:A:105:LEU:HA   | 1.79                     | 0.45              |
| 1:A:188:ASP:OD2  | 1:A:258:ASN:ND2  | 2.37                     | 0.45              |
| 1:A:429:VAL:O    | 1:A:430:PHE:C    | 2.57                     | 0.45              |
| 2:B:75:LEU:O     | 2:B:76:ILE:C     | 2.58                     | 0.45              |
| 3:C:8:ASP:HB3    | 3:C:72:THR:CG2   | 2.31                     | 0.45              |
| 3:C:41:PRO:O     | 3:C:42:TRP:C     | 2.59                     | 0.45              |
| 3:C:58:TRP:O     | 3:C:62:VAL:HG23  | 2.16                     | 0.45              |
| 3:C:136:ILE:HG21 | 3:C:181:PHE:CE2  | 2.51                     | 0.45              |
| 3:C:169:ALA:O    | 3:C:170:LEU:C    | 2.59                     | 0.45              |
| 1:G:551:PHE:CE1  | 1:G:555:PRO:HG3  | 2.51                     | 0.45              |
| 10:G:3031:HOH:O  | 3:I:104:HIS:HE1  | 1.99                     | 0.45              |
| 2:H:252:CYS:HB2  | 2:H:263:MET:CG   | 2.47                     | 0.45              |
| 1:A:173:VAL:O    | 1:A:174:LEU:CB   | 2.62                     | 0.45              |
| 1:A:189:LEU:HD21 | 3:C:30:PHE:HD1   | 1.80                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:389:PHE:CD2   | 1:A:390:LEU:HD23  | 2.51                     | 0.45              |
| 2:B:211:THR:CG2   | 2:B:212:GLY:N     | 2.79                     | 0.45              |
| 3:C:204:MET:O     | 3:C:205:ALA:C     | 2.59                     | 0.45              |
| 1:G:310:ILE:HG23  | 1:G:310:ILE:O     | 2.16                     | 0.45              |
| 1:G:431:GLY:O     | 1:G:434:ALA:HB3   | 2.16                     | 0.45              |
| 9:G:3012:3PE:H232 | 4:J:29:MET:CE     | 2.46                     | 0.45              |
| 2:H:211:THR:HG23  | 2:H:234:ARG:O     | 2.16                     | 0.45              |
| 1:A:137:ARG:N     | 9:A:2009:3PE:O12  | 2.49                     | 0.45              |
| 1:A:251:THR:HG22  | 3:C:97:TRP:CH2    | 2.51                     | 0.45              |
| 1:A:450:GLU:OE2   | 1:A:454:LYS:HE3   | 2.16                     | 0.45              |
| 2:B:97:ASN:C      | 2:B:97:ASN:OD1    | 2.59                     | 0.45              |
| 1:G:314:LEU:O     | 1:G:317:VAL:N     | 2.49                     | 0.45              |
| 1:G:396:VAL:O     | 1:G:399:ILE:N     | 2.47                     | 0.45              |
| 2:H:97:ASN:C      | 2:H:97:ASN:OD1    | 2.60                     | 0.45              |
| 2:H:206:VAL:HB    | 2:H:240:PHE:CE1   | 2.52                     | 0.45              |
| 1:A:486:TYR:HB2   | 1:A:487:PRO:CD    | 2.45                     | 0.45              |
| 8:A:1001:HEA:H201 | 8:A:1001:HEA:H253 | 1.99                     | 0.45              |
| 2:B:120:LEU:HD23  | 2:B:120:LEU:HA    | 1.85                     | 0.45              |
| 9:C:2010:3PE:H3F1 | 9:C:2010:3PE:H3I3 | 1.49                     | 0.45              |
| 9:C:2010:3PE:H2H2 | 9:C:2013:3PE:H3F1 | 1.99                     | 0.45              |
| 1:G:74:LYS:HD2    | 1:G:74:LYS:N      | 2.28                     | 0.45              |
| 1:G:279:LEU:HD23  | 1:G:280:TRP:N     | 2.28                     | 0.45              |
| 1:G:292:LEU:O     | 1:G:293:PRO:C     | 2.59                     | 0.45              |
| 1:G:337:THR:HG22  | 1:G:408:ARG:HH11  | 1.81                     | 0.45              |
| 3:I:238:VAL:HB    | 9:I:3008:3PE:P    | 2.56                     | 0.45              |
| 3:I:245:TRP:CZ2   | 9:I:3013:3PE:H231 | 2.51                     | 0.45              |
| 1:A:286:GLN:O     | 1:A:289:ILE:HB    | 2.16                     | 0.45              |
| 2:B:219:TRP:CD1   | 2:B:265:ILE:HD13  | 2.52                     | 0.45              |
| 1:G:131:PRO:HG2   | 3:I:9:TYR:CD2     | 2.50                     | 0.45              |
| 1:G:381:MET:O     | 1:G:384:ALA:HB3   | 2.16                     | 0.45              |
| 9:G:3012:3PE:H2I3 | 3:I:91:VAL:HG11   | 1.99                     | 0.45              |
| 2:H:68:ILE:HG22   | 2:H:69:THR:N      | 2.29                     | 0.45              |
| 1:A:24:THR:O      | 1:A:136:PRO:HB3   | 2.17                     | 0.45              |
| 1:A:284:HIS:N     | 1:A:285:PRO:CD    | 2.78                     | 0.45              |
| 9:A:2009:3PE:H381 | 9:A:2009:3PE:H251 | 1.97                     | 0.45              |
| 3:C:27:VAL:O      | 3:C:28:MET:C      | 2.58                     | 0.45              |
| 1:G:141:LEU:CB    | 3:I:18:PRO:HB3    | 2.45                     | 0.45              |
| 1:G:400:VAL:HG11  | 10:G:3109:HOH:O   | 2.16                     | 0.45              |
| 2:H:134:VAL:CG1   | 2:H:135:THR:N     | 2.80                     | 0.45              |
| 2:H:209:GLN:HB2   | 2:H:237:GLN:HG2   | 1.97                     | 0.45              |
| 3:I:223:CYS:O     | 3:I:224:LEU:C     | 2.57                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:J:30:VAL:O      | 4:J:33:ALA:HB3    | 2.17                     | 0.45              |
| 1:A:135:PHE:CD1   | 9:A:2009:3PE:H11  | 2.52                     | 0.45              |
| 1:A:359:THR:HG21  | 1:A:391:PHE:HE2   | 1.79                     | 0.45              |
| 2:B:61:ILE:HG22   | 10:B:1031:HOH:O   | 2.16                     | 0.45              |
| 2:B:276:ALA:HA    | 2:B:279:LEU:CD1   | 2.46                     | 0.45              |
| 3:C:71:HIS:O      | 3:C:76:ARG:HG3    | 2.17                     | 0.45              |
| 3:C:245:TRP:CZ2   | 9:C:2013:3PE:H231 | 2.52                     | 0.45              |
| 9:C:2013:3PE:C31  | 9:C:2013:3PE:H351 | 2.46                     | 0.45              |
| 4:D:44:LEU:HD23   | 9:D:2011:3PE:C32  | 2.45                     | 0.45              |
| 1:G:18:THR:HG22   | 1:G:19:ARG:N      | 2.30                     | 0.45              |
| 9:G:3009:3PE:H242 | 9:G:3009:3PE:C37  | 2.44                     | 0.45              |
| 2:H:120:LEU:HB2   | 2:H:121:PRO:CD    | 2.47                     | 0.45              |
| 3:I:84:ILE:O      | 3:I:85:LEU:C      | 2.59                     | 0.45              |
| 9:I:3010:3PE:H231 | 9:I:3010:3PE:H331 | 1.97                     | 0.45              |
| 1:A:92:GLY:HA2    | 1:A:484:ILE:CD1   | 2.47                     | 0.45              |
| 1:A:124:MET:C     | 1:A:124:MET:SD    | 2.99                     | 0.45              |
| 1:A:337:THR:HG22  | 1:A:408:ARG:NH1   | 2.32                     | 0.45              |
| 1:A:425:SER:O     | 1:A:429:VAL:HB    | 2.16                     | 0.45              |
| 1:A:535:ALA:HB1   | 1:A:540:TRP:NE1   | 2.32                     | 0.45              |
| 4:D:41:LEU:O      | 4:D:44:LEU:HB3    | 2.16                     | 0.45              |
| 3:I:226:ARG:HH12  | 9:I:3008:3PE:H12  | 1.82                     | 0.45              |
| 1:A:74:LYS:H      | 1:A:74:LYS:CD     | 2.24                     | 0.45              |
| 1:A:237:TRP:CH2   | 9:A:2012:3PE:H282 | 2.52                     | 0.45              |
| 1:A:291:VAL:CG2   | 1:A:295:PHE:CE1   | 3.00                     | 0.45              |
| 1:A:442:LYS:NZ    | 1:A:542:LEU:O     | 2.40                     | 0.45              |
| 1:A:463:GLY:CA    | 1:A:503:LEU:HD23  | 2.47                     | 0.45              |
| 1:A:486:TYR:N     | 1:A:486:TYR:CD1   | 2.85                     | 0.45              |
| 2:B:226:VAL:HA    | 10:B:1047:HOH:O   | 2.16                     | 0.45              |
| 3:C:40:GLY:HA2    | 3:C:41:PRO:HD2    | 1.78                     | 0.45              |
| 1:G:176:PRO:CB    | 1:G:177:PRO:HA    | 2.47                     | 0.45              |
| 1:G:497:SER:O     | 1:G:498:SER:C     | 2.58                     | 0.45              |
| 2:H:111:ILE:O     | 2:H:114:ALA:HB3   | 2.17                     | 0.45              |
| 3:I:55:MET:O      | 3:I:56:PHE:C      | 2.59                     | 0.45              |
| 1:A:50:TYR:O      | 1:A:53:MET:HB2    | 2.17                     | 0.45              |
| 1:A:147:VAL:HG12  | 1:A:148:ALA:N     | 2.32                     | 0.45              |
| 1:A:323:ILE:HD11  | 1:A:359:THR:OG1   | 2.16                     | 0.45              |
| 1:A:390:LEU:H     | 1:A:390:LEU:CD2   | 2.30                     | 0.45              |
| 1:A:470:PRO:O     | 1:A:473:PHE:N     | 2.50                     | 0.45              |
| 1:A:489:ALA:O     | 2:B:38:PRO:HA     | 2.16                     | 0.45              |
| 3:C:198:TYR:CD1   | 3:C:198:TYR:C     | 2.94                     | 0.45              |
| 1:G:390:LEU:O     | 1:G:393:VAL:HB    | 2.17                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:G:3012:3PE:H3E1 | 9:J:3011:3PE:H2F1 | 1.99                     | 0.45              |
| 3:I:210:GLY:O     | 3:I:211:PHE:C     | 2.59                     | 0.45              |
| 9:I:3013:3PE:O14  | 9:I:3013:3PE:C12  | 2.55                     | 0.45              |
| 4:J:44:LEU:HD23   | 9:J:3011:3PE:H322 | 1.99                     | 0.45              |
| 1:A:48:THR:HG22   | 1:A:102:HIS:CE1   | 2.52                     | 0.44              |
| 1:A:195:HIS:CD2   | 1:A:250:ILE:HD11  | 2.52                     | 0.44              |
| 1:A:239:ILE:HD11  | 1:A:289:ILE:HG21  | 1.99                     | 0.44              |
| 1:A:423:VAL:HG21  | 8:A:1002:HEA:C2C  | 2.47                     | 0.44              |
| 1:A:433:PHE:HE1   | 1:A:511:PHE:CZ    | 2.36                     | 0.44              |
| 1:A:547:PRO:O     | 1:A:550:THR:HG23  | 2.17                     | 0.44              |
| 2:B:109:ILE:O     | 2:B:113:VAL:HG23  | 2.17                     | 0.44              |
| 3:C:137:ASN:HD21  | 3:C:181:PHE:HB3   | 1.82                     | 0.44              |
| 3:C:252:VAL:HG12  | 9:C:2010:3PE:C3H  | 2.47                     | 0.44              |
| 3:C:256:PHE:O     | 3:C:257:LEU:C     | 2.59                     | 0.44              |
| 1:G:29:ILE:HD11   | 1:G:140:ASN:HA    | 1.98                     | 0.44              |
| 1:G:264:PHE:HA    | 1:G:271:ASP:N     | 2.31                     | 0.44              |
| 1:G:299:SER:O     | 1:G:300:HIS:C     | 2.60                     | 0.44              |
| 1:G:302:ILE:CG2   | 1:G:369:THR:HG21  | 2.40                     | 0.44              |
| 1:G:447:GLN:HG3   | 1:G:448:TYR:N     | 2.31                     | 0.44              |
| 2:H:249:PHE:HE1   | 2:H:266:THR:OG1   | 2.00                     | 0.44              |
| 3:I:129:ASP:O     | 3:I:134:PRO:HG2   | 2.17                     | 0.44              |
| 1:A:115:LEU:HD12  | 1:A:432:ILE:CG1   | 2.47                     | 0.44              |
| 9:A:2009:3PE:H3B2 | 9:A:2009:3PE:H2C2 | 1.98                     | 0.44              |
| 3:C:81:TRP:O      | 3:C:82:GLY:C      | 2.59                     | 0.44              |
| 1:G:112:ILE:H     | 1:G:113:PRO:HD2   | 1.82                     | 0.44              |
| 1:G:195:HIS:CD2   | 1:G:250:ILE:HD11  | 2.52                     | 0.44              |
| 1:G:243:LEU:HD21  | 10:G:3038:HOH:O   | 2.17                     | 0.44              |
| 1:G:266:PRO:HG2   | 2:H:232:PRO:C     | 2.42                     | 0.44              |
| 1:G:453:GLY:O     | 1:G:454:LYS:C     | 2.59                     | 0.44              |
| 1:G:515:ILE:O     | 1:G:516:PHE:C     | 2.58                     | 0.44              |
| 9:G:3012:3PE:H2I3 | 9:I:3010:3PE:H2H1 | 1.99                     | 0.44              |
| 2:H:76:ILE:O      | 2:H:77:LEU:C      | 2.60                     | 0.44              |
| 2:H:107:VAL:CG1   | 2:H:108:PRO:HD3   | 2.43                     | 0.44              |
| 2:H:173:SER:O     | 2:H:174:PRO:O     | 2.35                     | 0.44              |
| 2:H:205:THR:O     | 2:H:205:THR:HG22  | 2.16                     | 0.44              |
| 2:H:209:GLN:CD    | 2:H:235:LEU:HD22  | 2.41                     | 0.44              |
| 2:H:221:VAL:CB    | 2:H:224:PHE:HD2   | 2.30                     | 0.44              |
| 4:J:10:VAL:O      | 4:J:10:VAL:HG12   | 2.18                     | 0.44              |
| 1:A:110:VAL:HG12  | 1:A:111:VAL:N     | 2.32                     | 0.44              |
| 1:A:235:THR:HG22  | 1:A:236:ALA:N     | 2.32                     | 0.44              |
| 1:A:342:LEU:HD11  | 2:B:123:LEU:HG    | 1.98                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:136:VAL:HG21  | 2:B:198:MET:HE2   | 1.99                     | 0.44              |
| 3:C:81:TRP:O      | 3:C:84:ILE:N      | 2.51                     | 0.44              |
| 3:C:130:PRO:HB3   | 3:C:263:ILE:HD13  | 1.98                     | 0.44              |
| 1:G:31:VAL:O      | 1:G:32:LEU:C      | 2.59                     | 0.44              |
| 1:G:213:LEU:HD21  | 1:G:233:PHE:CZ    | 2.52                     | 0.44              |
| 1:G:227:LEU:HD23  | 1:G:227:LEU:HA    | 1.70                     | 0.44              |
| 1:G:247:ALA:HB2   | 9:G:3009:3PE:H3H2 | 1.99                     | 0.44              |
| 1:G:289:ILE:O     | 1:G:290:ILE:C     | 2.59                     | 0.44              |
| 1:G:297:ILE:O     | 1:G:298:VAL:C     | 2.60                     | 0.44              |
| 1:G:429:VAL:HG22  | 8:G:1001:HEA:H272 | 1.99                     | 0.44              |
| 1:G:436:ILE:HD11  | 8:G:1001:HEA:H251 | 1.99                     | 0.44              |
| 3:I:59:TRP:HD1    | 3:I:62:VAL:HG21   | 1.81                     | 0.44              |
| 3:I:74:VAL:O      | 3:I:77:LEU:N      | 2.51                     | 0.44              |
| 1:A:55:LEU:O      | 1:A:56:MET:C      | 2.59                     | 0.44              |
| 1:A:210:THR:O     | 1:A:211:THR:C     | 2.60                     | 0.44              |
| 1:A:307:LYS:HD3   | 1:A:374:SER:OG    | 2.18                     | 0.44              |
| 8:A:1002:HEA:HH A | 10:A:2047:HOH:O   | 2.17                     | 0.44              |
| 2:B:201:PRO:CB    | 2:B:204:LYS:HG3   | 2.47                     | 0.44              |
| 3:C:182:GLN:O     | 3:C:185:GLU:HB2   | 2.17                     | 0.44              |
| 3:C:231:HIS:O     | 9:C:2008:3PE:H121 | 2.18                     | 0.44              |
| 1:G:24:THR:O      | 1:G:136:PRO:HB3   | 2.17                     | 0.44              |
| 1:G:341:SER:H     | 1:G:344:GLN:CD    | 2.26                     | 0.44              |
| 1:G:539:GLU:O     | 1:G:542:LEU:HD12  | 2.17                     | 0.44              |
| 1:A:29:ILE:O      | 1:A:30:GLY:C      | 2.59                     | 0.44              |
| 1:A:235:THR:OG1   | 1:A:292:LEU:HB2   | 2.17                     | 0.44              |
| 1:A:390:LEU:HD13  | 1:A:426:LEU:HD13  | 1.99                     | 0.44              |
| 2:B:253:SER:O     | 2:B:254:GLU:HB2   | 2.17                     | 0.44              |
| 3:C:2:ALA:HB3     | 3:C:5:LYS:NZ      | 2.31                     | 0.44              |
| 3:C:25:ALA:HA     | 3:C:28:MET:HB3    | 2.00                     | 0.44              |
| 3:C:74:VAL:HG12   | 4:D:16:ILE:HG23   | 1.98                     | 0.44              |
| 3:C:211:PHE:O     | 3:C:215:VAL:HG23  | 2.17                     | 0.44              |
| 1:G:52:ARG:HD3    | 1:G:498:SER:OG    | 2.18                     | 0.44              |
| 1:G:243:LEU:HD22  | 1:G:282:PHE:CE1   | 2.53                     | 0.44              |
| 1:G:392:THR:O     | 1:G:393:VAL:C     | 2.60                     | 0.44              |
| 1:G:406:VAL:HG12  | 1:G:410:TYR:CE2   | 2.52                     | 0.44              |
| 9:G:3009:3PE:H221 | 3:I:58:TRP:NE1    | 2.33                     | 0.44              |
| 9:G:3009:3PE:O22  | 3:I:59:TRP:NE1    | 2.45                     | 0.44              |
| 2:H:51:ALA:HA     | 2:H:54:ILE:HD12   | 2.00                     | 0.44              |
| 2:H:192:LEU:HD23  | 2:H:192:LEU:HA    | 1.69                     | 0.44              |
| 1:A:70:SER:O      | 1:A:71:GLY:C      | 2.61                     | 0.44              |
| 1:A:98:MET:O      | 1:A:101:GLY:N     | 2.50                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:234:VAL:HG12  | 1:A:292:LEU:HD11  | 1.98                     | 0.44              |
| 1:A:367:ILE:HG22  | 1:A:368:ALA:N     | 2.31                     | 0.44              |
| 1:A:379:THR:HA    | 1:A:382:LEU:CD1   | 2.42                     | 0.44              |
| 1:A:504:SER:HB3   | 8:A:1001:HEA:H262 | 1.99                     | 0.44              |
| 9:A:2009:3PE:H291 | 9:A:2009:3PE:H3A1 | 2.00                     | 0.44              |
| 9:A:2012:3PE:C3E  | 9:D:2011:3PE:H2F1 | 2.48                     | 0.44              |
| 2:B:255:LEU:HB3   | 10:B:1011:HOH:O   | 2.18                     | 0.44              |
| 1:G:34:LEU:O      | 1:G:38:GLY:N      | 2.47                     | 0.44              |
| 1:G:70:SER:C      | 1:G:71:GLY:O      | 2.59                     | 0.44              |
| 2:H:209:GLN:HG3   | 2:H:235:LEU:HD22  | 2.00                     | 0.44              |
| 3:I:79:LEU:O      | 3:I:80:ARG:C      | 2.60                     | 0.44              |
| 1:A:177:PRO:O     | 1:A:178:LEU:C     | 2.61                     | 0.44              |
| 1:A:341:SER:OG    | 1:A:344:GLN:HG3   | 2.18                     | 0.44              |
| 1:A:367:ILE:HG13  | 2:B:76:ILE:HD13   | 1.99                     | 0.44              |
| 1:A:442:LYS:O     | 1:A:546:PRO:HD3   | 2.18                     | 0.44              |
| 2:B:142:GLN:NE2   | 10:B:1006:HOH:O   | 2.44                     | 0.44              |
| 2:B:211:THR:HG22  | 2:B:212:GLY:O     | 2.17                     | 0.44              |
| 1:G:37:GLY:O      | 1:G:110:VAL:HG13  | 2.18                     | 0.44              |
| 1:G:91:ASN:OD1    | 1:G:165:GLN:NE2   | 2.49                     | 0.44              |
| 1:G:390:LEU:CD1   | 1:G:426:LEU:HB3   | 2.48                     | 0.44              |
| 8:G:1001:HEA:HAA1 | 8:G:1001:HEA:HMA  | 1.80                     | 0.44              |
| 3:I:133:LEU:O     | 3:I:136:ILE:HB    | 2.18                     | 0.44              |
| 9:I:3013:3PE:H282 | 9:I:3013:3PE:H2B1 | 1.72                     | 0.44              |
| 1:A:209:ILE:HG21  | 3:C:85:LEU:CD2    | 2.48                     | 0.44              |
| 1:A:322:ALA:HB3   | 1:A:358:PRO:HB3   | 2.00                     | 0.44              |
| 3:C:28:MET:CA     | 3:C:47:GLY:HA3    | 2.48                     | 0.44              |
| 3:C:112:GLU:O     | 3:C:115:ILE:HD12  | 2.17                     | 0.44              |
| 3:C:226:ARG:HH22  | 9:C:2008:3PE:C12  | 2.30                     | 0.44              |
| 1:G:332:ALA:HB3   | 1:G:348:PHE:CE2   | 2.52                     | 0.44              |
| 1:G:390:LEU:HD23  | 1:G:390:LEU:H     | 1.83                     | 0.44              |
| 1:G:537:THR:HG21  | 10:G:3070:HOH:O   | 2.17                     | 0.44              |
| 3:I:66:SER:HB2    | 3:I:71:HIS:CE1    | 2.53                     | 0.44              |
| 3:I:87:ILE:O      | 3:I:88:MET:C      | 2.60                     | 0.44              |
| 3:I:96:ALA:O      | 3:I:97:TRP:C      | 2.60                     | 0.44              |
| 1:A:45:VAL:O      | 1:A:46:ALA:C      | 2.61                     | 0.44              |
| 1:A:307:LYS:HD3   | 1:A:374:SER:HG    | 1.82                     | 0.44              |
| 1:A:487:PRO:HG2   | 1:A:490:PHE:HE2   | 1.83                     | 0.44              |
| 9:A:2009:3PE:H361 | 9:C:2008:3PE:H292 | 1.99                     | 0.44              |
| 3:C:31:GLY:CA     | 3:C:43:MET:SD     | 3.06                     | 0.44              |
| 3:C:80:ARG:HH12   | 9:C:2013:3PE:H111 | 1.83                     | 0.44              |
| 4:D:31:THR:HG22   | 4:D:32:TRP:N      | 2.32                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:374:SER:HB2   | 2:H:85:GLU:HA     | 1.99                     | 0.44              |
| 2:H:272:GLU:HG3   | 10:H:1091:HOH:O   | 2.18                     | 0.44              |
| 3:I:17:TRP:O      | 3:I:20:MET:HB3    | 2.17                     | 0.44              |
| 9:I:3010:3PE:H3I3 | 9:I:3010:3PE:H3F1 | 1.60                     | 0.44              |
| 4:J:43:PHE:O      | 4:J:44:LEU:C      | 2.60                     | 0.44              |
| 1:A:102:HIS:CE1   | 8:A:1001:HEA:NC   | 2.85                     | 0.43              |
| 1:A:397:THR:HG21  | 10:A:2072:HOH:O   | 2.17                     | 0.43              |
| 2:B:116:GLY:O     | 2:B:117:ALA:C     | 2.60                     | 0.43              |
| 1:G:65:ALA:CB     | 1:G:89:THR:HB     | 2.46                     | 0.43              |
| 1:G:251:THR:O     | 1:G:252:MET:C     | 2.61                     | 0.43              |
| 1:G:299:SER:HB3   | 1:G:310:ILE:CD1   | 2.46                     | 0.43              |
| 1:G:409:TYR:CD1   | 1:G:409:TYR:C     | 2.96                     | 0.43              |
| 1:G:496:VAL:O     | 1:G:499:LEU:HB2   | 2.18                     | 0.43              |
| 8:G:1001:HEA:HBA1 | 10:G:3059:HOH:O   | 2.17                     | 0.43              |
| 3:I:8:ASP:HB3     | 3:I:72:THR:CG2    | 2.29                     | 0.43              |
| 1:A:178:LEU:HD23  | 2:B:255:LEU:O     | 2.17                     | 0.43              |
| 1:A:251:THR:O     | 1:A:252:MET:C     | 2.60                     | 0.43              |
| 1:A:296:GLY:O     | 1:A:297:ILE:C     | 2.58                     | 0.43              |
| 1:A:367:ILE:HD13  | 2:B:75:LEU:CB     | 2.48                     | 0.43              |
| 1:A:506:ALA:HA    | 1:A:509:LEU:HD12  | 1.98                     | 0.43              |
| 8:A:1001:HEA:HMA  | 8:A:1001:HEA:HAA1 | 1.53                     | 0.43              |
| 9:A:2009:3PE:C36  | 9:C:2008:3PE:H292 | 2.48                     | 0.43              |
| 2:B:84:HIS:O      | 2:B:87:ARG:N      | 2.46                     | 0.43              |
| 2:B:86:LYS:HD2    | 2:B:89:LYS:HZ3    | 1.83                     | 0.43              |
| 2:B:164:PRO:HA    | 2:B:168:GLY:O     | 2.18                     | 0.43              |
| 2:B:231:VAL:O     | 2:B:232:PRO:C     | 2.61                     | 0.43              |
| 3:C:112:GLU:HB2   | 3:C:116:ILE:HB    | 2.00                     | 0.43              |
| 1:G:122:TYR:C     | 1:G:122:TYR:CD1   | 2.96                     | 0.43              |
| 1:G:287:VAL:O     | 1:G:288:TYR:C     | 2.59                     | 0.43              |
| 1:G:341:SER:N     | 1:G:344:GLN:OE1   | 2.45                     | 0.43              |
| 1:G:481:ARG:O     | 1:G:482:ARG:HB2   | 2.18                     | 0.43              |
| 1:A:472:HIS:O     | 1:A:473:PHE:C     | 2.58                     | 0.43              |
| 2:B:98:SER:CB     | 2:B:99:PRO:HD3    | 2.28                     | 0.43              |
| 2:B:143:TRP:HZ2   | 2:B:257:GLY:HA3   | 1.82                     | 0.43              |
| 2:B:276:ALA:HA    | 2:B:279:LEU:HD12  | 2.01                     | 0.43              |
| 3:C:133:LEU:HD11  | 3:C:181:PHE:CD2   | 2.54                     | 0.43              |
| 3:C:201:ASN:HD22  | 3:C:201:ASN:HA    | 1.48                     | 0.43              |
| 1:G:71:GLY:HA3    | 1:G:74:LYS:HD3    | 2.01                     | 0.43              |
| 1:G:135:PHE:CE1   | 3:I:79:LEU:HD23   | 2.43                     | 0.43              |
| 1:G:488:GLU:O     | 1:G:489:ALA:C     | 2.58                     | 0.43              |
| 9:G:3009:3PE:H271 | 9:G:3009:3PE:H382 | 1.99                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:G:3065:HOH:O   | 2:H:260:HIS:HB3   | 2.17                     | 0.43              |
| 2:H:175:GLU:O     | 2:H:176:VAL:C     | 2.58                     | 0.43              |
| 2:H:241:ARG:HH21  | 2:H:243:GLU:HG2   | 1.83                     | 0.43              |
| 3:I:239:GLY:N     | 9:I:3008:3PE:H11  | 2.30                     | 0.43              |
| 2:B:248:PHE:HE2   | 2:B:269:VAL:HG12  | 1.82                     | 0.43              |
| 1:G:17:PHE:O      | 1:G:21:PHE:HB2    | 2.17                     | 0.43              |
| 1:G:384:ALA:O     | 1:G:388:LEU:HD23  | 2.19                     | 0.43              |
| 3:I:48:LEU:O      | 3:I:48:LEU:HG     | 2.16                     | 0.43              |
| 1:A:300:HIS:HB3   | 10:A:2020:HOH:O   | 2.17                     | 0.43              |
| 1:A:433:PHE:HD1   | 1:A:436:ILE:HD12  | 1.83                     | 0.43              |
| 1:A:473:PHE:O     | 1:A:474:LEU:C     | 2.61                     | 0.43              |
| 2:B:71:PHE:O      | 2:B:75:LEU:HD12   | 2.19                     | 0.43              |
| 2:B:142:GLN:HG3   | 2:B:214:ASP:OD2   | 2.18                     | 0.43              |
| 3:C:73:PRO:HG2    | 4:D:12:GLY:HA2    | 2.00                     | 0.43              |
| 3:C:136:ILE:HG21  | 3:C:181:PHE:HE2   | 1.83                     | 0.43              |
| 3:C:161:ARG:HH22  | 3:C:230:GLY:HA2   | 1.83                     | 0.43              |
| 9:C:2013:3PE:H2D2 | 9:C:2013:3PE:C3G  | 2.49                     | 0.43              |
| 4:D:33:ALA:O      | 4:D:36:VAL:HB     | 2.19                     | 0.43              |
| 1:G:239:ILE:CG1   | 1:G:289:ILE:HG12  | 2.48                     | 0.43              |
| 1:G:314:LEU:HA    | 1:G:314:LEU:HD12  | 1.70                     | 0.43              |
| 2:H:177:GLU:HA    | 2:H:180:LEU:HD12  | 2.00                     | 0.43              |
| 3:I:112:GLU:HB2   | 3:I:116:ILE:HB    | 2.01                     | 0.43              |
| 1:A:271:ASP:HB2   | 3:C:109:MET:SD    | 2.58                     | 0.43              |
| 1:A:387:PHE:CD1   | 1:A:388:LEU:N     | 2.87                     | 0.43              |
| 9:A:2009:3PE:H221 | 3:C:58:TRP:CZ2    | 2.53                     | 0.43              |
| 1:G:22:MET:HG2    | 3:I:16:ILE:CA     | 2.48                     | 0.43              |
| 1:G:33:TYR:OH     | 1:G:142:SER:HB2   | 2.18                     | 0.43              |
| 1:G:170:ILE:CG2   | 1:G:174:LEU:HA    | 2.47                     | 0.43              |
| 1:G:468:PHE:O     | 1:G:469:PHE:C     | 2.61                     | 0.43              |
| 3:I:226:ARG:HE    | 3:I:231:HIS:CD2   | 2.36                     | 0.43              |
| 3:I:256:PHE:CE1   | 9:J:3011:3PE:H391 | 2.53                     | 0.43              |
| 1:A:22:MET:SD     | 3:C:16:ILE:HD12   | 2.59                     | 0.43              |
| 1:A:95:TRP:HB2    | 1:A:484:ILE:CG1   | 2.47                     | 0.43              |
| 1:A:424:MET:HE2   | 1:A:424:MET:HB2   | 1.88                     | 0.43              |
| 1:A:442:LYS:HD2   | 1:A:442:LYS:HA    | 1.70                     | 0.43              |
| 2:B:35:ARG:HG3    | 2:B:36:PRO:HD2    | 2.00                     | 0.43              |
| 2:B:108:PRO:HA    | 2:B:111:ILE:HD12  | 2.01                     | 0.43              |
| 3:C:220:LEU:O     | 3:C:223:CYS:N     | 2.52                     | 0.43              |
| 1:G:98:MET:O      | 1:G:101:GLY:N     | 2.51                     | 0.43              |
| 1:G:195:HIS:O     | 1:G:198:GLY:N     | 2.51                     | 0.43              |
| 1:G:291:VAL:O     | 1:G:291:VAL:CG2   | 2.67                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:G:509:LEU:HG   | 1:G:509:LEU:H     | 1.56                     | 0.43              |
| 2:H:173:SER:H    | 2:H:176:VAL:HB    | 1.82                     | 0.43              |
| 1:A:141:LEU:HD11 | 1:A:145:LEU:HD11  | 2.00                     | 0.43              |
| 1:A:325:VAL:CG2  | 9:A:2012:3PE:H3B2 | 2.49                     | 0.43              |
| 1:A:367:ILE:HG13 | 2:B:76:ILE:CD1    | 2.49                     | 0.43              |
| 1:A:375:ILE:HD12 | 2:B:80:VAL:HA     | 2.01                     | 0.43              |
| 1:A:407:ASP:O    | 1:A:411:HIS:N     | 2.38                     | 0.43              |
| 3:C:85:LEU:HD23  | 3:C:88:MET:CE     | 2.48                     | 0.43              |
| 1:G:93:HIS:CD2   | 1:G:165:GLN:HB2   | 2.54                     | 0.43              |
| 2:H:120:LEU:HD23 | 2:H:120:LEU:HA    | 1.77                     | 0.43              |
| 2:H:129:ILE:HA   | 2:H:130:PRO:HD3   | 1.64                     | 0.43              |
| 2:H:192:LEU:HB3  | 2:H:249:PHE:CE2   | 2.54                     | 0.43              |
| 3:I:25:ALA:HA    | 3:I:28:MET:HB3    | 2.00                     | 0.43              |
| 1:A:84:ALA:O     | 1:A:85:VAL:C      | 2.61                     | 0.43              |
| 1:A:150:THR:O    | 1:A:153:ALA:HB3   | 2.19                     | 0.43              |
| 1:A:155:ALA:HB1  | 10:A:2080:HOH:O   | 2.18                     | 0.43              |
| 1:A:365:SER:O    | 1:A:366:TRP:C     | 2.62                     | 0.43              |
| 1:A:519:LEU:N    | 1:A:519:LEU:HD23  | 2.33                     | 0.43              |
| 1:A:556:LYS:O    | 1:A:559:ASP:HB2   | 2.19                     | 0.43              |
| 1:A:558:GLU:O    | 1:A:559:ASP:C     | 2.61                     | 0.43              |
| 3:C:72:THR:O     | 3:C:72:THR:HG22   | 2.15                     | 0.43              |
| 1:G:237:TRP:CZ3  | 9:G:3012:3PE:H2A1 | 2.54                     | 0.43              |
| 1:G:318:TYR:HD1  | 1:G:318:TYR:HA    | 1.65                     | 0.43              |
| 1:G:342:LEU:HD11 | 2:H:123:LEU:HG    | 2.01                     | 0.43              |
| 1:G:451:TRP:CG   | 1:G:452:ALA:N     | 2.87                     | 0.43              |
| 2:H:135:THR:O    | 2:H:150:PRO:HD2   | 2.19                     | 0.43              |
| 2:H:229:ASP:OD2  | 10:H:1050:HOH:O   | 2.21                     | 0.43              |
| 3:I:147:ALA:HB2  | 3:I:170:LEU:HD23  | 2.00                     | 0.43              |
| 1:A:243:LEU:CD2  | 1:A:282:PHE:CE1   | 3.01                     | 0.43              |
| 1:A:271:ASP:OD2  | 3:C:103:LYS:NZ    | 2.51                     | 0.43              |
| 1:A:530:TYR:CE2  | 1:A:531:TRP:NE1   | 2.87                     | 0.43              |
| 2:B:161:ILE:CD1  | 2:B:180:LEU:HD23  | 2.49                     | 0.43              |
| 3:C:72:THR:HG22  | 3:C:74:VAL:N      | 2.34                     | 0.43              |
| 1:G:292:LEU:O    | 1:G:295:PHE:HB2   | 2.19                     | 0.43              |
| 1:G:342:LEU:HD21 | 2:H:124:PHE:CE1   | 2.54                     | 0.43              |
| 1:G:342:LEU:HD11 | 2:H:124:PHE:CD1   | 2.54                     | 0.43              |
| 1:G:423:VAL:HG21 | 8:G:1002:HEA:C2C  | 2.48                     | 0.43              |
| 1:G:431:GLY:O    | 1:G:434:ALA:N     | 2.52                     | 0.43              |
| 1:G:433:PHE:CD1  | 1:G:436:ILE:HD12  | 2.53                     | 0.43              |
| 1:G:472:HIS:O    | 1:G:476:ARG:HG3   | 2.19                     | 0.43              |
| 2:H:194:THR:HG22 | 2:H:266:THR:OG1   | 2.18                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:20:MET:HE3    | 3:I:20:MET:HB2    | 1.85                     | 0.43              |
| 1:A:15:GLY:O      | 1:A:16:PHE:C      | 2.62                     | 0.42              |
| 1:A:70:SER:HB2    | 1:A:74:LYS:HB3    | 2.01                     | 0.42              |
| 1:A:88:CYS:SG     | 1:A:89:THR:N      | 2.90                     | 0.42              |
| 1:A:408:ARG:HG3   | 2:B:126:GLN:OE1   | 2.19                     | 0.42              |
| 1:A:409:TYR:C     | 1:A:409:TYR:HD1   | 2.26                     | 0.42              |
| 1:A:535:ALA:HB1   | 1:A:540:TRP:CD1   | 2.54                     | 0.42              |
| 2:B:137:LYS:HG2   | 2:B:138:VAL:N     | 2.22                     | 0.42              |
| 2:B:228:GLN:NE2   | 2:B:229:ASP:N     | 2.67                     | 0.42              |
| 2:B:283:ARG:HG3   | 2:B:283:ARG:HH11  | 1.83                     | 0.42              |
| 3:C:8:ASP:CG      | 3:C:72:THR:HG21   | 2.43                     | 0.42              |
| 1:G:48:THR:HG22   | 1:G:102:HIS:CE1   | 2.54                     | 0.42              |
| 1:G:155:ALA:O     | 1:G:158:PHE:N     | 2.39                     | 0.42              |
| 1:G:263:PHE:O     | 1:G:270:GLY:HA2   | 2.19                     | 0.42              |
| 2:H:119:SER:O     | 2:H:120:LEU:C     | 2.62                     | 0.42              |
| 3:I:197:ILE:HG13  | 3:I:198:TYR:N     | 2.34                     | 0.42              |
| 3:I:219:PHE:HE1   | 9:I:3008:3PE:H342 | 1.84                     | 0.42              |
| 1:A:29:ILE:HG21   | 1:A:139:ASN:HD21  | 1.83                     | 0.42              |
| 1:A:110:VAL:O     | 1:A:111:VAL:C     | 2.59                     | 0.42              |
| 1:A:249:ALA:O     | 1:A:252:MET:HG3   | 2.19                     | 0.42              |
| 1:A:263:PHE:CZ    | 3:C:200:ALA:HB1   | 2.54                     | 0.42              |
| 2:B:202:VAL:HG12  | 2:B:269:VAL:HG22  | 2.02                     | 0.42              |
| 3:C:135:LEU:HD12  | 3:C:135:LEU:HA    | 1.89                     | 0.42              |
| 3:C:144:SER:O     | 3:C:145:GLY:C     | 2.63                     | 0.42              |
| 1:G:45:VAL:O      | 1:G:46:ALA:C      | 2.61                     | 0.42              |
| 1:G:104:ILE:HG13  | 1:G:172:TRP:HA    | 2.00                     | 0.42              |
| 1:G:389:PHE:O     | 1:G:390:LEU:C     | 2.61                     | 0.42              |
| 1:G:422:TYR:O     | 1:G:426:LEU:HB2   | 2.19                     | 0.42              |
| 2:H:33:ILE:HD11   | 10:H:1146:HOH:O   | 2.19                     | 0.42              |
| 2:H:220:THR:HB    | 2:H:227:LYS:CB    | 2.48                     | 0.42              |
| 3:I:219:PHE:O     | 3:I:220:LEU:C     | 2.62                     | 0.42              |
| 1:A:115:LEU:CD1   | 1:A:432:ILE:CG1   | 2.95                     | 0.42              |
| 1:A:427:GLY:O     | 1:A:430:PHE:HB2   | 2.20                     | 0.42              |
| 2:B:174:PRO:O     | 2:B:175:GLU:C     | 2.62                     | 0.42              |
| 9:C:2010:3PE:H391 | 9:C:2010:3PE:H362 | 1.74                     | 0.42              |
| 1:G:26:HIS:NE2    | 1:G:27:LYS:HG3    | 2.34                     | 0.42              |
| 1:G:300:HIS:O     | 1:G:303:ALA:HB3   | 2.19                     | 0.42              |
| 1:G:325:VAL:O     | 1:G:327:GLY:N     | 2.52                     | 0.42              |
| 1:G:366:TRP:O     | 1:G:367:ILE:C     | 2.63                     | 0.42              |
| 3:I:40:GLY:HA2    | 3:I:41:PRO:HD2    | 1.76                     | 0.42              |
| 1:A:72:LEU:O      | 1:A:76:PHE:HB2    | 2.19                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:95:TRP:HE1    | 1:A:482:ARG:C     | 2.28                     | 0.42              |
| 1:A:99:ILE:HG21   | 1:A:482:ARG:HG2   | 2.00                     | 0.42              |
| 1:A:390:LEU:O     | 1:A:393:VAL:N     | 2.52                     | 0.42              |
| 2:B:136:VAL:CG1   | 2:B:137:LYS:N     | 2.82                     | 0.42              |
| 2:B:163:SER:HB2   | 2:B:165:ALA:HB3   | 2.00                     | 0.42              |
| 1:G:100:THR:HG23  | 1:G:104:ILE:HD12  | 2.02                     | 0.42              |
| 1:G:189:LEU:HD21  | 3:I:30:PHE:HD1    | 1.85                     | 0.42              |
| 1:G:217:ALA:O     | 1:G:218:PRO:C     | 2.63                     | 0.42              |
| 1:G:398:GLY:O     | 1:G:402:SER:HB3   | 2.18                     | 0.42              |
| 1:G:448:TYR:HD1   | 1:G:448:TYR:H     | 1.61                     | 0.42              |
| 1:G:454:LYS:O     | 1:G:457:PHE:N     | 2.52                     | 0.42              |
| 2:H:218:SER:HA    | 2:H:229:ASP:HA    | 2.01                     | 0.42              |
| 1:A:222:MET:O     | 1:A:224:LYS:N     | 2.52                     | 0.42              |
| 1:A:389:PHE:O     | 1:A:392:THR:N     | 2.46                     | 0.42              |
| 3:C:20:MET:HE3    | 3:C:20:MET:HB2    | 1.77                     | 0.42              |
| 4:D:10:VAL:HG12   | 4:D:13:SER:HB3    | 2.02                     | 0.42              |
| 1:G:61:GLN:O      | 1:G:83:SER:HB3    | 2.20                     | 0.42              |
| 1:G:63:MET:HE1    | 1:G:95:TRP:HB2    | 2.00                     | 0.42              |
| 1:G:70:SER:HB2    | 1:G:74:LYS:CB     | 2.49                     | 0.42              |
| 1:G:163:ASN:CG    | 2:H:258:ILE:HD11  | 2.45                     | 0.42              |
| 2:H:123:LEU:O     | 2:H:126:GLN:HG2   | 2.19                     | 0.42              |
| 2:H:283:ARG:HG3   | 2:H:283:ARG:HH11  | 1.84                     | 0.42              |
| 9:I:3013:3PE:H322 | 9:I:3013:3PE:H351 | 1.84                     | 0.42              |
| 1:A:130:ALA:HA    | 1:A:131:PRO:HD3   | 1.87                     | 0.42              |
| 1:A:222:MET:HB3   | 1:A:222:MET:HE2   | 1.81                     | 0.42              |
| 1:A:274:LEU:O     | 1:A:275:TYR:C     | 2.63                     | 0.42              |
| 1:A:314:LEU:O     | 1:A:315:PRO:C     | 2.62                     | 0.42              |
| 1:A:493:TRP:O     | 1:A:496:VAL:HB    | 2.20                     | 0.42              |
| 2:B:159:TYR:O     | 2:B:194:THR:HA    | 2.19                     | 0.42              |
| 3:C:83:PHE:O      | 3:C:86:PHE:HB3    | 2.19                     | 0.42              |
| 1:G:56:MET:HG3    | 1:G:495:PHE:CD1   | 2.54                     | 0.42              |
| 1:G:174:LEU:HD13  | 1:G:191:ILE:CD1   | 2.45                     | 0.42              |
| 1:G:222:MET:HE2   | 1:G:222:MET:HB3   | 1.92                     | 0.42              |
| 1:G:401:LEU:HD21  | 1:G:415:TYR:CD1   | 2.55                     | 0.42              |
| 1:A:235:THR:O     | 1:A:236:ALA:C     | 2.62                     | 0.42              |
| 1:A:361:ILE:O     | 1:A:362:LYS:C     | 2.61                     | 0.42              |
| 1:A:473:PHE:O     | 1:A:476:ARG:N     | 2.53                     | 0.42              |
| 2:B:176:VAL:O     | 2:B:177:GLU:C     | 2.63                     | 0.42              |
| 2:B:197:ALA:HB2   | 10:B:1022:HOH:O   | 2.20                     | 0.42              |
| 3:C:61:ASP:O      | 3:C:62:VAL:C      | 2.62                     | 0.42              |
| 3:C:107:TYR:OH    | 4:D:49:ALA:HA     | 2.19                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:126:LEU:HD23  | 10:G:3051:HOH:O   | 2.20                     | 0.42              |
| 1:G:225:VAL:HA    | 1:G:226:PRO:HD2   | 1.78                     | 0.42              |
| 1:G:390:LEU:HB2   | 1:G:426:LEU:O     | 2.19                     | 0.42              |
| 1:G:407:ASP:O     | 1:G:410:TYR:N     | 2.53                     | 0.42              |
| 1:A:34:LEU:HD23   | 1:A:34:LEU:HA     | 1.66                     | 0.42              |
| 1:A:116:PHE:CE2   | 1:A:208:MET:HE3   | 2.55                     | 0.42              |
| 1:A:304:THR:OG1   | 1:A:535:ALA:CA    | 2.67                     | 0.42              |
| 1:A:424:MET:HB3   | 8:A:1001:HEA:CBC  | 2.45                     | 0.42              |
| 2:B:98:SER:CB     | 2:B:99:PRO:CD     | 2.91                     | 0.42              |
| 2:B:235:LEU:HD11  | 4:J:9:HIS:H       | 1.84                     | 0.42              |
| 3:C:101:PHE:CZ    | 3:C:261:ILE:HA    | 2.55                     | 0.42              |
| 9:C:2010:3PE:H3F2 | 9:C:2010:3PE:H3C1 | 1.78                     | 0.42              |
| 1:G:29:ILE:HG22   | 1:G:30:GLY:N      | 2.35                     | 0.42              |
| 1:G:168:SER:OG    | 1:G:187:THR:OG1   | 2.26                     | 0.42              |
| 1:G:233:PHE:HE2   | 9:G:3012:3PE:H351 | 1.84                     | 0.42              |
| 1:G:467:THR:OG1   | 1:G:501:ALA:N     | 2.53                     | 0.42              |
| 1:G:483:TYR:OH    | 2:H:251:GLN:HB3   | 2.19                     | 0.42              |
| 8:G:1002:HEA:HAD2 | 10:G:3052:HOH:O   | 2.20                     | 0.42              |
| 9:G:3012:3PE:H2D2 | 4:J:33:ALA:CB     | 2.50                     | 0.42              |
| 2:H:136:VAL:HG11  | 2:H:147:TYR:HD2   | 1.84                     | 0.42              |
| 2:H:202:VAL:CG1   | 2:H:269:VAL:HG22  | 2.50                     | 0.42              |
| 3:I:8:ASP:CG      | 3:I:72:THR:HG21   | 2.45                     | 0.42              |
| 1:A:71:GLY:CA     | 1:A:74:LYS:HD3    | 2.50                     | 0.42              |
| 1:A:137:ARG:NH2   | 3:C:65:GLU:OE1    | 2.49                     | 0.42              |
| 1:A:466:LEU:O     | 1:A:467:THR:C     | 2.61                     | 0.42              |
| 2:B:84:HIS:CD2    | 2:B:86:LYS:H      | 2.30                     | 0.42              |
| 3:C:123:GLU:HG3   | 1:G:557:ARG:CZ    | 2.50                     | 0.42              |
| 1:G:111:VAL:HG13  | 1:G:290:ILE:HG23  | 1.98                     | 0.42              |
| 1:G:530:TYR:CE2   | 1:G:531:TRP:NE1   | 2.88                     | 0.42              |
| 3:I:32:ALA:O      | 3:I:36:MET:HG3    | 2.20                     | 0.42              |
| 9:I:3010:3PE:H322 | 9:J:3011:3PE:O32  | 2.19                     | 0.42              |
| 1:A:311:PHE:O     | 1:A:312:GLY:C     | 2.62                     | 0.42              |
| 1:A:396:VAL:HG11  | 2:B:65:ILE:CD1    | 2.47                     | 0.42              |
| 9:A:2009:3PE:H221 | 3:C:58:TRP:CE2    | 2.54                     | 0.42              |
| 9:A:2009:3PE:H372 | 9:A:2009:3PE:H3A2 | 1.68                     | 0.42              |
| 2:B:101:GLU:O     | 2:B:102:ILE:C     | 2.59                     | 0.42              |
| 2:B:192:LEU:HD13  | 2:B:249:PHE:CB    | 2.50                     | 0.42              |
| 2:B:206:VAL:O     | 2:B:206:VAL:HG12  | 2.13                     | 0.42              |
| 2:B:272:GLU:HG3   | 10:B:1024:HOH:O   | 2.19                     | 0.42              |
| 1:G:29:ILE:O      | 1:G:30:GLY:C      | 2.62                     | 0.42              |
| 1:G:94:LEU:O      | 1:G:97:VAL:N      | 2.53                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:147:VAL:HG12  | 1:G:148:ALA:N     | 2.35                     | 0.42              |
| 1:G:189:LEU:O     | 1:G:190:ALA:C     | 2.63                     | 0.42              |
| 1:G:442:LYS:HD3   | 1:G:540:TRP:CE3   | 2.55                     | 0.42              |
| 2:H:126:GLN:O     | 2:H:127:GLN:NE2   | 2.53                     | 0.42              |
| 3:I:169:ALA:O     | 3:I:170:LEU:C     | 2.63                     | 0.42              |
| 1:A:52:ARG:HD3    | 1:A:498:SER:OG    | 2.20                     | 0.41              |
| 1:A:57:ALA:HA     | 10:A:2032:HOH:O   | 2.19                     | 0.41              |
| 1:A:329:VAL:HB    | 1:A:347:TYR:OH    | 2.20                     | 0.41              |
| 2:B:160:MET:HE1   | 2:B:262:TYR:CD1   | 2.55                     | 0.41              |
| 3:C:213:VAL:O     | 3:C:214:ILE:C     | 2.64                     | 0.41              |
| 1:G:22:MET:SD     | 3:I:16:ILE:HB     | 2.60                     | 0.41              |
| 1:G:124:MET:C     | 1:G:124:MET:SD    | 3.03                     | 0.41              |
| 1:G:130:ALA:HB2   | 1:G:215:MET:O     | 2.20                     | 0.41              |
| 1:G:137:ARG:NE    | 9:G:3009:3PE:O14  | 2.46                     | 0.41              |
| 2:H:98:SER:CB     | 2:H:99:PRO:CD     | 2.94                     | 0.41              |
| 2:H:98:SER:O      | 2:H:99:PRO:C      | 2.61                     | 0.41              |
| 2:H:141:TYR:O     | 2:H:142:GLN:C     | 2.62                     | 0.41              |
| 3:I:152:HIS:CA    | 3:I:240:PHE:HE1   | 2.32                     | 0.41              |
| 1:A:40:VAL:HG11   | 1:A:105:LEU:HD22  | 2.01                     | 0.41              |
| 1:A:137:ARG:HB2   | 1:A:137:ARG:HE    | 1.63                     | 0.41              |
| 2:B:142:GLN:HB3   | 2:B:143:TRP:CD2   | 2.55                     | 0.41              |
| 2:B:145:TRP:CD1   | 2:B:263:MET:HE2   | 2.56                     | 0.41              |
| 3:C:33:VAL:HA     | 3:C:36:MET:HE2    | 2.01                     | 0.41              |
| 9:C:2013:3PE:H2B1 | 9:C:2013:3PE:H3D2 | 2.02                     | 0.41              |
| 1:G:302:ILE:CG2   | 1:G:369:THR:CG2   | 2.97                     | 0.41              |
| 1:A:85:VAL:O      | 1:A:88:CYS:N      | 2.49                     | 0.41              |
| 1:A:255:THR:HA    | 1:A:259:PHE:HD2   | 1.85                     | 0.41              |
| 1:A:354:VAL:O     | 1:A:356:ALA:N     | 2.53                     | 0.41              |
| 1:A:504:SER:O     | 1:A:507:SER:N     | 2.53                     | 0.41              |
| 1:A:517:TYR:O     | 1:A:520:THR:HB    | 2.20                     | 0.41              |
| 3:C:113:SER:HA    | 3:C:114:PRO:HA    | 1.64                     | 0.41              |
| 1:G:22:MET:HE3    | 1:G:22:MET:HB2    | 1.84                     | 0.41              |
| 1:G:62:PHE:CE2    | 1:G:82:PRO:HD3    | 2.55                     | 0.41              |
| 1:G:286:GLN:CA    | 1:G:286:GLN:HE21  | 2.33                     | 0.41              |
| 2:H:113:VAL:O     | 2:H:114:ALA:C     | 2.63                     | 0.41              |
| 2:H:164:PRO:CA    | 2:H:168:GLY:O     | 2.68                     | 0.41              |
| 2:H:173:SER:OG    | 2:H:176:VAL:HG23  | 2.19                     | 0.41              |
| 2:H:272:GLU:HG3   | 2:H:272:GLU:H     | 1.55                     | 0.41              |
| 2:H:278:TRP:O     | 2:H:279:LEU:C     | 2.63                     | 0.41              |
| 3:I:72:THR:HG22   | 3:I:74:VAL:N      | 2.34                     | 0.41              |
| 3:I:133:LEU:HA    | 3:I:136:ILE:HG12  | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:I:141:LEU:HD21 | 3:I:178:PHE:CD2  | 2.56                     | 0.41              |
| 3:I:149:THR:HG22 | 3:I:150:TRP:N    | 2.33                     | 0.41              |
| 1:A:182:GLU:HG3  | 1:A:183:SER:N    | 2.35                     | 0.41              |
| 1:A:516:PHE:O    | 1:A:517:TYR:C    | 2.63                     | 0.41              |
| 1:G:26:HIS:CD2   | 1:G:27:LYS:N     | 2.89                     | 0.41              |
| 1:G:116:PHE:HD1  | 1:G:235:THR:HG21 | 1.83                     | 0.41              |
| 1:G:241:LEU:HB3  | 3:I:92:MET:HE2   | 2.02                     | 0.41              |
| 1:G:342:LEU:O    | 1:G:343:THR:C    | 2.62                     | 0.41              |
| 2:H:70:ILE:O     | 2:H:71:PHE:C     | 2.63                     | 0.41              |
| 1:A:29:ILE:HG21  | 1:A:139:ASN:ND2  | 2.35                     | 0.41              |
| 1:A:161:GLY:N    | 1:A:165:GLN:O    | 2.53                     | 0.41              |
| 1:A:330:VAL:CG1  | 1:A:352:THR:HA   | 2.50                     | 0.41              |
| 1:A:332:ALA:O    | 1:A:333:HIS:C    | 2.62                     | 0.41              |
| 1:A:465:ASN:O    | 1:A:466:LEU:C    | 2.62                     | 0.41              |
| 1:A:476:ARG:O    | 2:B:43:PHE:HA    | 2.20                     | 0.41              |
| 2:B:68:ILE:O     | 2:B:71:PHE:HB3   | 2.20                     | 0.41              |
| 2:B:76:ILE:O     | 2:B:77:LEU:C     | 2.63                     | 0.41              |
| 2:B:161:ILE:HG21 | 2:B:180:LEU:HD23 | 2.01                     | 0.41              |
| 3:C:106:LEU:C    | 3:C:108:PRO:HD3  | 2.45                     | 0.41              |
| 1:G:15:GLY:N     | 1:G:18:THR:HB    | 2.35                     | 0.41              |
| 1:G:88:CYS:C     | 2:H:171:ARG:HH11 | 2.28                     | 0.41              |
| 1:G:139:ASN:O    | 1:G:142:SER:N    | 2.50                     | 0.41              |
| 1:G:442:LYS:HA   | 1:G:442:LYS:HD2  | 1.86                     | 0.41              |
| 2:H:70:ILE:O     | 2:H:73:THR:N     | 2.49                     | 0.41              |
| 2:H:206:VAL:HB   | 2:H:240:PHE:CD1  | 2.56                     | 0.41              |
| 1:A:133:MET:HE3  | 1:A:211:THR:OG1  | 2.20                     | 0.41              |
| 1:A:152:LEU:O    | 1:A:153:ALA:C    | 2.63                     | 0.41              |
| 1:A:242:ALA:C    | 1:A:243:LEU:HD23 | 2.45                     | 0.41              |
| 1:A:396:VAL:CG1  | 2:B:65:ILE:HB    | 2.51                     | 0.41              |
| 1:A:407:ASP:O    | 1:A:410:TYR:N    | 2.53                     | 0.41              |
| 1:A:408:ARG:NE   | 2:B:126:GLN:OE1  | 2.53                     | 0.41              |
| 1:A:479:MET:HA   | 1:A:480:PRO:HD3  | 1.89                     | 0.41              |
| 1:A:508:PHE:O    | 1:A:509:LEU:C    | 2.62                     | 0.41              |
| 2:B:115:ILE:O    | 2:B:116:GLY:C    | 2.63                     | 0.41              |
| 3:C:106:LEU:O    | 3:C:108:PRO:HD3  | 2.21                     | 0.41              |
| 3:C:108:PRO:HA   | 10:C:2014:HOH:O  | 2.21                     | 0.41              |
| 3:C:133:LEU:O    | 3:C:136:ILE:HB   | 2.21                     | 0.41              |
| 1:G:76:PHE:O     | 1:G:79:SER:HB2   | 2.21                     | 0.41              |
| 1:G:160:PRO:HG2  | 1:G:185:TYR:HE1  | 1.79                     | 0.41              |
| 1:G:311:PHE:CD1  | 1:G:311:PHE:C    | 2.98                     | 0.41              |
| 1:G:556:LYS:N    | 1:G:559:ASP:OD2  | 2.51                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:47:ALA:HB2    | 2:H:223:ALA:HB1   | 2.03                     | 0.41              |
| 2:H:144:TYR:HD2   | 2:H:145:TRP:O     | 2.02                     | 0.41              |
| 3:I:122:PRO:HG2   | 3:I:125:ILE:CD1   | 2.50                     | 0.41              |
| 1:A:81:TRP:CG     | 1:A:82:PRO:HD2    | 2.55                     | 0.41              |
| 1:A:88:CYS:C      | 2:B:171:ARG:HH11  | 2.27                     | 0.41              |
| 1:A:238:LEU:O     | 1:A:239:ILE:C     | 2.64                     | 0.41              |
| 1:A:379:THR:CA    | 1:A:382:LEU:HD12  | 2.45                     | 0.41              |
| 2:B:221:VAL:HG11  | 2:B:224:PHE:CE2   | 2.56                     | 0.41              |
| 3:C:186:TYR:O     | 3:C:189:ALA:N     | 2.54                     | 0.41              |
| 3:C:256:PHE:HZ    | 9:D:2011:3PE:H391 | 1.83                     | 0.41              |
| 1:G:243:LEU:HD22  | 1:G:282:PHE:HE1   | 1.86                     | 0.41              |
| 2:H:194:THR:HG22  | 2:H:266:THR:CB    | 2.49                     | 0.41              |
| 2:H:209:GLN:HA    | 2:H:236:ALA:O     | 2.20                     | 0.41              |
| 2:H:277:ALA:O     | 2:H:278:TRP:C     | 2.63                     | 0.41              |
| 3:I:83:PHE:CE2    | 3:I:242:ALA:HB1   | 2.56                     | 0.41              |
| 3:I:99:TRP:CZ2    | 9:I:3010:3PE:H222 | 2.55                     | 0.41              |
| 9:I:3010:3PE:H3C1 | 9:I:3010:3PE:H3F2 | 1.59                     | 0.41              |
| 1:A:232:ILE:HD13  | 1:A:232:ILE:HA    | 1.80                     | 0.41              |
| 1:G:56:MET:HG3    | 1:G:495:PHE:HD1   | 1.84                     | 0.41              |
| 1:G:316:MET:SD    | 1:G:365:SER:HB2   | 2.61                     | 0.41              |
| 1:G:367:ILE:HD13  | 2:H:75:LEU:CB     | 2.46                     | 0.41              |
| 1:G:556:LYS:O     | 1:G:559:ASP:HB2   | 2.21                     | 0.41              |
| 2:H:112:LEU:O     | 2:H:113:VAL:C     | 2.63                     | 0.41              |
| 2:H:145:TRP:HB2   | 10:H:1159:HOH:O   | 2.20                     | 0.41              |
| 3:I:253:VAL:HG22  | 9:I:3010:3PE:C3H  | 2.51                     | 0.41              |
| 9:I:3010:3PE:H362 | 9:I:3010:3PE:H391 | 1.81                     | 0.41              |
| 1:A:20:TRP:HE3    | 1:A:32:LEU:HD21   | 1.81                     | 0.41              |
| 1:A:26:HIS:CB     | 1:A:133:MET:HG2   | 2.50                     | 0.41              |
| 1:A:151:SER:O     | 1:A:152:LEU:C     | 2.64                     | 0.41              |
| 1:A:221:THR:HA    | 9:A:2012:3PE:H121 | 2.03                     | 0.41              |
| 1:A:326:LEU:O     | 1:A:330:VAL:HG22  | 2.21                     | 0.41              |
| 1:A:513:GLY:O     | 1:A:514:VAL:C     | 2.64                     | 0.41              |
| 2:B:202:VAL:HG22  | 10:B:1024:HOH:O   | 2.20                     | 0.41              |
| 2:B:235:LEU:HG    | 4:J:9:HIS:O       | 2.21                     | 0.41              |
| 3:C:160:ASN:O     | 3:C:164:VAL:HG23  | 2.20                     | 0.41              |
| 3:C:168:LEU:HB2   | 3:C:224:LEU:HD13  | 2.03                     | 0.41              |
| 3:C:222:VAL:HG11  | 9:C:2008:3PE:C35  | 2.50                     | 0.41              |
| 3:C:253:VAL:HG22  | 9:C:2010:3PE:C3I  | 2.51                     | 0.41              |
| 9:C:2013:3PE:H261 | 9:C:2013:3PE:C3A  | 2.45                     | 0.41              |
| 4:D:38:VAL:HG12   | 4:D:42:ILE:CD1    | 2.51                     | 0.41              |
| 4:D:44:LEU:HD21   | 9:D:2011:3PE:C3   | 2.50                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:63:MET:HE3    | 1:G:484:ILE:HD11  | 2.02                     | 0.41              |
| 1:G:213:LEU:CB    | 3:I:81:TRP:CH2    | 3.02                     | 0.41              |
| 1:G:237:TRP:CZ2   | 9:G:3012:3PE:H282 | 2.56                     | 0.41              |
| 1:G:280:TRP:CZ3   | 1:G:334:HIS:CE1   | 3.09                     | 0.41              |
| 1:G:307:LYS:HD3   | 1:G:374:SER:HG    | 1.84                     | 0.41              |
| 1:G:325:VAL:HG22  | 9:G:3012:3PE:C3D  | 2.51                     | 0.41              |
| 1:G:342:LEU:HD13  | 2:H:127:GLN:CB    | 2.35                     | 0.41              |
| 1:G:396:VAL:HG11  | 2:H:65:ILE:CD1    | 2.35                     | 0.41              |
| 1:G:422:TYR:CD2   | 1:G:426:LEU:HD12  | 2.56                     | 0.41              |
| 1:G:504:SER:O     | 1:G:507:SER:HB2   | 2.21                     | 0.41              |
| 8:G:1001:HEA:H11  | 8:G:1001:HEA:HHC  | 1.80                     | 0.41              |
| 8:G:1002:HEA:H241 | 2:H:112:LEU:HD21  | 2.03                     | 0.41              |
| 3:I:27:VAL:O      | 3:I:28:MET:C      | 2.63                     | 0.41              |
| 3:I:33:VAL:HA     | 3:I:36:MET:HE2    | 2.03                     | 0.41              |
| 3:I:41:PRO:O      | 3:I:42:TRP:C      | 2.63                     | 0.41              |
| 1:A:145:LEU:HD23  | 1:A:145:LEU:HA    | 1.89                     | 0.41              |
| 2:B:53:GLN:OE1    | 2:B:122:VAL:HG13  | 2.21                     | 0.41              |
| 2:B:272:GLU:HG3   | 2:B:272:GLU:H     | 1.68                     | 0.41              |
| 3:C:17:TRP:O      | 3:C:18:PRO:C      | 2.64                     | 0.41              |
| 3:C:51:VAL:O      | 3:C:54:THR:HB     | 2.21                     | 0.41              |
| 3:C:176:ALA:O     | 3:C:177:LEU:C     | 2.63                     | 0.41              |
| 1:G:26:HIS:HB3    | 1:G:132:ASP:OD1   | 2.20                     | 0.41              |
| 1:G:74:LYS:H      | 1:G:74:LYS:CD     | 2.31                     | 0.41              |
| 1:G:252:MET:HB3   | 1:G:263:PHE:CD2   | 2.56                     | 0.41              |
| 1:G:423:VAL:O     | 1:G:423:VAL:HG23  | 2.21                     | 0.41              |
| 1:G:459:MET:HB3   | 1:G:507:SER:OG    | 2.21                     | 0.41              |
| 2:H:194:THR:O     | 2:H:195:ASP:C     | 2.63                     | 0.41              |
| 3:I:36:MET:HE3    | 3:I:36:MET:HB2    | 1.96                     | 0.41              |
| 3:I:168:LEU:HB2   | 3:I:224:LEU:HD13  | 2.01                     | 0.41              |
| 3:I:245:TRP:CE2   | 9:I:3013:3PE:H231 | 2.55                     | 0.41              |
| 3:I:255:LEU:HD23  | 3:I:255:LEU:HA    | 1.73                     | 0.41              |
| 1:A:387:PHE:HD1   | 1:A:388:LEU:N     | 2.19                     | 0.40              |
| 1:A:447:GLN:O     | 1:A:518:THR:HG23  | 2.21                     | 0.40              |
| 1:A:477:GLN:HA    | 1:A:477:GLN:HE21  | 1.86                     | 0.40              |
| 10:A:2037:HOH:O   | 2:B:143:TRP:HH2   | 2.03                     | 0.40              |
| 2:B:57:LEU:O      | 2:B:58:ASP:C      | 2.62                     | 0.40              |
| 2:B:192:LEU:HD13  | 2:B:249:PHE:HB3   | 2.03                     | 0.40              |
| 3:C:28:MET:HA     | 3:C:47:GLY:HA3    | 2.03                     | 0.40              |
| 3:C:77:LEU:HA     | 3:C:80:ARG:HD3    | 2.03                     | 0.40              |
| 3:C:87:ILE:O      | 3:C:91:VAL:HG23   | 2.21                     | 0.40              |
| 3:C:161:ARG:HA    | 3:C:164:VAL:HB    | 2.03                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:432:ILE:O     | 1:G:433:PHE:C     | 2.64                     | 0.40              |
| 1:G:454:LYS:O     | 1:G:457:PHE:HB3   | 2.20                     | 0.40              |
| 1:G:494:ASN:ND2   | 10:G:3047:HOH:O   | 2.44                     | 0.40              |
| 1:G:502:PHE:O     | 1:G:503:LEU:C     | 2.63                     | 0.40              |
| 2:H:149:TYR:HA    | 2:H:150:PRO:HD2   | 1.83                     | 0.40              |
| 3:I:166:TRP:O     | 3:I:167:GLY:C     | 2.63                     | 0.40              |
| 3:I:199:GLY:O     | 3:I:203:PHE:HB2   | 2.21                     | 0.40              |
| 1:A:95:TRP:HB2    | 1:A:484:ILE:CD1   | 2.51                     | 0.40              |
| 1:A:195:HIS:O     | 1:A:196:LEU:C     | 2.62                     | 0.40              |
| 1:A:243:LEU:HD22  | 1:A:243:LEU:HA    | 1.89                     | 0.40              |
| 1:A:554:LEU:H     | 3:C:6:ASN:HD21    | 1.68                     | 0.40              |
| 2:B:61:ILE:CG2    | 10:B:1031:HOH:O   | 2.69                     | 0.40              |
| 3:C:109:MET:HE3   | 3:C:109:MET:HB3   | 1.86                     | 0.40              |
| 9:C:2013:3PE:H3H2 | 9:C:2013:3PE:H2E1 | 2.02                     | 0.40              |
| 1:G:109:PHE:HA    | 1:G:146:TYR:HE1   | 1.86                     | 0.40              |
| 1:G:125:PRO:O     | 1:G:126:LEU:C     | 2.64                     | 0.40              |
| 1:G:189:LEU:HD21  | 3:I:30:PHE:CD1    | 2.56                     | 0.40              |
| 1:G:234:VAL:CG1   | 1:G:292:LEU:HD11  | 2.51                     | 0.40              |
| 1:G:241:LEU:HD13  | 9:J:3011:3PE:H2I1 | 2.03                     | 0.40              |
| 1:G:421:HIS:HB3   | 1:G:468:PHE:CE2   | 2.57                     | 0.40              |
| 1:G:445:GLY:HA2   | 1:G:525:VAL:CG1   | 2.38                     | 0.40              |
| 1:G:483:TYR:CE1   | 2:H:261:ALA:HA    | 2.56                     | 0.40              |
| 1:G:513:GLY:O     | 1:G:516:PHE:N     | 2.54                     | 0.40              |
| 9:G:3009:3PE:C38  | 9:G:3009:3PE:H271 | 2.52                     | 0.40              |
| 2:H:175:GLU:H     | 2:H:175:GLU:CD    | 2.28                     | 0.40              |
| 2:H:219:TRP:CD1   | 2:H:265:ILE:CD1   | 3.04                     | 0.40              |
| 3:I:83:PHE:CE1    | 9:I:3008:3PE:H262 | 2.47                     | 0.40              |
| 3:I:226:ARG:O     | 3:I:227:VAL:C     | 2.63                     | 0.40              |
| 1:A:52:ARG:HG3    | 1:A:501:ALA:CB    | 2.51                     | 0.40              |
| 1:A:121:ASN:O     | 1:A:125:PRO:HG3   | 2.21                     | 0.40              |
| 1:A:152:LEU:O     | 1:A:155:ALA:N     | 2.54                     | 0.40              |
| 1:A:271:ASP:O     | 1:A:272:PRO:C     | 2.65                     | 0.40              |
| 1:A:316:MET:HG2   | 1:A:316:MET:H     | 1.71                     | 0.40              |
| 1:A:321:VAL:O     | 1:A:322:ALA:C     | 2.65                     | 0.40              |
| 1:A:488:GLU:O     | 1:A:490:PHE:N     | 2.54                     | 0.40              |
| 2:B:192:LEU:HB3   | 2:B:249:PHE:CG    | 2.55                     | 0.40              |
| 2:B:260:HIS:HB3   | 10:B:1034:HOH:O   | 2.20                     | 0.40              |
| 3:C:152:HIS:CD2   | 9:C:2013:3PE:H332 | 2.56                     | 0.40              |
| 1:G:15:GLY:O      | 1:G:16:PHE:C      | 2.64                     | 0.40              |
| 1:G:33:TYR:CE1    | 1:G:143:TYR:HB2   | 2.56                     | 0.40              |
| 1:G:319:ALA:O     | 1:G:322:ALA:N     | 2.54                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:488:GLU:O     | 1:G:490:PHE:N     | 2.55                     | 0.40              |
| 1:G:493:TRP:O     | 1:G:496:VAL:HB    | 2.21                     | 0.40              |
| 2:H:79:ALA:O      | 2:H:80:VAL:C      | 2.64                     | 0.40              |
| 2:H:211:THR:OG1   | 2:H:235:LEU:HD23  | 2.22                     | 0.40              |
| 3:I:122:PRO:HA    | 10:I:3045:HOH:O   | 2.19                     | 0.40              |
| 1:A:45:VAL:HA     | 1:A:48:THR:HG23   | 2.03                     | 0.40              |
| 1:A:265:GLN:O     | 1:A:266:PRO:C     | 2.63                     | 0.40              |
| 1:A:316:MET:SD    | 1:A:365:SER:HB2   | 2.61                     | 0.40              |
| 1:A:375:ILE:HD13  | 1:A:375:ILE:HG21  | 1.90                     | 0.40              |
| 1:A:457:PHE:CD2   | 1:A:457:PHE:C     | 2.97                     | 0.40              |
| 2:B:228:GLN:CD    | 2:B:229:ASP:H     | 2.28                     | 0.40              |
| 3:C:85:LEU:O      | 3:C:88:MET:N      | 2.53                     | 0.40              |
| 3:C:193:PHE:C     | 3:C:193:PHE:CD1   | 3.00                     | 0.40              |
| 3:I:72:THR:O      | 3:I:75:VAL:N      | 2.54                     | 0.40              |
| 3:C:57:GLY:O      | 3:C:58:TRP:C      | 2.65                     | 0.40              |
| 3:C:143:CYS:O     | 3:C:144:SER:C     | 2.64                     | 0.40              |
| 1:G:266:PRO:HG2   | 2:H:232:PRO:O     | 2.22                     | 0.40              |
| 1:G:322:ALA:O     | 1:G:326:LEU:HG    | 2.21                     | 0.40              |
| 1:G:385:LEU:O     | 1:G:388:LEU:N     | 2.54                     | 0.40              |
| 1:G:499:LEU:O     | 1:G:500:GLY:C     | 2.63                     | 0.40              |
| 1:G:507:SER:O     | 1:G:510:PHE:N     | 2.54                     | 0.40              |
| 2:H:185:TYR:HE1   | 2:H:247:ILE:HD13  | 1.86                     | 0.40              |
| 9:I:3010:3PE:H381 | 9:I:3010:3PE:H3B1 | 1.91                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed   | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|-----------|----------|-------------|----|
| 1   | A     | 545/566 (96%) | 416 (76%) | 106 (19%) | 23 (4%)  | 2           | 13 |
| 1   | G     | 545/566 (96%) | 403 (74%) | 112 (21%) | 30 (6%)  | 1           | 8  |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 2   | B     | 258/264 (98%)   | 203 (79%)  | 47 (18%)  | 8 (3%)   | 3           | 19 |
| 2   | H     | 258/264 (98%)   | 206 (80%)  | 44 (17%)  | 8 (3%)   | 3           | 19 |
| 3   | C     | 263/266 (99%)   | 217 (82%)  | 41 (16%)  | 5 (2%)   | 6           | 30 |
| 3   | I     | 263/266 (99%)   | 209 (80%)  | 49 (19%)  | 5 (2%)   | 6           | 30 |
| 4   | D     | 40/51 (78%)     | 26 (65%)   | 13 (32%)  | 1 (2%)   | 4           | 23 |
| 4   | J     | 40/51 (78%)     | 26 (65%)   | 12 (30%)  | 2 (5%)   | 1           | 10 |
| All | All   | 2212/2294 (96%) | 1706 (77%) | 424 (19%) | 82 (4%)  | 2           | 15 |

All (82) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 102 | HIS  |
| 1   | A     | 160 | PRO  |
| 1   | A     | 544 | SER  |
| 1   | A     | 545 | PRO  |
| 2   | B     | 254 | GLU  |
| 2   | B     | 264 | PRO  |
| 3   | C     | 73  | PRO  |
| 3   | C     | 195 | GLY  |
| 1   | G     | 58  | PRO  |
| 1   | G     | 102 | HIS  |
| 1   | G     | 160 | PRO  |
| 1   | G     | 544 | SER  |
| 1   | G     | 559 | ASP  |
| 3   | I     | 195 | GLY  |
| 1   | A     | 58  | PRO  |
| 1   | A     | 110 | VAL  |
| 1   | A     | 395 | GLY  |
| 1   | A     | 496 | VAL  |
| 2   | B     | 45  | PRO  |
| 2   | B     | 255 | LEU  |
| 1   | G     | 90  | PRO  |
| 1   | G     | 298 | VAL  |
| 1   | G     | 394 | GLY  |
| 1   | G     | 395 | GLY  |
| 1   | G     | 396 | VAL  |
| 1   | G     | 432 | ILE  |
| 1   | G     | 545 | PRO  |
| 1   | G     | 551 | PHE  |
| 3   | I     | 73  | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | I     | 194 | ALA  |
| 4   | J     | 33  | ALA  |
| 1   | A     | 90  | PRO  |
| 1   | A     | 103 | GLY  |
| 3   | C     | 42  | TRP  |
| 1   | G     | 103 | GLY  |
| 1   | G     | 176 | PRO  |
| 1   | G     | 211 | THR  |
| 1   | G     | 239 | ILE  |
| 1   | G     | 377 | LEU  |
| 1   | G     | 405 | SER  |
| 1   | G     | 462 | VAL  |
| 2   | H     | 45  | PRO  |
| 1   | A     | 71  | GLY  |
| 1   | A     | 394 | GLY  |
| 1   | A     | 405 | SER  |
| 1   | A     | 408 | ARG  |
| 1   | A     | 495 | PHE  |
| 3   | C     | 14  | PRO  |
| 1   | G     | 210 | THR  |
| 1   | G     | 393 | VAL  |
| 1   | G     | 408 | ARG  |
| 2   | H     | 120 | LEU  |
| 2   | H     | 187 | ARG  |
| 2   | H     | 255 | LEU  |
| 2   | H     | 264 | PRO  |
| 3   | I     | 243 | ALA  |
| 4   | J     | 10  | VAL  |
| 1   | A     | 39  | LEU  |
| 1   | A     | 284 | HIS  |
| 1   | A     | 377 | LEU  |
| 1   | A     | 393 | VAL  |
| 2   | B     | 121 | PRO  |
| 4   | D     | 33  | ALA  |
| 1   | G     | 82  | PRO  |
| 1   | G     | 156 | SER  |
| 1   | G     | 389 | PHE  |
| 2   | H     | 215 | VAL  |
| 2   | B     | 120 | LEU  |
| 2   | B     | 174 | PRO  |
| 1   | G     | 492 | THR  |
| 2   | H     | 121 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 239 | ILE  |
| 2   | B     | 215 | VAL  |
| 3   | C     | 111 | PRO  |
| 1   | G     | 431 | GLY  |
| 1   | G     | 480 | PRO  |
| 1   | A     | 111 | VAL  |
| 1   | A     | 432 | ILE  |
| 2   | H     | 33  | ILE  |
| 1   | A     | 396 | VAL  |
| 1   | G     | 330 | VAL  |
| 3   | I     | 133 | LEU  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 1   | A     | 446/459 (97%)   | 388 (87%)  | 58 (13%)  | 4           | 19 |
| 1   | G     | 446/459 (97%)   | 380 (85%)  | 66 (15%)  | 3           | 15 |
| 2   | B     | 216/220 (98%)   | 188 (87%)  | 28 (13%)  | 4           | 19 |
| 2   | H     | 216/220 (98%)   | 193 (89%)  | 23 (11%)  | 6           | 27 |
| 3   | C     | 215/216 (100%)  | 197 (92%)  | 18 (8%)   | 10          | 37 |
| 3   | I     | 215/216 (100%)  | 189 (88%)  | 26 (12%)  | 5           | 21 |
| 4   | D     | 30/37 (81%)     | 26 (87%)   | 4 (13%)   | 4           | 18 |
| 4   | J     | 30/37 (81%)     | 26 (87%)   | 4 (13%)   | 4           | 18 |
| All | All   | 1814/1864 (97%) | 1587 (88%) | 227 (12%) | 4           | 20 |

All (227) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 18  | THR  |
| 1   | A     | 29  | ILE  |
| 1   | A     | 52  | ARG  |
| 1   | A     | 80  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 85  | VAL  |
| 1   | A     | 89  | THR  |
| 1   | A     | 100 | THR  |
| 1   | A     | 111 | VAL  |
| 1   | A     | 113 | PRO  |
| 1   | A     | 137 | ARG  |
| 1   | A     | 142 | SER  |
| 1   | A     | 147 | VAL  |
| 1   | A     | 160 | PRO  |
| 1   | A     | 173 | VAL  |
| 1   | A     | 174 | LEU  |
| 1   | A     | 178 | LEU  |
| 1   | A     | 182 | GLU  |
| 1   | A     | 183 | SER  |
| 1   | A     | 208 | MET  |
| 1   | A     | 212 | PHE  |
| 1   | A     | 221 | THR  |
| 1   | A     | 231 | SER  |
| 1   | A     | 235 | THR  |
| 1   | A     | 239 | ILE  |
| 1   | A     | 243 | LEU  |
| 1   | A     | 250 | ILE  |
| 1   | A     | 251 | THR  |
| 1   | A     | 252 | MET  |
| 1   | A     | 264 | PHE  |
| 1   | A     | 273 | VAL  |
| 1   | A     | 282 | PHE  |
| 1   | A     | 304 | THR  |
| 1   | A     | 307 | LYS  |
| 1   | A     | 310 | ILE  |
| 1   | A     | 330 | VAL  |
| 1   | A     | 341 | SER  |
| 1   | A     | 343 | THR  |
| 1   | A     | 367 | ILE  |
| 1   | A     | 369 | THR  |
| 1   | A     | 382 | LEU  |
| 1   | A     | 388 | LEU  |
| 1   | A     | 390 | LEU  |
| 1   | A     | 397 | THR  |
| 1   | A     | 402 | SER  |
| 1   | A     | 412 | ASP  |
| 1   | A     | 419 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 424 | MET  |
| 1   | A     | 432 | ILE  |
| 1   | A     | 443 | MET  |
| 1   | A     | 477 | GLN  |
| 1   | A     | 492 | THR  |
| 1   | A     | 514 | VAL  |
| 1   | A     | 515 | ILE  |
| 1   | A     | 519 | LEU  |
| 1   | A     | 525 | VAL  |
| 1   | A     | 529 | ASN  |
| 1   | A     | 539 | GLU  |
| 1   | A     | 556 | LYS  |
| 2   | B     | 63  | VAL  |
| 2   | B     | 64  | ILE  |
| 2   | B     | 98  | SER  |
| 2   | B     | 99  | PRO  |
| 2   | B     | 104 | TRP  |
| 2   | B     | 110 | VAL  |
| 2   | B     | 121 | PRO  |
| 2   | B     | 123 | LEU  |
| 2   | B     | 125 | ASN  |
| 2   | B     | 134 | VAL  |
| 2   | B     | 137 | LYS  |
| 2   | B     | 149 | TYR  |
| 2   | B     | 158 | SER  |
| 2   | B     | 180 | LEU  |
| 2   | B     | 186 | SER  |
| 2   | B     | 198 | MET  |
| 2   | B     | 199 | VAL  |
| 2   | B     | 200 | VAL  |
| 2   | B     | 209 | GLN  |
| 2   | B     | 214 | ASP  |
| 2   | B     | 215 | VAL  |
| 2   | B     | 216 | ILE  |
| 2   | B     | 222 | PRO  |
| 2   | B     | 232 | PRO  |
| 2   | B     | 237 | GLN  |
| 2   | B     | 238 | LEU  |
| 2   | B     | 253 | SER  |
| 2   | B     | 272 | GLU  |
| 3   | C     | 16  | ILE  |
| 3   | C     | 20  | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 39  | SER  |
| 3   | C     | 45  | LEU  |
| 3   | C     | 48  | LEU  |
| 3   | C     | 63  | VAL  |
| 3   | C     | 72  | THR  |
| 3   | C     | 75  | VAL  |
| 3   | C     | 85  | LEU  |
| 3   | C     | 100 | SER  |
| 3   | C     | 103 | LYS  |
| 3   | C     | 125 | ILE  |
| 3   | C     | 136 | ILE  |
| 3   | C     | 149 | THR  |
| 3   | C     | 157 | HIS  |
| 3   | C     | 204 | MET  |
| 3   | C     | 231 | HIS  |
| 3   | C     | 236 | LYS  |
| 4   | D     | 16  | ILE  |
| 4   | D     | 21  | LYS  |
| 4   | D     | 31  | THR  |
| 4   | D     | 48  | ASN  |
| 1   | G     | 18  | THR  |
| 1   | G     | 25  | ASN  |
| 1   | G     | 29  | ILE  |
| 1   | G     | 31  | VAL  |
| 1   | G     | 80  | LEU  |
| 1   | G     | 85  | VAL  |
| 1   | G     | 89  | THR  |
| 1   | G     | 100 | THR  |
| 1   | G     | 106 | MET  |
| 1   | G     | 111 | VAL  |
| 1   | G     | 113 | PRO  |
| 1   | G     | 137 | ARG  |
| 1   | G     | 142 | SER  |
| 1   | G     | 147 | VAL  |
| 1   | G     | 160 | PRO  |
| 1   | G     | 173 | VAL  |
| 1   | G     | 174 | LEU  |
| 1   | G     | 176 | PRO  |
| 1   | G     | 178 | LEU  |
| 1   | G     | 183 | SER  |
| 1   | G     | 206 | ILE  |
| 1   | G     | 208 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 211 | THR  |
| 1   | G     | 212 | PHE  |
| 1   | G     | 221 | THR  |
| 1   | G     | 231 | SER  |
| 1   | G     | 235 | THR  |
| 1   | G     | 239 | ILE  |
| 1   | G     | 250 | ILE  |
| 1   | G     | 251 | THR  |
| 1   | G     | 252 | MET  |
| 1   | G     | 282 | PHE  |
| 1   | G     | 286 | GLN  |
| 1   | G     | 297 | ILE  |
| 1   | G     | 304 | THR  |
| 1   | G     | 307 | LYS  |
| 1   | G     | 310 | ILE  |
| 1   | G     | 330 | VAL  |
| 1   | G     | 341 | SER  |
| 1   | G     | 343 | THR  |
| 1   | G     | 363 | ILE  |
| 1   | G     | 367 | ILE  |
| 1   | G     | 369 | THR  |
| 1   | G     | 382 | LEU  |
| 1   | G     | 388 | LEU  |
| 1   | G     | 390 | LEU  |
| 1   | G     | 397 | THR  |
| 1   | G     | 400 | VAL  |
| 1   | G     | 402 | SER  |
| 1   | G     | 412 | ASP  |
| 1   | G     | 419 | HIS  |
| 1   | G     | 424 | MET  |
| 1   | G     | 432 | ILE  |
| 1   | G     | 443 | MET  |
| 1   | G     | 477 | GLN  |
| 1   | G     | 492 | THR  |
| 1   | G     | 509 | LEU  |
| 1   | G     | 514 | VAL  |
| 1   | G     | 515 | ILE  |
| 1   | G     | 519 | LEU  |
| 1   | G     | 525 | VAL  |
| 1   | G     | 529 | ASN  |
| 1   | G     | 537 | THR  |
| 1   | G     | 542 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 543 | THR  |
| 1   | G     | 556 | LYS  |
| 2   | H     | 45  | PRO  |
| 2   | H     | 52  | THR  |
| 2   | H     | 63  | VAL  |
| 2   | H     | 64  | ILE  |
| 2   | H     | 98  | SER  |
| 2   | H     | 111 | ILE  |
| 2   | H     | 134 | VAL  |
| 2   | H     | 149 | TYR  |
| 2   | H     | 158 | SER  |
| 2   | H     | 163 | SER  |
| 2   | H     | 180 | LEU  |
| 2   | H     | 186 | SER  |
| 2   | H     | 198 | MET  |
| 2   | H     | 199 | VAL  |
| 2   | H     | 200 | VAL  |
| 2   | H     | 209 | GLN  |
| 2   | H     | 216 | ILE  |
| 2   | H     | 221 | VAL  |
| 2   | H     | 228 | GLN  |
| 2   | H     | 237 | GLN  |
| 2   | H     | 238 | LEU  |
| 2   | H     | 253 | SER  |
| 2   | H     | 272 | GLU  |
| 3   | I     | 6   | ASN  |
| 3   | I     | 15  | SER  |
| 3   | I     | 16  | ILE  |
| 3   | I     | 20  | MET  |
| 3   | I     | 39  | SER  |
| 3   | I     | 45  | LEU  |
| 3   | I     | 48  | LEU  |
| 3   | I     | 63  | VAL  |
| 3   | I     | 68  | GLU  |
| 3   | I     | 72  | THR  |
| 3   | I     | 75  | VAL  |
| 3   | I     | 85  | LEU  |
| 3   | I     | 90  | GLU  |
| 3   | I     | 95  | SER  |
| 3   | I     | 100 | SER  |
| 3   | I     | 103 | LYS  |
| 3   | I     | 125 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | I     | 149 | THR  |
| 3   | I     | 155 | LEU  |
| 3   | I     | 157 | HIS  |
| 3   | I     | 180 | VAL  |
| 3   | I     | 196 | ASN  |
| 3   | I     | 204 | MET  |
| 3   | I     | 231 | HIS  |
| 3   | I     | 236 | LYS  |
| 3   | I     | 253 | VAL  |
| 4   | J     | 16  | ILE  |
| 4   | J     | 21  | LYS  |
| 4   | J     | 31  | THR  |
| 4   | J     | 48  | ASN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 25  | ASN  |
| 1   | A     | 26  | HIS  |
| 1   | A     | 91  | ASN  |
| 1   | A     | 96  | ASN  |
| 1   | A     | 165 | GLN  |
| 1   | A     | 286 | GLN  |
| 1   | A     | 345 | GLN  |
| 1   | A     | 403 | GLN  |
| 1   | A     | 494 | ASN  |
| 1   | A     | 549 | HIS  |
| 2   | B     | 55  | HIS  |
| 2   | B     | 84  | HIS  |
| 2   | B     | 178 | GLN  |
| 2   | B     | 209 | GLN  |
| 2   | B     | 237 | GLN  |
| 3   | C     | 10  | HIS  |
| 3   | C     | 159 | ASN  |
| 3   | C     | 160 | ASN  |
| 3   | C     | 201 | ASN  |
| 3   | C     | 231 | HIS  |
| 1   | G     | 25  | ASN  |
| 1   | G     | 26  | HIS  |
| 1   | G     | 163 | ASN  |
| 1   | G     | 286 | GLN  |
| 1   | G     | 345 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 465 | ASN  |
| 1   | G     | 494 | ASN  |
| 1   | G     | 534 | HIS  |
| 2   | H     | 55  | HIS  |
| 2   | H     | 84  | HIS  |
| 2   | H     | 178 | GLN  |
| 2   | H     | 209 | GLN  |
| 2   | H     | 237 | GLN  |
| 2   | H     | 251 | GLN  |
| 3   | I     | 152 | HIS  |
| 3   | I     | 153 | HIS  |
| 3   | I     | 159 | ASN  |
| 3   | I     | 160 | ASN  |
| 3   | I     | 201 | ASN  |
| 3   | I     | 212 | HIS  |
| 3   | I     | 231 | HIS  |
| 4   | J     | 9   | HIS  |
| 4   | J     | 18  | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 10 are monoatomic - leaving 16 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 9   | 3PE  | I     | 3008 | -    | 50,50,50     | 1.65 | 2 (4%)      | 53,55,55    | 1.14 | 3 (5%)      |
| 8   | HEA  | G     | 1002 | 1    | 67,67,67     | 1.31 | 9 (13%)     | 81,103,103  | 2.00 | 20 (24%)    |
| 9   | 3PE  | C     | 2008 | -    | 50,50,50     | 1.58 | 2 (4%)      | 53,55,55    | 1.20 | 6 (11%)     |
| 9   | 3PE  | G     | 3009 | -    | 50,50,50     | 1.50 | 3 (6%)      | 53,55,55    | 0.99 | 2 (3%)      |
| 8   | HEA  | A     | 1002 | 1    | 67,67,67     | 1.41 | 11 (16%)    | 81,103,103  | 2.22 | 24 (29%)    |
| 9   | 3PE  | I     | 3010 | -    | 50,50,50     | 1.61 | 4 (8%)      | 53,55,55    | 1.03 | 2 (3%)      |
| 9   | 3PE  | A     | 2009 | -    | 50,50,50     | 1.62 | 3 (6%)      | 53,55,55    | 1.13 | 3 (5%)      |
| 8   | HEA  | A     | 1001 | 1    | 67,67,67     | 1.39 | 10 (14%)    | 81,103,103  | 2.41 | 35 (43%)    |
| 9   | 3PE  | J     | 3011 | -    | 50,50,50     | 1.70 | 2 (4%)      | 53,55,55    | 1.54 | 7 (13%)     |
| 9   | 3PE  | I     | 3013 | -    | 50,50,50     | 1.63 | 3 (6%)      | 53,55,55    | 1.20 | 3 (5%)      |
| 9   | 3PE  | C     | 2010 | -    | 50,50,50     | 1.54 | 2 (4%)      | 53,55,55    | 1.15 | 3 (5%)      |
| 9   | 3PE  | D     | 2011 | -    | 50,50,50     | 1.50 | 3 (6%)      | 53,55,55    | 1.31 | 7 (13%)     |
| 9   | 3PE  | G     | 3012 | -    | 50,50,50     | 1.63 | 3 (6%)      | 53,55,55    | 1.25 | 5 (9%)      |
| 9   | 3PE  | A     | 2012 | -    | 50,50,50     | 1.62 | 3 (6%)      | 53,55,55    | 1.41 | 6 (11%)     |
| 9   | 3PE  | C     | 2013 | -    | 50,50,50     | 1.58 | 3 (6%)      | 53,55,55    | 1.31 | 3 (5%)      |
| 8   | HEA  | G     | 1001 | 1    | 67,67,67     | 1.46 | 10 (14%)    | 81,103,103  | 2.62 | 35 (43%)    |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions    | Rings |
|-----|------|-------|------|------|---------|-------------|-------|
| 9   | 3PE  | I     | 3008 | -    | -       | 32/54/54/54 | -     |
| 8   | HEA  | G     | 1002 | 1    | -       | 6/36/76/76  | -     |
| 9   | 3PE  | C     | 2008 | -    | -       | 35/54/54/54 | -     |
| 9   | 3PE  | G     | 3009 | -    | -       | 29/54/54/54 | -     |
| 8   | HEA  | A     | 1002 | 1    | -       | 9/36/76/76  | -     |
| 9   | 3PE  | I     | 3010 | -    | -       | 28/54/54/54 | -     |
| 9   | 3PE  | A     | 2009 | -    | -       | 28/54/54/54 | -     |
| 8   | HEA  | A     | 1001 | 1    | -       | 17/36/76/76 | -     |
| 9   | 3PE  | J     | 3011 | -    | -       | 22/54/54/54 | -     |
| 9   | 3PE  | I     | 3013 | -    | -       | 27/54/54/54 | -     |
| 9   | 3PE  | C     | 2010 | -    | -       | 22/54/54/54 | -     |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions    | Rings |
|-----|------|-------|------|------|---------|-------------|-------|
| 9   | 3PE  | D     | 2011 | -    | -       | 21/54/54/54 | -     |
| 9   | 3PE  | G     | 3012 | -    | -       | 22/54/54/54 | -     |
| 9   | 3PE  | A     | 2012 | -    | -       | 21/54/54/54 | -     |
| 9   | 3PE  | C     | 2013 | -    | -       | 26/54/54/54 | -     |
| 8   | HEA  | G     | 1001 | 1    | -       | 16/36/76/76 | -     |

All (73) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 9   | J     | 3011 | 3PE  | O21-C21 | 8.32  | 1.57        | 1.34     |
| 9   | I     | 3013 | 3PE  | O31-C31 | 7.71  | 1.55        | 1.33     |
| 9   | A     | 2009 | 3PE  | O21-C21 | 7.63  | 1.55        | 1.34     |
| 9   | I     | 3008 | 3PE  | O21-C21 | 7.63  | 1.55        | 1.34     |
| 9   | G     | 3012 | 3PE  | O31-C31 | 7.57  | 1.55        | 1.33     |
| 9   | C     | 2010 | 3PE  | O21-C21 | 7.55  | 1.55        | 1.34     |
| 9   | C     | 2013 | 3PE  | O31-C31 | 7.51  | 1.55        | 1.33     |
| 9   | A     | 2012 | 3PE  | O31-C31 | 7.48  | 1.55        | 1.33     |
| 9   | I     | 3008 | 3PE  | O31-C31 | 7.47  | 1.55        | 1.33     |
| 9   | I     | 3010 | 3PE  | O31-C31 | 7.44  | 1.55        | 1.33     |
| 9   | G     | 3012 | 3PE  | O21-C21 | 7.40  | 1.55        | 1.34     |
| 9   | I     | 3013 | 3PE  | O21-C21 | 7.37  | 1.55        | 1.34     |
| 9   | C     | 2008 | 3PE  | O31-C31 | 7.28  | 1.54        | 1.33     |
| 9   | C     | 2008 | 3PE  | O21-C21 | 7.26  | 1.54        | 1.34     |
| 9   | C     | 2013 | 3PE  | O21-C21 | 7.25  | 1.54        | 1.34     |
| 9   | J     | 3011 | 3PE  | O31-C31 | 7.23  | 1.54        | 1.33     |
| 9   | D     | 2011 | 3PE  | O21-C21 | 7.21  | 1.54        | 1.34     |
| 9   | I     | 3010 | 3PE  | O21-C21 | 7.16  | 1.54        | 1.34     |
| 9   | A     | 2012 | 3PE  | O21-C21 | 7.09  | 1.54        | 1.34     |
| 9   | A     | 2009 | 3PE  | O31-C31 | 6.97  | 1.53        | 1.33     |
| 9   | G     | 3009 | 3PE  | O31-C31 | 6.82  | 1.53        | 1.33     |
| 9   | G     | 3009 | 3PE  | O21-C21 | 6.79  | 1.53        | 1.34     |
| 9   | C     | 2010 | 3PE  | O31-C31 | 6.69  | 1.52        | 1.33     |
| 9   | D     | 2011 | 3PE  | O31-C31 | 6.53  | 1.52        | 1.33     |
| 8   | G     | 1001 | HEA  | C1D-ND  | -4.39 | 1.32        | 1.40     |
| 8   | A     | 1002 | HEA  | C4C-NC  | -4.18 | 1.31        | 1.39     |
| 8   | G     | 1001 | HEA  | C4C-NC  | -4.07 | 1.31        | 1.39     |
| 8   | A     | 1002 | HEA  | C1D-ND  | -3.97 | 1.33        | 1.40     |
| 8   | G     | 1001 | HEA  | CAC-C3C | -3.46 | 1.38        | 1.47     |
| 8   | A     | 1001 | HEA  | C4C-NC  | -3.36 | 1.33        | 1.39     |
| 8   | A     | 1001 | HEA  | CAC-C3C | -3.34 | 1.38        | 1.47     |
| 8   | A     | 1001 | HEA  | C16-C15 | -3.30 | 1.44        | 1.51     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 8   | A     | 1001 | HEA  | FE-ND   | -3.08 | 1.85        | 1.94     |
| 8   | G     | 1002 | HEA  | C1D-ND  | -3.04 | 1.35        | 1.40     |
| 8   | G     | 1002 | HEA  | CMA-C3A | 3.01  | 1.52        | 1.45     |
| 8   | G     | 1001 | HEA  | FE-ND   | -2.94 | 1.85        | 1.94     |
| 8   | A     | 1002 | HEA  | C1A-NA  | -2.92 | 1.34        | 1.39     |
| 8   | A     | 1002 | HEA  | CAC-C3C | -2.85 | 1.39        | 1.47     |
| 9   | A     | 2012 | 3PE  | O21-C2  | -2.85 | 1.39        | 1.46     |
| 8   | G     | 1001 | HEA  | FE-NB   | 2.82  | 2.03        | 1.94     |
| 8   | A     | 1002 | HEA  | FE-ND   | -2.80 | 1.86        | 1.94     |
| 8   | A     | 1001 | HEA  | C1D-ND  | -2.73 | 1.35        | 1.40     |
| 8   | A     | 1001 | HEA  | C1A-NA  | -2.65 | 1.34        | 1.39     |
| 8   | G     | 1001 | HEA  | C4D-ND  | -2.57 | 1.33        | 1.38     |
| 8   | G     | 1001 | HEA  | C1A-NA  | -2.52 | 1.34        | 1.39     |
| 8   | G     | 1002 | HEA  | C4C-NC  | -2.52 | 1.34        | 1.39     |
| 8   | A     | 1002 | HEA  | C3C-C2C | -2.48 | 1.32        | 1.41     |
| 8   | A     | 1002 | HEA  | FE-NB   | 2.45  | 2.02        | 1.94     |
| 8   | G     | 1002 | HEA  | CAC-C3C | -2.44 | 1.40        | 1.47     |
| 8   | G     | 1002 | HEA  | C4D-ND  | -2.42 | 1.34        | 1.38     |
| 9   | D     | 2011 | 3PE  | O21-C2  | -2.40 | 1.41        | 1.46     |
| 8   | G     | 1001 | HEA  | CMA-C3A | 2.37  | 1.50        | 1.45     |
| 8   | A     | 1002 | HEA  | C4D-ND  | -2.35 | 1.34        | 1.38     |
| 8   | A     | 1001 | HEA  | C3C-C2C | -2.33 | 1.33        | 1.41     |
| 8   | A     | 1001 | HEA  | C4D-ND  | -2.33 | 1.34        | 1.38     |
| 8   | A     | 1001 | HEA  | CMA-C3A | 2.31  | 1.50        | 1.45     |
| 8   | G     | 1001 | HEA  | C3C-C2C | -2.31 | 1.33        | 1.41     |
| 8   | G     | 1002 | HEA  | CHC-C1C | -2.30 | 1.34        | 1.39     |
| 9   | G     | 3009 | 3PE  | O21-C2  | -2.29 | 1.41        | 1.46     |
| 9   | I     | 3010 | 3PE  | O32-C31 | 2.27  | 1.29        | 1.22     |
| 9   | I     | 3013 | 3PE  | O32-C31 | 2.22  | 1.29        | 1.22     |
| 8   | G     | 1002 | HEA  | FE-NB   | 2.16  | 2.01        | 1.94     |
| 8   | G     | 1002 | HEA  | FE-ND   | -2.14 | 1.88        | 1.94     |
| 9   | G     | 3012 | 3PE  | O21-C2  | -2.14 | 1.41        | 1.46     |
| 9   | I     | 3010 | 3PE  | C32-C31 | 2.07  | 1.56        | 1.50     |
| 8   | G     | 1001 | HEA  | C22-C23 | 2.06  | 1.38        | 1.32     |
| 8   | A     | 1002 | HEA  | C3A-C2A | -2.06 | 1.32        | 1.37     |
| 8   | A     | 1002 | HEA  | C14-C15 | 2.05  | 1.37        | 1.33     |
| 9   | C     | 2013 | 3PE  | O32-C31 | 2.05  | 1.28        | 1.22     |
| 8   | A     | 1002 | HEA  | CMA-C3A | 2.05  | 1.49        | 1.45     |
| 9   | A     | 2009 | 3PE  | C32-C31 | 2.03  | 1.56        | 1.50     |
| 8   | A     | 1001 | HEA  | FE-NB   | 2.02  | 2.01        | 1.94     |
| 8   | G     | 1002 | HEA  | C1A-NA  | -2.01 | 1.35        | 1.39     |

All (164) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 8   | G     | 1001 | HEA  | CHB-C1B-NB  | -7.09 | 116.80      | 124.42   |
| 8   | G     | 1001 | HEA  | CMB-C2B-C1B | 6.94  | 135.88      | 125.03   |
| 8   | A     | 1002 | HEA  | CMC-C2C-C1C | 6.85  | 135.85      | 125.42   |
| 9   | C     | 2013 | 3PE  | C2-O21-C21  | -6.63 | 101.93      | 117.80   |
| 8   | A     | 1002 | HEA  | C13-C14-C15 | -6.50 | 112.75      | 127.62   |
| 9   | J     | 3011 | 3PE  | C2-O21-C21  | -6.41 | 102.44      | 117.80   |
| 8   | A     | 1001 | HEA  | CMB-C2B-C1B | 6.41  | 135.06      | 125.03   |
| 8   | G     | 1002 | HEA  | CMB-C2B-C1B | 6.22  | 134.75      | 125.03   |
| 8   | A     | 1001 | HEA  | CMB-C2B-C3B | -6.19 | 118.30      | 130.28   |
| 8   | A     | 1001 | HEA  | CAA-C2A-C1A | 6.05  | 137.16      | 124.85   |
| 8   | G     | 1001 | HEA  | CMB-C2B-C3B | -6.01 | 118.65      | 130.28   |
| 8   | G     | 1001 | HEA  | C4B-NB-C1B  | -5.91 | 98.21       | 105.21   |
| 8   | G     | 1001 | HEA  | CHA-C1A-NA  | -5.90 | 118.03      | 124.45   |
| 8   | G     | 1002 | HEA  | C13-C14-C15 | -5.76 | 114.44      | 127.62   |
| 8   | G     | 1001 | HEA  | C3B-C4B-NB  | 5.66  | 116.34      | 109.84   |
| 9   | I     | 3013 | 3PE  | C2-O21-C21  | -5.58 | 104.44      | 117.80   |
| 8   | A     | 1002 | HEA  | C3C-C4C-NC  | 5.43  | 114.38      | 109.80   |
| 8   | G     | 1002 | HEA  | CMB-C2B-C3B | -5.24 | 120.14      | 130.28   |
| 9   | I     | 3008 | 3PE  | C2-O21-C21  | -5.07 | 105.67      | 117.80   |
| 8   | A     | 1002 | HEA  | CMB-C2B-C1B | 4.76  | 132.47      | 125.03   |
| 8   | A     | 1001 | HEA  | C3B-C4B-NB  | 4.66  | 115.20      | 109.84   |
| 8   | G     | 1001 | HEA  | CBA-CAA-C2A | 4.57  | 125.16      | 112.53   |
| 8   | A     | 1002 | HEA  | CMB-C2B-C3B | -4.54 | 121.50      | 130.28   |
| 9   | A     | 2012 | 3PE  | C3-C2-C1    | -4.45 | 101.41      | 111.78   |
| 8   | G     | 1001 | HEA  | C3C-C4C-NC  | 4.43  | 113.53      | 109.80   |
| 8   | A     | 1002 | HEA  | C2A-C1A-NA  | 4.41  | 114.58      | 110.32   |
| 8   | A     | 1002 | HEA  | CHA-C1A-NA  | -4.38 | 119.68      | 124.45   |
| 9   | A     | 2012 | 3PE  | O21-C21-O22 | 4.36  | 133.91      | 123.70   |
| 8   | A     | 1001 | HEA  | C27-C19-C18 | -4.34 | 112.47      | 123.63   |
| 8   | A     | 1001 | HEA  | CHB-C1B-NB  | -4.30 | 119.80      | 124.42   |
| 8   | G     | 1001 | HEA  | C2B-C1B-NB  | 4.26  | 114.83      | 109.90   |
| 8   | A     | 1001 | HEA  | CHA-C1A-NA  | -4.23 | 119.85      | 124.45   |
| 8   | G     | 1001 | HEA  | CAA-C2A-C1A | 4.10  | 133.18      | 124.85   |
| 9   | G     | 3012 | 3PE  | O21-C21-O22 | 4.08  | 133.24      | 123.70   |
| 8   | A     | 1001 | HEA  | C4B-NB-C1B  | -4.03 | 100.44      | 105.21   |
| 9   | C     | 2008 | 3PE  | C2-O21-C21  | -4.02 | 108.17      | 117.80   |
| 9   | G     | 3009 | 3PE  | C3-C2-C1    | -3.97 | 102.52      | 111.78   |
| 8   | G     | 1002 | HEA  | O11-C11-C3B | -3.97 | 103.98      | 111.26   |
| 8   | A     | 1001 | HEA  | C21-C22-C23 | -3.97 | 114.41      | 127.64   |
| 8   | G     | 1002 | HEA  | C3D-C4D-ND  | 3.97  | 114.18      | 110.35   |
| 9   | D     | 2011 | 3PE  | C3-C2-C1    | -3.93 | 102.61      | 111.78   |
| 8   | G     | 1001 | HEA  | C21-C22-C23 | -3.89 | 114.68      | 127.64   |
| 8   | G     | 1001 | HEA  | C13-C14-C15 | -3.87 | 118.77      | 127.62   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 8   | G     | 1001 | HEA  | C2A-C1A-NA  | 3.85  | 114.04      | 110.32   |
| 8   | A     | 1002 | HEA  | CHB-C1B-NB  | -3.72 | 120.42      | 124.42   |
| 8   | A     | 1002 | HEA  | CMC-C2C-C3C | -3.72 | 117.81      | 126.55   |
| 9   | J     | 3011 | 3PE  | C3-C2-C1    | -3.67 | 103.23      | 111.78   |
| 9   | A     | 2009 | 3PE  | C3-C2-C1    | -3.62 | 103.35      | 111.78   |
| 8   | A     | 1001 | HEA  | C2A-C1A-NA  | 3.60  | 113.80      | 110.32   |
| 8   | A     | 1002 | HEA  | C3B-C4B-NB  | 3.58  | 113.96      | 109.84   |
| 8   | G     | 1002 | HEA  | CHB-C1B-NB  | -3.57 | 120.58      | 124.42   |
| 8   | G     | 1001 | HEA  | C27-C19-C20 | 3.52  | 121.34      | 115.23   |
| 9   | A     | 2012 | 3PE  | O21-C2-C1   | 3.49  | 120.85      | 108.34   |
| 8   | A     | 1001 | HEA  | C1D-C2D-C3D | -3.23 | 103.58      | 106.98   |
| 8   | A     | 1001 | HEA  | C27-C19-C20 | 3.23  | 120.83      | 115.23   |
| 8   | A     | 1002 | HEA  | C3D-C4D-ND  | 3.19  | 113.44      | 110.35   |
| 8   | G     | 1001 | HEA  | OMA-CMA-C3A | 3.18  | 132.81      | 125.62   |
| 8   | A     | 1001 | HEA  | C3C-C4C-NC  | 3.14  | 112.44      | 109.80   |
| 8   | G     | 1001 | HEA  | C2D-C1D-ND  | 3.14  | 113.45      | 109.84   |
| 8   | A     | 1001 | HEA  | CMD-C2D-C1D | 3.13  | 129.93      | 125.03   |
| 8   | A     | 1002 | HEA  | C4B-NB-C1B  | -3.13 | 101.50      | 105.21   |
| 8   | G     | 1001 | HEA  | C25-C23-C22 | -3.07 | 113.45      | 122.66   |
| 9   | A     | 2012 | 3PE  | O21-C21-C22 | -3.07 | 104.85      | 111.48   |
| 8   | A     | 1001 | HEA  | C13-C12-C11 | 3.05  | 119.26      | 114.39   |
| 8   | G     | 1002 | HEA  | CAD-C3D-C4D | 3.04  | 129.99      | 124.70   |
| 8   | G     | 1002 | HEA  | C27-C19-C20 | 3.00  | 120.43      | 115.23   |
| 9   | D     | 2011 | 3PE  | C2-O21-C21  | -2.99 | 110.65      | 117.80   |
| 8   | A     | 1001 | HEA  | C13-C14-C15 | -2.97 | 120.82      | 127.62   |
| 9   | G     | 3012 | 3PE  | C3-O31-C31  | -2.96 | 106.31      | 117.12   |
| 9   | C     | 2010 | 3PE  | O21-C21-O22 | 2.96  | 130.62      | 123.70   |
| 8   | A     | 1002 | HEA  | C17-C16-C15 | -2.93 | 103.48      | 113.19   |
| 8   | G     | 1001 | HEA  | C17-C18-C19 | -2.90 | 120.99      | 127.62   |
| 9   | C     | 2008 | 3PE  | C3-O31-C31  | -2.87 | 106.64      | 117.12   |
| 8   | G     | 1002 | HEA  | C12-C13-C14 | 2.87  | 119.70      | 112.16   |
| 8   | G     | 1002 | HEA  | C4B-NB-C1B  | -2.83 | 101.86      | 105.21   |
| 8   | A     | 1002 | HEA  | CAD-C3D-C4D | 2.83  | 129.62      | 124.70   |
| 8   | A     | 1001 | HEA  | CHC-C4B-C3B | -2.82 | 118.69      | 125.80   |
| 8   | G     | 1001 | HEA  | CHC-C4B-C3B | -2.81 | 118.70      | 125.80   |
| 9   | C     | 2010 | 3PE  | C2-O21-C21  | -2.81 | 111.08      | 117.80   |
| 8   | A     | 1001 | HEA  | CHC-C1C-C2C | -2.77 | 119.38      | 127.43   |
| 9   | A     | 2012 | 3PE  | C3-O31-C31  | -2.75 | 107.05      | 117.12   |
| 8   | G     | 1001 | HEA  | CAD-C3D-C4D | 2.75  | 129.50      | 124.70   |
| 8   | A     | 1001 | HEA  | C2D-C1D-ND  | 2.73  | 112.98      | 109.84   |
| 8   | A     | 1001 | HEA  | C26-C15-C14 | -2.73 | 116.61      | 123.63   |
| 8   | G     | 1002 | HEA  | C2B-C1B-NB  | 2.73  | 113.06      | 109.90   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 8   | A     | 1002 | HEA  | C4A-NA-C1A  | -2.70 | 101.42      | 105.82   |
| 8   | A     | 1001 | HEA  | C16-C15-C14 | 2.69  | 127.21      | 121.17   |
| 8   | G     | 1001 | HEA  | C16-C17-C18 | -2.68 | 98.77       | 112.02   |
| 8   | G     | 1001 | HEA  | CMD-C2D-C1D | 2.67  | 129.21      | 125.03   |
| 8   | G     | 1002 | HEA  | O2D-CGD-CBD | 2.67  | 122.43      | 114.00   |
| 9   | I     | 3010 | 3PE  | O31-C31-O32 | 2.62  | 130.19      | 123.63   |
| 9   | G     | 3012 | 3PE  | C3-C2-C1    | -2.60 | 105.72      | 111.78   |
| 8   | G     | 1002 | HEA  | C12-C11-C3B | 2.57  | 116.14      | 112.12   |
| 8   | G     | 1001 | HEA  | C27-C19-C18 | -2.57 | 117.04      | 123.63   |
| 8   | A     | 1001 | HEA  | C2B-C1B-NB  | 2.55  | 112.86      | 109.90   |
| 8   | A     | 1001 | HEA  | O2A-CGA-O1A | -2.55 | 116.77      | 123.33   |
| 8   | G     | 1001 | HEA  | C1D-C2D-C3D | -2.55 | 104.30      | 106.98   |
| 8   | G     | 1002 | HEA  | C2A-C1A-NA  | 2.54  | 112.77      | 110.32   |
| 8   | A     | 1002 | HEA  | C12-C13-C14 | 2.53  | 118.81      | 112.16   |
| 9   | G     | 3012 | 3PE  | C2-O21-C21  | -2.52 | 111.77      | 117.80   |
| 8   | A     | 1001 | HEA  | O11-C11-C12 | 2.51  | 115.79      | 109.14   |
| 8   | G     | 1001 | HEA  | C1A-CHA-C4D | 2.49  | 131.32      | 126.02   |
| 8   | G     | 1001 | HEA  | C24-C23-C22 | 2.49  | 130.13      | 122.66   |
| 8   | A     | 1001 | HEA  | C20-C19-C18 | 2.46  | 126.69      | 121.17   |
| 8   | G     | 1002 | HEA  | C3B-C4B-NB  | 2.46  | 112.67      | 109.84   |
| 9   | A     | 2009 | 3PE  | C33-C32-C31 | -2.46 | 104.69      | 113.69   |
| 8   | A     | 1001 | HEA  | C2C-C1C-NC  | 2.45  | 114.07      | 110.14   |
| 8   | A     | 1002 | HEA  | C2D-C1D-ND  | 2.44  | 112.64      | 109.84   |
| 9   | C     | 2013 | 3PE  | C23-C22-C21 | -2.43 | 104.78      | 113.69   |
| 8   | A     | 1001 | HEA  | CBA-CAA-C2A | 2.42  | 119.23      | 112.53   |
| 9   | C     | 2010 | 3PE  | O21-C2-C3   | -2.42 | 99.66       | 108.34   |
| 9   | D     | 2011 | 3PE  | C2D-C2C-C2B | -2.42 | 102.14      | 114.37   |
| 8   | G     | 1002 | HEA  | C17-C16-C15 | -2.42 | 105.17      | 113.19   |
| 8   | A     | 1002 | HEA  | O11-C11-C3B | -2.41 | 106.83      | 111.26   |
| 9   | I     | 3008 | 3PE  | O31-C3-C2   | 2.41  | 115.34      | 108.40   |
| 8   | A     | 1002 | HEA  | CBA-CAA-C2A | 2.38  | 119.12      | 112.53   |
| 9   | A     | 2009 | 3PE  | O31-C31-O32 | 2.37  | 129.55      | 123.63   |
| 8   | A     | 1002 | HEA  | CAA-C2A-C1A | 2.35  | 129.63      | 124.85   |
| 8   | G     | 1002 | HEA  | O2D-CGD-O1D | -2.35 | 117.30      | 123.33   |
| 9   | C     | 2008 | 3PE  | O21-C21-O22 | 2.35  | 129.19      | 123.70   |
| 8   | G     | 1001 | HEA  | C4A-C3A-C2A | -2.34 | 104.78      | 106.81   |
| 8   | A     | 1002 | HEA  | C2B-C1B-NB  | 2.34  | 112.60      | 109.90   |
| 8   | G     | 1001 | HEA  | C4A-NA-C1A  | -2.33 | 102.02      | 105.82   |
| 8   | A     | 1001 | HEA  | C4C-NC-C1C  | -2.33 | 102.03      | 105.82   |
| 8   | G     | 1002 | HEA  | C3A-C2A-C1A | -2.32 | 104.85      | 107.05   |
| 9   | J     | 3011 | 3PE  | O21-C21-O22 | -2.32 | 118.28      | 123.70   |
| 8   | G     | 1002 | HEA  | C17-C18-C19 | -2.32 | 122.31      | 127.62   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 9   | J     | 3011 | 3PE  | P-O13-C11   | -2.32 | 110.23      | 121.26   |
| 8   | A     | 1001 | HEA  | C16-C17-C18 | -2.30 | 100.64      | 112.02   |
| 8   | A     | 1002 | HEA  | C4C-NC-C1C  | -2.30 | 102.07      | 105.82   |
| 9   | I     | 3010 | 3PE  | C2-O21-C21  | -2.30 | 112.30      | 117.80   |
| 8   | G     | 1001 | HEA  | C12-C11-C3B | -2.29 | 108.54      | 112.12   |
| 9   | C     | 2008 | 3PE  | O21-C2-C3   | -2.28 | 100.17      | 108.34   |
| 8   | A     | 1001 | HEA  | C3C-C2C-C1C | -2.27 | 104.50      | 107.17   |
| 9   | J     | 3011 | 3PE  | C2D-C2C-C2B | -2.26 | 102.94      | 114.37   |
| 9   | I     | 3008 | 3PE  | C3-O31-C31  | -2.23 | 108.96      | 117.12   |
| 8   | A     | 1001 | HEA  | C1C-CHC-C4B | -2.23 | 121.01      | 126.25   |
| 9   | D     | 2011 | 3PE  | O32-C31-C32 | -2.23 | 115.07      | 123.78   |
| 8   | A     | 1001 | HEA  | CHB-C4A-NA  | -2.22 | 122.03      | 124.45   |
| 9   | D     | 2011 | 3PE  | C2E-C2D-C2C | -2.22 | 103.15      | 114.37   |
| 8   | A     | 1002 | HEA  | CHB-C4A-NA  | -2.22 | 122.04      | 124.45   |
| 9   | A     | 2012 | 3PE  | C2E-C2D-C2C | -2.21 | 103.20      | 114.37   |
| 9   | J     | 3011 | 3PE  | P-O11-C1    | -2.20 | 108.77      | 121.35   |
| 9   | G     | 3009 | 3PE  | O21-C21-C22 | 2.19  | 116.23      | 111.48   |
| 9   | C     | 2008 | 3PE  | O31-C3-C2   | 2.16  | 114.61      | 108.40   |
| 9   | I     | 3013 | 3PE  | O31-C3-C2   | 2.14  | 114.58      | 108.40   |
| 8   | G     | 1001 | HEA  | C16-C15-C14 | 2.14  | 125.97      | 121.17   |
| 8   | G     | 1001 | HEA  | C4A-CHB-C1B | 2.13  | 130.55      | 126.02   |
| 9   | D     | 2011 | 3PE  | P-O13-C11   | -2.13 | 111.13      | 121.26   |
| 8   | A     | 1001 | HEA  | C17-C16-C15 | 2.12  | 120.21      | 113.19   |
| 8   | G     | 1002 | HEA  | CBA-CAA-C2A | 2.12  | 118.39      | 112.53   |
| 8   | G     | 1001 | HEA  | CHB-C1B-C2B | 2.11  | 128.36      | 125.03   |
| 9   | G     | 3012 | 3PE  | O21-C2-C1   | 2.10  | 115.89      | 108.34   |
| 8   | A     | 1001 | HEA  | C24-C23-C22 | 2.08  | 128.91      | 122.66   |
| 8   | A     | 1001 | HEA  | C4A-NA-C1A  | -2.08 | 102.42      | 105.82   |
| 8   | A     | 1002 | HEA  | C4C-C3C-C2C | -2.07 | 104.73      | 107.30   |
| 9   | J     | 3011 | 3PE  | O22-C21-C22 | 2.06  | 131.85      | 123.78   |
| 9   | C     | 2008 | 3PE  | O22-C21-C22 | -2.06 | 115.72      | 123.78   |
| 9   | I     | 3013 | 3PE  | C23-C22-C21 | -2.05 | 106.20      | 113.69   |
| 8   | G     | 1001 | HEA  | CBD-CAD-C3D | -2.03 | 106.92      | 112.53   |
| 9   | D     | 2011 | 3PE  | P-O11-C1    | -2.03 | 109.74      | 121.35   |
| 8   | G     | 1001 | HEA  | C4C-C3C-C2C | -2.02 | 104.79      | 107.30   |
| 9   | C     | 2013 | 3PE  | C3-O31-C31  | -2.01 | 109.75      | 117.12   |
| 8   | G     | 1001 | HEA  | CMC-C2C-C1C | 2.00  | 128.47      | 125.42   |

There are no chirality outliers.

All (361) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 8   | A     | 1001 | HEA  | C11-C12-C13-C14 |
| 8   | A     | 1002 | HEA  | C2A-C3A-CMA-OMA |
| 8   | G     | 1001 | HEA  | C12-C11-C3B-C2B |
| 8   | G     | 1001 | HEA  | C11-C12-C13-C14 |
| 9   | A     | 2009 | 3PE  | C1-O11-P-O12    |
| 9   | A     | 2009 | 3PE  | C1-O11-P-O13    |
| 9   | A     | 2009 | 3PE  | C1-O11-P-O14    |
| 9   | A     | 2009 | 3PE  | C11-O13-P-O11   |
| 9   | A     | 2009 | 3PE  | C11-O13-P-O12   |
| 9   | A     | 2009 | 3PE  | C11-O13-P-O14   |
| 9   | A     | 2009 | 3PE  | O13-C11-C12-N   |
| 9   | A     | 2012 | 3PE  | C1-O11-P-O14    |
| 9   | C     | 2008 | 3PE  | C1-O11-P-O12    |
| 9   | C     | 2008 | 3PE  | C1-O11-P-O13    |
| 9   | C     | 2008 | 3PE  | O13-C11-C12-N   |
| 9   | C     | 2010 | 3PE  | C1-O11-P-O12    |
| 9   | C     | 2010 | 3PE  | C1-O11-P-O13    |
| 9   | C     | 2010 | 3PE  | C1-O11-P-O14    |
| 9   | C     | 2010 | 3PE  | O13-C11-C12-N   |
| 9   | C     | 2013 | 3PE  | C1-O11-P-O13    |
| 9   | C     | 2013 | 3PE  | C12-C11-O13-P   |
| 9   | C     | 2013 | 3PE  | O13-C11-C12-N   |
| 9   | C     | 2013 | 3PE  | O22-C21-O21-C2  |
| 9   | C     | 2013 | 3PE  | C22-C21-O21-C2  |
| 9   | D     | 2011 | 3PE  | C11-O13-P-O11   |
| 9   | D     | 2011 | 3PE  | C11-O13-P-O12   |
| 9   | G     | 3009 | 3PE  | C1-O11-P-O12    |
| 9   | G     | 3009 | 3PE  | C11-O13-P-O11   |
| 9   | G     | 3009 | 3PE  | C11-O13-P-O12   |
| 9   | G     | 3009 | 3PE  | C11-O13-P-O14   |
| 9   | G     | 3009 | 3PE  | O13-C11-C12-N   |
| 9   | G     | 3012 | 3PE  | C1-O11-P-O13    |
| 9   | G     | 3012 | 3PE  | C1-O11-P-O14    |
| 9   | G     | 3012 | 3PE  | O13-C11-C12-N   |
| 9   | G     | 3012 | 3PE  | O11-C1-C2-O21   |
| 9   | I     | 3008 | 3PE  | C1-O11-P-O12    |
| 9   | I     | 3008 | 3PE  | O13-C11-C12-N   |
| 9   | I     | 3010 | 3PE  | C1-O11-P-O12    |
| 9   | I     | 3010 | 3PE  | C1-O11-P-O13    |
| 9   | I     | 3010 | 3PE  | C1-O11-P-O14    |
| 9   | I     | 3010 | 3PE  | O13-C11-C12-N   |
| 9   | I     | 3013 | 3PE  | C1-O11-P-O13    |
| 9   | I     | 3013 | 3PE  | C12-C11-O13-P   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 9   | I     | 3013 | 3PE  | O13-C11-C12-N   |
| 9   | I     | 3013 | 3PE  | C22-C21-O21-C2  |
| 9   | J     | 3011 | 3PE  | C11-O13-P-O11   |
| 9   | J     | 3011 | 3PE  | C11-O13-P-O12   |
| 9   | I     | 3008 | 3PE  | O32-C31-O31-C3  |
| 9   | C     | 2008 | 3PE  | O32-C31-O31-C3  |
| 9   | I     | 3013 | 3PE  | O22-C21-O21-C2  |
| 8   | A     | 1001 | HEA  | C3A-C2A-CAA-CBA |
| 8   | G     | 1001 | HEA  | C3A-C2A-CAA-CBA |
| 9   | C     | 2008 | 3PE  | C32-C31-O31-C3  |
| 9   | I     | 3008 | 3PE  | C32-C31-O31-C3  |
| 8   | A     | 1001 | HEA  | C1A-C2A-CAA-CBA |
| 8   | G     | 1001 | HEA  | C1A-C2A-CAA-CBA |
| 9   | C     | 2010 | 3PE  | C38-C39-C3A-C3B |
| 9   | I     | 3010 | 3PE  | C38-C39-C3A-C3B |
| 8   | A     | 1001 | HEA  | C27-C19-C20-C21 |
| 8   | G     | 1001 | HEA  | C27-C19-C20-C21 |
| 8   | A     | 1001 | HEA  | C18-C19-C20-C21 |
| 8   | G     | 1001 | HEA  | C18-C19-C20-C21 |
| 9   | I     | 3013 | 3PE  | C32-C33-C34-C35 |
| 9   | C     | 2013 | 3PE  | C32-C33-C34-C35 |
| 9   | A     | 2009 | 3PE  | C3B-C3C-C3D-C3E |
| 9   | G     | 3009 | 3PE  | C3B-C3C-C3D-C3E |
| 9   | D     | 2011 | 3PE  | C31-C32-C33-C34 |
| 9   | J     | 3011 | 3PE  | C21-C22-C23-C24 |
| 9   | D     | 2011 | 3PE  | C21-C22-C23-C24 |
| 9   | C     | 2010 | 3PE  | C21-C22-C23-C24 |
| 9   | G     | 3009 | 3PE  | C31-C32-C33-C34 |
| 9   | A     | 2009 | 3PE  | C29-C2A-C2B-C2C |
| 9   | D     | 2011 | 3PE  | C28-C29-C2A-C2B |
| 9   | I     | 3008 | 3PE  | C36-C37-C38-C39 |
| 9   | A     | 2009 | 3PE  | C25-C26-C27-C28 |
| 9   | G     | 3012 | 3PE  | C26-C27-C28-C29 |
| 9   | C     | 2008 | 3PE  | C2D-C2E-C2F-C2G |
| 9   | C     | 2013 | 3PE  | C3D-C3E-C3F-C3G |
| 9   | C     | 2013 | 3PE  | C22-C23-C24-C25 |
| 9   | D     | 2011 | 3PE  | C26-C27-C28-C29 |
| 9   | A     | 2009 | 3PE  | C24-C25-C26-C27 |
| 9   | C     | 2008 | 3PE  | C26-C27-C28-C29 |
| 9   | G     | 3012 | 3PE  | C23-C24-C25-C26 |
| 8   | A     | 1001 | HEA  | C4C-C3C-CAC-CBC |
| 9   | J     | 3011 | 3PE  | C31-C32-C33-C34 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 9   | A     | 2012 | 3PE  | C23-C24-C25-C26 |
| 9   | A     | 2009 | 3PE  | C39-C3A-C3B-C3C |
| 9   | C     | 2008 | 3PE  | C27-C28-C29-C2A |
| 9   | I     | 3008 | 3PE  | C3A-C3B-C3C-C3D |
| 9   | I     | 3008 | 3PE  | C26-C27-C28-C29 |
| 9   | J     | 3011 | 3PE  | C26-C27-C28-C29 |
| 9   | G     | 3009 | 3PE  | C29-C2A-C2B-C2C |
| 9   | G     | 3009 | 3PE  | C25-C26-C27-C28 |
| 9   | I     | 3008 | 3PE  | C38-C39-C3A-C3B |
| 9   | I     | 3008 | 3PE  | C27-C28-C29-C2A |
| 9   | I     | 3008 | 3PE  | C32-C33-C34-C35 |
| 9   | I     | 3010 | 3PE  | C3F-C3G-C3H-C3I |
| 9   | A     | 2012 | 3PE  | C28-C29-C2A-C2B |
| 9   | G     | 3009 | 3PE  | C39-C3A-C3B-C3C |
| 9   | G     | 3009 | 3PE  | C24-C25-C26-C27 |
| 9   | I     | 3013 | 3PE  | C3D-C3E-C3F-C3G |
| 9   | A     | 2012 | 3PE  | C26-C27-C28-C29 |
| 9   | A     | 2009 | 3PE  | C3D-C3E-C3F-C3G |
| 9   | C     | 2010 | 3PE  | C3F-C3G-C3H-C3I |
| 9   | C     | 2013 | 3PE  | C39-C3A-C3B-C3C |
| 9   | A     | 2009 | 3PE  | C3E-C3F-C3G-C3H |
| 9   | I     | 3010 | 3PE  | C2E-C2F-C2G-C2H |
| 9   | C     | 2008 | 3PE  | C2A-C2B-C2C-C2D |
| 9   | C     | 2013 | 3PE  | C37-C38-C39-C3A |
| 9   | I     | 3013 | 3PE  | C22-C23-C24-C25 |
| 9   | I     | 3010 | 3PE  | C26-C27-C28-C29 |
| 9   | C     | 2008 | 3PE  | C3A-C3B-C3C-C3D |
| 9   | A     | 2009 | 3PE  | C36-C37-C38-C39 |
| 9   | C     | 2008 | 3PE  | C23-C24-C25-C26 |
| 9   | C     | 2008 | 3PE  | C36-C37-C38-C39 |
| 9   | G     | 3009 | 3PE  | C3D-C3E-C3F-C3G |
| 9   | D     | 2011 | 3PE  | C36-C37-C38-C39 |
| 9   | I     | 3013 | 3PE  | C36-C37-C38-C39 |
| 9   | J     | 3011 | 3PE  | C33-C34-C35-C36 |
| 9   | I     | 3008 | 3PE  | C2A-C2B-C2C-C2D |
| 9   | G     | 3009 | 3PE  | C23-C24-C25-C26 |
| 9   | I     | 3010 | 3PE  | C2A-C2B-C2C-C2D |
| 9   | I     | 3010 | 3PE  | C22-C21-O21-C2  |
| 9   | D     | 2011 | 3PE  | C29-C2A-C2B-C2C |
| 9   | J     | 3011 | 3PE  | C27-C28-C29-C2A |
| 9   | C     | 2008 | 3PE  | C24-C25-C26-C27 |
| 9   | G     | 3012 | 3PE  | C3B-C3C-C3D-C3E |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 9   | I     | 3008 | 3PE  | C24-C25-C26-C27 |
| 9   | I     | 3010 | 3PE  | C21-C22-C23-C24 |
| 9   | I     | 3013 | 3PE  | C2C-C2D-C2E-C2F |
| 9   | A     | 2012 | 3PE  | O11-C1-C2-O21   |
| 9   | I     | 3008 | 3PE  | C2D-C2E-C2F-C2G |
| 9   | G     | 3009 | 3PE  | C21-C22-C23-C24 |
| 9   | C     | 2010 | 3PE  | C36-C37-C38-C39 |
| 9   | G     | 3012 | 3PE  | C28-C29-C2A-C2B |
| 9   | C     | 2013 | 3PE  | C36-C37-C38-C39 |
| 9   | G     | 3009 | 3PE  | C3E-C3F-C3G-C3H |
| 9   | I     | 3008 | 3PE  | C2E-C2F-C2G-C2H |
| 9   | C     | 2013 | 3PE  | C2C-C2D-C2E-C2F |
| 9   | C     | 2008 | 3PE  | C22-C21-O21-C2  |
| 9   | A     | 2009 | 3PE  | C2B-C2C-C2D-C2E |
| 9   | C     | 2008 | 3PE  | C32-C33-C34-C35 |
| 9   | I     | 3008 | 3PE  | C23-C24-C25-C26 |
| 9   | G     | 3009 | 3PE  | C2E-C2F-C2G-C2H |
| 9   | D     | 2011 | 3PE  | C27-C28-C29-C2A |
| 9   | D     | 2011 | 3PE  | C2B-C2C-C2D-C2E |
| 9   | I     | 3010 | 3PE  | C28-C29-C2A-C2B |
| 9   | A     | 2012 | 3PE  | O11-C1-C2-C3    |
| 9   | C     | 2008 | 3PE  | O11-C1-C2-C3    |
| 9   | C     | 2013 | 3PE  | O11-C1-C2-C3    |
| 9   | I     | 3013 | 3PE  | O11-C1-C2-C3    |
| 9   | I     | 3013 | 3PE  | C39-C3A-C3B-C3C |
| 9   | C     | 2010 | 3PE  | C26-C27-C28-C29 |
| 9   | C     | 2013 | 3PE  | C2E-C2F-C2G-C2H |
| 9   | G     | 3012 | 3PE  | C31-C32-C33-C34 |
| 9   | A     | 2009 | 3PE  | C1-C2-C3-O31    |
| 9   | I     | 3013 | 3PE  | C1-C2-C3-O31    |
| 9   | D     | 2011 | 3PE  | C33-C34-C35-C36 |
| 9   | I     | 3013 | 3PE  | C25-C26-C27-C28 |
| 9   | C     | 2008 | 3PE  | C38-C39-C3A-C3B |
| 9   | C     | 2010 | 3PE  | C2E-C2F-C2G-C2H |
| 9   | D     | 2011 | 3PE  | C32-C31-O31-C3  |
| 9   | A     | 2009 | 3PE  | C23-C24-C25-C26 |
| 9   | G     | 3009 | 3PE  | C36-C37-C38-C39 |
| 9   | I     | 3008 | 3PE  | C34-C35-C36-C37 |
| 9   | A     | 2009 | 3PE  | C2E-C2F-C2G-C2H |
| 9   | A     | 2012 | 3PE  | C3B-C3C-C3D-C3E |
| 9   | J     | 3011 | 3PE  | C36-C37-C38-C39 |
| 9   | J     | 3011 | 3PE  | C2B-C2C-C2D-C2E |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 9   | A     | 2009 | 3PE  | C22-C21-O21-C2  |
| 9   | C     | 2010 | 3PE  | C28-C29-C2A-C2B |
| 9   | I     | 3010 | 3PE  | O22-C21-O21-C2  |
| 9   | C     | 2008 | 3PE  | C34-C35-C36-C37 |
| 9   | G     | 3009 | 3PE  | C2B-C2C-C2D-C2E |
| 9   | C     | 2010 | 3PE  | C2A-C2B-C2C-C2D |
| 9   | I     | 3013 | 3PE  | C37-C38-C39-C3A |
| 9   | J     | 3011 | 3PE  | C3E-C3F-C3G-C3H |
| 9   | G     | 3012 | 3PE  | C34-C35-C36-C37 |
| 9   | D     | 2011 | 3PE  | C3B-C3C-C3D-C3E |
| 9   | G     | 3009 | 3PE  | C22-C21-O21-C2  |
| 9   | A     | 2012 | 3PE  | C3E-C3F-C3G-C3H |
| 9   | J     | 3011 | 3PE  | C3F-C3G-C3H-C3I |
| 9   | I     | 3008 | 3PE  | C29-C2A-C2B-C2C |
| 9   | C     | 2008 | 3PE  | C29-C2A-C2B-C2C |
| 9   | A     | 2009 | 3PE  | O21-C2-C3-O31   |
| 9   | C     | 2010 | 3PE  | C32-C31-O31-C3  |
| 9   | I     | 3013 | 3PE  | C2E-C2F-C2G-C2H |
| 9   | C     | 2010 | 3PE  | C23-C24-C25-C26 |
| 8   | A     | 1001 | HEA  | C3B-C11-C12-C13 |
| 8   | G     | 1001 | HEA  | C3B-C11-C12-C13 |
| 9   | A     | 2012 | 3PE  | C34-C35-C36-C37 |
| 9   | J     | 3011 | 3PE  | C3B-C3C-C3D-C3E |
| 9   | J     | 3011 | 3PE  | C29-C2A-C2B-C2C |
| 9   | I     | 3008 | 3PE  | C2F-C2G-C2H-C2I |
| 9   | D     | 2011 | 3PE  | C3E-C3F-C3G-C3H |
| 8   | G     | 1001 | HEA  | C4C-C3C-CAC-CBC |
| 9   | C     | 2013 | 3PE  | C29-C2A-C2B-C2C |
| 9   | G     | 3012 | 3PE  | O11-C1-C2-C3    |
| 9   | I     | 3008 | 3PE  | O11-C1-C2-C3    |
| 9   | I     | 3013 | 3PE  | C3B-C3C-C3D-C3E |
| 9   | D     | 2011 | 3PE  | C3F-C3G-C3H-C3I |
| 9   | D     | 2011 | 3PE  | O32-C31-O31-C3  |
| 9   | I     | 3010 | 3PE  | C32-C33-C34-C35 |
| 9   | C     | 2013 | 3PE  | C25-C26-C27-C28 |
| 9   | C     | 2008 | 3PE  | C2E-C2F-C2G-C2H |
| 9   | C     | 2008 | 3PE  | C2F-C2G-C2H-C2I |
| 9   | C     | 2013 | 3PE  | C1-C2-C3-O31    |
| 9   | G     | 3009 | 3PE  | C1-C2-C3-O31    |
| 9   | G     | 3012 | 3PE  | C1-C2-C3-O31    |
| 9   | G     | 3012 | 3PE  | C24-C25-C26-C27 |
| 9   | C     | 2010 | 3PE  | O32-C31-O31-C3  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 9   | C     | 2008 | 3PE  | O11-C1-C2-O21   |
| 9   | I     | 3008 | 3PE  | O11-C1-C2-O21   |
| 9   | I     | 3010 | 3PE  | O11-C1-C2-O21   |
| 9   | I     | 3013 | 3PE  | O11-C1-C2-O21   |
| 9   | G     | 3012 | 3PE  | C29-C2A-C2B-C2C |
| 9   | C     | 2008 | 3PE  | O21-C2-C3-O31   |
| 9   | G     | 3009 | 3PE  | O21-C2-C3-O31   |
| 9   | G     | 3012 | 3PE  | C3E-C3F-C3G-C3H |
| 9   | A     | 2012 | 3PE  | C37-C38-C39-C3A |
| 9   | I     | 3013 | 3PE  | C35-C36-C37-C38 |
| 9   | C     | 2013 | 3PE  | C3B-C3C-C3D-C3E |
| 8   | G     | 1002 | HEA  | C15-C16-C17-C18 |
| 9   | J     | 3011 | 3PE  | C32-C31-O31-C3  |
| 8   | G     | 1001 | HEA  | C26-C15-C16-C17 |
| 9   | C     | 2008 | 3PE  | C3C-C3D-C3E-C3F |
| 9   | I     | 3013 | 3PE  | C34-C35-C36-C37 |
| 9   | C     | 2008 | 3PE  | O22-C21-O21-C2  |
| 9   | G     | 3009 | 3PE  | O22-C21-O21-C2  |
| 9   | G     | 3012 | 3PE  | C27-C28-C29-C2A |
| 8   | G     | 1001 | HEA  | C14-C15-C16-C17 |
| 9   | A     | 2012 | 3PE  | C24-C25-C26-C27 |
| 9   | C     | 2010 | 3PE  | C32-C33-C34-C35 |
| 9   | D     | 2011 | 3PE  | C3A-C3B-C3C-C3D |
| 9   | C     | 2013 | 3PE  | C33-C34-C35-C36 |
| 9   | A     | 2009 | 3PE  | O22-C21-O21-C2  |
| 9   | C     | 2010 | 3PE  | O11-C1-C2-O21   |
| 9   | C     | 2013 | 3PE  | O11-C1-C2-O21   |
| 8   | A     | 1002 | HEA  | C15-C16-C17-C18 |
| 9   | C     | 2013 | 3PE  | C35-C36-C37-C38 |
| 9   | I     | 3013 | 3PE  | O21-C2-C3-O31   |
| 9   | A     | 2012 | 3PE  | C29-C2A-C2B-C2C |
| 9   | J     | 3011 | 3PE  | O32-C31-O31-C3  |
| 9   | A     | 2012 | 3PE  | C27-C28-C29-C2A |
| 9   | I     | 3013 | 3PE  | C33-C34-C35-C36 |
| 9   | A     | 2009 | 3PE  | C38-C39-C3A-C3B |
| 9   | C     | 2008 | 3PE  | C3B-C3C-C3D-C3E |
| 9   | I     | 3010 | 3PE  | O11-C1-C2-C3    |
| 9   | C     | 2008 | 3PE  | C2C-C2D-C2E-C2F |
| 9   | C     | 2013 | 3PE  | C34-C35-C36-C37 |
| 9   | G     | 3009 | 3PE  | C38-C39-C3A-C3B |
| 9   | I     | 3008 | 3PE  | C2C-C2D-C2E-C2F |
| 9   | J     | 3011 | 3PE  | C24-C25-C26-C27 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 9   | I     | 3013 | 3PE  | C3A-C3B-C3C-C3D |
| 9   | A     | 2009 | 3PE  | C33-C34-C35-C36 |
| 8   | A     | 1002 | HEA  | C4A-C3A-CMA-OMA |
| 9   | C     | 2013 | 3PE  | O21-C2-C3-O31   |
| 9   | I     | 3008 | 3PE  | O21-C2-C3-O31   |
| 9   | I     | 3010 | 3PE  | C23-C24-C25-C26 |
| 9   | C     | 2008 | 3PE  | C1-C2-C3-O31    |
| 9   | G     | 3012 | 3PE  | C39-C3A-C3B-C3C |
| 9   | C     | 2010 | 3PE  | C22-C21-O21-C2  |
| 9   | I     | 3010 | 3PE  | C32-C31-O31-C3  |
| 9   | G     | 3009 | 3PE  | C34-C35-C36-C37 |
| 8   | A     | 1001 | HEA  | O11-C11-C3B-C2B |
| 8   | G     | 1001 | HEA  | O11-C11-C3B-C2B |
| 9   | A     | 2012 | 3PE  | C1-O11-P-O12    |
| 9   | A     | 2012 | 3PE  | C1-O11-P-O13    |
| 9   | A     | 2012 | 3PE  | O13-C11-C12-N   |
| 9   | C     | 2008 | 3PE  | C1-O11-P-O14    |
| 9   | C     | 2008 | 3PE  | C11-O13-P-O14   |
| 9   | C     | 2013 | 3PE  | C1-O11-P-O14    |
| 9   | C     | 2013 | 3PE  | C11-O13-P-O14   |
| 9   | G     | 3009 | 3PE  | C1-O11-P-O13    |
| 9   | G     | 3009 | 3PE  | C1-O11-P-O14    |
| 9   | G     | 3012 | 3PE  | C1-O11-P-O12    |
| 9   | I     | 3008 | 3PE  | C1-O11-P-O13    |
| 9   | I     | 3008 | 3PE  | C1-O11-P-O14    |
| 9   | I     | 3013 | 3PE  | C1-O11-P-O14    |
| 9   | I     | 3008 | 3PE  | C3C-C3D-C3E-C3F |
| 8   | A     | 1001 | HEA  | C2C-C3C-CAC-CBC |
| 9   | A     | 2012 | 3PE  | C39-C3A-C3B-C3C |
| 9   | I     | 3010 | 3PE  | O32-C31-O31-C3  |
| 9   | A     | 2012 | 3PE  | C38-C39-C3A-C3B |
| 9   | J     | 3011 | 3PE  | C3A-C3B-C3C-C3D |
| 9   | I     | 3013 | 3PE  | C31-C32-C33-C34 |
| 9   | A     | 2009 | 3PE  | O11-C1-C2-C3    |
| 9   | A     | 2012 | 3PE  | C31-C32-C33-C34 |
| 9   | C     | 2010 | 3PE  | O22-C21-O21-C2  |
| 9   | G     | 3009 | 3PE  | C33-C34-C35-C36 |
| 9   | G     | 3012 | 3PE  | C37-C38-C39-C3A |
| 8   | A     | 1001 | HEA  | C26-C15-C16-C17 |
| 9   | I     | 3010 | 3PE  | C3C-C3D-C3E-C3F |
| 9   | I     | 3010 | 3PE  | C36-C37-C38-C39 |
| 9   | D     | 2011 | 3PE  | C2A-C2B-C2C-C2D |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 9   | G     | 3012 | 3PE  | C38-C39-C3A-C3B |
| 9   | C     | 2008 | 3PE  | C37-C38-C39-C3A |
| 9   | I     | 3008 | 3PE  | C1-C2-C3-O31    |
| 8   | A     | 1001 | HEA  | C12-C11-C3B-C2B |
| 8   | A     | 1002 | HEA  | CAD-CBD-CGD-O2D |
| 9   | A     | 2009 | 3PE  | C34-C35-C36-C37 |
| 9   | G     | 3012 | 3PE  | C2D-C2E-C2F-C2G |
| 8   | A     | 1002 | HEA  | CAD-CBD-CGD-O1D |
| 9   | C     | 2008 | 3PE  | C1-C2-O21-C21   |
| 9   | C     | 2008 | 3PE  | C3-C2-O21-C21   |
| 9   | I     | 3008 | 3PE  | C3-C2-O21-C21   |
| 8   | G     | 1001 | HEA  | C2C-C3C-CAC-CBC |
| 8   | A     | 1001 | HEA  | O11-C11-C12-C13 |
| 8   | G     | 1001 | HEA  | O11-C11-C12-C13 |
| 9   | I     | 3008 | 3PE  | C3F-C3G-C3H-C3I |
| 9   | G     | 3012 | 3PE  | C36-C37-C38-C39 |
| 9   | G     | 3009 | 3PE  | O11-C1-C2-C3    |
| 8   | A     | 1001 | HEA  | C14-C15-C16-C17 |
| 9   | J     | 3011 | 3PE  | C2D-C2E-C2F-C2G |
| 9   | A     | 2012 | 3PE  | C2A-C2B-C2C-C2D |
| 9   | I     | 3013 | 3PE  | C2A-C2B-C2C-C2D |
| 9   | J     | 3011 | 3PE  | C23-C24-C25-C26 |
| 8   | G     | 1002 | HEA  | CAA-CBA-CGA-O2A |
| 8   | G     | 1002 | HEA  | CAD-CBD-CGD-O2D |
| 8   | G     | 1002 | HEA  | C26-C15-C16-C17 |
| 9   | I     | 3010 | 3PE  | C2C-C2D-C2E-C2F |
| 9   | C     | 2013 | 3PE  | C3A-C3B-C3C-C3D |
| 9   | I     | 3010 | 3PE  | C1-C2-C3-O31    |
| 9   | I     | 3008 | 3PE  | O22-C21-O21-C2  |
| 9   | J     | 3011 | 3PE  | C28-C29-C2A-C2B |
| 8   | A     | 1002 | HEA  | C11-C12-C13-C14 |
| 9   | I     | 3008 | 3PE  | C3B-C3C-C3D-C3E |
| 8   | G     | 1002 | HEA  | CAD-CBD-CGD-O1D |
| 8   | A     | 1002 | HEA  | CAA-CBA-CGA-O2A |
| 9   | D     | 2011 | 3PE  | C34-C35-C36-C37 |
| 9   | C     | 2008 | 3PE  | C3F-C3G-C3H-C3I |
| 8   | G     | 1002 | HEA  | CAA-CBA-CGA-O1A |
| 8   | A     | 1001 | HEA  | CAA-CBA-CGA-O2A |
| 8   | G     | 1001 | HEA  | CAA-CBA-CGA-O2A |
| 9   | I     | 3013 | 3PE  | C29-C2A-C2B-C2C |
| 8   | A     | 1002 | HEA  | CAA-CBA-CGA-O1A |
| 8   | A     | 1001 | HEA  | CAA-CBA-CGA-O1A |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 9   | A     | 2009 | 3PE  | C37-C38-C39-C3A |
| 9   | J     | 3011 | 3PE  | C2A-C2B-C2C-C2D |
| 8   | G     | 1001 | HEA  | CAA-CBA-CGA-O1A |
| 8   | A     | 1002 | HEA  | C20-C21-C22-C23 |
| 9   | I     | 3008 | 3PE  | C22-C21-O21-C2  |
| 9   | I     | 3010 | 3PE  | O31-C31-C32-C33 |
| 9   | I     | 3008 | 3PE  | C37-C38-C39-C3A |
| 9   | A     | 2009 | 3PE  | C31-C32-C33-C34 |
| 9   | C     | 2008 | 3PE  | C21-C22-C23-C24 |
| 9   | I     | 3010 | 3PE  | O21-C2-C3-O31   |
| 9   | G     | 3009 | 3PE  | C37-C38-C39-C3A |
| 9   | I     | 3010 | 3PE  | C31-C32-C33-C34 |
| 9   | D     | 2011 | 3PE  | C24-C25-C26-C27 |
| 9   | C     | 2010 | 3PE  | O31-C31-C32-C33 |
| 9   | I     | 3010 | 3PE  | O21-C21-C22-C23 |
| 9   | I     | 3010 | 3PE  | O32-C31-C32-C33 |
| 9   | A     | 2012 | 3PE  | C36-C37-C38-C39 |
| 9   | C     | 2010 | 3PE  | O21-C21-C22-C23 |
| 8   | A     | 1001 | HEA  | O11-C11-C3B-C4B |
| 8   | G     | 1001 | HEA  | O11-C11-C3B-C4B |
| 9   | D     | 2011 | 3PE  | O21-C21-C22-C23 |
| 8   | A     | 1001 | HEA  | C16-C17-C18-C19 |
| 9   | J     | 3011 | 3PE  | O21-C21-C22-C23 |
| 9   | C     | 2010 | 3PE  | C25-C26-C27-C28 |

There are no ring outliers.

16 monomers are involved in 280 short contacts:

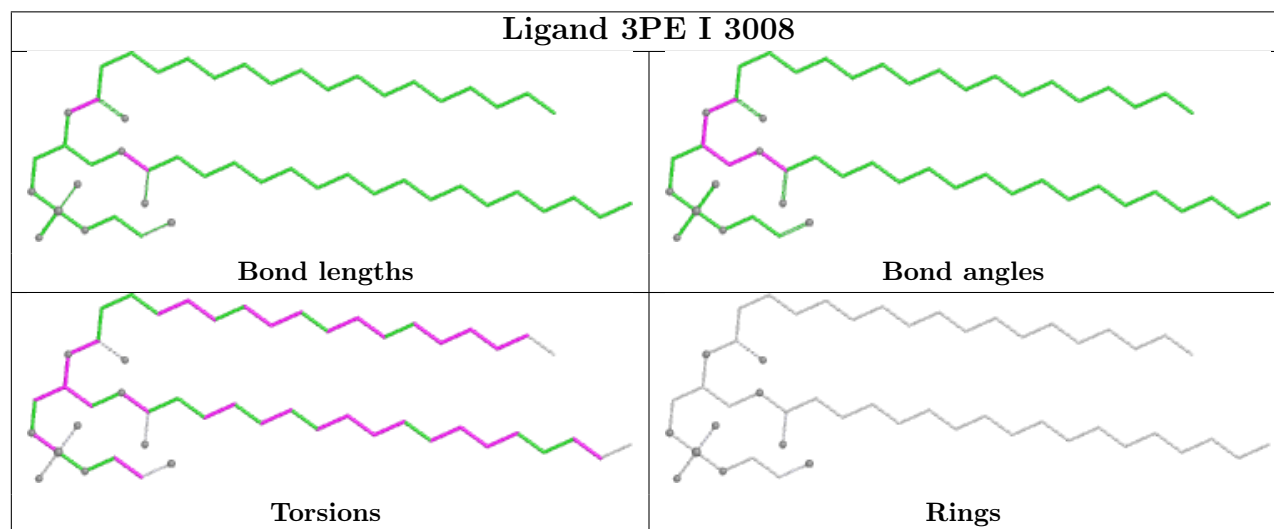
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 9   | I     | 3008 | 3PE  | 13      | 0            |
| 8   | G     | 1002 | HEA  | 15      | 0            |
| 9   | C     | 2008 | 3PE  | 13      | 0            |
| 9   | G     | 3009 | 3PE  | 20      | 0            |
| 8   | A     | 1002 | HEA  | 19      | 0            |
| 9   | I     | 3010 | 3PE  | 24      | 0            |
| 9   | A     | 2009 | 3PE  | 18      | 0            |
| 8   | A     | 1001 | HEA  | 18      | 0            |
| 9   | J     | 3011 | 3PE  | 12      | 0            |
| 9   | I     | 3013 | 3PE  | 22      | 0            |
| 9   | C     | 2010 | 3PE  | 24      | 0            |
| 9   | D     | 2011 | 3PE  | 17      | 0            |
| 9   | G     | 3012 | 3PE  | 22      | 0            |

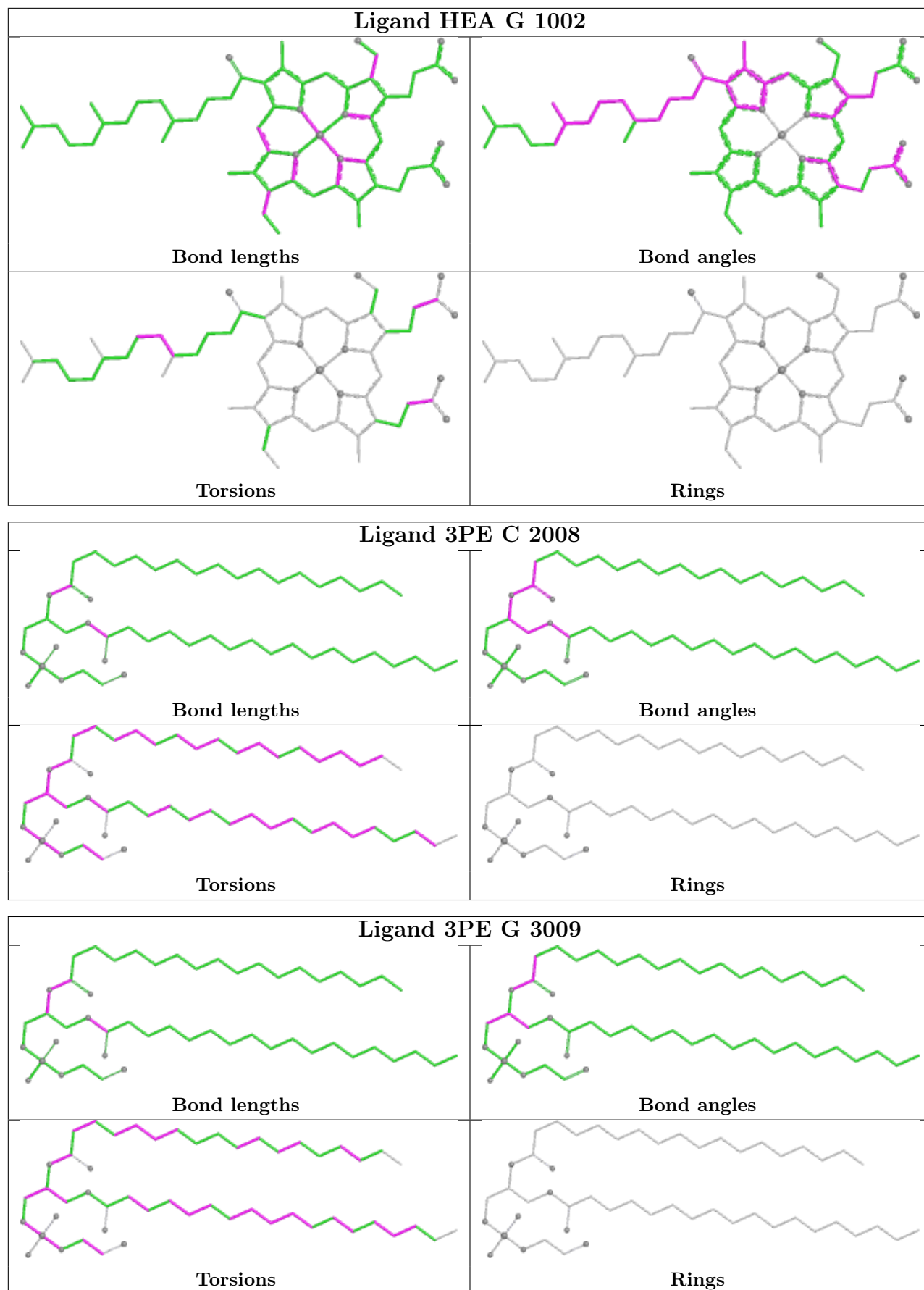
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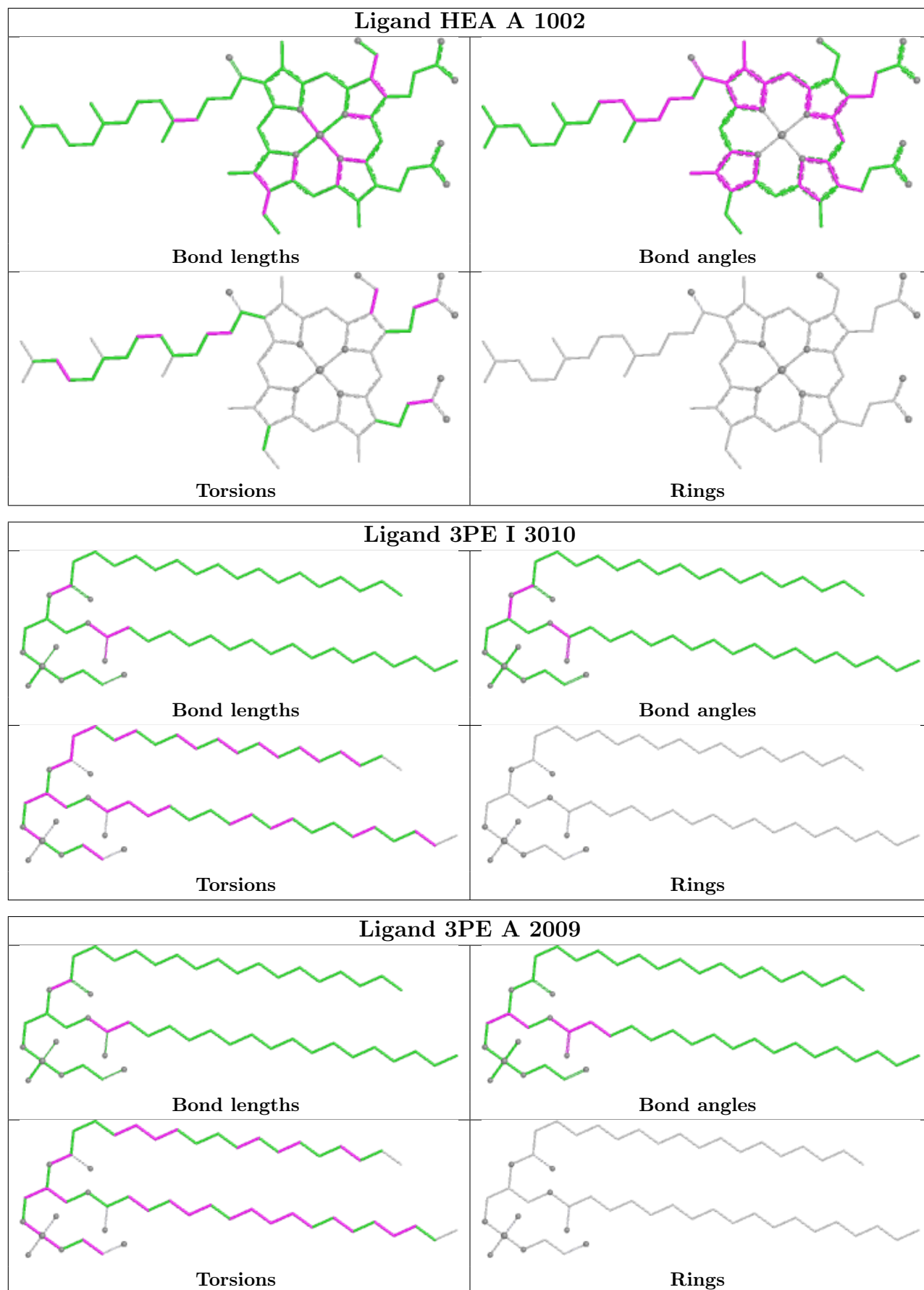
*Continued from previous page...*

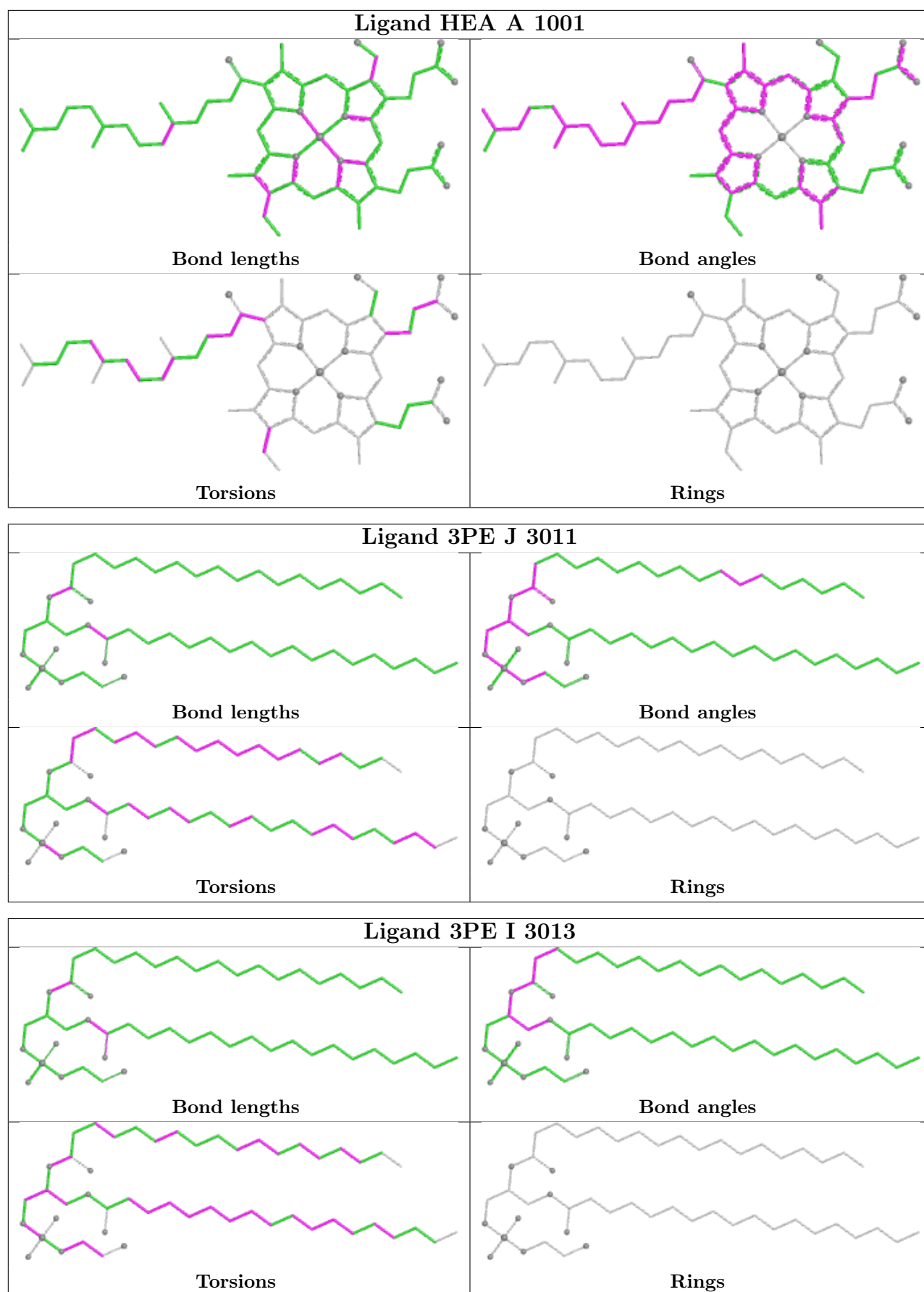
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 9   | A     | 2012 | 3PE  | 20      | 0            |
| 9   | C     | 2013 | 3PE  | 21      | 0            |
| 8   | G     | 1001 | HEA  | 23      | 0            |

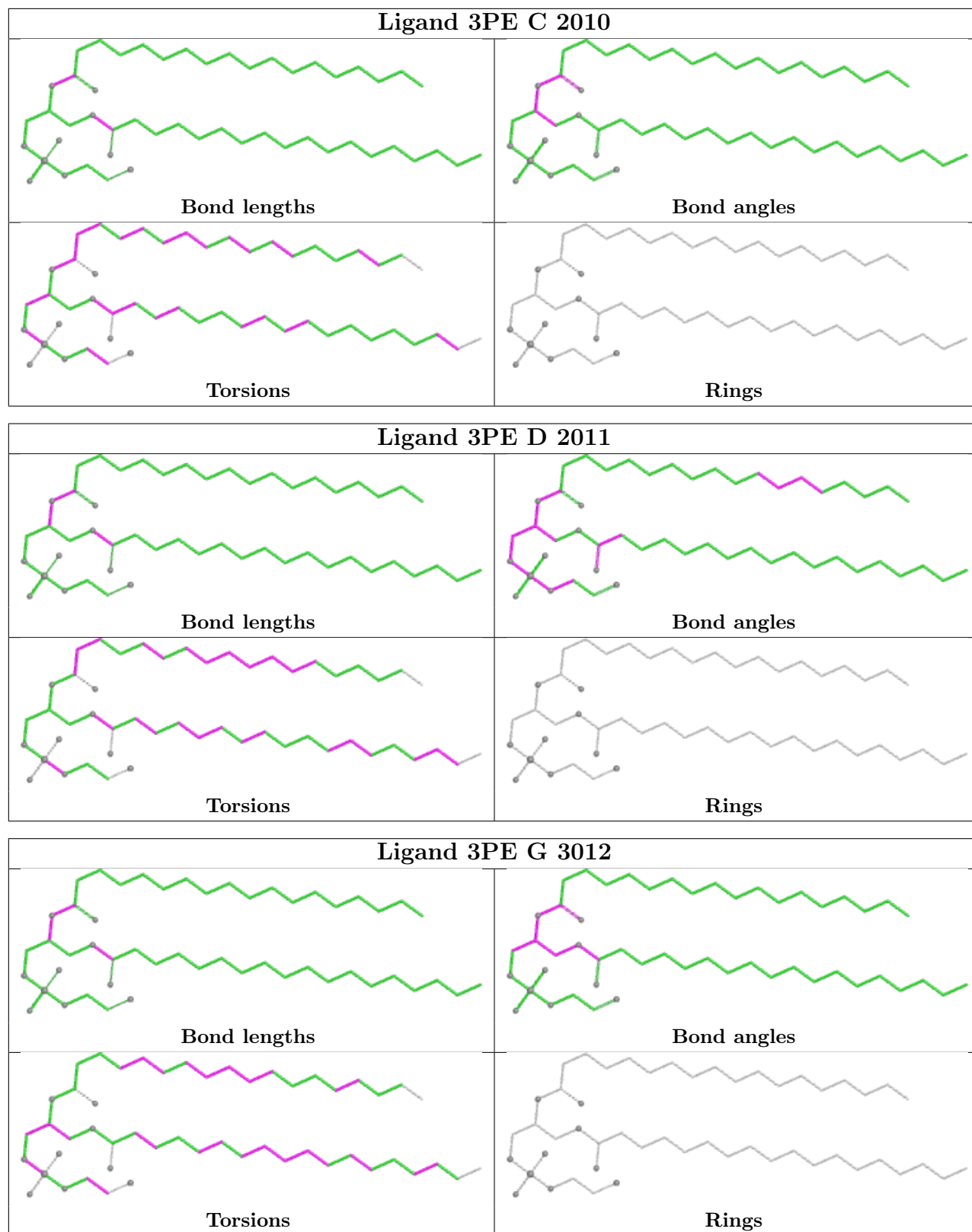
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

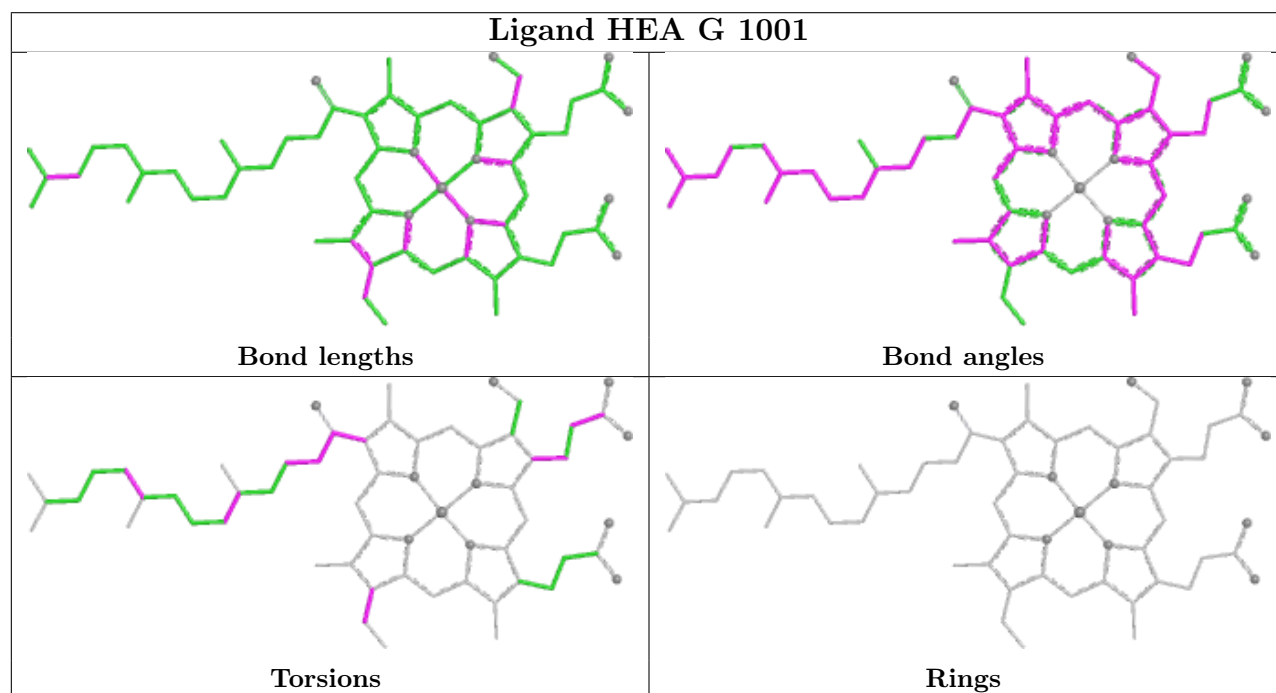
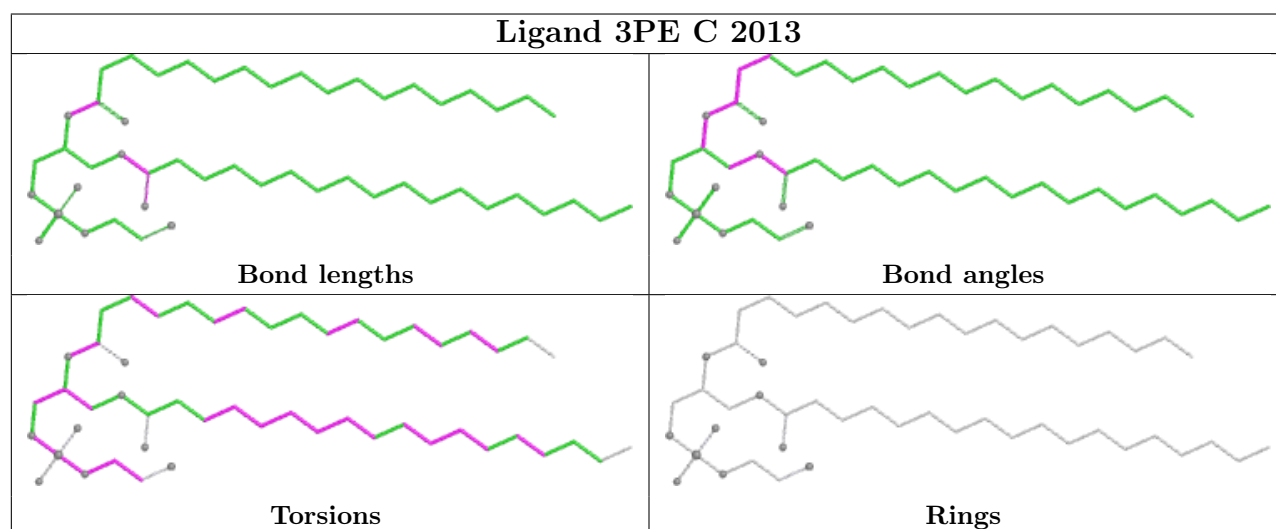
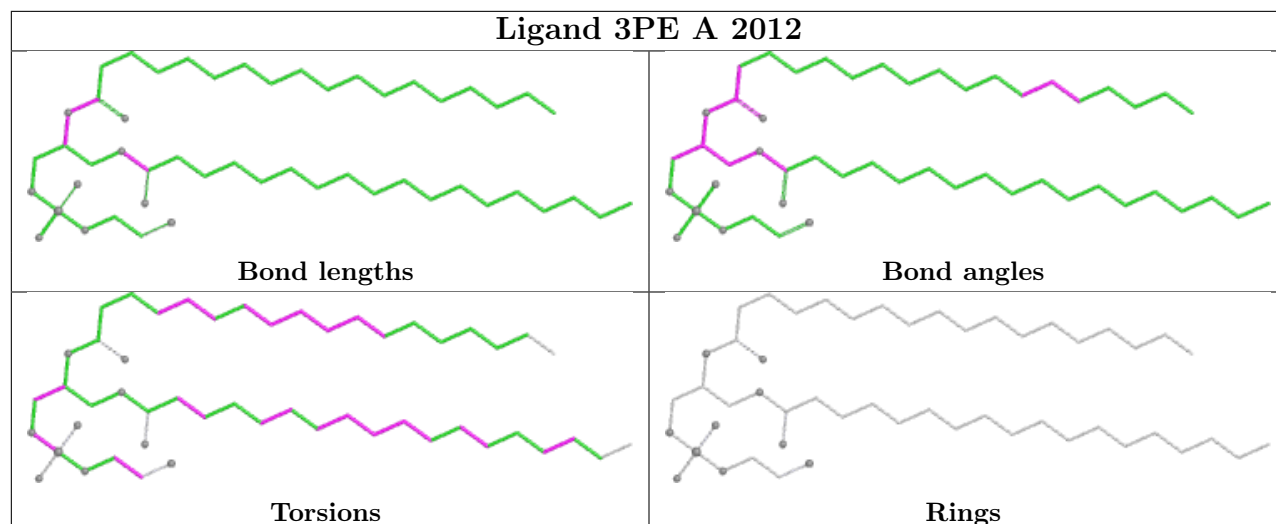












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.