



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 07:46 PM UTC

PDB ID : 3ML6 / pdb\_00003ml6  
Title : a complex between Dishevelled2 and clathrin adaptor AP-2  
Authors : Yu, A.; Xing, Y.; Harrison, S.C.; Kirchhausen, T.L.  
Deposited on : 2010-04-16  
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

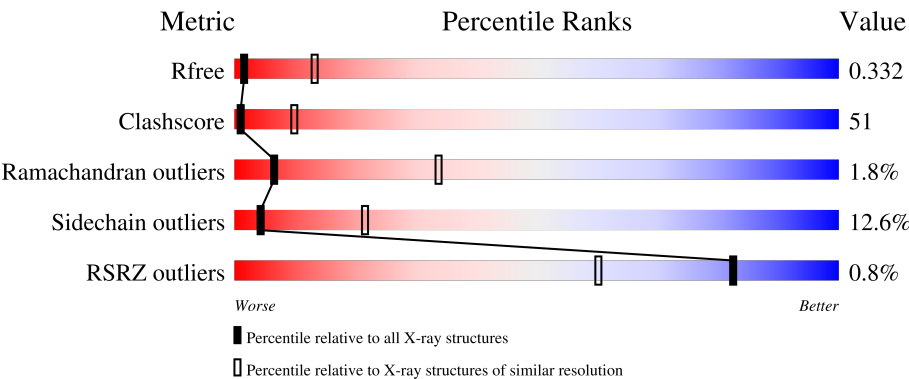
|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                             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

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1085 (3.54-3.46)                                      |
| Clashscore            | 190562                      | 1140 (3.54-3.46)                                      |
| Ramachandran outliers | 187476                      | 1113 (3.54-3.46)                                      |
| Sidechain outliers    | 187428                      | 1114 (3.54-3.46)                                      |
| RSRZ outliers         | 180081                      | 1084 (3.54-3.46)                                      |

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

| Mol | Chain | Length | Quality of chain                               |
|-----|-------|--------|------------------------------------------------|
| 1   | A     | 385    | <div><div>2%</div><div>31%48%12%9%</div></div> |
| 1   | B     | 385    | <div><div>%</div><div>32%47%9%12%</div></div>  |
| 1   | C     | 385    | <div><div>%</div><div>30%53%8%9%</div></div>   |
| 1   | D     | 385    | <div><div>%</div><div>27%50%10%13%</div></div> |
| 1   | E     | 385    | <div><div></div><div>29%50%9%12%</div></div>   |

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| Mol | Chain | Length | Quality of chain                                                                                                                                                                  |
|-----|-------|--------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 1   | F     | 385    | <div><div><div>%</div><div><div></div><div>33%</div></div><div><div></div><div>48%</div></div><div><div></div><div>8%</div></div><div><div></div><div>12%</div></div></div></div> |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 16319 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 Chimeric complex between protein Dishevelled2 homolog dvl-2 and clathrin adaptor AP-2 complex subunit mu.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 351      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2787  | 1790 | 480 | 498 | 19 |         |         |       |
| 1   | B     | 339      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2695  | 1732 | 466 | 478 | 19 |         |         |       |
| 1   | C     | 350      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2780  | 1785 | 479 | 497 | 19 |         |         |       |
| 1   | D     | 336      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2668  | 1716 | 460 | 473 | 19 |         |         |       |
| 1   | E     | 338      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2686  | 1725 | 463 | 479 | 19 |         |         |       |
| 1   | F     | 340      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2703  | 1736 | 467 | 481 | 19 |         |         |       |

There are 150 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 415     | GLY      | -      | expression tag | UNP Q60838 |
| A     | 416     | ALA      | -      | expression tag | UNP Q60838 |
| A     | 1147    | GLY      | -      | linker         | UNP P84092 |
| A     | 1148    | PRO      | -      | linker         | UNP P84092 |
| A     | 1149    | ARG      | -      | linker         | UNP P84092 |
| A     | 1150    | PRO      | -      | linker         | UNP P84092 |
| A     | 1151    | TYR      | -      | linker         | UNP P84092 |
| A     | 1152    | SER      | -      | linker         | UNP P84092 |
| A     | 1153    | PRO      | -      | linker         | UNP P84092 |
| A     | 1154    | GLN      | -      | linker         | UNP P84092 |
| A     | 1155    | PRO      | -      | linker         | UNP P84092 |
| A     | 1156    | PRO      | -      | linker         | UNP P84092 |
| A     | 1157    | PRO      | -      | linker         | UNP P84092 |
| A     | 1158    | TYR      | -      | linker         | UNP P84092 |
| A     | 1159    | HIS      | -      | linker         | UNP P84092 |
| A     | 1160    | GLU      | -      | linker         | UNP P84092 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 1161    | LEU      | -      | linker         | UNP P84092 |
| A     | 1162    | GLU      | -      | linker         | UNP P84092 |
| A     | 1163    | PHE      | -      | linker         | UNP P84092 |
| A     | 1164    | GLY      | -      | linker         | UNP P84092 |
| A     | 1165    | GLY      | -      | linker         | UNP P84092 |
| A     | 1166    | SER      | -      | linker         | UNP P84092 |
| A     | 1167    | GLY      | -      | linker         | UNP P84092 |
| A     | 1168    | GLY      | -      | linker         | UNP P84092 |
| A     | 1169    | SER      | -      | linker         | UNP P84092 |
| B     | 415     | GLY      | -      | expression tag | UNP Q60838 |
| B     | 416     | ALA      | -      | expression tag | UNP Q60838 |
| B     | 1147    | GLY      | -      | linker         | UNP P84092 |
| B     | 1148    | PRO      | -      | linker         | UNP P84092 |
| B     | 1149    | ARG      | -      | linker         | UNP P84092 |
| B     | 1150    | PRO      | -      | linker         | UNP P84092 |
| B     | 1151    | TYR      | -      | linker         | UNP P84092 |
| B     | 1152    | SER      | -      | linker         | UNP P84092 |
| B     | 1153    | PRO      | -      | linker         | UNP P84092 |
| B     | 1154    | GLN      | -      | linker         | UNP P84092 |
| B     | 1155    | PRO      | -      | linker         | UNP P84092 |
| B     | 1156    | PRO      | -      | linker         | UNP P84092 |
| B     | 1157    | PRO      | -      | linker         | UNP P84092 |
| B     | 1158    | TYR      | -      | linker         | UNP P84092 |
| B     | 1159    | HIS      | -      | linker         | UNP P84092 |
| B     | 1160    | GLU      | -      | linker         | UNP P84092 |
| B     | 1161    | LEU      | -      | linker         | UNP P84092 |
| B     | 1162    | GLU      | -      | linker         | UNP P84092 |
| B     | 1163    | PHE      | -      | linker         | UNP P84092 |
| B     | 1164    | GLY      | -      | linker         | UNP P84092 |
| B     | 1165    | GLY      | -      | linker         | UNP P84092 |
| B     | 1166    | SER      | -      | linker         | UNP P84092 |
| B     | 1167    | GLY      | -      | linker         | UNP P84092 |
| B     | 1168    | GLY      | -      | linker         | UNP P84092 |
| B     | 1169    | SER      | -      | linker         | UNP P84092 |
| C     | 415     | GLY      | -      | expression tag | UNP Q60838 |
| C     | 416     | ALA      | -      | expression tag | UNP Q60838 |
| C     | 1147    | GLY      | -      | linker         | UNP P84092 |
| C     | 1148    | PRO      | -      | linker         | UNP P84092 |
| C     | 1149    | ARG      | -      | linker         | UNP P84092 |
| C     | 1150    | PRO      | -      | linker         | UNP P84092 |
| C     | 1151    | TYR      | -      | linker         | UNP P84092 |
| C     | 1152    | SER      | -      | linker         | UNP P84092 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| C     | 1153    | PRO      | -      | linker         | UNP P84092 |
| C     | 1154    | GLN      | -      | linker         | UNP P84092 |
| C     | 1155    | PRO      | -      | linker         | UNP P84092 |
| C     | 1156    | PRO      | -      | linker         | UNP P84092 |
| C     | 1157    | PRO      | -      | linker         | UNP P84092 |
| C     | 1158    | TYR      | -      | linker         | UNP P84092 |
| C     | 1159    | HIS      | -      | linker         | UNP P84092 |
| C     | 1160    | GLU      | -      | linker         | UNP P84092 |
| C     | 1161    | LEU      | -      | linker         | UNP P84092 |
| C     | 1162    | GLU      | -      | linker         | UNP P84092 |
| C     | 1163    | PHE      | -      | linker         | UNP P84092 |
| C     | 1164    | GLY      | -      | linker         | UNP P84092 |
| C     | 1165    | GLY      | -      | linker         | UNP P84092 |
| C     | 1166    | SER      | -      | linker         | UNP P84092 |
| C     | 1167    | GLY      | -      | linker         | UNP P84092 |
| C     | 1168    | GLY      | -      | linker         | UNP P84092 |
| C     | 1169    | SER      | -      | linker         | UNP P84092 |
| D     | 415     | GLY      | -      | expression tag | UNP Q60838 |
| D     | 416     | ALA      | -      | expression tag | UNP Q60838 |
| D     | 1147    | GLY      | -      | linker         | UNP P84092 |
| D     | 1148    | PRO      | -      | linker         | UNP P84092 |
| D     | 1149    | ARG      | -      | linker         | UNP P84092 |
| D     | 1150    | PRO      | -      | linker         | UNP P84092 |
| D     | 1151    | TYR      | -      | linker         | UNP P84092 |
| D     | 1152    | SER      | -      | linker         | UNP P84092 |
| D     | 1153    | PRO      | -      | linker         | UNP P84092 |
| D     | 1154    | GLN      | -      | linker         | UNP P84092 |
| D     | 1155    | PRO      | -      | linker         | UNP P84092 |
| D     | 1156    | PRO      | -      | linker         | UNP P84092 |
| D     | 1157    | PRO      | -      | linker         | UNP P84092 |
| D     | 1158    | TYR      | -      | linker         | UNP P84092 |
| D     | 1159    | HIS      | -      | linker         | UNP P84092 |
| D     | 1160    | GLU      | -      | linker         | UNP P84092 |
| D     | 1161    | LEU      | -      | linker         | UNP P84092 |
| D     | 1162    | GLU      | -      | linker         | UNP P84092 |
| D     | 1163    | PHE      | -      | linker         | UNP P84092 |
| D     | 1164    | GLY      | -      | linker         | UNP P84092 |
| D     | 1165    | GLY      | -      | linker         | UNP P84092 |
| D     | 1166    | SER      | -      | linker         | UNP P84092 |
| D     | 1167    | GLY      | -      | linker         | UNP P84092 |
| D     | 1168    | GLY      | -      | linker         | UNP P84092 |
| D     | 1169    | SER      | -      | linker         | UNP P84092 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| E     | 415     | GLY      | -      | expression tag | UNP Q60838 |
| E     | 416     | ALA      | -      | expression tag | UNP Q60838 |
| E     | 1147    | GLY      | -      | linker         | UNP P84092 |
| E     | 1148    | PRO      | -      | linker         | UNP P84092 |
| E     | 1149    | ARG      | -      | linker         | UNP P84092 |
| E     | 1150    | PRO      | -      | linker         | UNP P84092 |
| E     | 1151    | TYR      | -      | linker         | UNP P84092 |
| E     | 1152    | SER      | -      | linker         | UNP P84092 |
| E     | 1153    | PRO      | -      | linker         | UNP P84092 |
| E     | 1154    | GLN      | -      | linker         | UNP P84092 |
| E     | 1155    | PRO      | -      | linker         | UNP P84092 |
| E     | 1156    | PRO      | -      | linker         | UNP P84092 |
| E     | 1157    | PRO      | -      | linker         | UNP P84092 |
| E     | 1158    | TYR      | -      | linker         | UNP P84092 |
| E     | 1159    | HIS      | -      | linker         | UNP P84092 |
| E     | 1160    | GLU      | -      | linker         | UNP P84092 |
| E     | 1161    | LEU      | -      | linker         | UNP P84092 |
| E     | 1162    | GLU      | -      | linker         | UNP P84092 |
| E     | 1163    | PHE      | -      | linker         | UNP P84092 |
| E     | 1164    | GLY      | -      | linker         | UNP P84092 |
| E     | 1165    | GLY      | -      | linker         | UNP P84092 |
| E     | 1166    | SER      | -      | linker         | UNP P84092 |
| E     | 1167    | GLY      | -      | linker         | UNP P84092 |
| E     | 1168    | GLY      | -      | linker         | UNP P84092 |
| E     | 1169    | SER      | -      | linker         | UNP P84092 |
| F     | 415     | GLY      | -      | expression tag | UNP Q60838 |
| F     | 416     | ALA      | -      | expression tag | UNP Q60838 |
| F     | 1147    | GLY      | -      | linker         | UNP P84092 |
| F     | 1148    | PRO      | -      | linker         | UNP P84092 |
| F     | 1149    | ARG      | -      | linker         | UNP P84092 |
| F     | 1150    | PRO      | -      | linker         | UNP P84092 |
| F     | 1151    | TYR      | -      | linker         | UNP P84092 |
| F     | 1152    | SER      | -      | linker         | UNP P84092 |
| F     | 1153    | PRO      | -      | linker         | UNP P84092 |
| F     | 1154    | GLN      | -      | linker         | UNP P84092 |
| F     | 1155    | PRO      | -      | linker         | UNP P84092 |
| F     | 1156    | PRO      | -      | linker         | UNP P84092 |
| F     | 1157    | PRO      | -      | linker         | UNP P84092 |
| F     | 1158    | TYR      | -      | linker         | UNP P84092 |
| F     | 1159    | HIS      | -      | linker         | UNP P84092 |
| F     | 1160    | GLU      | -      | linker         | UNP P84092 |
| F     | 1161    | LEU      | -      | linker         | UNP P84092 |

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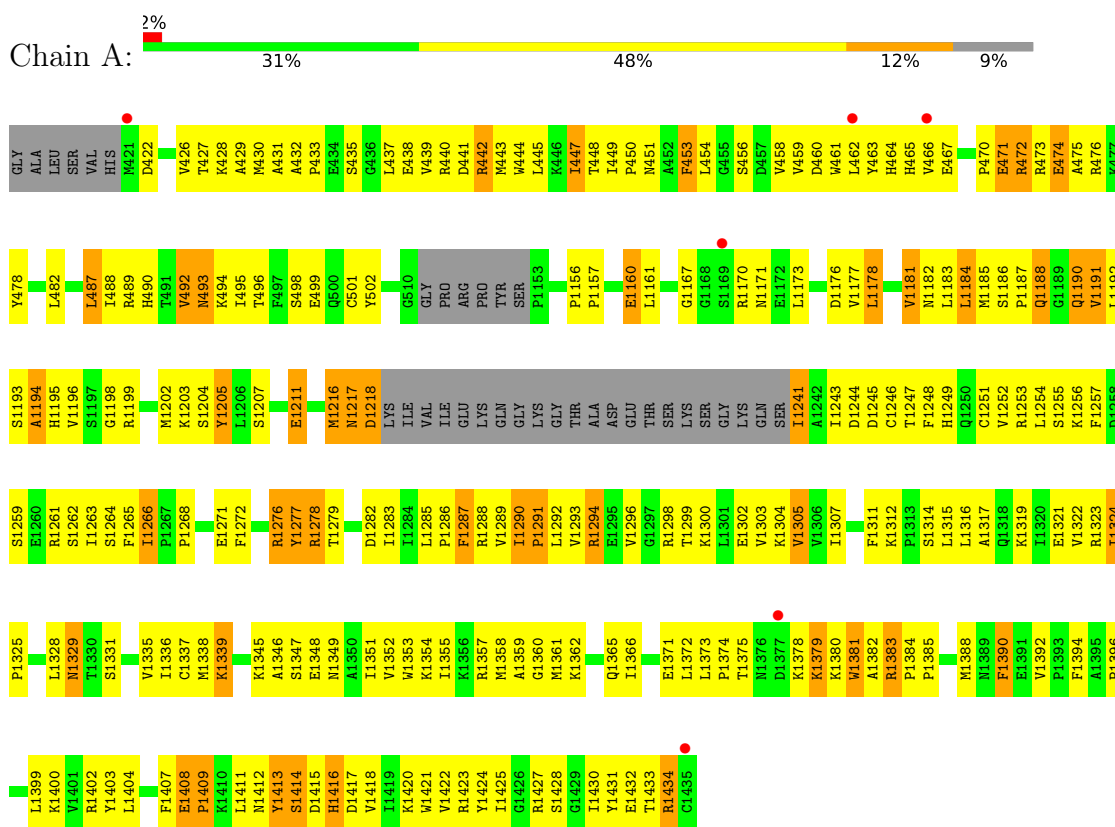
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| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| F     | 1162    | GLU      | -      | linker  | UNP P84092 |
| F     | 1163    | PHE      | -      | linker  | UNP P84092 |
| F     | 1164    | GLY      | -      | linker  | UNP P84092 |
| F     | 1165    | GLY      | -      | linker  | UNP P84092 |
| F     | 1166    | SER      | -      | linker  | UNP P84092 |
| F     | 1167    | GLY      | -      | linker  | UNP P84092 |
| F     | 1168    | GLY      | -      | linker  | UNP P84092 |
| F     | 1169    | SER      | -      | linker  | UNP P84092 |

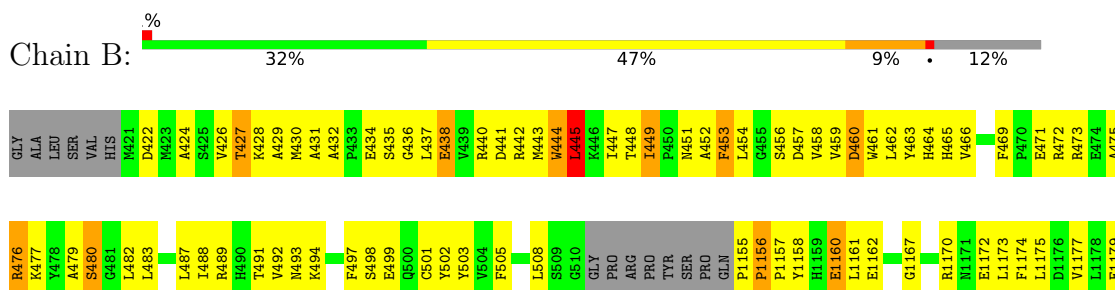
### 3 Residue-property plots

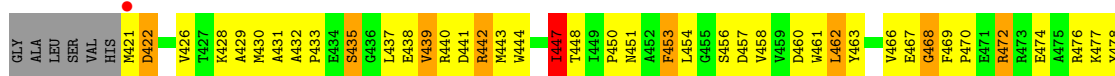
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

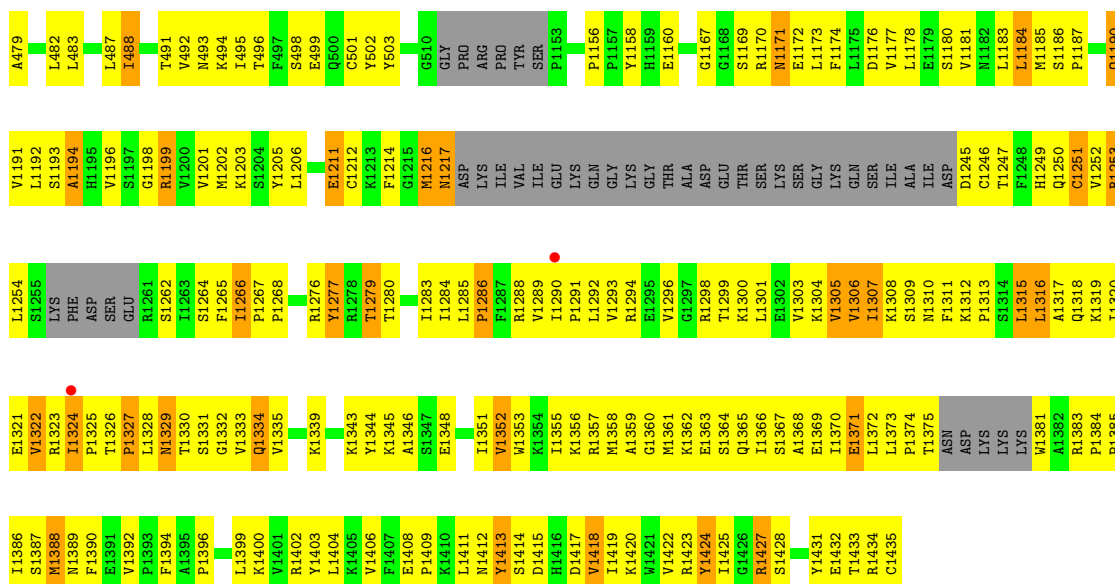
- Molecule 1: Chimeric complex between protein Dishevelled2 homolog dvl-2 and clathrin adaptor AP-2 complex subunit mu



- Molecule 1: Chimeric complex between protein Dishevelled2 homolog dvl-2 and clathrin adaptor AP-2 complex subunit mu

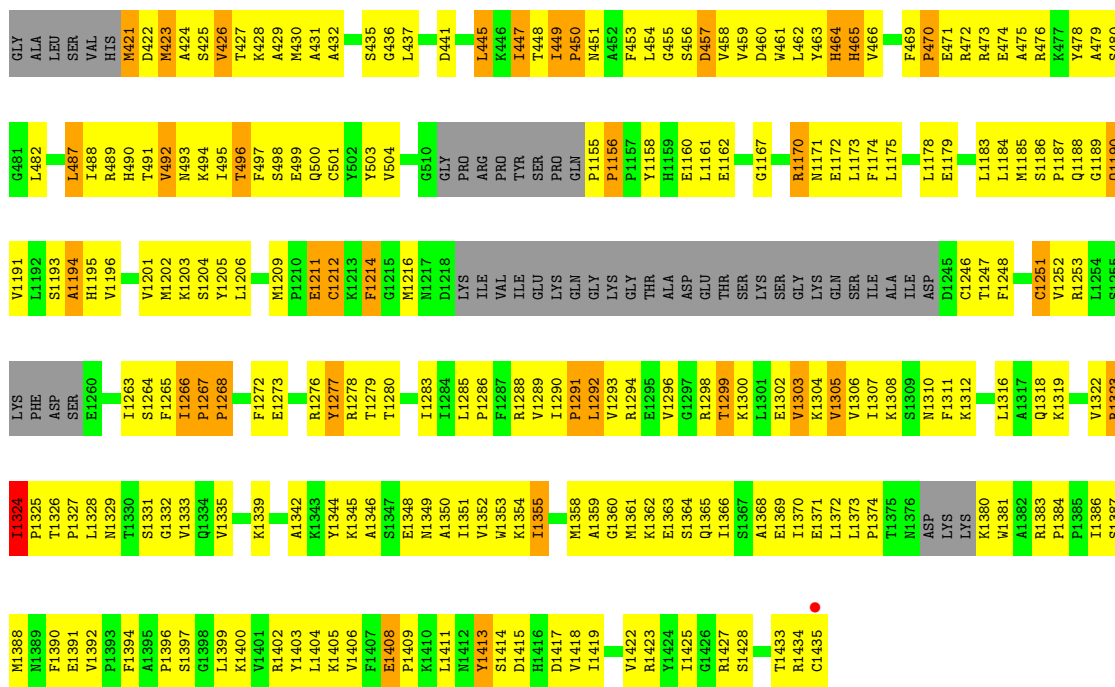






- Molecule 1: Chimeric complex between protein Dishevelled2 homolog dvl-2 and clathrin adaptor AP-2 complex subunit mu

Chain E: 29% 50% 9% 12%



- Molecule 1: Chimeric complex between protein Dishevelled2 homolog dvl-2 and clathrin adaptor AP-2 complex subunit mu

Chain F: 33% 48% 8% 12%



|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| V1392 | P1393 | F1394 | A1395 | P1396 | L1399 | K1400 | V1401 | R1402 | Y1403 | L1404 | K1405 | V1406 | F1407 | E1408 | P1409 | K1410 | L1411 | N1412 | Y1413 | S1414 | D1415 | H1416 | D1417 | V1418 | I1419 | K1420 | W1421 | V1422 | R1423 | Y1424 | I1425 | G1426 | R1427 | S1428 | E1432 | I1433 | R1434 | C1435 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| V1322 | R1323 | T1324 | P1325 | T1326 | P1327 | L1328 | N1329 | T1330 | S1331 | G1332 | V1333 | Q1334 | V1335 | K1339 | A1342 | K1345 | A1346 | S1347 | E1348 | I1351 | V1352 | W1353 | K1354 | R1357 | M1358 | A1359 | G1360 | M1361 | K1362 | E1363 | S1364 | Q1365 | I1366 | I1370 | E1371 | L1372 | L1373 | F1374 | T1375 | K1379 | K1380 | W1381 | A1382 | R1383 | P1384 | P1385 | I1386 | S1387 | M1388 | F1389 | F1390 | E1391 |       |       |       |       |       |       |
| C1251 | V1252 | R1253 | L1254 | S1255 | LYS   | PHE   | ASP   | SER   | GLU   | R1261 | S1262 | I1263 | S1264 | F1265 | I1266 | P1267 | P1268 | F1272 | R1276 | Y1277 | R1278 | T1279 | T1283 | I1284 | L1285 | P1286 | F1287 | R1288 | V1289 | I1290 | P1291 | L1292 | V1293 | R1294 | E1295 | V1296 | G1297 | R1298 | T1299 | K1300 | L1301 | E1302 | V1303 | I1307 | N1310 | F1311 | K1312 | L1316 | A1317 | Q1318 | K1319 | T1320 | E1321 |       |       |       |       |       |
| M1185 | S1186 | P1187 | Q1188 | G1189 | Q1190 | V1191 | L1192 | R1193 | A1194 | H1195 | V1196 | S1197 | G1198 | R1199 | V1200 | F1201 | L1206 | E1211 | G1212 | K1213 | F1214 | G1215 | M1216 | N1217 | D1218 | LYS   | ILE   | VAL   | ILE   | GLU   | LYS   | GLN   | GLY   | LYS   | GLY   | THR   | ALA   | ASP   | GLU   | THR   | SER   | LYS   | SER   | GLY   | LYS   | GLN   | SER   | ILE   | ALA   | ILE   | ASP   | D1245 | C1246 | T1247 | F1248 | H1249 | L1183 | Q1250 |
| Y478  | L482  | L487  | I488  | R489  | R490  | T491  | V492  | R493  | V494  | L495  | T496  | S498  | E499  | O500  | C501  | Y502  | Y503  | Y504  | F505  | G506  | B507  | G510  | GLY   | PRO   | ARG   | PRO   | TYR   | SER   | PRO   | GLN   | P1155 | P1156 | P1157 | Y1158 | H1159 | E1160 | G1167 | R1170 | H1171 | E1172 | L1173 | F1174 | L1175 | D1176 | V1177 | L1178 | E1179 | S1180 | V1181 | N1182 | L1184 |       |       |       |       |       |       |       |

## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | C 1 2 1                                                     | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 292.37Å 98.14Å 171.32Å<br>90.00° 121.97° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 49.07 – 3.50<br>49.07 – 3.50                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 98.3 (49.07-3.50)<br>98.3 (49.07-3.50)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.11                                                        | Depositor        |
| $R_{sym}$                                                               | 0.11                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.97 (at 3.48Å)                                             | Xtriage          |
| Refinement program                                                      | CNS 1.2                                                     | Depositor        |
| R, $R_{free}$                                                           | 0.308 , 0.335<br>0.308 , 0.332                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2576 reflections (5.01%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 107.5                                                       | Xtriage          |
| Anisotropy                                                              | 0.646                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.35 , 85.8                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.90                                                        | EDS              |
| Total number of atoms                                                   | 16319                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 117.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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     | 0.64         | 0/2851         | 1.02        | 13/3845 (0.3%)  |
| 1   | B     | 0.58         | 0/2756         | 1.01        | 15/3714 (0.4%)  |
| 1   | C     | 0.59         | 1/2844 (0.0%)  | 1.02        | 14/3835 (0.4%)  |
| 1   | D     | 0.59         | 1/2729 (0.0%)  | 1.01        | 12/3680 (0.3%)  |
| 1   | E     | 0.61         | 1/2746 (0.0%)  | 1.02        | 14/3701 (0.4%)  |
| 1   | F     | 0.58         | 0/2764         | 0.98        | 10/3725 (0.3%)  |
| All | All   | 0.60         | 3/16690 (0.0%) | 1.01        | 78/22500 (0.3%) |

All (3) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1   | E     | 1170 | ARG  | C-O   | -7.73 | 1.14        | 1.23     |
| 1   | C     | 461  | TRP  | C-N   | -6.28 | 1.26        | 1.33     |
| 1   | D     | 421  | MET  | CG-SD | 6.13  | 1.96        | 1.80     |

All (78) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 1   | E     | 1170 | ARG  | CA-C-O | -10.70 | 109.17      | 121.16   |
| 1   | A     | 1381 | TRP  | N-CA-C | 9.49   | 122.57      | 108.14   |
| 1   | E     | 1408 | GLU  | CA-C-O | 8.58   | 130.36      | 119.54   |
| 1   | B     | 1155 | PRO  | CA-C-N | 8.20   | 128.82      | 120.38   |
| 1   | B     | 1155 | PRO  | C-N-CA | 8.20   | 128.82      | 120.38   |
| 1   | C     | 1257 | PHE  | N-CA-C | -8.18  | 103.40      | 112.72   |
| 1   | C     | 461  | TRP  | O-C-N  | -8.13  | 113.50      | 122.12   |
| 1   | C     | 461  | TRP  | CA-C-N | 7.91   | 131.21      | 120.54   |
| 1   | C     | 461  | TRP  | C-N-CA | 7.91   | 131.21      | 120.54   |
| 1   | A     | 1261 | ARG  | N-CA-C | -7.57  | 102.55      | 112.24   |
| 1   | B     | 1156 | PRO  | CA-C-N | 7.49   | 127.93      | 119.92   |
| 1   | B     | 1156 | PRO  | C-N-CA | 7.49   | 127.93      | 119.92   |
| 1   | A     | 1156 | PRO  | CA-C-N | 7.15   | 127.57      | 119.92   |
| 1   | A     | 1156 | PRO  | C-N-CA | 7.15   | 127.57      | 119.92   |
| 1   | E     | 1156 | PRO  | CA-C-N | 7.05   | 127.47      | 119.92   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | E     | 1156 | PRO  | C-N-CA  | 7.05  | 127.47      | 119.92   |
| 1   | F     | 1156 | PRO  | CA-C-N  | 7.04  | 127.45      | 119.92   |
| 1   | F     | 1156 | PRO  | C-N-CA  | 7.04  | 127.45      | 119.92   |
| 1   | C     | 1156 | PRO  | CA-C-N  | 7.01  | 127.42      | 119.92   |
| 1   | C     | 1156 | PRO  | C-N-CA  | 7.01  | 127.42      | 119.92   |
| 1   | D     | 1156 | PRO  | CA-C-N  | 7.01  | 127.42      | 119.92   |
| 1   | D     | 1156 | PRO  | C-N-CA  | 7.01  | 127.42      | 119.92   |
| 1   | B     | 1413 | TYR  | N-CA-C  | 6.44  | 119.11      | 110.35   |
| 1   | D     | 1413 | TYR  | N-CA-C  | 6.42  | 119.08      | 110.35   |
| 1   | E     | 1266 | ILE  | CA-C-N  | 6.29  | 126.86      | 120.38   |
| 1   | E     | 1266 | ILE  | C-N-CA  | 6.29  | 126.86      | 120.38   |
| 1   | C     | 1266 | ILE  | CA-C-N  | 6.21  | 126.78      | 120.38   |
| 1   | C     | 1266 | ILE  | C-N-CA  | 6.21  | 126.78      | 120.38   |
| 1   | E     | 1413 | TYR  | N-CA-C  | 6.20  | 119.24      | 110.50   |
| 1   | A     | 1413 | TYR  | N-CA-C  | 6.15  | 119.17      | 110.50   |
| 1   | A     | 1266 | ILE  | CA-C-N  | 6.13  | 126.69      | 120.38   |
| 1   | A     | 1266 | ILE  | C-N-CA  | 6.13  | 126.69      | 120.38   |
| 1   | B     | 1266 | ILE  | CA-C-N  | 6.06  | 126.62      | 120.38   |
| 1   | B     | 1266 | ILE  | C-N-CA  | 6.06  | 126.62      | 120.38   |
| 1   | D     | 1266 | ILE  | CA-C-N  | 6.05  | 126.61      | 120.38   |
| 1   | D     | 1266 | ILE  | C-N-CA  | 6.05  | 126.61      | 120.38   |
| 1   | F     | 1266 | ILE  | CA-C-N  | 6.03  | 126.59      | 120.38   |
| 1   | F     | 1266 | ILE  | C-N-CA  | 6.03  | 126.59      | 120.38   |
| 1   | F     | 445  | LEU  | CB-CA-C | -6.02 | 109.65      | 116.63   |
| 1   | D     | 468  | GLY  | N-CA-C  | -6.02 | 106.67      | 115.63   |
| 1   | F     | 1268 | PRO  | N-CA-C  | -6.01 | 102.39      | 111.41   |
| 1   | A     | 1408 | GLU  | CA-C-O  | 5.91  | 126.99      | 119.54   |
| 1   | C     | 1413 | TYR  | N-CA-C  | 5.91  | 119.02      | 110.28   |
| 1   | E     | 1268 | PRO  | N-CA-C  | -5.89 | 102.57      | 111.41   |
| 1   | A     | 445  | LEU  | CB-CA-C | -5.83 | 109.86      | 116.63   |
| 1   | B     | 445  | LEU  | CB-CA-C | -5.80 | 109.90      | 116.63   |
| 1   | B     | 1412 | ASN  | N-CA-C  | 5.80  | 119.54      | 112.23   |
| 1   | C     | 1324 | ILE  | CA-C-N  | 5.78  | 127.34      | 120.23   |
| 1   | C     | 1324 | ILE  | C-N-CA  | 5.78  | 127.34      | 120.23   |
| 1   | C     | 1267 | PRO  | N-CA-C  | 5.78  | 117.75      | 110.70   |
| 1   | B     | 1324 | ILE  | CA-C-N  | 5.73  | 127.28      | 120.23   |
| 1   | B     | 1324 | ILE  | C-N-CA  | 5.73  | 127.28      | 120.23   |
| 1   | F     | 1413 | TYR  | N-CA-C  | 5.64  | 118.45      | 110.50   |
| 1   | D     | 1412 | ASN  | N-CA-C  | 5.62  | 119.32      | 112.23   |
| 1   | A     | 1268 | PRO  | N-CA-C  | -5.58 | 103.04      | 111.41   |
| 1   | B     | 1267 | PRO  | N-CA-C  | 5.55  | 117.47      | 110.70   |
| 1   | B     | 1268 | PRO  | N-CA-C  | -5.50 | 103.16      | 111.41   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | A     | 1324 | ILE  | CA-C-N   | 5.47  | 126.95      | 120.23   |
| 1   | A     | 1324 | ILE  | C-N-CA   | 5.47  | 126.95      | 120.23   |
| 1   | D     | 1268 | PRO  | N-CA-C   | -5.45 | 103.24      | 111.41   |
| 1   | D     | 1267 | PRO  | N-CA-C   | 5.36  | 117.24      | 110.70   |
| 1   | E     | 1324 | ILE  | CA-C-N   | 5.30  | 126.75      | 120.23   |
| 1   | E     | 1324 | ILE  | C-N-CA   | 5.30  | 126.75      | 120.23   |
| 1   | F     | 1412 | ASN  | N-CA-C   | 5.28  | 119.82      | 112.90   |
| 1   | E     | 1267 | PRO  | N-CA-C   | 5.27  | 117.13      | 110.70   |
| 1   | F     | 1324 | ILE  | CA-C-N   | 5.26  | 126.69      | 120.23   |
| 1   | F     | 1324 | ILE  | C-N-CA   | 5.26  | 126.69      | 120.23   |
| 1   | D     | 1184 | LEU  | CA-CB-CG | 5.24  | 134.62      | 116.30   |
| 1   | D     | 1324 | ILE  | CA-C-N   | 5.22  | 126.65      | 120.23   |
| 1   | D     | 1324 | ILE  | C-N-CA   | 5.22  | 126.65      | 120.23   |
| 1   | E     | 449  | ILE  | CA-C-N   | 5.22  | 125.62      | 119.99   |
| 1   | E     | 449  | ILE  | C-N-CA   | 5.22  | 125.62      | 119.99   |
| 1   | C     | 1261 | ARG  | N-CA-C   | -5.20 | 105.60      | 113.51   |
| 1   | A     | 1282 | ASP  | N-CA-C   | 5.17  | 118.86      | 112.24   |
| 1   | C     | 1268 | PRO  | N-CA-C   | -5.07 | 103.48      | 111.34   |
| 1   | B     | 449  | ILE  | CA-C-N   | 5.01  | 125.79      | 120.13   |
| 1   | B     | 449  | ILE  | C-N-CA   | 5.01  | 125.79      | 120.13   |
| 1   | E     | 1170 | ARG  | O-C-N    | 5.00  | 128.99      | 122.89   |

There are no chirality outliers.

There are no planarity outliers.

## 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     | 2787  | 0        | 2835     | 290     | 0            |
| 1   | B     | 2695  | 0        | 2751     | 279     | 0            |
| 1   | C     | 2780  | 0        | 2826     | 298     | 0            |
| 1   | D     | 2668  | 0        | 2716     | 283     | 0            |
| 1   | E     | 2686  | 0        | 2730     | 280     | 0            |
| 1   | F     | 2703  | 0        | 2755     | 292     | 0            |
| All | All   | 16319 | 0        | 16613    | 1679    | 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 51.

All (1679) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1244:ASP:OD1  | 1:A:1279:THR:HA   | 1.24                     | 1.37              |
| 1:C:462:LEU:O     | 1:C:466:VAL:HB    | 1.22                     | 1.28              |
| 1:C:458:VAL:O     | 1:C:462:LEU:HG    | 1.28                     | 1.24              |
| 1:C:462:LEU:O     | 1:C:466:VAL:CB    | 1.94                     | 1.15              |
| 1:A:462:LEU:O     | 1:A:466:VAL:HB    | 1.43                     | 1.14              |
| 1:A:430:MET:HE2   | 1:A:437:LEU:HD22  | 1.12                     | 1.11              |
| 1:C:1256:LYS:HG3  | 1:C:1259:SER:HB2  | 1.17                     | 1.10              |
| 1:D:1293:VAL:HG22 | 1:D:1303:VAL:HG22 | 1.25                     | 1.10              |
| 1:A:1217:ASN:HD21 | 1:A:1400:LYS:HB2  | 1.04                     | 1.10              |
| 1:A:1294:ARG:HB3  | 1:A:1294:ARG:HH11 | 1.15                     | 1.05              |
| 1:A:442:ARG:HH11  | 1:A:442:ARG:CG    | 1.70                     | 1.04              |
| 1:C:1183:LEU:HD12 | 1:C:1184:LEU:H    | 1.22                     | 1.04              |
| 1:D:430:MET:HE2   | 1:D:437:LEU:HD22  | 1.37                     | 1.04              |
| 1:F:462:LEU:O     | 1:F:466:VAL:HB    | 1.56                     | 1.03              |
| 1:C:459:VAL:HA    | 1:C:462:LEU:HD12  | 1.41                     | 1.03              |
| 1:A:1196:VAL:HG23 | 1:A:1283:ILE:HD13 | 1.36                     | 1.01              |
| 1:C:1406:VAL:HG11 | 1:C:1418:VAL:HG21 | 1.41                     | 1.00              |
| 1:F:1323:ARG:HH12 | 1:F:1352:VAL:HG22 | 1.26                     | 1.00              |
| 1:C:1253:ARG:HH12 | 1:C:1266:ILE:HD11 | 1.27                     | 1.00              |
| 1:A:1328:LEU:HB2  | 1:A:1381:TRP:HH2  | 1.21                     | 1.00              |
| 1:C:1244:ASP:OD2  | 1:C:1280:THR:HG23 | 1.62                     | 0.99              |
| 1:A:442:ARG:HH11  | 1:A:442:ARG:HG3   | 1.23                     | 0.99              |
| 1:A:1253:ARG:HD2  | 1:A:1264:SER:OG   | 1.63                     | 0.99              |
| 1:D:1183:LEU:HD21 | 1:D:1285:LEU:HD23 | 1.44                     | 0.98              |
| 1:D:1324:ILE:HD12 | 1:D:1386:ILE:HG12 | 1.43                     | 0.98              |
| 1:E:430:MET:HE1   | 1:E:458:VAL:HG23  | 1.46                     | 0.98              |
| 1:A:1184:LEU:HD22 | 1:A:1192:LEU:HD12 | 1.47                     | 0.96              |
| 1:C:440:ARG:HG2   | 1:C:442:ARG:HH11  | 1.32                     | 0.95              |
| 1:E:1293:VAL:HG12 | 1:E:1303:VAL:HG13 | 1.48                     | 0.95              |
| 1:B:476:ARG:HH21  | 1:B:476:ARG:HB3   | 1.29                     | 0.95              |
| 1:E:462:LEU:O     | 1:E:466:VAL:HB    | 1.65                     | 0.95              |
| 1:A:1182:ASN:HD22 | 1:A:1195:HIS:CE1  | 1.85                     | 0.94              |
| 1:D:1196:VAL:CG2  | 1:D:1279:THR:HG22 | 1.97                     | 0.94              |
| 1:C:1243:ILE:HA   | 1:C:1279:THR:HG22 | 1.47                     | 0.94              |
| 1:B:464:HIS:ND1   | 1:B:465:HIS:NE2   | 2.14                     | 0.93              |
| 1:F:1183:LEU:HD12 | 1:F:1184:LEU:H    | 1.28                     | 0.93              |
| 1:A:1183:LEU:HD11 | 1:A:1191:VAL:HG22 | 1.50                     | 0.93              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:1187:PRO:HD3  | 1:E:1434:ARG:HD3  | 1.50                     | 0.93              |
| 1:B:491:THR:HG22  | 1:B:492:VAL:HG13  | 1.49                     | 0.93              |
| 1:D:1333:VAL:HG22 | 1:D:1370:ILE:HG22 | 1.50                     | 0.93              |
| 1:B:464:HIS:ND1   | 1:B:465:HIS:CD2   | 2.37                     | 0.92              |
| 1:D:1217:ASN:HD21 | 1:D:1400:LYS:N    | 1.68                     | 0.92              |
| 1:A:1244:ASP:OD1  | 1:A:1279:THR:CA   | 2.16                     | 0.91              |
| 1:C:1256:LYS:CG   | 1:C:1259:SER:HB2  | 2.00                     | 0.91              |
| 1:C:458:VAL:O     | 1:C:462:LEU:CG    | 2.19                     | 0.91              |
| 1:A:1294:ARG:HB3  | 1:A:1294:ARG:NH1  | 1.85                     | 0.91              |
| 1:E:1298:ARG:NH1  | 1:E:1374:PRO:HG3  | 1.87                     | 0.90              |
| 1:D:1253:ARG:HH21 | 1:D:1253:ARG:HB2  | 1.36                     | 0.90              |
| 1:B:1253:ARG:HH21 | 1:B:1253:ARG:HG3  | 1.36                     | 0.90              |
| 1:D:1356:LYS:HD3  | 1:D:1357:ARG:HH12 | 1.34                     | 0.90              |
| 1:F:430:MET:HE2   | 1:F:437:LEU:HD22  | 1.51                     | 0.90              |
| 1:F:1390:PHE:CE1  | 1:F:1428:SER:HB3  | 2.07                     | 0.90              |
| 1:C:1174:PHE:HD2  | 1:C:1203:LYS:HD2  | 1.34                     | 0.90              |
| 1:F:1408:GLU:HG2  | 1:F:1411:LEU:HB2  | 1.54                     | 0.90              |
| 1:D:1180:SER:HB2  | 1:D:1427:ARG:HE   | 1.36                     | 0.90              |
| 1:D:1325:PRO:HG3  | 1:D:1384:PRO:O    | 1.70                     | 0.90              |
| 1:C:1246:CYS:HB2  | 1:C:1276:ARG:O    | 1.73                     | 0.89              |
| 1:D:1290:ILE:HB   | 1:D:1306:VAL:HG12 | 1.55                     | 0.89              |
| 1:F:1187:PRO:HD3  | 1:F:1434:ARG:HB2  | 1.53                     | 0.89              |
| 1:E:1339:LYS:HZ1  | 1:E:1364:SER:HA   | 1.35                     | 0.89              |
| 1:A:462:LEU:HD11  | 1:A:478:TYR:HD2   | 1.39                     | 0.88              |
| 1:E:458:VAL:O     | 1:E:462:LEU:HB2   | 1.72                     | 0.88              |
| 1:A:1289:VAL:HB   | 1:A:1433:THR:HG21 | 1.55                     | 0.88              |
| 1:B:1312:LYS:HB2  | 1:B:1315:LEU:HD13 | 1.55                     | 0.88              |
| 1:F:1294:ARG:NH2  | 1:F:1302:GLU:HG3  | 1.87                     | 0.88              |
| 1:A:441:ASP:OD1   | 1:A:450:PRO:HA    | 1.73                     | 0.88              |
| 1:E:1408:GLU:HG2  | 1:E:1411:LEU:HB2  | 1.56                     | 0.87              |
| 1:A:1217:ASN:ND2  | 1:A:1400:LYS:HB2  | 1.90                     | 0.87              |
| 1:C:479:ALA:HA    | 1:C:482:LEU:HD12  | 1.55                     | 0.87              |
| 1:B:1305:VAL:HG21 | 1:B:1324:ILE:HD11 | 1.57                     | 0.87              |
| 1:E:1327:PRO:HA   | 1:E:1381:TRP:CE2  | 2.10                     | 0.87              |
| 1:B:462:LEU:O     | 1:B:466:VAL:HB    | 1.75                     | 0.86              |
| 1:B:1161:LEU:HB2  | 1:F:1422:VAL:HG23 | 1.56                     | 0.86              |
| 1:A:1378:LYS:HE3  | 1:A:1381:TRP:CZ2  | 2.11                     | 0.86              |
| 1:E:462:LEU:HD22  | 1:E:475:ALA:O     | 1.74                     | 0.86              |
| 1:E:1186:SER:HA   | 1:E:1434:ARG:HD2  | 1.57                     | 0.86              |
| 1:F:1217:ASN:HD21 | 1:F:1400:LYS:N    | 1.73                     | 0.86              |
| 1:A:1294:ARG:HH11 | 1:A:1294:ARG:CB   | 1.89                     | 0.85              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:476:ARG:HD2   | 1:B:499:GLU:OE2   | 1.76                     | 0.85              |
| 1:A:472:ARG:HH21  | 1:A:472:ARG:HG3   | 1.41                     | 0.85              |
| 1:A:1379:LYS:H    | 1:A:1379:LYS:HD2  | 1.40                     | 0.85              |
| 1:B:1390:PHE:CE1  | 1:B:1428:SER:HB3  | 2.12                     | 0.84              |
| 1:C:1256:LYS:HG3  | 1:C:1259:SER:CB   | 2.04                     | 0.84              |
| 1:C:472:ARG:HG2   | 1:C:472:ARG:HH21  | 1.42                     | 0.84              |
| 1:D:430:MET:HE1   | 1:D:458:VAL:HG13  | 1.56                     | 0.84              |
| 1:F:498:SER:HB2   | 1:F:501:CYS:SG    | 2.17                     | 0.84              |
| 1:C:1256:LYS:HB2  | 1:C:1260:GLU:HG3  | 1.58                     | 0.84              |
| 1:C:1174:PHE:HE1  | 1:C:1421:TRP:CD1  | 1.94                     | 0.84              |
| 1:C:1399:LEU:HD23 | 1:C:1400:LYS:N    | 1.92                     | 0.84              |
| 1:E:498:SER:HB2   | 1:E:501:CYS:SG    | 2.17                     | 0.84              |
| 1:A:1294:ARG:HH12 | 1:A:1302:GLU:HG3  | 1.41                     | 0.84              |
| 1:A:1422:VAL:HG21 | 1:E:1161:LEU:HD13 | 1.60                     | 0.83              |
| 1:B:1323:ARG:NH1  | 1:B:1323:ARG:HB2  | 1.93                     | 0.83              |
| 1:D:1301:LEU:HB3  | 1:D:1370:ILE:HG13 | 1.60                     | 0.83              |
| 1:A:1390:PHE:CE1  | 1:A:1428:SER:HB3  | 2.12                     | 0.83              |
| 1:C:440:ARG:HG2   | 1:C:442:ARG:NH1   | 1.92                     | 0.83              |
| 1:B:430:MET:HE2   | 1:B:437:LEU:HD22  | 1.58                     | 0.83              |
| 1:A:1378:LYS:HE3  | 1:A:1381:TRP:HZ2  | 1.40                     | 0.83              |
| 1:E:463:TYR:HB2   | 1:E:475:ALA:CB    | 2.09                     | 0.83              |
| 1:A:460:ASP:HA    | 1:A:463:TYR:CE2   | 2.14                     | 0.83              |
| 1:B:1294:ARG:HH12 | 1:B:1302:GLU:HG3  | 1.45                     | 0.82              |
| 1:F:422:ASP:O     | 1:F:426:VAL:HG23  | 1.79                     | 0.82              |
| 1:D:1171:ASN:O    | 1:D:1418:VAL:HG13 | 1.80                     | 0.82              |
| 1:A:430:MET:HE2   | 1:A:437:LEU:CD2   | 2.04                     | 0.82              |
| 1:C:1171:ASN:O    | 1:C:1418:VAL:HG13 | 1.80                     | 0.82              |
| 1:C:1318:GLN:HE21 | 1:C:1357:ARG:NH1  | 1.78                     | 0.82              |
| 1:C:1217:ASN:ND2  | 1:C:1400:LYS:HB2  | 1.95                     | 0.82              |
| 1:E:1160:GLU:HB3  | 1:E:1167:GLY:HA3  | 1.61                     | 0.82              |
| 1:F:1408:GLU:CG   | 1:F:1411:LEU:HB2  | 2.09                     | 0.82              |
| 1:A:1161:LEU:HB2  | 1:E:1422:VAL:HG23 | 1.63                     | 0.81              |
| 1:B:442:ARG:NH2   | 1:B:453:PHE:HA    | 1.95                     | 0.81              |
| 1:B:464:HIS:HD1   | 1:B:465:HIS:CD2   | 1.97                     | 0.81              |
| 1:B:1408:GLU:HG2  | 1:B:1411:LEU:HB2  | 1.63                     | 0.81              |
| 1:C:1249:HIS:CE1  | 1:C:1268:PRO:HG2  | 2.15                     | 0.81              |
| 1:F:1329:ASN:ND2  | 1:F:1372:LEU:HB3  | 1.96                     | 0.81              |
| 1:A:1173:LEU:HD12 | 1:A:1173:LEU:O    | 1.81                     | 0.81              |
| 1:B:453:PHE:HZ    | 1:B:488:ILE:HD12  | 1.45                     | 0.81              |
| 1:E:1183:LEU:HD22 | 1:E:1285:LEU:HD22 | 1.62                     | 0.80              |
| 1:C:1293:VAL:HG12 | 1:C:1303:VAL:HG13 | 1.64                     | 0.80              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:462:LEU:O     | 1:A:466:VAL:CB    | 2.28                     | 0.80              |
| 1:B:422:ASP:O     | 1:B:426:VAL:HG23  | 1.81                     | 0.80              |
| 1:B:1161:LEU:HD13 | 1:F:1422:VAL:HG21 | 1.63                     | 0.80              |
| 1:D:458:VAL:O     | 1:D:462:LEU:HB2   | 1.79                     | 0.80              |
| 1:C:1249:HIS:HE1  | 1:C:1268:PRO:HG2  | 1.45                     | 0.80              |
| 1:F:1357:ARG:HG2  | 1:F:1357:ARG:HH11 | 1.46                     | 0.80              |
| 1:A:1305:VAL:HG12 | 1:A:1366:ILE:HG22 | 1.62                     | 0.80              |
| 1:C:422:ASP:O     | 1:C:426:VAL:HG23  | 1.80                     | 0.80              |
| 1:D:1408:GLU:HG2  | 1:D:1411:LEU:HB2  | 1.64                     | 0.80              |
| 1:E:1203:LYS:HB3  | 1:E:1205:TYR:HE1  | 1.46                     | 0.80              |
| 1:E:1339:LYS:NZ   | 1:E:1364:SER:HA   | 1.96                     | 0.80              |
| 1:C:462:LEU:O     | 1:C:466:VAL:CG2   | 2.29                     | 0.80              |
| 1:C:1183:LEU:HD12 | 1:C:1184:LEU:N    | 1.95                     | 0.79              |
| 1:D:1183:LEU:CD2  | 1:D:1285:LEU:HD23 | 2.13                     | 0.79              |
| 1:D:1339:LYS:HD2  | 1:D:1364:SER:OG   | 1.81                     | 0.79              |
| 1:A:1339:LYS:HB3  | 1:A:1339:LYS:NZ   | 1.97                     | 0.79              |
| 1:A:1345:LYS:HA   | 1:A:1345:LYS:HE2  | 1.64                     | 0.79              |
| 1:F:1160:GLU:HB3  | 1:F:1167:GLY:HA3  | 1.64                     | 0.79              |
| 1:E:463:TYR:HB2   | 1:E:475:ALA:HB2   | 1.65                     | 0.79              |
| 1:C:1160:GLU:HB3  | 1:C:1167:GLY:HA3  | 1.64                     | 0.79              |
| 1:A:1337:CYS:HB3  | 1:A:1366:ILE:HG13 | 1.64                     | 0.78              |
| 1:F:1177:VAL:HB   | 1:F:1424:TYR:HD1  | 1.47                     | 0.78              |
| 1:B:473:ARG:O     | 1:B:477:LYS:HG3   | 1.84                     | 0.78              |
| 1:C:1178:LEU:N    | 1:C:1178:LEU:HD12 | 1.99                     | 0.78              |
| 1:E:1331:SER:HB3  | 1:E:1373:LEU:HG   | 1.64                     | 0.78              |
| 1:F:1213:LYS:CE   | 1:F:1262:SER:OG   | 2.31                     | 0.78              |
| 1:B:430:MET:CE    | 1:B:437:LEU:HD22  | 2.14                     | 0.78              |
| 1:D:1301:LEU:HB2  | 1:D:1372:LEU:HD11 | 1.64                     | 0.78              |
| 1:A:442:ARG:HD2   | 1:A:502:TYR:CZ    | 2.19                     | 0.78              |
| 1:B:1276:ARG:HG3  | 1:B:1277:TYR:N    | 1.98                     | 0.78              |
| 1:E:1173:LEU:C    | 1:E:1173:LEU:HD12 | 2.09                     | 0.78              |
| 1:E:1323:ARG:HB3  | 1:E:1387:SER:OG   | 1.83                     | 0.78              |
| 1:D:1217:ASN:ND2  | 1:D:1400:LYS:HB2  | 1.99                     | 0.77              |
| 1:B:462:LEU:HD13  | 1:B:475:ALA:O     | 1.85                     | 0.77              |
| 1:B:1214:PHE:HE1  | 1:B:1401:VAL:HG13 | 1.50                     | 0.77              |
| 1:C:1324:ILE:HG23 | 1:C:1386:ILE:HD11 | 1.64                     | 0.77              |
| 1:F:1324:ILE:HD12 | 1:F:1386:ILE:CG2  | 2.14                     | 0.77              |
| 1:B:463:TYR:HB2   | 1:B:475:ALA:HB2   | 1.65                     | 0.77              |
| 1:D:1253:ARG:HB2  | 1:D:1253:ARG:NH2  | 1.98                     | 0.77              |
| 1:A:1394:PHE:O    | 1:A:1396:PRO:HD3  | 1.85                     | 0.77              |
| 1:A:1434:ARG:HG2  | 1:A:1434:ARG:HH11 | 1.49                     | 0.77              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:422:ASP:OD1   | 1:E:423:MET:HE3   | 1.84                     | 0.77              |
| 1:B:1323:ARG:HB2  | 1:B:1323:ARG:HH11 | 1.49                     | 0.77              |
| 1:A:430:MET:HE1   | 1:A:458:VAL:HG13  | 1.65                     | 0.76              |
| 1:D:1298:ARG:HH22 | 1:D:1372:LEU:CD2  | 1.97                     | 0.76              |
| 1:D:1312:LYS:HE3  | 1:D:1315:LEU:HD11 | 1.67                     | 0.76              |
| 1:C:1176:ASP:HB3  | 1:C:1178:LEU:HD11 | 1.67                     | 0.76              |
| 1:C:1290:ILE:HB   | 1:C:1306:VAL:HG12 | 1.67                     | 0.76              |
| 1:A:1328:LEU:HB2  | 1:A:1381:TRP:CH2  | 2.14                     | 0.76              |
| 1:D:1253:ARG:HH21 | 1:D:1253:ARG:CB   | 1.99                     | 0.76              |
| 1:A:438:GLU:OE2   | 1:A:440:ARG:NH2   | 2.18                     | 0.76              |
| 1:C:1214:PHE:HD2  | 1:C:1214:PHE:C    | 1.94                     | 0.76              |
| 1:C:1318:GLN:HE21 | 1:C:1357:ARG:HH11 | 1.30                     | 0.76              |
| 1:D:1434:ARG:HH11 | 1:D:1434:ARG:HG3  | 1.49                     | 0.76              |
| 1:D:1301:LEU:CB   | 1:D:1370:ILE:HG13 | 2.15                     | 0.76              |
| 1:A:422:ASP:O     | 1:A:426:VAL:HG23  | 1.86                     | 0.76              |
| 1:D:1187:PRO:HD3  | 1:D:1434:ARG:HB2  | 1.67                     | 0.76              |
| 1:E:1172:GLU:HB3  | 1:E:1419:ILE:HB   | 1.68                     | 0.76              |
| 1:E:1318:GLN:HE21 | 1:E:1319:LYS:HE3  | 1.51                     | 0.76              |
| 1:D:1301:LEU:HB3  | 1:D:1370:ILE:CG1  | 2.15                     | 0.76              |
| 1:B:1344:TYR:CE2  | 1:B:1346:ALA:HB2  | 2.20                     | 0.75              |
| 1:D:1408:GLU:OE2  | 1:D:1409:PRO:HD2  | 1.87                     | 0.75              |
| 1:E:1325:PRO:HG3  | 1:E:1384:PRO:O    | 1.86                     | 0.75              |
| 1:C:1217:ASN:HD21 | 1:C:1400:LYS:HB2  | 1.49                     | 0.75              |
| 1:D:1289:VAL:HB   | 1:D:1433:THR:HG21 | 1.68                     | 0.75              |
| 1:E:464:HIS:HB3   | 1:E:465:HIS:HD2   | 1.50                     | 0.75              |
| 1:C:1209:MET:HE2  | 1:C:1410:LYS:NZ   | 2.01                     | 0.75              |
| 1:F:491:THR:HG22  | 1:F:492:VAL:HG13  | 1.68                     | 0.75              |
| 1:F:1186:SER:HA   | 1:F:1434:ARG:HG3  | 1.67                     | 0.75              |
| 1:C:1331:SER:HB3  | 1:C:1373:LEU:HD21 | 1.68                     | 0.75              |
| 1:D:1330:THR:HG21 | 1:D:1344:TYR:OH   | 1.87                     | 0.75              |
| 1:C:1296:VAL:HB   | 1:C:1300:LYS:HB3  | 1.67                     | 0.74              |
| 1:A:1335:VAL:C    | 1:A:1336:ILE:HD12 | 2.12                     | 0.74              |
| 1:A:1392:VAL:HB   | 1:A:1394:PHE:CE2  | 2.23                     | 0.74              |
| 1:E:422:ASP:O     | 1:E:426:VAL:HG23  | 1.87                     | 0.74              |
| 1:B:457:ASP:HA    | 1:B:460:ASP:OD2   | 1.87                     | 0.74              |
| 1:B:1425:ILE:O    | 1:B:1425:ILE:HG22 | 1.86                     | 0.74              |
| 1:C:1214:PHE:C    | 1:C:1214:PHE:CD2  | 2.65                     | 0.74              |
| 1:E:1394:PHE:O    | 1:E:1396:PRO:HD3  | 1.86                     | 0.74              |
| 1:F:1319:LYS:HE3  | 1:F:1391:GLU:OE1  | 1.87                     | 0.74              |
| 1:B:463:TYR:HE1   | 1:B:469:PHE:O     | 1.70                     | 0.74              |
| 1:C:1183:LEU:HD23 | 1:C:1431:TYR:CE1  | 2.22                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:1160:GLU:HB3  | 1:D:1167:GLY:HA3  | 1.70                     | 0.74              |
| 1:C:1333:VAL:HG22 | 1:C:1370:ILE:HG12 | 1.68                     | 0.74              |
| 1:D:433:PRO:HD3   | 1:D:1254:LEU:O    | 1.87                     | 0.74              |
| 1:C:430:MET:HE1   | 1:C:458:VAL:HG23  | 1.69                     | 0.74              |
| 1:C:1357:ARG:HH11 | 1:C:1357:ARG:HB3  | 1.51                     | 0.74              |
| 1:E:1422:VAL:HG12 | 1:E:1423:ARG:N    | 2.01                     | 0.74              |
| 1:B:459:VAL:HA    | 1:B:462:LEU:HD12  | 1.70                     | 0.74              |
| 1:C:459:VAL:HG21  | 1:C:499:GLU:OE1   | 1.88                     | 0.74              |
| 1:E:1383:ARG:HD2  | 1:E:1435:CYS:SG   | 2.28                     | 0.74              |
| 1:F:1213:LYS:HE3  | 1:F:1262:SER:OG   | 1.87                     | 0.74              |
| 1:B:1173:LEU:HD11 | 1:B:1420:LYS:HG2  | 1.68                     | 0.73              |
| 1:B:1322:VAL:HG22 | 1:B:1388:MET:HE3  | 1.70                     | 0.73              |
| 1:B:1419:ILE:HD12 | 1:B:1419:ILE:N    | 2.03                     | 0.73              |
| 1:D:1356:LYS:HB3  | 1:D:1357:ARG:NH1  | 2.03                     | 0.73              |
| 1:B:1308:LYS:HG2  | 1:B:1363:GLU:HG2  | 1.70                     | 0.73              |
| 1:C:1422:VAL:HG12 | 1:C:1423:ARG:N    | 2.03                     | 0.73              |
| 1:D:440:ARG:HG2   | 1:D:442:ARG:NH1   | 2.03                     | 0.73              |
| 1:F:1188:GLN:NE2  | 1:F:1188:GLN:H    | 1.85                     | 0.73              |
| 1:F:1192:LEU:HD11 | 1:F:1434:ARG:HE   | 1.51                     | 0.73              |
| 1:E:455:GLY:O     | 1:E:458:VAL:HG12  | 1.89                     | 0.73              |
| 1:A:490:HIS:CE1   | 1:A:494:LYS:HE2   | 2.23                     | 0.73              |
| 1:B:1333:VAL:HG11 | 1:B:1344:TYR:CG   | 2.23                     | 0.73              |
| 1:C:1318:GLN:HG2  | 1:C:1357:ARG:HB2  | 1.70                     | 0.73              |
| 1:F:1217:ASN:HD21 | 1:F:1400:LYS:H    | 1.34                     | 0.73              |
| 1:F:1422:VAL:HG12 | 1:F:1423:ARG:N    | 2.01                     | 0.73              |
| 1:B:442:ARG:HG2   | 1:B:502:TYR:CZ    | 2.24                     | 0.73              |
| 1:B:1160:GLU:HB3  | 1:B:1167:GLY:HA3  | 1.69                     | 0.73              |
| 1:F:1402:ARG:HG3  | 1:F:1402:ARG:HH11 | 1.52                     | 0.73              |
| 1:B:1408:GLU:CB   | 1:B:1413:TYR:CE2  | 2.72                     | 0.72              |
| 1:D:1322:VAL:HG23 | 1:D:1353:TRP:HB3  | 1.71                     | 0.72              |
| 1:E:430:MET:HE2   | 1:E:437:LEU:HD22  | 1.71                     | 0.72              |
| 1:F:1284:ILE:HG12 | 1:F:1396:PRO:O    | 1.88                     | 0.72              |
| 1:A:1160:GLU:HB3  | 1:A:1167:GLY:HA3  | 1.71                     | 0.72              |
| 1:A:1278:ARG:HH11 | 1:A:1278:ARG:HG3  | 1.53                     | 0.72              |
| 1:B:1302:GLU:OE2  | 1:B:1369:GLU:HG2  | 1.89                     | 0.72              |
| 1:A:1312:LYS:HB2  | 1:A:1315:LEU:HD12 | 1.71                     | 0.72              |
| 1:B:440:ARG:HG2   | 1:B:441:ASP:H     | 1.54                     | 0.72              |
| 1:A:1322:VAL:HG22 | 1:A:1388:MET:HE3  | 1.71                     | 0.72              |
| 1:A:1408:GLU:HG2  | 1:A:1411:LEU:HB2  | 1.71                     | 0.72              |
| 1:A:1241:ILE:HD11 | 1:A:1399:LEU:HA   | 1.72                     | 0.72              |
| 1:D:1318:GLN:HG2  | 1:D:1357:ARG:HB3  | 1.70                     | 0.72              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1422:VAL:HG23 | 1:E:1161:LEU:HB2  | 1.72                     | 0.72              |
| 1:C:1409:PRO:HG2  | 1:C:1410:LYS:HD2  | 1.71                     | 0.72              |
| 1:B:1425:ILE:HD11 | 1:F:1156:PRO:CG   | 2.20                     | 0.72              |
| 1:F:1329:ASN:HD21 | 1:F:1372:LEU:HB3  | 1.55                     | 0.72              |
| 1:A:1434:ARG:HH11 | 1:A:1434:ARG:CG   | 2.03                     | 0.71              |
| 1:E:422:ASP:OD2   | 1:E:424:ALA:HB3   | 1.90                     | 0.71              |
| 1:F:1217:ASN:ND2  | 1:F:1400:LYS:H    | 1.89                     | 0.71              |
| 1:B:443:MET:HE3   | 1:B:448:THR:HG23  | 1.71                     | 0.71              |
| 1:C:440:ARG:H     | 1:C:442:ARG:NH1   | 1.87                     | 0.71              |
| 1:C:462:LEU:HD11  | 1:C:479:ALA:HB2   | 1.73                     | 0.71              |
| 1:C:1209:MET:HE2  | 1:C:1410:LYS:HZ1  | 1.54                     | 0.71              |
| 1:D:1217:ASN:ND2  | 1:D:1400:LYS:N    | 2.38                     | 0.71              |
| 1:E:470:PRO:CG    | 1:E:474:GLU:HG3   | 2.20                     | 0.71              |
| 1:F:1425:ILE:O    | 1:F:1425:ILE:HG22 | 1.89                     | 0.71              |
| 1:D:1158:TYR:HB2  | 1:D:1170:ARG:HD2  | 1.71                     | 0.71              |
| 1:D:1324:ILE:HG22 | 1:D:1351:ILE:HB   | 1.73                     | 0.70              |
| 1:D:444:TRP:O     | 1:D:447:ILE:HG13  | 1.90                     | 0.70              |
| 1:A:1204:SER:C    | 1:A:1205:TYR:HD2  | 1.98                     | 0.70              |
| 1:E:462:LEU:HD22  | 1:E:475:ALA:CA    | 2.21                     | 0.70              |
| 1:E:1305:VAL:HG21 | 1:E:1324:ILE:HD13 | 1.73                     | 0.70              |
| 1:D:1187:PRO:HD3  | 1:D:1434:ARG:CB   | 2.21                     | 0.70              |
| 1:D:1301:LEU:HB3  | 1:D:1370:ILE:CD1  | 2.22                     | 0.70              |
| 1:D:1170:ARG:HH11 | 1:D:1172:GLU:CD   | 2.00                     | 0.70              |
| 1:D:1298:ARG:HH22 | 1:D:1372:LEU:HD22 | 1.56                     | 0.70              |
| 1:D:1308:LYS:HE2  | 1:D:1363:GLU:OE2  | 1.91                     | 0.70              |
| 1:C:1211:GLU:HG3  | 1:C:1253:ARG:NH1  | 2.07                     | 0.70              |
| 1:D:443:MET:HE2   | 1:D:448:THR:OG1   | 1.92                     | 0.70              |
| 1:D:1217:ASN:ND2  | 1:D:1400:LYS:H    | 1.90                     | 0.70              |
| 1:F:1293:VAL:HG12 | 1:F:1303:VAL:HG22 | 1.73                     | 0.70              |
| 1:F:1187:PRO:CD   | 1:F:1434:ARG:HB2  | 2.21                     | 0.69              |
| 1:C:1177:VAL:C    | 1:C:1178:LEU:HD12 | 2.16                     | 0.69              |
| 1:E:1294:ARG:NH2  | 1:E:1302:GLU:HG3  | 2.07                     | 0.69              |
| 1:A:1294:ARG:HH12 | 1:A:1302:GLU:CG   | 2.05                     | 0.69              |
| 1:D:1305:VAL:HG23 | 1:D:1366:ILE:CG2  | 2.22                     | 0.69              |
| 1:E:1298:ARG:HD2  | 1:E:1374:PRO:HA   | 1.74                     | 0.69              |
| 1:F:1263:ILE:HD12 | 1:F:1263:ILE:N    | 2.07                     | 0.69              |
| 1:F:1324:ILE:HD12 | 1:F:1386:ILE:HG21 | 1.73                     | 0.69              |
| 1:A:476:ARG:NH2   | 1:A:476:ARG:HG2   | 2.08                     | 0.69              |
| 1:D:440:ARG:HG2   | 1:D:442:ARG:CZ    | 2.22                     | 0.69              |
| 1:E:1305:VAL:HG23 | 1:E:1366:ILE:HG23 | 1.73                     | 0.69              |
| 1:C:1357:ARG:NH1  | 1:C:1357:ARG:HB3  | 2.08                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:1333:VAL:CG2  | 1:D:1370:ILE:HG22 | 2.22                     | 0.69              |
| 1:E:1187:PRO:HD3  | 1:E:1434:ARG:CD   | 2.20                     | 0.69              |
| 1:F:1375:THR:OG1  | 1:F:1379:LYS:HD3  | 1.92                     | 0.69              |
| 1:E:487:LEU:N     | 1:E:487:LEU:HD23  | 2.06                     | 0.69              |
| 1:F:1211:GLU:HA   | 1:F:1266:ILE:HD13 | 1.74                     | 0.69              |
| 1:F:1214:PHE:HD1  | 1:F:1215:GLY:N    | 1.90                     | 0.69              |
| 1:A:1161:LEU:HD13 | 1:E:1422:VAL:HG21 | 1.75                     | 0.69              |
| 1:A:1278:ARG:HG3  | 1:A:1278:ARG:NH1  | 2.07                     | 0.69              |
| 1:B:1211:GLU:HA   | 1:B:1266:ILE:HD13 | 1.74                     | 0.69              |
| 1:C:498:SER:HB3   | 1:C:501:CYS:SG    | 2.33                     | 0.69              |
| 1:F:1213:LYS:HE2  | 1:F:1262:SER:OG   | 1.93                     | 0.69              |
| 1:B:1158:TYR:CE1  | 1:F:1174:PHE:HD2  | 2.11                     | 0.69              |
| 1:D:1394:PHE:O    | 1:D:1396:PRO:HD3  | 1.91                     | 0.69              |
| 1:F:1178:LEU:HD22 | 1:F:1427:ARG:NH1  | 2.08                     | 0.69              |
| 1:A:1304:LYS:HD2  | 1:A:1365:GLN:NE2  | 2.08                     | 0.68              |
| 1:A:1380:LYS:HB3  | 1:D:477:LYS:HE3   | 1.75                     | 0.68              |
| 1:B:1253:ARG:O    | 1:B:1263:ILE:HD11 | 1.93                     | 0.68              |
| 1:D:1329:ASN:ND2  | 1:D:1372:LEU:HD23 | 2.07                     | 0.68              |
| 1:F:1196:VAL:HG23 | 1:F:1283:ILE:HD13 | 1.75                     | 0.68              |
| 1:C:490:HIS:NE2   | 1:C:494:LYS:HB3   | 2.08                     | 0.68              |
| 1:D:1217:ASN:HD21 | 1:D:1400:LYS:H    | 1.41                     | 0.68              |
| 1:D:1285:LEU:HD12 | 1:D:1285:LEU:N    | 2.08                     | 0.68              |
| 1:E:1339:LYS:NZ   | 1:E:1363:GLU:O    | 2.27                     | 0.68              |
| 1:F:1357:ARG:HG2  | 1:F:1357:ARG:NH1  | 2.07                     | 0.68              |
| 1:A:476:ARG:HG2   | 1:A:476:ARG:HH21  | 1.57                     | 0.68              |
| 1:A:1339:LYS:HB3  | 1:A:1339:LYS:HZ2  | 1.59                     | 0.68              |
| 1:C:1406:VAL:HG11 | 1:C:1418:VAL:CG2  | 2.22                     | 0.68              |
| 1:F:1217:ASN:ND2  | 1:F:1400:LYS:N    | 2.42                     | 0.68              |
| 1:B:1425:ILE:HD11 | 1:F:1156:PRO:HG2  | 1.76                     | 0.68              |
| 1:E:447:ILE:HG22  | 1:E:448:THR:H     | 1.59                     | 0.68              |
| 1:E:462:LEU:HD22  | 1:E:475:ALA:C     | 2.18                     | 0.68              |
| 1:B:1268:PRO:HD2  | 1:B:1272:PHE:CE2  | 2.29                     | 0.68              |
| 1:C:1408:GLU:HG2  | 1:C:1411:LEU:HB2  | 1.75                     | 0.68              |
| 1:A:487:LEU:N     | 1:A:487:LEU:HD23  | 2.08                     | 0.68              |
| 1:B:1294:ARG:HH12 | 1:B:1302:GLU:CG   | 2.07                     | 0.68              |
| 1:C:1180:SER:HB2  | 1:C:1427:ARG:NH1  | 2.08                     | 0.68              |
| 1:D:442:ARG:HD3   | 1:D:502:TYR:CZ    | 2.29                     | 0.68              |
| 1:D:1320:ILE:HG23 | 1:D:1388:MET:HE2  | 1.75                     | 0.68              |
| 1:F:1359:ALA:HB3  | 1:F:1362:LYS:HD2  | 1.74                     | 0.68              |
| 1:A:1184:LEU:CD2  | 1:A:1192:LEU:HD12 | 2.21                     | 0.67              |
| 1:C:1170:ARG:HH22 | 1:C:1205:TYR:HD2  | 1.42                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:424:ALA:O     | 1:B:428:LYS:HG3   | 1.93                     | 0.67              |
| 1:C:471:GLU:HG2   | 1:C:473:ARG:NH2   | 2.09                     | 0.67              |
| 1:C:463:TYR:CZ    | 1:C:464:HIS:ND1   | 2.63                     | 0.67              |
| 1:C:1174:PHE:CE1  | 1:C:1421:TRP:CD1  | 2.80                     | 0.67              |
| 1:D:1280:THR:HA   | 1:D:1283:ILE:HD11 | 1.74                     | 0.67              |
| 1:C:1293:VAL:CG1  | 1:C:1303:VAL:HG13 | 2.23                     | 0.67              |
| 1:B:1406:VAL:HG23 | 1:B:1415:ASP:OD1  | 1.94                     | 0.67              |
| 1:F:1185:MET:HE2  | 1:F:1433:THR:HG23 | 1.77                     | 0.67              |
| 1:F:1331:SER:HB2  | 1:F:1373:LEU:HD22 | 1.75                     | 0.67              |
| 1:F:1345:LYS:CE   | 1:F:1352:VAL:HG21 | 2.24                     | 0.67              |
| 1:E:1211:GLU:HA   | 1:E:1266:ILE:HD13 | 1.75                     | 0.67              |
| 1:E:1293:VAL:CG1  | 1:E:1303:VAL:HG13 | 2.23                     | 0.67              |
| 1:D:1301:LEU:HD12 | 1:D:1372:LEU:HD21 | 1.75                     | 0.67              |
| 1:F:1289:VAL:HG22 | 1:F:1307:ILE:HG22 | 1.76                     | 0.67              |
| 1:A:492:VAL:HG21  | 1:C:1338:MET:HB3  | 1.76                     | 0.66              |
| 1:E:454:LEU:HB3   | 1:E:457:ASP:OD2   | 1.95                     | 0.66              |
| 1:A:492:VAL:HG13  | 1:C:1338:MET:HG2  | 1.76                     | 0.66              |
| 1:B:464:HIS:CE1   | 1:B:465:HIS:NE2   | 2.62                     | 0.66              |
| 1:C:447:ILE:HG22  | 1:C:448:THR:N     | 2.10                     | 0.66              |
| 1:D:1323:ARG:HB2  | 1:D:1387:SER:OG   | 1.95                     | 0.66              |
| 1:E:1323:ARG:HH11 | 1:E:1323:ARG:HB2  | 1.58                     | 0.66              |
| 1:B:462:LEU:CD1   | 1:B:479:ALA:HB2   | 2.25                     | 0.66              |
| 1:D:1315:LEU:C    | 1:D:1316:LEU:HD23 | 2.20                     | 0.66              |
| 1:D:1326:THR:HG21 | 1:D:1344:TYR:CE1  | 2.31                     | 0.66              |
| 1:E:1335:VAL:HG12 | 1:E:1368:ALA:HB2  | 1.77                     | 0.66              |
| 1:F:1187:PRO:HD3  | 1:F:1434:ARG:CB   | 2.25                     | 0.66              |
| 1:A:1336:ILE:HD12 | 1:A:1336:ILE:N    | 2.10                     | 0.66              |
| 1:D:1183:LEU:HD12 | 1:D:1193:SER:O    | 1.95                     | 0.66              |
| 1:D:1196:VAL:HG21 | 1:D:1279:THR:HG22 | 1.75                     | 0.66              |
| 1:D:1246:CYS:HB2  | 1:D:1276:ARG:O    | 1.96                     | 0.66              |
| 1:D:1298:ARG:HH22 | 1:D:1372:LEU:HB3  | 1.60                     | 0.66              |
| 1:E:1408:GLU:CG   | 1:E:1411:LEU:HB2  | 2.26                     | 0.66              |
| 1:B:1216:MET:N    | 1:B:1216:MET:HE2  | 2.11                     | 0.66              |
| 1:B:1408:GLU:CB   | 1:B:1413:TYR:HE2  | 2.09                     | 0.66              |
| 1:C:469:PHE:HZ    | 1:C:478:TYR:CD2   | 2.12                     | 0.66              |
| 1:C:483:LEU:HD22  | 1:C:488:ILE:HB    | 1.76                     | 0.66              |
| 1:D:1434:ARG:HG3  | 1:D:1434:ARG:NH1  | 2.11                     | 0.66              |
| 1:C:1378:LYS:HG2  | 1:C:1379:LYS:H    | 1.60                     | 0.66              |
| 1:D:1331:SER:HB3  | 1:D:1373:LEU:HG   | 1.77                     | 0.66              |
| 1:D:1345:LYS:HD2  | 1:D:1352:VAL:HG21 | 1.77                     | 0.66              |
| 1:F:1311:PHE:CE1  | 1:F:1360:GLY:HA2  | 2.31                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:478:TYR:O     | 1:D:482:LEU:HD12  | 1.95                     | 0.66              |
| 1:D:1386:ILE:HG13 | 1:D:1435:CYS:SG   | 2.36                     | 0.66              |
| 1:F:1293:VAL:HG21 | 1:F:1383:ARG:NH1  | 2.10                     | 0.66              |
| 1:A:447:ILE:HG22  | 1:A:448:THR:N     | 2.09                     | 0.66              |
| 1:C:447:ILE:CG2   | 1:C:448:THR:N     | 2.59                     | 0.66              |
| 1:D:1305:VAL:HG23 | 1:D:1366:ILE:HG23 | 1.76                     | 0.66              |
| 1:D:441:ASP:OD1   | 1:D:450:PRO:HA    | 1.96                     | 0.65              |
| 1:D:1298:ARG:HH22 | 1:D:1372:LEU:CB   | 2.09                     | 0.65              |
| 1:E:1183:LEU:HD11 | 1:E:1191:VAL:HG13 | 1.78                     | 0.65              |
| 1:A:453:PHE:N     | 1:A:453:PHE:CD2   | 2.64                     | 0.65              |
| 1:A:1290:ILE:HD12 | 1:A:1290:ILE:N    | 2.11                     | 0.65              |
| 1:B:454:LEU:HG    | 1:B:456:SER:H     | 1.61                     | 0.65              |
| 1:D:1176:ASP:CG   | 1:D:1423:ARG:HH21 | 2.05                     | 0.65              |
| 1:F:448:THR:HG22  | 1:F:448:THR:O     | 1.97                     | 0.65              |
| 1:F:1294:ARG:HB3  | 1:F:1294:ARG:HH11 | 1.60                     | 0.65              |
| 1:E:1324:ILE:HD12 | 1:E:1386:ILE:HG21 | 1.77                     | 0.65              |
| 1:B:1170:ARG:HA   | 1:F:1421:TRP:CZ3  | 2.31                     | 0.65              |
| 1:B:1338:MET:HB3  | 1:E:492:VAL:HG21  | 1.79                     | 0.65              |
| 1:C:471:GLU:HG3   | 1:C:472:ARG:N     | 2.11                     | 0.65              |
| 1:D:443:MET:HG3   | 1:D:447:ILE:O     | 1.97                     | 0.65              |
| 1:A:1204:SER:C    | 1:A:1205:TYR:CD2  | 2.75                     | 0.65              |
| 1:B:458:VAL:O     | 1:B:462:LEU:HG    | 1.96                     | 0.65              |
| 1:D:1250:GLN:HG3  | 1:D:1251:CYS:N    | 2.12                     | 0.65              |
| 1:D:1343:LYS:HE3  | 1:D:1345:LYS:HZ3  | 1.61                     | 0.65              |
| 1:A:447:ILE:HG22  | 1:A:448:THR:H     | 1.61                     | 0.65              |
| 1:C:455:GLY:O     | 1:C:458:VAL:HG12  | 1.97                     | 0.65              |
| 1:C:1331:SER:HB3  | 1:C:1373:LEU:CD2  | 2.27                     | 0.65              |
| 1:D:1321:GLU:O    | 1:D:1388:MET:HE3  | 1.96                     | 0.65              |
| 1:E:1342:ALA:HB2  | 1:E:1353:TRP:CD1  | 2.32                     | 0.65              |
| 1:F:1384:PRO:O    | 1:F:1435:CYS:SG   | 2.54                     | 0.65              |
| 1:B:442:ARG:HH21  | 1:B:453:PHE:HA    | 1.62                     | 0.65              |
| 1:C:1306:VAL:HG23 | 1:C:1365:GLN:HB2  | 1.79                     | 0.65              |
| 1:C:1326:THR:HG22 | 1:C:1370:ILE:HD11 | 1.79                     | 0.65              |
| 1:D:462:LEU:HD23  | 1:D:466:VAL:HG21  | 1.77                     | 0.65              |
| 1:D:1357:ARG:HG2  | 1:D:1357:ARG:HH11 | 1.61                     | 0.65              |
| 1:E:466:VAL:CG1   | 1:E:469:PHE:HE2   | 2.10                     | 0.65              |
| 1:F:1217:ASN:ND2  | 1:F:1400:LYS:HB2  | 2.12                     | 0.65              |
| 1:A:472:ARG:HG3   | 1:A:472:ARG:NH2   | 2.11                     | 0.65              |
| 1:D:440:ARG:O     | 1:D:442:ARG:NH1   | 2.30                     | 0.65              |
| 1:D:491:THR:HG22  | 1:D:492:VAL:HG13  | 1.78                     | 0.65              |
| 1:F:1312:LYS:HB2  | 1:F:1312:LYS:NZ   | 2.11                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:1422:VAL:HG12 | 1:D:1423:ARG:N    | 2.11                     | 0.64              |
| 1:F:458:VAL:O     | 1:F:462:LEU:HB2   | 1.97                     | 0.64              |
| 1:F:1295:GLU:OE2  | 1:F:1301:LEU:HD13 | 1.98                     | 0.64              |
| 1:D:1319:LYS:O    | 1:D:1390:PHE:HA   | 1.98                     | 0.64              |
| 1:E:441:ASP:OD1   | 1:E:450:PRO:HA    | 1.97                     | 0.64              |
| 1:F:1293:VAL:CG2  | 1:F:1383:ARG:NH1  | 2.60                     | 0.64              |
| 1:C:462:LEU:CD1   | 1:C:479:ALA:HB2   | 2.27                     | 0.64              |
| 1:C:1202:MET:HE2  | 1:C:1272:PHE:CZ   | 2.32                     | 0.64              |
| 1:C:467:GLU:HA    | 1:C:467:GLU:OE2   | 1.96                     | 0.64              |
| 1:C:1174:PHE:CD2  | 1:C:1203:LYS:HD2  | 2.26                     | 0.64              |
| 1:D:1326:THR:HB   | 1:D:1327:PRO:HD2  | 1.79                     | 0.64              |
| 1:E:464:HIS:HB3   | 1:E:465:HIS:CD2   | 2.32                     | 0.64              |
| 1:A:487:LEU:O     | 1:A:488:ILE:HD13  | 1.96                     | 0.64              |
| 1:D:1323:ARG:O    | 1:D:1386:ILE:HG23 | 1.98                     | 0.64              |
| 1:F:1186:SER:HA   | 1:F:1434:ARG:CG   | 2.28                     | 0.64              |
| 1:A:1183:LEU:HB3  | 1:A:1431:TYR:CD1  | 2.33                     | 0.64              |
| 1:B:1325:PRO:HG3  | 1:B:1384:PRO:O    | 1.97                     | 0.64              |
| 1:C:1202:MET:HE3  | 1:C:1204:SER:HB2  | 1.80                     | 0.64              |
| 1:E:1435:CYS:SG   | 1:E:1435:CYS:O    | 2.56                     | 0.64              |
| 1:B:428:LYS:O     | 1:B:431:ALA:HB3   | 1.97                     | 0.64              |
| 1:B:1170:ARG:NH1  | 1:B:1172:GLU:OE1  | 2.31                     | 0.64              |
| 1:E:1327:PRO:HG3  | 1:E:1381:TRP:CE3  | 2.33                     | 0.64              |
| 1:E:1359:ALA:HB3  | 1:E:1362:LYS:HD2  | 1.80                     | 0.64              |
| 1:C:1331:SER:HB3  | 1:C:1373:LEU:CG   | 2.28                     | 0.64              |
| 1:D:1172:GLU:HB3  | 1:D:1419:ILE:HB   | 1.81                     | 0.64              |
| 1:D:1356:LYS:HB3  | 1:D:1357:ARG:HH11 | 1.62                     | 0.64              |
| 1:E:1183:LEU:HD12 | 1:E:1193:SER:O    | 1.98                     | 0.64              |
| 1:D:1359:ALA:HB3  | 1:D:1362:LYS:HE2  | 1.79                     | 0.63              |
| 1:E:1171:ASN:O    | 1:E:1418:VAL:HG13 | 1.98                     | 0.63              |
| 1:A:1422:VAL:HG12 | 1:A:1423:ARG:H    | 1.63                     | 0.63              |
| 1:B:1315:LEU:HD12 | 1:B:1315:LEU:N    | 2.13                     | 0.63              |
| 1:B:1311:PHE:CE1  | 1:B:1360:GLY:HA2  | 2.33                     | 0.63              |
| 1:C:463:TYR:CE2   | 1:C:464:HIS:ND1   | 2.62                     | 0.63              |
| 1:E:1332:GLY:HA3  | 1:E:1371:GLU:OE1  | 1.98                     | 0.63              |
| 1:A:1187:PRO:HD3  | 1:A:1434:ARG:HB3  | 1.80                     | 0.63              |
| 1:C:1202:MET:HE2  | 1:C:1272:PHE:CE1  | 2.33                     | 0.63              |
| 1:B:453:PHE:CZ    | 1:B:488:ILE:HD12  | 2.30                     | 0.63              |
| 1:D:483:LEU:HD12  | 1:D:483:LEU:O     | 1.98                     | 0.63              |
| 1:E:1185:MET:SD   | 1:E:1189:GLY:HA2  | 2.39                     | 0.63              |
| 1:F:1192:LEU:CD1  | 1:F:1434:ARG:HE   | 2.11                     | 0.63              |
| 1:F:1345:LYS:HE3  | 1:F:1352:VAL:HG21 | 1.80                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:434:GLU:OE1   | 1:B:434:GLU:HA    | 1.99                     | 0.63              |
| 1:D:453:PHE:N     | 1:D:453:PHE:CD2   | 2.67                     | 0.63              |
| 1:F:1298:ARG:NH2  | 1:F:1379:LYS:HD2  | 2.13                     | 0.63              |
| 1:F:1327:PRO:HG3  | 1:F:1381:TRP:CE3  | 2.33                     | 0.63              |
| 1:F:460:ASP:O     | 1:F:464:HIS:HD2   | 1.81                     | 0.63              |
| 1:B:462:LEU:O     | 1:B:466:VAL:CB    | 2.46                     | 0.63              |
| 1:C:1305:VAL:HG21 | 1:C:1324:ILE:HD13 | 1.81                     | 0.63              |
| 1:F:1183:LEU:HD22 | 1:F:1285:LEU:HD22 | 1.81                     | 0.63              |
| 1:C:1404:LEU:HD23 | 1:C:1404:LEU:C    | 2.24                     | 0.62              |
| 1:F:1186:SER:OG   | 1:F:1188:GLN:NE2  | 2.31                     | 0.62              |
| 1:F:1294:ARG:HB3  | 1:F:1294:ARG:NH1  | 2.13                     | 0.62              |
| 1:B:483:LEU:HD13  | 1:B:503:TYR:CE1   | 2.35                     | 0.62              |
| 1:D:476:ARG:HH11  | 1:D:499:GLU:HB2   | 1.64                     | 0.62              |
| 1:D:1184:LEU:HB3  | 1:D:1193:SER:HB3  | 1.79                     | 0.62              |
| 1:E:1327:PRO:HA   | 1:E:1381:TRP:NE1  | 2.14                     | 0.62              |
| 1:F:1394:PHE:CD1  | 1:F:1394:PHE:C    | 2.77                     | 0.62              |
| 1:A:459:VAL:O     | 1:A:463:TYR:CD2   | 2.51                     | 0.62              |
| 1:A:1171:ASN:HD21 | 1:A:1207:SER:H    | 1.46                     | 0.62              |
| 1:B:1312:LYS:HB2  | 1:B:1315:LEU:CD1  | 2.27                     | 0.62              |
| 1:D:495:ILE:HG13  | 1:D:496:THR:N     | 2.14                     | 0.62              |
| 1:C:471:GLU:HG3   | 1:C:472:ARG:H     | 1.64                     | 0.62              |
| 1:E:462:LEU:CD2   | 1:E:475:ALA:HA    | 2.30                     | 0.62              |
| 1:A:442:ARG:HH11  | 1:A:442:ARG:HG2   | 1.62                     | 0.62              |
| 1:D:1301:LEU:HB3  | 1:D:1370:ILE:HD11 | 1.81                     | 0.62              |
| 1:F:1294:ARG:CZ   | 1:F:1302:GLU:HG3  | 2.29                     | 0.62              |
| 1:D:1392:VAL:HB   | 1:D:1394:PHE:CE2  | 2.34                     | 0.62              |
| 1:E:1291:PRO:O    | 1:E:1292:LEU:HD12 | 1.99                     | 0.62              |
| 1:E:1381:TRP:CZ3  | 1:E:1383:ARG:HG2  | 2.34                     | 0.62              |
| 1:C:461:TRP:CD1   | 1:C:465:HIS:CD2   | 2.88                     | 0.62              |
| 1:C:1172:GLU:HB3  | 1:C:1419:ILE:HB   | 1.81                     | 0.62              |
| 1:D:1298:ARG:NH2  | 1:D:1372:LEU:HB3  | 2.15                     | 0.62              |
| 1:E:1319:LYS:O    | 1:E:1390:PHE:HA   | 2.00                     | 0.62              |
| 1:F:1184:LEU:HB3  | 1:F:1193:SER:HB3  | 1.80                     | 0.62              |
| 1:B:449:ILE:HG22  | 1:B:452:ALA:HB2   | 1.81                     | 0.62              |
| 1:B:476:ARG:HB3   | 1:B:476:ARG:NH2   | 2.09                     | 0.62              |
| 1:D:1203:LYS:HB3  | 1:D:1205:TYR:HE2  | 1.65                     | 0.62              |
| 1:F:430:MET:CE    | 1:F:437:LEU:HD22  | 2.26                     | 0.62              |
| 1:F:1185:MET:HE1  | 1:F:1289:VAL:O    | 1.99                     | 0.62              |
| 1:A:1187:PRO:HD3  | 1:A:1434:ARG:CB   | 2.30                     | 0.62              |
| 1:A:1329:ASN:ND2  | 1:A:1372:LEU:HD22 | 2.15                     | 0.62              |
| 1:B:430:MET:HE2   | 1:B:437:LEU:HB2   | 1.82                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:472:ARG:O     | 1:E:472:ARG:HD3   | 2.00                     | 0.62              |
| 1:B:1319:LYS:O    | 1:B:1390:PHE:HA   | 2.00                     | 0.62              |
| 1:F:1192:LEU:HD11 | 1:F:1434:ARG:NE   | 2.15                     | 0.62              |
| 1:A:1170:ARG:NH1  | 1:A:1205:TYR:CD1  | 2.60                     | 0.61              |
| 1:A:1276:ARG:CZ   | 1:A:1276:ARG:HB2  | 2.30                     | 0.61              |
| 1:A:1427:ARG:HG2  | 1:A:1427:ARG:HH11 | 1.64                     | 0.61              |
| 1:F:1325:PRO:HG3  | 1:F:1384:PRO:O    | 2.00                     | 0.61              |
| 1:F:1422:VAL:HG12 | 1:F:1423:ARG:H    | 1.63                     | 0.61              |
| 1:A:1422:VAL:HG12 | 1:A:1423:ARG:N    | 2.15                     | 0.61              |
| 1:A:437:LEU:H     | 1:A:461:TRP:CD1   | 2.18                     | 0.61              |
| 1:B:1408:GLU:HB3  | 1:B:1413:TYR:CE2  | 2.35                     | 0.61              |
| 1:E:1196:VAL:HG23 | 1:E:1283:ILE:HD13 | 1.82                     | 0.61              |
| 1:E:1298:ARG:HG2  | 1:E:1298:ARG:HH21 | 1.64                     | 0.61              |
| 1:F:1158:TYR:HB2  | 1:F:1170:ARG:HD2  | 1.82                     | 0.61              |
| 1:A:462:LEU:HD11  | 1:A:478:TYR:CD2   | 2.28                     | 0.61              |
| 1:A:1170:ARG:HH12 | 1:A:1205:TYR:HD1  | 1.40                     | 0.61              |
| 1:A:428:LYS:O     | 1:A:431:ALA:HB3   | 2.00                     | 0.61              |
| 1:A:1188:GLN:NE2  | 1:D:422:ASP:OD1   | 2.33                     | 0.61              |
| 1:B:480:SER:OG    | 1:B:497:PHE:HB3   | 2.00                     | 0.61              |
| 1:E:1184:LEU:HB2  | 1:E:1193:SER:HB3  | 1.83                     | 0.61              |
| 1:C:1356:LYS:H    | 1:C:1356:LYS:HD2  | 1.64                     | 0.61              |
| 1:F:491:THR:HG22  | 1:F:492:VAL:CG1   | 2.30                     | 0.61              |
| 1:E:1325:PRO:O    | 1:E:1381:TRP:HH2  | 1.83                     | 0.61              |
| 1:E:1318:GLN:NE2  | 1:E:1319:LYS:HE3  | 2.16                     | 0.61              |
| 1:A:1305:VAL:HG11 | 1:A:1324:ILE:HD11 | 1.82                     | 0.61              |
| 1:A:1255:SER:CB   | 1:A:1263:ILE:HA   | 2.30                     | 0.60              |
| 1:C:1276:ARG:HH11 | 1:C:1276:ARG:HG3  | 1.66                     | 0.60              |
| 1:C:1329:ASN:ND2  | 1:C:1372:LEU:HB3  | 2.16                     | 0.60              |
| 1:A:462:LEU:HD23  | 1:A:475:ALA:CB    | 2.31                     | 0.60              |
| 1:C:1214:PHE:HD2  | 1:C:1215:GLY:N    | 1.99                     | 0.60              |
| 1:D:1183:LEU:HD11 | 1:D:1191:VAL:CG1  | 2.31                     | 0.60              |
| 1:F:428:LYS:O     | 1:F:431:ALA:HB3   | 2.01                     | 0.60              |
| 1:B:447:ILE:HG22  | 1:B:448:THR:N     | 2.16                     | 0.60              |
| 1:C:427:THR:HG21  | 1:C:487:LEU:HB3   | 1.83                     | 0.60              |
| 1:D:1184:LEU:HA   | 1:D:1432:GLU:O    | 2.02                     | 0.60              |
| 1:A:1328:LEU:HD12 | 1:A:1349:ASN:ND2  | 2.15                     | 0.60              |
| 1:D:1277:TYR:HD2  | 1:D:1277:TYR:N    | 2.00                     | 0.60              |
| 1:C:1214:PHE:CD2  | 1:C:1215:GLY:N    | 2.70                     | 0.60              |
| 1:D:1186:SER:HA   | 1:D:1434:ARG:HB2  | 1.83                     | 0.60              |
| 1:F:1333:VAL:HG13 | 1:F:1370:ILE:HG12 | 1.83                     | 0.60              |
| 1:D:1424:TYR:N    | 1:D:1424:TYR:CD2  | 2.68                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:423:MET:HA    | 1:E:478:TYR:OH    | 2.01                     | 0.60              |
| 1:A:442:ARG:HG3   | 1:A:442:ARG:NH1   | 2.03                     | 0.60              |
| 1:B:483:LEU:HD13  | 1:B:503:TYR:HE1   | 1.65                     | 0.60              |
| 1:C:1316:LEU:HD13 | 1:C:1357:ARG:HD2  | 1.84                     | 0.60              |
| 1:E:465:HIS:CD2   | 1:E:465:HIS:N     | 2.68                     | 0.60              |
| 1:F:1402:ARG:HG3  | 1:F:1402:ARG:NH1  | 2.17                     | 0.60              |
| 1:D:1425:ILE:HG22 | 1:D:1425:ILE:O    | 2.00                     | 0.60              |
| 1:A:442:ARG:CG    | 1:A:442:ARG:NH1   | 2.41                     | 0.60              |
| 1:B:447:ILE:HG22  | 1:B:448:THR:H     | 1.67                     | 0.60              |
| 1:B:1253:ARG:HG3  | 1:B:1253:ARG:NH2  | 2.06                     | 0.60              |
| 1:F:1298:ARG:O    | 1:F:1372:LEU:HD12 | 2.01                     | 0.60              |
| 1:B:1338:MET:HE2  | 1:E:491:THR:HB    | 1.84                     | 0.59              |
| 1:A:467:GLU:HA    | 1:A:467:GLU:OE2   | 2.02                     | 0.59              |
| 1:C:1331:SER:CB   | 1:C:1373:LEU:HD21 | 2.32                     | 0.59              |
| 1:C:1422:VAL:HG12 | 1:C:1423:ARG:H    | 1.66                     | 0.59              |
| 1:D:1356:LYS:CD   | 1:D:1357:ARG:HH12 | 2.12                     | 0.59              |
| 1:D:1359:ALA:HB3  | 1:D:1362:LYS:CE   | 2.31                     | 0.59              |
| 1:E:470:PRO:HG2   | 1:E:471:GLU:H     | 1.67                     | 0.59              |
| 1:E:1214:PHE:C    | 1:E:1214:PHE:CD2  | 2.80                     | 0.59              |
| 1:B:1198:GLY:O    | 1:B:1276:ARG:HD3  | 2.02                     | 0.59              |
| 1:F:1298:ARG:NH1  | 1:F:1375:THR:OG1  | 2.35                     | 0.59              |
| 1:A:492:VAL:CG1   | 1:C:1338:MET:HG2  | 2.33                     | 0.59              |
| 1:A:1276:ARG:HH11 | 1:A:1276:ARG:HG3  | 1.68                     | 0.59              |
| 1:D:430:MET:HE2   | 1:D:437:LEU:CD2   | 2.25                     | 0.59              |
| 1:D:498:SER:HB2   | 1:D:501:CYS:SG    | 2.41                     | 0.59              |
| 1:D:1158:TYR:HB2  | 1:D:1170:ARG:CD   | 2.32                     | 0.59              |
| 1:A:462:LEU:HD23  | 1:A:475:ALA:HB1   | 1.83                     | 0.59              |
| 1:B:442:ARG:HG2   | 1:B:502:TYR:CE2   | 2.38                     | 0.59              |
| 1:F:440:ARG:NH2   | 1:F:440:ARG:HB3   | 2.17                     | 0.59              |
| 1:A:1408:GLU:CG   | 1:A:1411:LEU:HB2  | 2.33                     | 0.59              |
| 1:B:440:ARG:HG2   | 1:B:441:ASP:N     | 2.17                     | 0.59              |
| 1:E:1422:VAL:HG12 | 1:E:1423:ARG:H    | 1.68                     | 0.59              |
| 1:A:1176:ASP:HB3  | 1:A:1178:LEU:HD21 | 1.85                     | 0.59              |
| 1:A:1425:ILE:HG22 | 1:A:1425:ILE:O    | 2.03                     | 0.59              |
| 1:F:1290:ILE:HD12 | 1:F:1290:ILE:N    | 2.18                     | 0.59              |
| 1:F:1390:PHE:CZ   | 1:F:1428:SER:HB3  | 2.38                     | 0.59              |
| 1:A:1243:ILE:HD12 | 1:A:1277:TYR:HD1  | 1.67                     | 0.59              |
| 1:B:443:MET:HE3   | 1:B:448:THR:CG2   | 2.31                     | 0.59              |
| 1:F:1394:PHE:O    | 1:F:1396:PRO:HD3  | 2.02                     | 0.59              |
| 1:A:1183:LEU:HG   | 1:A:1184:LEU:N    | 2.17                     | 0.59              |
| 1:A:1211:GLU:OE2  | 1:A:1253:ARG:NH2  | 2.36                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1319:LYS:O    | 1:C:1390:PHE:HA   | 2.03                     | 0.59              |
| 1:E:1279:THR:HG22 | 1:E:1280:THR:N    | 2.18                     | 0.59              |
| 1:F:1324:ILE:HD12 | 1:F:1386:ILE:HG23 | 1.84                     | 0.59              |
| 1:B:1216:MET:HE2  | 1:B:1216:MET:H    | 1.66                     | 0.58              |
| 1:B:1305:VAL:HG21 | 1:B:1324:ILE:CD1  | 2.30                     | 0.58              |
| 1:D:428:LYS:O     | 1:D:431:ALA:HB3   | 2.02                     | 0.58              |
| 1:D:1185:MET:HB3  | 1:D:1433:THR:HG22 | 1.85                     | 0.58              |
| 1:E:1186:SER:HA   | 1:E:1434:ARG:CD   | 2.30                     | 0.58              |
| 1:C:1187:PRO:HB2  | 1:C:1188:GLN:NE2  | 2.19                     | 0.58              |
| 1:C:1394:PHE:O    | 1:C:1396:PRO:HD3  | 2.03                     | 0.58              |
| 1:B:1187:PRO:HB2  | 1:B:1188:GLN:HE21 | 1.68                     | 0.58              |
| 1:C:497:PHE:O     | 1:C:497:PHE:CD1   | 2.55                     | 0.58              |
| 1:C:1178:LEU:N    | 1:C:1178:LEU:CD1  | 2.66                     | 0.58              |
| 1:B:453:PHE:CD2   | 1:B:453:PHE:N     | 2.71                     | 0.58              |
| 1:B:462:LEU:HD11  | 1:B:479:ALA:HB2   | 1.85                     | 0.58              |
| 1:C:489:ARG:HH21  | 1:C:1410:LYS:CE   | 2.16                     | 0.58              |
| 1:A:1173:LEU:HD22 | 1:A:1404:LEU:HD23 | 1.85                     | 0.58              |
| 1:B:1280:THR:HA   | 1:B:1283:ILE:HD11 | 1.84                     | 0.58              |
| 1:D:1298:ARG:NH2  | 1:D:1372:LEU:HD22 | 2.19                     | 0.58              |
| 1:E:1423:ARG:CD   | 1:E:1425:ILE:HD11 | 2.33                     | 0.58              |
| 1:E:1423:ARG:NE   | 1:E:1425:ILE:HD11 | 2.18                     | 0.58              |
| 1:F:1415:ASP:OD2  | 1:F:1420:LYS:NZ   | 2.36                     | 0.58              |
| 1:A:1298:ARG:O    | 1:A:1298:ARG:HD3  | 2.04                     | 0.58              |
| 1:D:1292:LEU:HD12 | 1:D:1304:LYS:CE   | 2.34                     | 0.58              |
| 1:E:1279:THR:HG22 | 1:E:1280:THR:H    | 1.67                     | 0.58              |
| 1:A:1241:ILE:CD1  | 1:A:1399:LEU:HA   | 2.33                     | 0.58              |
| 1:B:1408:GLU:HB2  | 1:B:1413:TYR:CE2  | 2.38                     | 0.58              |
| 1:E:1188:GLN:HB2  | 1:E:1190:GLN:HE21 | 1.67                     | 0.58              |
| 1:A:1287:PHE:N    | 1:A:1287:PHE:HD1  | 2.02                     | 0.58              |
| 1:A:1408:GLU:OE2  | 1:A:1409:PRO:HD2  | 2.04                     | 0.58              |
| 1:D:1422:VAL:HG12 | 1:D:1423:ARG:H    | 1.66                     | 0.58              |
| 1:A:1361:MET:O    | 1:A:1362:LYS:HG3  | 2.03                     | 0.58              |
| 1:B:463:TYR:HB2   | 1:B:475:ALA:CB    | 2.33                     | 0.58              |
| 1:C:1399:LEU:HD23 | 1:C:1399:LEU:C    | 2.29                     | 0.58              |
| 1:D:472:ARG:HH21  | 1:D:472:ARG:HG3   | 1.69                     | 0.58              |
| 1:D:451:ASN:ND2   | 1:D:1264:SER:HB3  | 2.19                     | 0.57              |
| 1:E:462:LEU:CD2   | 1:E:475:ALA:O     | 2.50                     | 0.57              |
| 1:F:1185:MET:O    | 1:F:1434:ARG:HG3  | 2.04                     | 0.57              |
| 1:B:1246:CYS:SG   | 1:B:1276:ARG:O    | 2.62                     | 0.57              |
| 1:C:453:PHE:CE1   | 1:C:503:TYR:HB2   | 2.40                     | 0.57              |
| 1:C:483:LEU:HG    | 1:C:497:PHE:HD2   | 1.68                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1187:PRO:HD3  | 1:C:1434:ARG:HB2  | 1.86                     | 0.57              |
| 1:D:1335:VAL:HG12 | 1:D:1368:ALA:HB2  | 1.86                     | 0.57              |
| 1:E:428:LYS:O     | 1:E:431:ALA:HB3   | 2.04                     | 0.57              |
| 1:E:458:VAL:O     | 1:E:462:LEU:CB    | 2.47                     | 0.57              |
| 1:F:437:LEU:H     | 1:F:461:TRP:CD1   | 2.22                     | 0.57              |
| 1:A:449:ILE:HD12  | 1:A:1407:PHE:CZ   | 2.40                     | 0.57              |
| 1:A:1403:TYR:CD1  | 1:A:1403:TYR:C    | 2.82                     | 0.57              |
| 1:B:1338:MET:CE   | 1:E:491:THR:HB    | 2.34                     | 0.57              |
| 1:F:1181:VAL:HG11 | 1:F:1396:PRO:HB3  | 1.86                     | 0.57              |
| 1:B:449:ILE:CG2   | 1:B:452:ALA:HB2   | 2.35                     | 0.57              |
| 1:C:428:LYS:O     | 1:C:431:ALA:HB3   | 2.04                     | 0.57              |
| 1:E:1381:TRP:CE3  | 1:E:1383:ARG:HG2  | 2.39                     | 0.57              |
| 1:B:437:LEU:H     | 1:B:461:TRP:CD1   | 2.22                     | 0.57              |
| 1:C:1185:MET:HE1  | 1:C:1289:VAL:O    | 2.04                     | 0.57              |
| 1:B:1252:VAL:HG22 | 1:B:1263:ILE:HG13 | 1.85                     | 0.57              |
| 1:D:1304:LYS:HG3  | 1:D:1365:GLN:HE21 | 1.68                     | 0.57              |
| 1:E:491:THR:HG22  | 1:E:492:VAL:HG13  | 1.87                     | 0.57              |
| 1:A:1183:LEU:HD11 | 1:A:1191:VAL:CG2  | 2.29                     | 0.57              |
| 1:A:1287:PHE:N    | 1:A:1287:PHE:CD1  | 2.73                     | 0.57              |
| 1:C:1276:ARG:HG2  | 1:C:1277:TYR:N    | 2.20                     | 0.57              |
| 1:E:470:PRO:HG2   | 1:E:474:GLU:HG3   | 1.85                     | 0.57              |
| 1:B:1173:LEU:O    | 1:B:1173:LEU:HD12 | 2.04                     | 0.57              |
| 1:D:1324:ILE:HD12 | 1:D:1386:ILE:CG1  | 2.28                     | 0.57              |
| 1:F:1183:LEU:HD12 | 1:F:1184:LEU:N    | 2.08                     | 0.57              |
| 1:A:459:VAL:O     | 1:A:463:TYR:HD2   | 1.87                     | 0.57              |
| 1:B:488:ILE:HG22  | 1:B:503:TYR:HD1   | 1.70                     | 0.57              |
| 1:B:1408:GLU:HB3  | 1:B:1413:TYR:CD2  | 2.39                     | 0.57              |
| 1:C:1329:ASN:OD1  | 1:C:1372:LEU:HD22 | 2.05                     | 0.57              |
| 1:F:1394:PHE:C    | 1:F:1394:PHE:HD1  | 2.11                     | 0.57              |
| 1:C:1253:ARG:NH1  | 1:C:1266:ILE:HD11 | 2.10                     | 0.56              |
| 1:D:1173:LEU:C    | 1:D:1173:LEU:HD12 | 2.29                     | 0.56              |
| 1:E:489:ARG:NH2   | 1:E:1409:PRO:HG3  | 2.20                     | 0.56              |
| 1:E:1328:LEU:HA   | 1:E:1349:ASN:HD21 | 1.69                     | 0.56              |
| 1:F:1381:TRP:CZ3  | 1:F:1383:ARG:HG2  | 2.40                     | 0.56              |
| 1:B:1187:PRO:HD3  | 1:B:1434:ARG:HB2  | 1.85                     | 0.56              |
| 1:D:1290:ILE:HG22 | 1:D:1290:ILE:O    | 2.05                     | 0.56              |
| 1:E:471:GLU:OE2   | 1:E:473:ARG:HB2   | 2.04                     | 0.56              |
| 1:F:1250:GLN:HG3  | 1:F:1251:CYS:N    | 2.20                     | 0.56              |
| 1:A:1392:VAL:HB   | 1:A:1394:PHE:HE2  | 1.66                     | 0.56              |
| 1:B:463:TYR:HD1   | 1:B:469:PHE:CB    | 2.18                     | 0.56              |
| 1:B:1329:ASN:OD1  | 1:B:1372:LEU:HD22 | 2.05                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1216:MET:HE3  | 1:C:1261:ARG:O    | 2.06                     | 0.56              |
| 1:C:1381:TRP:CH2  | 1:C:1383:ARG:HG2  | 2.40                     | 0.56              |
| 1:D:440:ARG:HG2   | 1:D:442:ARG:NH2   | 2.21                     | 0.56              |
| 1:D:1277:TYR:N    | 1:D:1277:TYR:CD2  | 2.71                     | 0.56              |
| 1:D:1298:ARG:NH2  | 1:D:1372:LEU:CB   | 2.68                     | 0.56              |
| 1:D:1331:SER:OG   | 1:D:1371:GLU:HB3  | 2.04                     | 0.56              |
| 1:E:495:ILE:HG23  | 1:E:496:THR:N     | 2.21                     | 0.56              |
| 1:F:460:ASP:C     | 1:F:464:HIS:HD2   | 2.14                     | 0.56              |
| 1:F:1319:LYS:O    | 1:F:1390:PHE:HA   | 2.05                     | 0.56              |
| 1:F:1324:ILE:CD1  | 1:F:1386:ILE:HG21 | 2.34                     | 0.56              |
| 1:A:1399:LEU:C    | 1:A:1399:LEU:HD23 | 2.30                     | 0.56              |
| 1:B:471:GLU:HG3   | 1:B:472:ARG:N     | 2.21                     | 0.56              |
| 1:B:1202:MET:SD   | 1:B:1272:PHE:CZ   | 2.98                     | 0.56              |
| 1:C:462:LEU:HD13  | 1:C:475:ALA:O     | 2.05                     | 0.56              |
| 1:D:1217:ASN:HD22 | 1:D:1400:LYS:HB2  | 1.69                     | 0.56              |
| 1:D:1324:ILE:HG23 | 1:D:1324:ILE:O    | 2.04                     | 0.56              |
| 1:E:1422:VAL:CG1  | 1:E:1423:ARG:N    | 2.68                     | 0.56              |
| 1:A:1247:THR:C    | 1:A:1248:PHE:CD1  | 2.84                     | 0.56              |
| 1:B:1156:PRO:HG2  | 1:F:1425:ILE:HD11 | 1.88                     | 0.56              |
| 1:B:1326:THR:HG21 | 1:B:1344:TYR:CE1  | 2.40                     | 0.56              |
| 1:A:462:LEU:CD1   | 1:A:478:TYR:HD2   | 2.16                     | 0.56              |
| 1:C:422:ASP:OD1   | 1:C:425:SER:HB2   | 2.06                     | 0.56              |
| 1:B:498:SER:HB3   | 1:B:501:CYS:SG    | 2.45                     | 0.56              |
| 1:A:1211:GLU:OE2  | 1:A:1253:ARG:CZ   | 2.53                     | 0.56              |
| 1:A:1331:SER:HB3  | 1:A:1373:LEU:HG   | 1.88                     | 0.56              |
| 1:B:1338:MET:HB3  | 1:E:492:VAL:CG2   | 2.36                     | 0.56              |
| 1:C:1317:ALA:HB2  | 1:C:1392:VAL:HG12 | 1.87                     | 0.56              |
| 1:D:1171:ASN:O    | 1:D:1418:VAL:CG1  | 2.53                     | 0.56              |
| 1:E:462:LEU:CD2   | 1:E:475:ALA:CA    | 2.84                     | 0.56              |
| 1:F:425:SER:HA    | 1:F:428:LYS:HD3   | 1.88                     | 0.56              |
| 1:A:495:ILE:HG23  | 1:A:496:THR:N     | 2.20                     | 0.56              |
| 1:C:426:VAL:HG21  | 1:C:478:TYR:OH    | 2.06                     | 0.56              |
| 1:C:1277:TYR:N    | 1:C:1277:TYR:HD2  | 2.03                     | 0.56              |
| 1:C:1288:ARG:NH1  | 1:C:1290:ILE:HD11 | 2.21                     | 0.56              |
| 1:C:1325:PRO:HG3  | 1:C:1384:PRO:O    | 2.06                     | 0.56              |
| 1:E:436:GLY:HA3   | 1:E:465:HIS:HE1   | 1.71                     | 0.56              |
| 1:F:1317:ALA:HB2  | 1:F:1392:VAL:HG12 | 1.88                     | 0.56              |
| 1:C:1277:TYR:N    | 1:C:1277:TYR:CD2  | 2.74                     | 0.55              |
| 1:A:1322:VAL:HB   | 1:A:1353:TRP:HB3  | 1.88                     | 0.55              |
| 1:B:1333:VAL:HG21 | 1:B:1351:ILE:HD11 | 1.87                     | 0.55              |
| 1:D:460:ASP:O     | 1:D:463:TYR:N     | 2.34                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:1175:LEU:HD11 | 1:E:1404:LEU:HD22 | 1.88                     | 0.55              |
| 1:F:1268:PRO:HD2  | 1:F:1272:PHE:CE1  | 2.41                     | 0.55              |
| 1:A:472:ARG:O     | 1:A:472:ARG:HD3   | 2.06                     | 0.55              |
| 1:C:1212:CYS:SG   | 1:C:1406:VAL:HG23 | 2.46                     | 0.55              |
| 1:E:453:PHE:CE1   | 1:E:503:TYR:HB2   | 2.42                     | 0.55              |
| 1:B:1333:VAL:HG11 | 1:B:1344:TYR:CD2  | 2.42                     | 0.55              |
| 1:C:1299:THR:HB   | 1:C:1371:GLU:OE2  | 2.06                     | 0.55              |
| 1:C:1413:TYR:HB2  | 1:C:1417:ASP:HB2  | 1.88                     | 0.55              |
| 1:E:1206:LEU:HD23 | 1:E:1406:VAL:HG11 | 1.87                     | 0.55              |
| 1:E:1296:VAL:HB   | 1:E:1300:LYS:HB3  | 1.88                     | 0.55              |
| 1:E:1324:ILE:HD12 | 1:E:1386:ILE:CG2  | 2.36                     | 0.55              |
| 1:F:478:TYR:CE1   | 1:F:482:LEU:HD21  | 2.41                     | 0.55              |
| 1:B:438:GLU:O     | 1:B:438:GLU:HG3   | 2.05                     | 0.55              |
| 1:C:1422:VAL:CG1  | 1:C:1423:ARG:N    | 2.70                     | 0.55              |
| 1:F:1183:LEU:CD1  | 1:F:1184:LEU:H    | 2.11                     | 0.55              |
| 1:F:1422:VAL:CG1  | 1:F:1423:ARG:N    | 2.68                     | 0.55              |
| 1:A:1413:TYR:HB2  | 1:A:1417:ASP:HB2  | 1.88                     | 0.55              |
| 1:C:447:ILE:CG2   | 1:C:448:THR:H     | 2.19                     | 0.55              |
| 1:C:1253:ARG:HH12 | 1:C:1266:ILE:CD1  | 2.11                     | 0.55              |
| 1:D:1211:GLU:OE1  | 1:D:1266:ILE:HD11 | 2.06                     | 0.55              |
| 1:F:440:ARG:HG2   | 1:F:441:ASP:N     | 2.21                     | 0.55              |
| 1:F:443:MET:HG3   | 1:F:447:ILE:O     | 2.07                     | 0.55              |
| 1:F:1183:LEU:CD1  | 1:F:1191:VAL:HG13 | 2.36                     | 0.55              |
| 1:B:1413:TYR:HB2  | 1:B:1417:ASP:HB2  | 1.87                     | 0.55              |
| 1:C:472:ARG:HG2   | 1:C:472:ARG:NH2   | 2.16                     | 0.55              |
| 1:D:1298:ARG:HH12 | 1:D:1329:ASN:ND2  | 2.03                     | 0.55              |
| 1:E:421:MET:HG3   | 1:E:422:ASP:H     | 1.71                     | 0.55              |
| 1:E:1305:VAL:HG23 | 1:E:1366:ILE:CG2  | 2.36                     | 0.55              |
| 1:A:1182:ASN:ND2  | 1:A:1195:HIS:CE1  | 2.67                     | 0.55              |
| 1:C:476:ARG:NH1   | 1:C:499:GLU:HG3   | 2.22                     | 0.55              |
| 1:C:1294:ARG:O    | 1:C:1301:LEU:HD12 | 2.06                     | 0.55              |
| 1:D:439:VAL:HG22  | 1:D:453:PHE:CD2   | 2.42                     | 0.55              |
| 1:E:1214:PHE:CE2  | 1:E:1216:MET:HE3  | 2.40                     | 0.55              |
| 1:F:1214:PHE:HD1  | 1:F:1214:PHE:C    | 2.15                     | 0.55              |
| 1:B:501:CYS:SG    | 1:B:503:TYR:HE2   | 2.29                     | 0.55              |
| 1:E:1323:ARG:HH11 | 1:E:1323:ARG:CB   | 2.20                     | 0.55              |
| 1:F:1214:PHE:C    | 1:F:1214:PHE:CD1  | 2.85                     | 0.55              |
| 1:F:1262:SER:C    | 1:F:1263:ILE:HD12 | 2.32                     | 0.55              |
| 1:A:471:GLU:H     | 1:A:474:GLU:HG3   | 1.72                     | 0.55              |
| 1:A:1173:LEU:HD12 | 1:A:1173:LEU:C    | 2.30                     | 0.55              |
| 1:B:1294:ARG:HB3  | 1:B:1294:ARG:NH1  | 2.22                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:1356:LYS:HD3  | 1:D:1357:ARG:NH1  | 2.13                     | 0.55              |
| 1:F:454:LEU:HD23  | 1:F:456:SER:OG    | 2.07                     | 0.55              |
| 1:C:1288:ARG:HH11 | 1:C:1290:ILE:HD11 | 1.72                     | 0.54              |
| 1:D:1291:PRO:HA   | 1:D:1305:VAL:HG12 | 1.89                     | 0.54              |
| 1:F:1252:VAL:HG13 | 1:F:1263:ILE:CG2  | 2.37                     | 0.54              |
| 1:F:1284:ILE:CG1  | 1:F:1396:PRO:HA   | 2.36                     | 0.54              |
| 1:C:433:PRO:HG2   | 1:C:1256:LYS:HE2  | 1.89                     | 0.54              |
| 1:D:1286:PRO:HG2  | 1:D:1390:PHE:CE1  | 2.42                     | 0.54              |
| 1:D:1322:VAL:CG2  | 1:D:1353:TRP:HB3  | 2.36                     | 0.54              |
| 1:F:1381:TRP:CE3  | 1:F:1383:ARG:HG2  | 2.42                     | 0.54              |
| 1:C:1425:ILE:O    | 1:C:1425:ILE:HG23 | 2.06                     | 0.54              |
| 1:D:430:MET:HB3   | 1:D:437:LEU:HD23  | 1.89                     | 0.54              |
| 1:D:495:ILE:HG13  | 1:D:496:THR:H     | 1.73                     | 0.54              |
| 1:D:495:ILE:HG13  | 1:D:496:THR:HG23  | 1.88                     | 0.54              |
| 1:D:1357:ARG:NH1  | 1:D:1357:ARG:HG2  | 2.22                     | 0.54              |
| 1:F:426:VAL:O     | 1:F:429:ALA:HB3   | 2.08                     | 0.54              |
| 1:A:442:ARG:HG2   | 1:A:442:ARG:NH1   | 2.21                     | 0.54              |
| 1:B:1272:PHE:C    | 1:B:1272:PHE:CD1  | 2.85                     | 0.54              |
| 1:B:1290:ILE:O    | 1:B:1290:ILE:HG22 | 2.07                     | 0.54              |
| 1:B:1408:GLU:CG   | 1:B:1411:LEU:HB2  | 2.36                     | 0.54              |
| 1:B:1419:ILE:N    | 1:B:1419:ILE:CD1  | 2.70                     | 0.54              |
| 1:C:440:ARG:N     | 1:C:442:ARG:NH1   | 2.55                     | 0.54              |
| 1:F:1263:ILE:N    | 1:F:1263:ILE:CD1  | 2.71                     | 0.54              |
| 1:A:1323:ARG:HH11 | 1:A:1323:ARG:HG3  | 1.73                     | 0.54              |
| 1:F:1181:VAL:CG1  | 1:F:1396:PRO:CB   | 2.85                     | 0.54              |
| 1:F:1324:ILE:O    | 1:F:1324:ILE:HG22 | 2.07                     | 0.54              |
| 1:C:1273:GLU:OE2  | 1:C:1276:ARG:NH2  | 2.41                     | 0.54              |
| 1:E:1286:PRO:O    | 1:E:1310:ASN:HB3  | 2.07                     | 0.54              |
| 1:E:1323:ARG:HH12 | 1:E:1352:VAL:HG13 | 1.73                     | 0.54              |
| 1:B:463:TYR:HD1   | 1:B:469:PHE:HB2   | 1.71                     | 0.54              |
| 1:E:479:ALA:HB3   | 1:E:497:PHE:HE2   | 1.72                     | 0.54              |
| 1:F:1216:MET:HE1  | 1:F:1263:ILE:HD13 | 1.88                     | 0.54              |
| 1:B:430:MET:HE2   | 1:B:437:LEU:CD2   | 2.34                     | 0.54              |
| 1:B:488:ILE:CG2   | 1:B:503:TYR:HD1   | 2.19                     | 0.54              |
| 1:C:1288:ARG:HH11 | 1:C:1290:ILE:CD1  | 2.20                     | 0.54              |
| 1:D:1264:SER:O    | 1:D:1265:PHE:HB3  | 2.08                     | 0.54              |
| 1:E:447:ILE:HG22  | 1:E:448:THR:N     | 2.21                     | 0.54              |
| 1:E:449:ILE:HD13  | 1:E:491:THR:HG21  | 1.90                     | 0.54              |
| 1:F:463:TYR:HB2   | 1:F:475:ALA:HB2   | 1.90                     | 0.54              |
| 1:A:458:VAL:O     | 1:A:462:LEU:HB2   | 2.07                     | 0.54              |
| 1:A:1184:LEU:CB   | 1:A:1193:SER:OG   | 2.56                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1359:ALA:HB3  | 1:A:1362:LYS:HD3  | 1.90                     | 0.54              |
| 1:D:1183:LEU:HB2  | 1:D:1431:TYR:CE2  | 2.43                     | 0.54              |
| 1:E:490:HIS:CD2   | 1:E:494:LYS:HB3   | 2.43                     | 0.54              |
| 1:B:451:ASN:HD21  | 1:B:1213:LYS:HG3  | 1.73                     | 0.54              |
| 1:C:489:ARG:HH21  | 1:C:1410:LYS:HE3  | 1.73                     | 0.54              |
| 1:F:1286:PRO:O    | 1:F:1310:ASN:HB3  | 2.07                     | 0.54              |
| 1:F:1322:VAL:HB   | 1:F:1353:TRP:HB3  | 1.90                     | 0.54              |
| 1:F:1401:VAL:H    | 1:F:1424:TYR:HH   | 1.54                     | 0.54              |
| 1:B:1434:ARG:HH11 | 1:B:1434:ARG:HG3  | 1.73                     | 0.53              |
| 1:C:453:PHE:HE1   | 1:C:503:TYR:HB2   | 1.72                     | 0.53              |
| 1:D:1317:ALA:HB2  | 1:D:1392:VAL:HG12 | 1.90                     | 0.53              |
| 1:F:1312:LYS:HB2  | 1:F:1312:LYS:HZ2  | 1.73                     | 0.53              |
| 1:F:1408:GLU:OE2  | 1:F:1410:LYS:HB2  | 2.08                     | 0.53              |
| 1:A:1286:PRO:C    | 1:A:1287:PHE:HD1  | 2.16                     | 0.53              |
| 1:D:432:ALA:HB3   | 1:D:435:SER:OG    | 2.09                     | 0.53              |
| 1:D:479:ALA:HA    | 1:D:482:LEU:HD12  | 1.90                     | 0.53              |
| 1:E:426:VAL:O     | 1:E:429:ALA:HB3   | 2.07                     | 0.53              |
| 1:E:1359:ALA:HB3  | 1:E:1362:LYS:CE   | 2.38                     | 0.53              |
| 1:A:494:LYS:NZ    | 1:C:1338:MET:O    | 2.39                     | 0.53              |
| 1:A:1244:ASP:HB2  | 1:A:1278:ARG:O    | 2.09                     | 0.53              |
| 1:C:427:THR:OG1   | 1:C:487:LEU:HD23  | 2.08                     | 0.53              |
| 1:C:1323:ARG:HB3  | 1:C:1387:SER:OG   | 2.09                     | 0.53              |
| 1:F:1408:GLU:HG3  | 1:F:1411:LEU:HB2  | 1.89                     | 0.53              |
| 1:A:1253:ARG:HB2  | 1:A:1264:SER:OG   | 2.08                     | 0.53              |
| 1:B:1294:ARG:HB3  | 1:B:1294:ARG:HH11 | 1.73                     | 0.53              |
| 1:C:490:HIS:CD2   | 1:C:494:LYS:HB3   | 2.42                     | 0.53              |
| 1:C:1202:MET:HE1  | 1:C:1267:PRO:HB3  | 1.90                     | 0.53              |
| 1:E:1293:VAL:HG21 | 1:E:1383:ARG:HH11 | 1.73                     | 0.53              |
| 1:F:1307:ILE:HG21 | 1:F:1388:MET:HE1  | 1.90                     | 0.53              |
| 1:B:1277:TYR:N    | 1:B:1277:TYR:CD2  | 2.77                     | 0.53              |
| 1:B:1341:LYS:NZ   | 1:B:1343:LYS:HE3  | 2.24                     | 0.53              |
| 1:B:1358:MET:HE2  | 1:B:1364:SER:OG   | 2.08                     | 0.53              |
| 1:B:1384:PRO:O    | 1:B:1435:CYS:SG   | 2.66                     | 0.53              |
| 1:D:1309:SER:OG   | 1:D:1358:MET:SD   | 2.67                     | 0.53              |
| 1:E:1345:LYS:NZ   | 1:E:1354:LYS:NZ   | 2.56                     | 0.53              |
| 1:E:1399:LEU:HD23 | 1:E:1400:LYS:N    | 2.23                     | 0.53              |
| 1:F:1277:TYR:N    | 1:F:1277:TYR:CD2  | 2.76                     | 0.53              |
| 1:A:1375:THR:CG2  | 1:A:1378:LYS:HD3  | 2.38                     | 0.53              |
| 1:C:1183:LEU:HD22 | 1:C:1285:LEU:HD22 | 1.91                     | 0.53              |
| 1:E:1206:LEU:CD2  | 1:E:1406:VAL:HG11 | 2.38                     | 0.53              |
| 1:A:1408:GLU:CD   | 1:A:1409:PRO:HD2  | 2.34                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1318:GLN:NE2  | 1:C:1357:ARG:NH1  | 2.51                     | 0.53              |
| 1:D:437:LEU:H     | 1:D:461:TRP:CD1   | 2.27                     | 0.53              |
| 1:E:1333:VAL:HG22 | 1:E:1370:ILE:HG13 | 1.91                     | 0.53              |
| 1:F:1188:GLN:NE2  | 1:F:1190:GLN:HG2  | 2.24                     | 0.53              |
| 1:F:1361:MET:HA   | 1:F:1361:MET:HE3  | 1.91                     | 0.53              |
| 1:D:1324:ILE:CG2  | 1:D:1351:ILE:HB   | 2.36                     | 0.53              |
| 1:E:1298:ARG:CD   | 1:E:1374:PRO:HA   | 2.39                     | 0.53              |
| 1:F:1402:ARG:O    | 1:F:1403:TYR:HB3  | 2.09                     | 0.53              |
| 1:B:1202:MET:SD   | 1:B:1272:PHE:HZ   | 2.31                     | 0.53              |
| 1:C:462:LEU:O     | 1:C:466:VAL:HG23  | 2.09                     | 0.53              |
| 1:D:1289:VAL:O    | 1:D:1291:PRO:HD3  | 2.08                     | 0.53              |
| 1:D:1292:LEU:HD12 | 1:D:1304:LYS:HE2  | 1.91                     | 0.53              |
| 1:E:504:VAL:HB    | 1:E:1211:GLU:OE1  | 2.09                     | 0.53              |
| 1:A:1241:ILE:O    | 1:A:1241:ILE:HG22 | 2.08                     | 0.53              |
| 1:C:1276:ARG:HB2  | 1:C:1276:ARG:CZ   | 2.38                     | 0.53              |
| 1:C:1288:ARG:NH1  | 1:C:1290:ILE:CD1  | 2.71                     | 0.53              |
| 1:E:466:VAL:HG11  | 1:E:469:PHE:HE2   | 1.74                     | 0.53              |
| 1:F:1217:ASN:HD22 | 1:F:1400:LYS:HB2  | 1.74                     | 0.53              |
| 1:B:1175:LEU:HD21 | 1:B:1202:MET:HE3  | 1.91                     | 0.52              |
| 1:D:422:ASP:O     | 1:D:426:VAL:HG23  | 2.09                     | 0.52              |
| 1:D:1196:VAL:HG23 | 1:D:1279:THR:HG22 | 1.90                     | 0.52              |
| 1:D:1424:TYR:N    | 1:D:1424:TYR:HD2  | 2.05                     | 0.52              |
| 1:E:491:THR:HG22  | 1:E:492:VAL:CG1   | 2.39                     | 0.52              |
| 1:C:426:VAL:O     | 1:C:429:ALA:HB3   | 2.09                     | 0.52              |
| 1:E:1319:LYS:HD2  | 1:E:1391:GLU:OE2  | 2.09                     | 0.52              |
| 1:A:1434:ARG:CG   | 1:A:1434:ARG:NH1  | 2.65                     | 0.52              |
| 1:B:489:ARG:NH1   | 1:B:1211:GLU:HB2  | 2.25                     | 0.52              |
| 1:B:1341:LYS:HZ2  | 1:B:1343:LYS:HE3  | 1.74                     | 0.52              |
| 1:C:1214:PHE:CE2  | 1:C:1216:MET:HE2  | 2.45                     | 0.52              |
| 1:C:1345:LYS:HD2  | 1:C:1352:VAL:HG21 | 1.91                     | 0.52              |
| 1:F:1298:ARG:HH21 | 1:F:1298:ARG:HG3  | 1.74                     | 0.52              |
| 1:A:1185:MET:HE1  | 1:A:1288:ARG:HD2  | 1.91                     | 0.52              |
| 1:A:1317:ALA:HB2  | 1:A:1392:VAL:HG12 | 1.92                     | 0.52              |
| 1:C:1174:PHE:HD1  | 1:C:1421:TRP:HB2  | 1.73                     | 0.52              |
| 1:C:1339:LYS:NZ   | 1:C:1358:MET:HE2  | 2.24                     | 0.52              |
| 1:E:462:LEU:HD13  | 1:E:479:ALA:HB2   | 1.91                     | 0.52              |
| 1:B:1342:ALA:HB2  | 1:B:1353:TRP:CD1  | 2.44                     | 0.52              |
| 1:F:1177:VAL:HB   | 1:F:1424:TYR:CD1  | 2.35                     | 0.52              |
| 1:D:1183:LEU:HD11 | 1:D:1191:VAL:HG13 | 1.92                     | 0.52              |
| 1:D:1301:LEU:O    | 1:D:1370:ILE:HG12 | 2.09                     | 0.52              |
| 1:E:1203:LYS:HB3  | 1:E:1205:TYR:CE1  | 2.37                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:1329:ASN:OD1  | 1:E:1372:LEU:HD22 | 2.10                     | 0.52              |
| 1:F:1323:ARG:NH1  | 1:F:1352:VAL:HG22 | 2.09                     | 0.52              |
| 1:B:426:VAL:O     | 1:B:429:ALA:HB3   | 2.09                     | 0.52              |
| 1:B:1300:LYS:NZ   | 1:B:1302:GLU:OE1  | 2.38                     | 0.52              |
| 1:B:1322:VAL:HB   | 1:B:1353:TRP:HB3  | 1.91                     | 0.52              |
| 1:C:487:LEU:H     | 1:C:487:LEU:HD12  | 1.73                     | 0.52              |
| 1:D:1206:LEU:HD22 | 1:D:1406:VAL:HG11 | 1.90                     | 0.52              |
| 1:B:1198:GLY:C    | 1:B:1277:TYR:CE2  | 2.87                     | 0.52              |
| 1:A:487:LEU:HD23  | 1:A:487:LEU:H     | 1.74                     | 0.52              |
| 1:A:1329:ASN:ND2  | 1:A:1372:LEU:HD13 | 2.25                     | 0.52              |
| 1:B:1252:VAL:HG22 | 1:B:1263:ILE:CG1  | 2.40                     | 0.52              |
| 1:C:1211:GLU:HG3  | 1:C:1253:ARG:HH11 | 1.73                     | 0.52              |
| 1:E:1324:ILE:CG2  | 1:E:1324:ILE:O    | 2.57                     | 0.52              |
| 1:C:423:MET:HE1   | 1:C:485:ALA:HB2   | 1.91                     | 0.52              |
| 1:C:1201:VAL:HG12 | 1:C:1202:MET:N    | 2.23                     | 0.52              |
| 1:D:1320:ILE:HG23 | 1:D:1388:MET:CE   | 2.39                     | 0.52              |
| 1:E:458:VAL:CG1   | 1:E:459:VAL:N     | 2.73                     | 0.52              |
| 1:E:1214:PHE:C    | 1:E:1214:PHE:HD2  | 2.18                     | 0.52              |
| 1:E:1264:SER:O    | 1:E:1265:PHE:HB3  | 2.10                     | 0.52              |
| 1:F:1294:ARG:HH11 | 1:F:1294:ARG:CB   | 2.22                     | 0.52              |
| 1:A:1423:ARG:HB2  | 1:E:1158:TYR:CD1  | 2.44                     | 0.51              |
| 1:C:1322:VAL:HB   | 1:C:1353:TRP:HB3  | 1.91                     | 0.51              |
| 1:A:430:MET:O     | 1:A:435:SER:OG    | 2.28                     | 0.51              |
| 1:A:449:ILE:HD12  | 1:A:1407:PHE:CE1  | 2.45                     | 0.51              |
| 1:B:1170:ARG:HA   | 1:F:1421:TRP:CH2  | 2.46                     | 0.51              |
| 1:B:1422:VAL:HG22 | 1:B:1423:ARG:H    | 1.75                     | 0.51              |
| 1:D:1181:VAL:CG1  | 1:D:1396:PRO:HB3  | 2.41                     | 0.51              |
| 1:F:1293:VAL:HG23 | 1:F:1383:ARG:HH12 | 1.74                     | 0.51              |
| 1:B:473:ARG:HH21  | 1:B:473:ARG:HG3   | 1.75                     | 0.51              |
| 1:C:449:ILE:HG22  | 1:C:452:ALA:HB2   | 1.92                     | 0.51              |
| 1:C:1299:THR:O    | 1:C:1371:GLU:HA   | 2.11                     | 0.51              |
| 1:D:1392:VAL:HB   | 1:D:1394:PHE:HE2  | 1.76                     | 0.51              |
| 1:F:1331:SER:HB2  | 1:F:1373:LEU:CD2  | 2.40                     | 0.51              |
| 1:D:1183:LEU:HD11 | 1:D:1191:VAL:HG11 | 1.93                     | 0.51              |
| 1:F:1158:TYR:O    | 1:F:1159:HIS:CD2  | 2.64                     | 0.51              |
| 1:F:1335:VAL:CG1  | 1:F:1351:ILE:HD13 | 2.41                     | 0.51              |
| 1:A:1253:ARG:CD   | 1:A:1264:SER:OG   | 2.49                     | 0.51              |
| 1:C:427:THR:CG2   | 1:C:482:LEU:HD22  | 2.41                     | 0.51              |
| 1:D:1183:LEU:HD21 | 1:D:1285:LEU:CD2  | 2.29                     | 0.51              |
| 1:A:1296:VAL:O    | 1:A:1300:LYS:HB2  | 2.11                     | 0.51              |
| 1:C:1331:SER:HB3  | 1:C:1373:LEU:HG   | 1.92                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:F:1214:PHE:CD1  | 1:F:1215:GLY:N    | 2.74                     | 0.51              |
| 1:D:426:VAL:O     | 1:D:429:ALA:HB3   | 2.11                     | 0.51              |
| 1:D:439:VAL:O     | 1:D:439:VAL:HG12  | 2.10                     | 0.51              |
| 1:D:1289:VAL:HG22 | 1:D:1307:ILE:CG2  | 2.40                     | 0.51              |
| 1:E:1268:PRO:HD2  | 1:E:1272:PHE:CE1  | 2.45                     | 0.51              |
| 1:F:1296:VAL:HB   | 1:F:1300:LYS:HB2  | 1.93                     | 0.51              |
| 1:A:454:LEU:HG    | 1:A:456:SER:H     | 1.76                     | 0.51              |
| 1:A:1185:MET:CE   | 1:A:1288:ARG:HD2  | 2.41                     | 0.51              |
| 1:D:1178:LEU:HD23 | 1:D:1425:ILE:HB   | 1.93                     | 0.51              |
| 1:F:1284:ILE:HD11 | 1:F:1396:PRO:HA   | 1.93                     | 0.51              |
| 1:F:1298:ARG:NH1  | 1:F:1375:THR:HG23 | 2.26                     | 0.51              |
| 1:F:1422:VAL:CG1  | 1:F:1423:ARG:H    | 2.24                     | 0.51              |
| 1:A:1319:LYS:O    | 1:A:1390:PHE:HA   | 2.11                     | 0.51              |
| 1:C:434:GLU:OE2   | 1:C:1256:LYS:NZ   | 2.38                     | 0.51              |
| 1:D:454:LEU:HB3   | 1:D:457:ASP:OD2   | 2.11                     | 0.51              |
| 1:D:1285:LEU:N    | 1:D:1285:LEU:CD1  | 2.73                     | 0.51              |
| 1:E:1253:ARG:HG3  | 1:E:1253:ARG:HH21 | 1.76                     | 0.51              |
| 1:F:462:LEU:HD12  | 1:F:475:ALA:O     | 2.11                     | 0.51              |
| 1:D:1413:TYR:HB2  | 1:D:1417:ASP:HB2  | 1.91                     | 0.51              |
| 1:A:426:VAL:O     | 1:A:429:ALA:HB3   | 2.11                     | 0.50              |
| 1:C:495:ILE:HG23  | 1:C:496:THR:HG23  | 1.94                     | 0.50              |
| 1:C:1359:ALA:HB3  | 1:C:1362:LYS:HE2  | 1.92                     | 0.50              |
| 1:D:1324:ILE:O    | 1:D:1324:ILE:CG2  | 2.58                     | 0.50              |
| 1:E:1179:GLU:OE2  | 1:E:1397:SER:OG   | 2.24                     | 0.50              |
| 1:E:1300:LYS:HE2  | 1:E:1369:GLU:OE2  | 2.11                     | 0.50              |
| 1:A:1338:MET:HE2  | 1:F:492:VAL:HG13  | 1.93                     | 0.50              |
| 1:B:1359:ALA:HB3  | 1:B:1362:LYS:HD2  | 1.92                     | 0.50              |
| 1:C:430:MET:HE2   | 1:C:437:LEU:HD22  | 1.92                     | 0.50              |
| 1:E:487:LEU:HD23  | 1:E:487:LEU:H     | 1.75                     | 0.50              |
| 1:F:1329:ASN:OD1  | 1:F:1372:LEU:HD22 | 2.12                     | 0.50              |
| 1:C:460:ASP:HA    | 1:C:463:TYR:HE1   | 1.75                     | 0.50              |
| 1:C:1174:PHE:CD1  | 1:C:1421:TRP:HB2  | 2.47                     | 0.50              |
| 1:C:1375:THR:HG22 | 1:C:1378:LYS:H    | 1.75                     | 0.50              |
| 1:B:1394:PHE:CD1  | 1:B:1394:PHE:C    | 2.90                     | 0.50              |
| 1:C:443:MET:HG3   | 1:C:447:ILE:O     | 2.11                     | 0.50              |
| 1:C:1315:LEU:N    | 1:C:1315:LEU:HD23 | 2.26                     | 0.50              |
| 1:E:1170:ARG:NH2  | 1:E:1205:TYR:CD2  | 2.79                     | 0.50              |
| 1:E:1178:LEU:HB3  | 1:E:1427:ARG:HH12 | 1.76                     | 0.50              |
| 1:E:1370:ILE:HD12 | 1:E:1370:ILE:N    | 2.25                     | 0.50              |
| 1:F:440:ARG:O     | 1:F:442:ARG:HD3   | 2.11                     | 0.50              |
| 1:A:1183:LEU:HB3  | 1:A:1431:TYR:CE1  | 2.47                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1184:LEU:HB2  | 1:A:1193:SER:OG   | 2.12                     | 0.50              |
| 1:C:1287:PHE:HB2  | 1:C:1388:MET:HE1  | 1.93                     | 0.50              |
| 1:D:1216:MET:HA   | 1:D:1402:ARG:HG3  | 1.92                     | 0.50              |
| 1:E:479:ALA:HB3   | 1:E:497:PHE:CE2   | 2.47                     | 0.50              |
| 1:E:1305:VAL:HG11 | 1:E:1324:ILE:HD11 | 1.94                     | 0.50              |
| 1:F:1284:ILE:HG13 | 1:F:1396:PRO:HA   | 1.94                     | 0.50              |
| 1:A:1202:MET:O    | 1:A:1271:GLU:HA   | 2.11                     | 0.50              |
| 1:B:1249:HIS:CD2  | 1:B:1272:PHE:HB2  | 2.47                     | 0.50              |
| 1:D:1296:VAL:HB   | 1:D:1300:LYS:HB2  | 1.94                     | 0.50              |
| 1:E:1186:SER:CA   | 1:E:1434:ARG:HD2  | 2.37                     | 0.50              |
| 1:E:1327:PRO:HA   | 1:E:1381:TRP:CZ2  | 2.47                     | 0.50              |
| 1:E:1345:LYS:NZ   | 1:E:1354:LYS:HZ1  | 2.09                     | 0.50              |
| 1:F:441:ASP:OD1   | 1:F:450:PRO:HA    | 2.11                     | 0.50              |
| 1:F:1177:VAL:HG21 | 1:F:1424:TYR:HE1  | 1.77                     | 0.50              |
| 1:A:1161:LEU:HB2  | 1:E:1422:VAL:CG2  | 2.38                     | 0.50              |
| 1:A:1298:ARG:HH21 | 1:A:1374:PRO:HA   | 1.77                     | 0.50              |
| 1:C:1287:PHE:N    | 1:C:1287:PHE:CD1  | 2.80                     | 0.50              |
| 1:C:1335:VAL:HG12 | 1:C:1368:ALA:HB2  | 1.93                     | 0.50              |
| 1:D:1198:GLY:C    | 1:D:1277:TYR:CE2  | 2.90                     | 0.50              |
| 1:E:1195:HIS:CE1  | 1:E:1278:ARG:HH12 | 2.29                     | 0.50              |
| 1:B:1323:ARG:HH11 | 1:B:1323:ARG:CB   | 2.22                     | 0.50              |
| 1:B:1415:ASP:OD2  | 1:B:1420:LYS:NZ   | 2.43                     | 0.50              |
| 1:C:463:TYR:CG    | 1:C:464:HIS:N     | 2.80                     | 0.50              |
| 1:C:1288:ARG:HH11 | 1:C:1288:ARG:HG2  | 1.76                     | 0.50              |
| 1:E:1247:THR:C    | 1:E:1248:PHE:CD1  | 2.90                     | 0.50              |
| 1:E:1299:THR:HG22 | 1:E:1300:LYS:HD2  | 1.93                     | 0.50              |
| 1:E:1392:VAL:HB   | 1:E:1394:PHE:CE2  | 2.47                     | 0.50              |
| 1:E:1419:ILE:HD12 | 1:E:1419:ILE:N    | 2.26                     | 0.50              |
| 1:F:498:SER:HB2   | 1:F:501:CYS:HG    | 1.76                     | 0.50              |
| 1:A:463:TYR:HB3   | 1:A:475:ALA:HB2   | 1.94                     | 0.50              |
| 1:C:495:ILE:HG23  | 1:C:496:THR:N     | 2.27                     | 0.50              |
| 1:E:458:VAL:HG13  | 1:E:459:VAL:N     | 2.27                     | 0.50              |
| 1:E:462:LEU:HD22  | 1:E:475:ALA:HB1   | 1.92                     | 0.50              |
| 1:F:1183:LEU:HD22 | 1:F:1285:LEU:CD2  | 2.42                     | 0.50              |
| 1:F:1413:TYR:HB2  | 1:F:1417:ASP:HB2  | 1.94                     | 0.49              |
| 1:A:1205:TYR:CD2  | 1:A:1205:TYR:N    | 2.79                     | 0.49              |
| 1:C:1419:ILE:HD12 | 1:C:1419:ILE:N    | 2.26                     | 0.49              |
| 1:A:1293:VAL:HG12 | 1:A:1303:VAL:HG13 | 1.94                     | 0.49              |
| 1:A:1392:VAL:HB   | 1:A:1394:PHE:CD2  | 2.47                     | 0.49              |
| 1:D:1185:MET:HG3  | 1:D:1191:VAL:HG22 | 1.94                     | 0.49              |
| 1:D:1324:ILE:CD1  | 1:D:1386:ILE:HG12 | 2.30                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:1306:VAL:HG22 | 1:E:1365:GLN:HB2  | 1.93                     | 0.49              |
| 1:B:1284:ILE:O    | 1:B:1286:PRO:HD3  | 2.12                     | 0.49              |
| 1:C:489:ARG:HD2   | 1:C:1410:LYS:HE2  | 1.93                     | 0.49              |
| 1:D:440:ARG:HG2   | 1:D:442:ARG:HH12  | 1.76                     | 0.49              |
| 1:D:1294:ARG:O    | 1:D:1301:LEU:HD23 | 2.12                     | 0.49              |
| 1:A:472:ARG:NH2   | 1:A:472:ARG:CG    | 2.76                     | 0.49              |
| 1:A:1328:LEU:HD13 | 1:A:1381:TRP:CZ3  | 2.48                     | 0.49              |
| 1:A:1345:LYS:HA   | 1:A:1345:LYS:CE   | 2.37                     | 0.49              |
| 1:C:458:VAL:CG1   | 1:C:459:VAL:N     | 2.76                     | 0.49              |
| 1:C:1264:SER:O    | 1:C:1265:PHE:HB3  | 2.12                     | 0.49              |
| 1:D:494:LYS:HE2   | 1:D:498:SER:OG    | 2.13                     | 0.49              |
| 1:D:1249:HIS:O    | 1:D:1252:VAL:HG23 | 2.11                     | 0.49              |
| 1:B:1158:TYR:HD1  | 1:F:1421:TRP:HB3  | 1.78                     | 0.49              |
| 1:B:1390:PHE:CD1  | 1:B:1390:PHE:C    | 2.91                     | 0.49              |
| 1:B:1413:TYR:HA   | 1:B:1417:ASP:OD2  | 2.12                     | 0.49              |
| 1:B:1421:TRP:CH2  | 1:F:1170:ARG:HA   | 2.48                     | 0.49              |
| 1:C:427:THR:HG23  | 1:C:482:LEU:HD22  | 1.94                     | 0.49              |
| 1:D:1180:SER:CB   | 1:D:1427:ARG:HE   | 2.16                     | 0.49              |
| 1:E:1183:LEU:HD11 | 1:E:1191:VAL:CG1  | 2.42                     | 0.49              |
| 1:F:461:TRP:C     | 1:F:461:TRP:CE3   | 2.91                     | 0.49              |
| 1:A:1329:ASN:OD1  | 1:A:1378:LYS:HD2  | 2.13                     | 0.49              |
| 1:F:439:VAL:HG13  | 1:F:453:PHE:HD2   | 1.77                     | 0.49              |
| 1:F:1293:VAL:HG23 | 1:F:1383:ARG:NH1  | 2.27                     | 0.49              |
| 1:F:1408:GLU:CD   | 1:F:1409:PRO:HD2  | 2.38                     | 0.49              |
| 1:B:458:VAL:O     | 1:B:462:LEU:CG    | 2.60                     | 0.49              |
| 1:B:1394:PHE:O    | 1:B:1396:PRO:HD3  | 2.13                     | 0.49              |
| 1:F:440:ARG:HG2   | 1:F:441:ASP:H     | 1.77                     | 0.49              |
| 1:F:1323:ARG:HG3  | 1:F:1323:ARG:HH11 | 1.76                     | 0.49              |
| 1:B:502:TYR:C     | 1:B:503:TYR:HD2   | 2.21                     | 0.49              |
| 1:B:1375:THR:HG23 | 1:B:1375:THR:O    | 2.12                     | 0.49              |
| 1:C:1185:MET:HE2  | 1:C:1433:THR:CG2  | 2.42                     | 0.49              |
| 1:D:1181:VAL:HG11 | 1:D:1396:PRO:HB3  | 1.95                     | 0.49              |
| 1:D:1250:GLN:HG3  | 1:D:1251:CYS:H    | 1.76                     | 0.49              |
| 1:A:1182:ASN:HB2  | 1:A:1195:HIS:CE1  | 2.46                     | 0.49              |
| 1:B:1422:VAL:HG22 | 1:B:1423:ARG:N    | 2.28                     | 0.49              |
| 1:C:430:MET:HB3   | 1:C:437:LEU:CD2   | 2.43                     | 0.49              |
| 1:C:1174:PHE:CE1  | 1:C:1421:TRP:HD1  | 2.27                     | 0.49              |
| 1:D:440:ARG:C     | 1:D:442:ARG:HH12  | 2.20                     | 0.49              |
| 1:E:459:VAL:HG11  | 1:E:472:ARG:HE    | 1.78                     | 0.49              |
| 1:A:1328:LEU:HD13 | 1:A:1381:TRP:HZ3  | 1.78                     | 0.48              |
| 1:B:483:LEU:HD12  | 1:B:488:ILE:O     | 2.13                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1277:TYR:N    | 1:B:1277:TYR:HD2  | 2.11                     | 0.48              |
| 1:B:1421:TRP:CZ3  | 1:F:1170:ARG:CB   | 2.96                     | 0.48              |
| 1:C:472:ARG:NH2   | 1:C:472:ARG:CG    | 2.74                     | 0.48              |
| 1:E:461:TRP:CE3   | 1:E:461:TRP:C     | 2.91                     | 0.48              |
| 1:E:490:HIS:NE2   | 1:E:494:LYS:HB3   | 2.28                     | 0.48              |
| 1:E:1173:LEU:HD12 | 1:E:1173:LEU:O    | 2.12                     | 0.48              |
| 1:E:1298:ARG:HH21 | 1:E:1298:ARG:CG   | 2.26                     | 0.48              |
| 1:E:1390:PHE:CE1  | 1:E:1428:SER:HB3  | 2.48                     | 0.48              |
| 1:E:1413:TYR:HB2  | 1:E:1417:ASP:HB2  | 1.95                     | 0.48              |
| 1:F:1277:TYR:CE1  | 1:F:1399:LEU:HD12 | 2.48                     | 0.48              |
| 1:A:430:MET:CE    | 1:A:437:LEU:HD22  | 2.08                     | 0.48              |
| 1:C:440:ARG:HG2   | 1:C:442:ARG:HD2   | 1.95                     | 0.48              |
| 1:C:1244:ASP:OD2  | 1:C:1280:THR:CG2  | 2.48                     | 0.48              |
| 1:E:1359:ALA:HB3  | 1:E:1362:LYS:CD   | 2.43                     | 0.48              |
| 1:F:1289:VAL:O    | 1:F:1291:PRO:HD3  | 2.12                     | 0.48              |
| 1:A:433:PRO:HG3   | 1:A:1256:LYS:HB2  | 1.94                     | 0.48              |
| 1:C:1251:CYS:SG   | 1:C:1268:PRO:HD3  | 2.54                     | 0.48              |
| 1:E:457:ASP:HA    | 1:E:460:ASP:OD2   | 2.14                     | 0.48              |
| 1:A:1205:TYR:HD2  | 1:A:1205:TYR:N    | 2.11                     | 0.48              |
| 1:B:440:ARG:HB3   | 1:B:442:ARG:NH1   | 2.29                     | 0.48              |
| 1:B:1252:VAL:O    | 1:B:1252:VAL:CG1  | 2.62                     | 0.48              |
| 1:B:1360:GLY:O    | 1:B:1361:MET:C    | 2.56                     | 0.48              |
| 1:B:1382:ALA:O    | 1:B:1384:PRO:HD3  | 2.13                     | 0.48              |
| 1:C:1276:ARG:HH11 | 1:C:1276:ARG:CG   | 2.26                     | 0.48              |
| 1:C:1381:TRP:CZ3  | 1:C:1383:ARG:HG2  | 2.49                     | 0.48              |
| 1:C:1422:VAL:CG1  | 1:C:1423:ARG:H    | 2.26                     | 0.48              |
| 1:D:447:ILE:HG22  | 1:D:1414:SER:OG   | 2.14                     | 0.48              |
| 1:D:479:ALA:HA    | 1:D:482:LEU:CD1   | 2.43                     | 0.48              |
| 1:D:1343:LYS:HE3  | 1:D:1345:LYS:NZ   | 2.27                     | 0.48              |
| 1:F:1287:PHE:HD1  | 1:F:1388:MET:SD   | 2.36                     | 0.48              |
| 1:A:1173:LEU:HD22 | 1:A:1404:LEU:CD2  | 2.44                     | 0.48              |
| 1:B:494:LYS:NZ    | 1:B:498:SER:HB2   | 2.29                     | 0.48              |
| 1:C:1178:LEU:HG   | 1:C:1425:ILE:CG2  | 2.44                     | 0.48              |
| 1:E:1326:THR:HG21 | 1:E:1344:TYR:CE1  | 2.49                     | 0.48              |
| 1:A:447:ILE:CG2   | 1:A:448:THR:N     | 2.77                     | 0.48              |
| 1:D:1217:ASN:ND2  | 1:D:1400:LYS:CB   | 2.76                     | 0.48              |
| 1:E:1178:LEU:C    | 1:E:1427:ARG:HH12 | 2.21                     | 0.48              |
| 1:F:423:MET:HA    | 1:F:478:TYR:OH    | 2.14                     | 0.48              |
| 1:C:460:ASP:HA    | 1:C:463:TYR:CE1   | 2.48                     | 0.48              |
| 1:C:1343:LYS:HG2  | 1:C:1344:TYR:N    | 2.28                     | 0.48              |
| 1:D:1170:ARG:NH1  | 1:D:1172:GLU:CD   | 2.69                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:1277:TYR:CD2  | 1:E:1277:TYR:N    | 2.82                     | 0.48              |
| 1:A:1247:THR:O    | 1:A:1248:PHE:CD1  | 2.67                     | 0.48              |
| 1:A:1291:PRO:HA   | 1:A:1305:VAL:HG23 | 1.96                     | 0.48              |
| 1:A:1422:VAL:CG2  | 1:E:1161:LEU:HB2  | 2.42                     | 0.48              |
| 1:B:1249:HIS:ND1  | 1:B:1250:GLN:HG3  | 2.29                     | 0.48              |
| 1:C:1183:LEU:CD1  | 1:C:1184:LEU:N    | 2.72                     | 0.48              |
| 1:E:1423:ARG:HD2  | 1:E:1425:ILE:HD11 | 1.94                     | 0.48              |
| 1:F:478:TYR:CZ    | 1:F:482:LEU:HD21  | 2.49                     | 0.48              |
| 1:F:1404:LEU:C    | 1:F:1404:LEU:CD2  | 2.86                     | 0.48              |
| 1:A:1311:PHE:O    | 1:A:1312:LYS:C    | 2.57                     | 0.48              |
| 1:B:1185:MET:SD   | 1:B:1288:ARG:HD2  | 2.54                     | 0.48              |
| 1:C:1329:ASN:HD21 | 1:C:1372:LEU:HB3  | 1.78                     | 0.48              |
| 1:D:467:GLU:HG2   | 1:D:468:GLY:N     | 2.29                     | 0.48              |
| 1:D:1320:ILE:CG2  | 1:D:1388:MET:CE   | 2.91                     | 0.48              |
| 1:F:424:ALA:O     | 1:F:428:LYS:HG3   | 2.14                     | 0.48              |
| 1:F:1360:GLY:O    | 1:F:1361:MET:C    | 2.57                     | 0.48              |
| 1:A:1177:VAL:HB   | 1:A:1424:TYR:HD1  | 1.79                     | 0.47              |
| 1:A:1304:LYS:HD2  | 1:A:1365:GLN:HE22 | 1.79                     | 0.47              |
| 1:C:1211:GLU:CG   | 1:C:1253:ARG:HH11 | 2.27                     | 0.47              |
| 1:E:1422:VAL:CG1  | 1:E:1423:ARG:H    | 2.26                     | 0.47              |
| 1:F:1322:VAL:HG22 | 1:F:1388:MET:HE2  | 1.95                     | 0.47              |
| 1:B:1296:VAL:O    | 1:B:1300:LYS:HB2  | 2.14                     | 0.47              |
| 1:E:1253:ARG:HG3  | 1:E:1253:ARG:NH2  | 2.30                     | 0.47              |
| 1:E:1300:LYS:HG3  | 1:E:1369:GLU:OE2  | 2.14                     | 0.47              |
| 1:F:1185:MET:HE2  | 1:F:1433:THR:CG2  | 2.43                     | 0.47              |
| 1:A:1184:LEU:HA   | 1:A:1432:GLU:O    | 2.14                     | 0.47              |
| 1:A:1277:TYR:N    | 1:A:1277:TYR:CD2  | 2.82                     | 0.47              |
| 1:A:1360:GLY:O    | 1:A:1361:MET:C    | 2.56                     | 0.47              |
| 1:A:1421:TRP:CZ3  | 1:E:1170:ARG:HB2  | 2.50                     | 0.47              |
| 1:B:1326:THR:HG21 | 1:B:1344:TYR:HE1  | 1.79                     | 0.47              |
| 1:E:422:ASP:O     | 1:E:426:VAL:CG2   | 2.60                     | 0.47              |
| 1:E:1293:VAL:CG2  | 1:E:1383:ARG:NH1  | 2.77                     | 0.47              |
| 1:E:1299:THR:O    | 1:E:1371:GLU:HA   | 2.14                     | 0.47              |
| 1:A:498:SER:HB3   | 1:A:501:CYS:SG    | 2.54                     | 0.47              |
| 1:A:1298:ARG:NH2  | 1:A:1375:THR:H    | 2.12                     | 0.47              |
| 1:A:1299:THR:O    | 1:A:1371:GLU:HA   | 2.13                     | 0.47              |
| 1:B:1158:TYR:CE2  | 1:F:1423:ARG:CZ   | 2.98                     | 0.47              |
| 1:B:1305:VAL:CG2  | 1:B:1324:ILE:HD11 | 2.37                     | 0.47              |
| 1:E:1322:VAL:HG22 | 1:E:1388:MET:HE3  | 1.96                     | 0.47              |
| 1:E:1360:GLY:O    | 1:E:1361:MET:C    | 2.57                     | 0.47              |
| 1:F:1177:VAL:HG21 | 1:F:1424:TYR:CE1  | 2.49                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:F:1390:PHE:C    | 1:F:1390:PHE:CD1  | 2.92                     | 0.47              |
| 1:A:1289:VAL:HG22 | 1:A:1307:ILE:HG22 | 1.96                     | 0.47              |
| 1:B:1377:ASP:OD2  | 1:B:1379:LYS:HE3  | 2.13                     | 0.47              |
| 1:D:461:TRP:O     | 1:D:461:TRP:CE3   | 2.67                     | 0.47              |
| 1:D:1360:GLY:O    | 1:D:1361:MET:C    | 2.58                     | 0.47              |
| 1:E:1413:TYR:HA   | 1:E:1417:ASP:OD2  | 2.14                     | 0.47              |
| 1:F:1296:VAL:O    | 1:F:1300:LYS:HB2  | 2.15                     | 0.47              |
| 1:A:489:ARG:HH12  | 1:A:1211:GLU:HB2  | 1.80                     | 0.47              |
| 1:A:1218:ASP:HA   | 1:A:1241:ILE:HB   | 1.97                     | 0.47              |
| 1:B:463:TYR:CD1   | 1:B:469:PHE:HB2   | 2.49                     | 0.47              |
| 1:C:463:TYR:OH    | 1:C:464:HIS:CE1   | 2.67                     | 0.47              |
| 1:C:1287:PHE:N    | 1:C:1287:PHE:HD1  | 2.13                     | 0.47              |
| 1:C:1360:GLY:O    | 1:C:1361:MET:C    | 2.58                     | 0.47              |
| 1:D:456:SER:HA    | 1:D:499:GLU:CG    | 2.45                     | 0.47              |
| 1:D:1181:VAL:CG1  | 1:D:1396:PRO:CB   | 2.93                     | 0.47              |
| 1:E:466:VAL:CG1   | 1:E:469:PHE:CE2   | 2.95                     | 0.47              |
| 1:F:1182:ASN:HB2  | 1:F:1195:HIS:CE1  | 2.50                     | 0.47              |
| 1:F:1250:GLN:CG   | 1:F:1251:CYS:N    | 2.77                     | 0.47              |
| 1:A:476:ARG:HH21  | 1:A:476:ARG:CG    | 2.24                     | 0.47              |
| 1:A:482:LEU:N     | 1:A:482:LEU:HD23  | 2.28                     | 0.47              |
| 1:A:1277:TYR:N    | 1:A:1277:TYR:HD2  | 2.12                     | 0.47              |
| 1:A:1298:ARG:O    | 1:A:1372:LEU:HB2  | 2.15                     | 0.47              |
| 1:A:1421:TRP:CH2  | 1:E:1170:ARG:HA   | 2.49                     | 0.47              |
| 1:B:1299:THR:O    | 1:B:1371:GLU:HA   | 2.14                     | 0.47              |
| 1:C:1290:ILE:N    | 1:C:1290:ILE:HD12 | 2.30                     | 0.47              |
| 1:C:1298:ARG:O    | 1:C:1372:LEU:HD12 | 2.15                     | 0.47              |
| 1:C:1326:THR:HG22 | 1:C:1370:ILE:CD1  | 2.44                     | 0.47              |
| 1:D:1181:VAL:HG12 | 1:D:1196:VAL:HG12 | 1.95                     | 0.47              |
| 1:D:1353:TRP:CZ3  | 1:D:1366:ILE:HB   | 2.50                     | 0.47              |
| 1:D:1413:TYR:HA   | 1:D:1417:ASP:OD2  | 2.13                     | 0.47              |
| 1:E:497:PHE:C     | 1:E:497:PHE:CD1   | 2.93                     | 0.47              |
| 1:E:1178:LEU:HB3  | 1:E:1427:ARG:NH1  | 2.29                     | 0.47              |
| 1:F:460:ASP:O     | 1:F:464:HIS:CD2   | 2.66                     | 0.47              |
| 1:F:498:SER:O     | 1:F:503:TYR:OH    | 2.31                     | 0.47              |
| 1:B:1408:GLU:O    | 1:B:1411:LEU:O    | 2.33                     | 0.47              |
| 1:C:1402:ARG:O    | 1:C:1403:TYR:HB3  | 2.15                     | 0.47              |
| 1:C:1427:ARG:CG   | 1:C:1428:SER:N    | 2.77                     | 0.47              |
| 1:D:1329:ASN:HD22 | 1:D:1372:LEU:HD23 | 1.77                     | 0.47              |
| 1:F:441:ASP:C     | 1:F:442:ARG:HD3   | 2.39                     | 0.47              |
| 1:F:453:PHE:HZ    | 1:F:488:ILE:HD12  | 1.80                     | 0.47              |
| 1:C:489:ARG:NH2   | 1:C:1410:LYS:HE3  | 2.29                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1408:GLU:HG2  | 1:C:1411:LEU:CB   | 2.44                     | 0.47              |
| 1:D:1187:PRO:CD   | 1:D:1434:ARG:HB2  | 2.41                     | 0.47              |
| 1:E:1305:VAL:HG21 | 1:E:1324:ILE:CD1  | 2.41                     | 0.47              |
| 1:F:495:ILE:HG13  | 1:F:496:THR:H     | 1.78                     | 0.47              |
| 1:F:1277:TYR:N    | 1:F:1277:TYR:HD2  | 2.12                     | 0.47              |
| 1:A:443:MET:HG3   | 1:A:447:ILE:O     | 2.15                     | 0.47              |
| 1:A:1181:VAL:HG23 | 1:A:1196:VAL:HG22 | 1.96                     | 0.47              |
| 1:A:1193:SER:O    | 1:A:1194:ALA:HB2  | 2.14                     | 0.47              |
| 1:B:428:LYS:HE2   | 1:B:508:LEU:O     | 2.15                     | 0.47              |
| 1:B:444:TRP:C     | 1:B:445:LEU:HG    | 2.40                     | 0.47              |
| 1:B:1264:SER:O    | 1:B:1265:PHE:HB3  | 2.14                     | 0.47              |
| 1:C:497:PHE:O     | 1:C:497:PHE:HD1   | 1.98                     | 0.47              |
| 1:C:1188:GLN:CD   | 1:C:1188:GLN:N    | 2.73                     | 0.47              |
| 1:C:1330:THR:HG21 | 1:C:1344:TYR:OH   | 2.15                     | 0.47              |
| 1:E:426:VAL:HG21  | 1:E:478:TYR:OH    | 2.15                     | 0.47              |
| 1:F:461:TRP:CE3   | 1:F:461:TRP:O     | 2.67                     | 0.47              |
| 1:F:505:PHE:HB2   | 1:F:1253:ARG:NH2  | 2.30                     | 0.47              |
| 1:F:1276:ARG:HG2  | 1:F:1277:TYR:N    | 2.30                     | 0.47              |
| 1:A:442:ARG:HD2   | 1:A:502:TYR:OH    | 2.15                     | 0.46              |
| 1:B:427:THR:HG21  | 1:B:487:LEU:HB3   | 1.97                     | 0.46              |
| 1:B:454:LEU:O     | 1:B:458:VAL:HG23  | 2.14                     | 0.46              |
| 1:B:1199:ARG:N    | 1:B:1277:TYR:HE2  | 2.13                     | 0.46              |
| 1:C:1290:ILE:O    | 1:C:1290:ILE:HG22 | 2.14                     | 0.46              |
| 1:C:1399:LEU:C    | 1:C:1399:LEU:CD2  | 2.88                     | 0.46              |
| 1:D:1389:ASN:HA   | 1:D:1428:SER:OG   | 2.15                     | 0.46              |
| 1:E:1201:VAL:HG12 | 1:E:1202:MET:N    | 2.30                     | 0.46              |
| 1:E:1322:VAL:HB   | 1:E:1353:TRP:HB3  | 1.95                     | 0.46              |
| 1:B:440:ARG:HD2   | 1:B:441:ASP:O     | 2.14                     | 0.46              |
| 1:B:501:CYS:SG    | 1:B:503:TYR:CE2   | 3.06                     | 0.46              |
| 1:B:1193:SER:O    | 1:B:1194:ALA:HB2  | 2.16                     | 0.46              |
| 1:B:1251:CYS:SG   | 1:B:1268:PRO:HD3  | 2.55                     | 0.46              |
| 1:B:1325:PRO:O    | 1:B:1381:TRP:HH2  | 1.98                     | 0.46              |
| 1:C:1403:TYR:CD1  | 1:C:1403:TYR:C    | 2.93                     | 0.46              |
| 1:D:1296:VAL:O    | 1:D:1300:LYS:HB2  | 2.15                     | 0.46              |
| 1:F:495:ILE:HG13  | 1:F:496:THR:N     | 2.31                     | 0.46              |
| 1:F:1404:LEU:C    | 1:F:1404:LEU:HD23 | 2.40                     | 0.46              |
| 1:A:437:LEU:N     | 1:A:461:TRP:CD1   | 2.83                     | 0.46              |
| 1:A:1276:ARG:HH11 | 1:A:1276:ARG:CG   | 2.27                     | 0.46              |
| 1:C:1263:ILE:HD11 | 1:C:1274:LEU:HD21 | 1.96                     | 0.46              |
| 1:C:1265:PHE:HE1  | 1:C:1267:PRO:HB3  | 1.81                     | 0.46              |
| 1:C:1365:GLN:HG2  | 1:C:1366:ILE:N    | 2.31                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:1381:TRP:CD2  | 1:D:1381:TRP:O    | 2.68                     | 0.46              |
| 1:E:1355:ILE:O    | 1:E:1355:ILE:HG22 | 2.15                     | 0.46              |
| 1:F:440:ARG:NH2   | 1:F:440:ARG:CB    | 2.78                     | 0.46              |
| 1:A:460:ASP:HA    | 1:A:463:TYR:HE2   | 1.77                     | 0.46              |
| 1:A:1379:LYS:HD2  | 1:A:1379:LYS:N    | 2.19                     | 0.46              |
| 1:A:1383:ARG:H    | 1:A:1383:ARG:NH1  | 2.14                     | 0.46              |
| 1:B:473:ARG:CZ    | 1:B:473:ARG:HB2   | 2.45                     | 0.46              |
| 1:B:1366:ILE:O    | 1:B:1366:ILE:HG23 | 2.15                     | 0.46              |
| 1:D:1316:LEU:HD23 | 1:D:1316:LEU:N    | 2.30                     | 0.46              |
| 1:E:1311:PHE:O    | 1:E:1312:LYS:C    | 2.57                     | 0.46              |
| 1:A:461:TRP:CD1   | 1:A:465:HIS:CD2   | 3.04                     | 0.46              |
| 1:A:1339:LYS:HB3  | 1:A:1339:LYS:HZ3  | 1.78                     | 0.46              |
| 1:F:1173:LEU:HD12 | 1:F:1173:LEU:O    | 2.15                     | 0.46              |
| 1:F:1247:THR:O    | 1:F:1248:PHE:CD2  | 2.69                     | 0.46              |
| 1:F:1323:ARG:HH12 | 1:F:1352:VAL:CG2  | 2.11                     | 0.46              |
| 1:F:1323:ARG:O    | 1:F:1386:ILE:HG23 | 2.15                     | 0.46              |
| 1:F:1413:TYR:HA   | 1:F:1417:ASP:OD2  | 2.16                     | 0.46              |
| 1:A:489:ARG:NH1   | 1:A:1211:GLU:HB2  | 2.30                     | 0.46              |
| 1:A:492:VAL:CG2   | 1:C:1338:MET:HB3  | 2.45                     | 0.46              |
| 1:A:1321:GLU:OE1  | 1:A:1354:LYS:HE3  | 2.16                     | 0.46              |
| 1:B:473:ARG:HH21  | 1:B:473:ARG:CG    | 2.28                     | 0.46              |
| 1:B:1201:VAL:HG12 | 1:B:1202:MET:N    | 2.29                     | 0.46              |
| 1:B:1268:PRO:HD2  | 1:B:1272:PHE:CD2  | 2.50                     | 0.46              |
| 1:B:1434:ARG:HG3  | 1:B:1434:ARG:NH1  | 2.28                     | 0.46              |
| 1:C:1252:VAL:HA   | 1:C:1265:PHE:HB3  | 1.97                     | 0.46              |
| 1:D:1304:LYS:HG3  | 1:D:1367:SER:OG   | 2.14                     | 0.46              |
| 1:E:1173:LEU:C    | 1:E:1173:LEU:CD1  | 2.82                     | 0.46              |
| 1:A:1186:SER:HA   | 1:A:1434:ARG:HB2  | 1.98                     | 0.46              |
| 1:B:1172:GLU:HB3  | 1:B:1419:ILE:HB   | 1.97                     | 0.46              |
| 1:B:1286:PRO:O    | 1:B:1310:ASN:HB3  | 2.16                     | 0.46              |
| 1:C:497:PHE:CD1   | 1:C:497:PHE:C     | 2.94                     | 0.46              |
| 1:C:1211:GLU:CG   | 1:C:1253:ARG:NH1  | 2.78                     | 0.46              |
| 1:D:1324:ILE:HG21 | 1:D:1351:ILE:HD12 | 1.96                     | 0.46              |
| 1:F:1264:SER:O    | 1:F:1265:PHE:HB3  | 2.14                     | 0.46              |
| 1:A:1402:ARG:O    | 1:A:1403:TYR:HB3  | 2.16                     | 0.46              |
| 1:C:433:PRO:CG    | 1:C:1256:LYS:HE2  | 2.46                     | 0.46              |
| 1:C:1217:ASN:HD21 | 1:C:1400:LYS:CB   | 2.23                     | 0.46              |
| 1:C:1294:ARG:NH2  | 1:C:1302:GLU:OE2  | 2.48                     | 0.46              |
| 1:D:1300:LYS:HD3  | 1:D:1300:LYS:HA   | 1.72                     | 0.46              |
| 1:E:480:SER:HB2   | 1:E:497:PHE:HD2   | 1.81                     | 0.46              |
| 1:F:447:ILE:HG22  | 1:F:448:THR:H     | 1.81                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1316:LEU:CD2  | 1:A:1359:ALA:HA   | 2.45                     | 0.46              |
| 1:C:1276:ARG:CG   | 1:C:1277:TYR:N    | 2.79                     | 0.46              |
| 1:D:1199:ARG:N    | 1:D:1277:TYR:HE2  | 2.14                     | 0.46              |
| 1:D:1315:LEU:HD23 | 1:D:1315:LEU:N    | 2.31                     | 0.46              |
| 1:D:1390:PHE:CE2  | 1:D:1428:SER:HB3  | 2.51                     | 0.46              |
| 1:D:1408:GLU:CG   | 1:D:1411:LEU:HB2  | 2.38                     | 0.46              |
| 1:E:1202:MET:HE2  | 1:E:1204:SER:HB2  | 1.97                     | 0.46              |
| 1:E:1246:CYS:HB2  | 1:E:1276:ARG:O    | 2.16                     | 0.46              |
| 1:F:1410:LYS:HD3  | 1:F:1410:LYS:HA   | 1.71                     | 0.46              |
| 1:A:447:ILE:CG2   | 1:A:448:THR:H     | 2.26                     | 0.46              |
| 1:A:1252:VAL:HG12 | 1:A:1253:ARG:O    | 2.16                     | 0.46              |
| 1:B:431:ALA:O     | 1:B:432:ALA:C     | 2.59                     | 0.46              |
| 1:B:1322:VAL:HG22 | 1:B:1388:MET:CE   | 2.42                     | 0.46              |
| 1:B:1371:GLU:O    | 1:B:1372:LEU:HD23 | 2.16                     | 0.46              |
| 1:C:1390:PHE:HD1  | 1:C:1391:GLU:N    | 2.14                     | 0.46              |
| 1:D:1216:MET:C    | 1:D:1402:ARG:HG3  | 2.41                     | 0.46              |
| 1:E:449:ILE:HD13  | 1:E:491:THR:CG2   | 2.46                     | 0.46              |
| 1:E:462:LEU:HD22  | 1:E:475:ALA:CB    | 2.45                     | 0.46              |
| 1:F:1188:GLN:HE21 | 1:F:1190:GLN:HG2  | 1.79                     | 0.46              |
| 1:F:1328:LEU:N    | 1:F:1328:LEU:HD23 | 2.31                     | 0.46              |
| 1:A:498:SER:OG    | 1:A:499:GLU:N     | 2.48                     | 0.45              |
| 1:B:1425:ILE:O    | 1:B:1425:ILE:CG2  | 2.57                     | 0.45              |
| 1:C:461:TRP:CD1   | 1:C:465:HIS:HD2   | 2.34                     | 0.45              |
| 1:C:1287:PHE:CE2  | 1:C:1320:ILE:HD13 | 2.51                     | 0.45              |
| 1:D:1176:ASP:CG   | 1:D:1423:ARG:NH2  | 2.74                     | 0.45              |
| 1:D:1202:MET:CE   | 1:D:1404:LEU:HD21 | 2.46                     | 0.45              |
| 1:E:1335:VAL:HG11 | 1:E:1351:ILE:HG21 | 1.98                     | 0.45              |
| 1:A:1264:SER:O    | 1:A:1265:PHE:HB3  | 2.15                     | 0.45              |
| 1:A:1316:LEU:HD22 | 1:A:1359:ALA:HA   | 1.98                     | 0.45              |
| 1:C:1173:LEU:HD11 | 1:C:1404:LEU:HD13 | 1.97                     | 0.45              |
| 1:C:1342:ALA:HB2  | 1:C:1353:TRP:CD1  | 2.52                     | 0.45              |
| 1:D:461:TRP:CE3   | 1:D:461:TRP:C     | 2.95                     | 0.45              |
| 1:E:1280:THR:HA   | 1:E:1283:ILE:HD11 | 1.98                     | 0.45              |
| 1:E:1335:VAL:HG12 | 1:E:1368:ALA:CB   | 2.46                     | 0.45              |
| 1:F:1298:ARG:O    | 1:F:1372:LEU:HB2  | 2.16                     | 0.45              |
| 1:B:1186:SER:HB3  | 1:B:1190:GLN:HB2  | 1.99                     | 0.45              |
| 1:B:1292:LEU:C    | 1:B:1292:LEU:HD12 | 2.41                     | 0.45              |
| 1:C:490:HIS:CE1   | 1:C:494:LYS:HB3   | 2.51                     | 0.45              |
| 1:C:1298:ARG:O    | 1:C:1372:LEU:HB2  | 2.16                     | 0.45              |
| 1:D:437:LEU:HD12  | 1:D:438:GLU:N     | 2.31                     | 0.45              |
| 1:D:1288:ARG:NH1  | 1:D:1310:ASN:OD1  | 2.48                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:F:1311:PHE:O    | 1:F:1312:LYS:C    | 2.60                     | 0.45              |
| 1:F:1335:VAL:HG12 | 1:F:1351:ILE:HD13 | 1.97                     | 0.45              |
| 1:F:1414:SER:O    | 1:F:1415:ASP:C    | 2.59                     | 0.45              |
| 1:A:444:TRP:CE2   | 1:C:1338:MET:HE2  | 2.52                     | 0.45              |
| 1:B:1331:SER:OG   | 1:B:1371:GLU:HB3  | 2.16                     | 0.45              |
| 1:B:1344:TYR:CD2  | 1:B:1344:TYR:O    | 2.69                     | 0.45              |
| 1:C:437:LEU:H     | 1:C:461:TRP:CD1   | 2.35                     | 0.45              |
| 1:C:469:PHE:CE1   | 1:C:475:ALA:HA    | 2.51                     | 0.45              |
| 1:C:1289:VAL:O    | 1:C:1291:PRO:HD3  | 2.17                     | 0.45              |
| 1:E:1359:ALA:HB3  | 1:E:1362:LYS:NZ   | 2.32                     | 0.45              |
| 1:F:456:SER:HA    | 1:F:499:GLU:HG2   | 1.99                     | 0.45              |
| 1:F:1299:THR:O    | 1:F:1371:GLU:HA   | 2.17                     | 0.45              |
| 1:C:1182:ASN:OD1  | 1:C:1430:ILE:N    | 2.49                     | 0.45              |
| 1:D:442:ARG:HD3   | 1:D:502:TYR:CE1   | 2.51                     | 0.45              |
| 1:D:482:LEU:HD23  | 1:D:487:LEU:HD12  | 1.97                     | 0.45              |
| 1:D:1286:PRO:HG2  | 1:D:1390:PHE:HE1  | 1.82                     | 0.45              |
| 1:B:1290:ILE:HD12 | 1:B:1290:ILE:N    | 2.31                     | 0.45              |
| 1:B:1330:THR:HG23 | 1:B:1370:ILE:HG23 | 1.97                     | 0.45              |
| 1:C:506:GLY:O     | 1:C:1253:ARG:NH2  | 2.49                     | 0.45              |
| 1:D:456:SER:OG    | 1:D:457:ASP:N     | 2.50                     | 0.45              |
| 1:D:1290:ILE:HB   | 1:D:1306:VAL:CG1  | 2.36                     | 0.45              |
| 1:A:1183:LEU:HG   | 1:A:1184:LEU:H    | 1.81                     | 0.45              |
| 1:A:1288:ARG:HH12 | 1:A:1290:ILE:HG13 | 1.80                     | 0.45              |
| 1:B:430:MET:HE2   | 1:B:437:LEU:CB    | 2.46                     | 0.45              |
| 1:B:1187:PRO:HD3  | 1:B:1434:ARG:CB   | 2.46                     | 0.45              |
| 1:B:1365:GLN:HG2  | 1:B:1366:ILE:N    | 2.31                     | 0.45              |
| 1:F:1181:VAL:CG1  | 1:F:1396:PRO:HB3  | 2.46                     | 0.45              |
| 1:A:1203:LYS:HB3  | 1:A:1205:TYR:HE2  | 1.82                     | 0.45              |
| 1:A:1266:ILE:O    | 1:A:1266:ILE:HG22 | 2.16                     | 0.45              |
| 1:A:1345:LYS:HB3  | 1:A:1348:GLU:OE2  | 2.17                     | 0.45              |
| 1:B:442:ARG:NH2   | 1:B:452:ALA:O     | 2.49                     | 0.45              |
| 1:D:1381:TRP:O    | 1:D:1381:TRP:CG   | 2.70                     | 0.45              |
| 1:E:471:GLU:HG2   | 1:E:472:ARG:N     | 2.32                     | 0.45              |
| 1:E:497:PHE:CE1   | 1:E:498:SER:O     | 2.70                     | 0.45              |
| 1:B:1179:GLU:OE2  | 1:B:1277:TYR:OH   | 2.26                     | 0.45              |
| 1:C:1267:PRO:HA   | 1:C:1268:PRO:HD3  | 1.90                     | 0.45              |
| 1:E:1195:HIS:CE1  | 1:E:1278:ARG:NH1  | 2.85                     | 0.45              |
| 1:F:1298:ARG:HH12 | 1:F:1375:THR:H    | 1.64                     | 0.45              |
| 1:F:1316:LEU:CD2  | 1:F:1357:ARG:HD2  | 2.47                     | 0.45              |
| 1:F:1321:GLU:OE1  | 1:F:1354:LYS:HG2  | 2.17                     | 0.45              |
| 1:F:1324:ILE:O    | 1:F:1324:ILE:CG2  | 2.63                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1173:LEU:C    | 1:A:1173:LEU:CD1  | 2.90                     | 0.45              |
| 1:A:1311:PHE:CE1  | 1:A:1360:GLY:HA2  | 2.51                     | 0.45              |
| 1:B:1402:ARG:O    | 1:B:1403:TYR:HB3  | 2.17                     | 0.45              |
| 1:D:1335:VAL:HG12 | 1:D:1368:ALA:CB   | 2.47                     | 0.45              |
| 1:F:1434:ARG:NH1  | 1:F:1434:ARG:HG2  | 2.32                     | 0.45              |
| 1:A:1249:HIS:CD2  | 1:A:1272:PHE:HD2  | 2.35                     | 0.44              |
| 1:A:1375:THR:HG22 | 1:A:1378:LYS:HD3  | 1.99                     | 0.44              |
| 1:A:1422:VAL:O    | 1:E:1158:TYR:HD1  | 2.01                     | 0.44              |
| 1:B:502:TYR:C     | 1:B:503:TYR:CD2   | 2.95                     | 0.44              |
| 1:B:1352:VAL:HG11 | 1:B:1354:LYS:HE3  | 1.99                     | 0.44              |
| 1:C:1187:PRO:HD3  | 1:C:1434:ARG:CB   | 2.46                     | 0.44              |
| 1:D:1192:LEU:CD1  | 1:D:1434:ARG:HH22 | 2.31                     | 0.44              |
| 1:D:1402:ARG:O    | 1:D:1403:TYR:HB3  | 2.16                     | 0.44              |
| 1:E:453:PHE:HZ    | 1:E:488:ILE:HD12  | 1.82                     | 0.44              |
| 1:F:1172:GLU:HB2  | 1:F:1419:ILE:O    | 2.17                     | 0.44              |
| 1:F:1307:ILE:CG2  | 1:F:1388:MET:HE1  | 2.47                     | 0.44              |
| 1:A:1171:ASN:ND2  | 1:A:1207:SER:H    | 2.14                     | 0.44              |
| 1:A:1413:TYR:HA   | 1:A:1417:ASP:OD2  | 2.18                     | 0.44              |
| 1:E:1267:PRO:HA   | 1:E:1268:PRO:HD3  | 1.89                     | 0.44              |
| 1:E:1327:PRO:HG3  | 1:E:1381:TRP:CD2  | 2.51                     | 0.44              |
| 1:B:463:TYR:CE1   | 1:B:469:PHE:O     | 2.61                     | 0.44              |
| 1:B:1174:PHE:HB2  | 1:B:1203:LYS:HB2  | 1.99                     | 0.44              |
| 1:C:458:VAL:HG13  | 1:C:459:VAL:N     | 2.32                     | 0.44              |
| 1:D:1299:THR:O    | 1:D:1371:GLU:HA   | 2.18                     | 0.44              |
| 1:E:1161:LEU:HD12 | 1:E:1162:GLU:N    | 2.32                     | 0.44              |
| 1:E:1286:PRO:HG2  | 1:E:1390:PHE:CZ   | 2.52                     | 0.44              |
| 1:F:442:ARG:HB3   | 1:F:502:TYR:CE2   | 2.52                     | 0.44              |
| 1:F:1206:LEU:HD22 | 1:F:1406:VAL:HG11 | 1.99                     | 0.44              |
| 1:C:1280:THR:HA   | 1:C:1283:ILE:HD11 | 1.99                     | 0.44              |
| 1:C:1287:PHE:CZ   | 1:C:1320:ILE:HD13 | 2.52                     | 0.44              |
| 1:D:1298:ARG:HE   | 1:D:1375:THR:H    | 1.64                     | 0.44              |
| 1:F:463:TYR:HB2   | 1:F:475:ALA:CB    | 2.48                     | 0.44              |
| 1:B:1330:THR:HG23 | 1:B:1370:ILE:CG2  | 2.48                     | 0.44              |
| 1:B:1390:PHE:CZ   | 1:B:1428:SER:HB3  | 2.52                     | 0.44              |
| 1:D:469:PHE:HZ    | 1:D:478:TYR:CG    | 2.36                     | 0.44              |
| 1:E:476:ARG:NH2   | 1:E:476:ARG:HG2   | 2.32                     | 0.44              |
| 1:E:1324:ILE:HG22 | 1:E:1351:ILE:HB   | 1.99                     | 0.44              |
| 1:E:1346:ALA:C    | 1:E:1348:GLU:N    | 2.75                     | 0.44              |
| 1:E:1369:GLU:C    | 1:E:1370:ILE:HD12 | 2.43                     | 0.44              |
| 1:A:1173:LEU:CD2  | 1:A:1404:LEU:HD23 | 2.47                     | 0.44              |
| 1:A:1183:LEU:HB3  | 1:A:1431:TYR:HD1  | 1.82                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1186:SER:OG   | 1:A:1190:GLN:HB2  | 2.17                     | 0.44              |
| 1:A:1328:LEU:HD22 | 1:A:1381:TRP:CZ3  | 2.53                     | 0.44              |
| 1:B:453:PHE:HZ    | 1:B:488:ILE:CD1   | 2.24                     | 0.44              |
| 1:C:1193:SER:O    | 1:C:1194:ALA:HB2  | 2.18                     | 0.44              |
| 1:D:1201:VAL:HG12 | 1:D:1202:MET:N    | 2.31                     | 0.44              |
| 1:E:1402:ARG:O    | 1:E:1403:TYR:HB3  | 2.17                     | 0.44              |
| 1:F:1188:GLN:H    | 1:F:1188:GLN:CD   | 2.25                     | 0.44              |
| 1:F:1407:PHE:CD2  | 1:F:1407:PHE:C    | 2.96                     | 0.44              |
| 1:A:430:MET:HB3   | 1:A:437:LEU:HD23  | 1.98                     | 0.44              |
| 1:A:1245:ASP:O    | 1:A:1246:CYS:HB3  | 2.18                     | 0.44              |
| 1:B:1315:LEU:N    | 1:B:1315:LEU:CD1  | 2.80                     | 0.44              |
| 1:B:1338:MET:HE2  | 1:E:492:VAL:HG13  | 1.98                     | 0.44              |
| 1:D:1170:ARG:NH1  | 1:D:1172:GLU:CG   | 2.80                     | 0.44              |
| 1:E:1170:ARG:NH2  | 1:E:1205:TYR:HD2  | 2.16                     | 0.44              |
| 1:F:442:ARG:CB    | 1:F:502:TYR:CE2   | 3.01                     | 0.44              |
| 1:F:1293:VAL:HG21 | 1:F:1383:ARG:HH11 | 1.81                     | 0.44              |
| 1:A:495:ILE:CG2   | 1:A:496:THR:N     | 2.81                     | 0.44              |
| 1:A:1288:ARG:NH1  | 1:A:1290:ILE:HG13 | 2.32                     | 0.44              |
| 1:A:1380:LYS:O    | 1:A:1381:TRP:HB3  | 2.18                     | 0.44              |
| 1:B:1311:PHE:O    | 1:B:1312:LYS:C    | 2.60                     | 0.44              |
| 1:B:1346:ALA:C    | 1:B:1348:GLU:N    | 2.75                     | 0.44              |
| 1:B:1390:PHE:C    | 1:B:1390:PHE:HD1  | 2.24                     | 0.44              |
| 1:B:1425:ILE:HD11 | 1:F:1156:PRO:HG3  | 1.95                     | 0.44              |
| 1:C:1260:GLU:O    | 1:C:1261:ARG:CB   | 2.66                     | 0.44              |
| 1:C:1346:ALA:C    | 1:C:1348:GLU:N    | 2.74                     | 0.44              |
| 1:D:1170:ARG:NH1  | 1:D:1172:GLU:OE2  | 2.50                     | 0.44              |
| 1:D:1184:LEU:HD23 | 1:D:1184:LEU:O    | 2.18                     | 0.44              |
| 1:F:1188:GLN:CD   | 1:F:1188:GLN:N    | 2.76                     | 0.44              |
| 1:F:1276:ARG:CG   | 1:F:1277:TYR:N    | 2.81                     | 0.44              |
| 1:F:1366:ILE:O    | 1:F:1366:ILE:HG23 | 2.18                     | 0.44              |
| 1:A:431:ALA:O     | 1:A:432:ALA:C     | 2.61                     | 0.44              |
| 1:D:1326:THR:CG2  | 1:D:1344:TYR:CE1  | 2.99                     | 0.44              |
| 1:E:1298:ARG:HB3  | 1:E:1298:ARG:CZ   | 2.47                     | 0.44              |
| 1:E:1326:THR:HG23 | 1:E:1350:ALA:HA   | 1.99                     | 0.44              |
| 1:A:433:PRO:HD3   | 1:A:1254:LEU:O    | 2.18                     | 0.43              |
| 1:A:1307:ILE:CD1  | 1:A:1358:MET:HE1  | 2.48                     | 0.43              |
| 1:C:423:MET:CE    | 1:C:485:ALA:HB2   | 2.48                     | 0.43              |
| 1:C:1183:LEU:HD22 | 1:C:1285:LEU:CD2  | 2.47                     | 0.43              |
| 1:D:1311:PHE:O    | 1:D:1312:LYS:C    | 2.61                     | 0.43              |
| 1:E:471:GLU:HG2   | 1:E:472:ARG:H     | 1.83                     | 0.43              |
| 1:B:1392:VAL:O    | 1:B:1392:VAL:HG23 | 2.17                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:469:PHE:HZ    | 1:C:478:TYR:HD2   | 1.61                     | 0.43              |
| 1:C:1249:HIS:O    | 1:C:1252:VAL:HG23 | 2.17                     | 0.43              |
| 1:D:1289:VAL:HG22 | 1:D:1307:ILE:HG23 | 2.00                     | 0.43              |
| 1:E:431:ALA:O     | 1:E:432:ALA:C     | 2.61                     | 0.43              |
| 1:E:495:ILE:HG23  | 1:E:496:THR:HG22  | 1.99                     | 0.43              |
| 1:E:1293:VAL:HG21 | 1:E:1383:ARG:NH1  | 2.33                     | 0.43              |
| 1:E:1298:ARG:O    | 1:E:1372:LEU:HB2  | 2.18                     | 0.43              |
| 1:F:431:ALA:O     | 1:F:432:ALA:C     | 2.60                     | 0.43              |
| 1:F:1403:TYR:CD1  | 1:F:1403:TYR:C    | 2.95                     | 0.43              |
| 1:F:1408:GLU:HG3  | 1:F:1411:LEU:N    | 2.33                     | 0.43              |
| 1:A:1256:LYS:HE2  | 1:A:1259:SER:HB2  | 1.99                     | 0.43              |
| 1:A:1328:LEU:CD1  | 1:A:1349:ASN:ND2  | 2.81                     | 0.43              |
| 1:B:437:LEU:N     | 1:B:461:TRP:CD1   | 2.87                     | 0.43              |
| 1:B:1248:PHE:HB3  | 1:B:1252:VAL:HG11 | 1.99                     | 0.43              |
| 1:C:1206:LEU:HD13 | 1:C:1406:VAL:CG2  | 2.48                     | 0.43              |
| 1:A:1336:ILE:N    | 1:A:1336:ILE:CD1  | 2.80                     | 0.43              |
| 1:B:457:ASP:HA    | 1:B:460:ASP:CG    | 2.41                     | 0.43              |
| 1:B:1252:VAL:HA   | 1:B:1265:PHE:HB3  | 2.01                     | 0.43              |
| 1:C:442:ARG:HG2   | 1:C:502:TYR:CE1   | 2.53                     | 0.43              |
| 1:C:1254:LEU:N    | 1:C:1254:LEU:HD23 | 2.33                     | 0.43              |
| 1:C:1331:SER:OG   | 1:C:1371:GLU:HB3  | 2.18                     | 0.43              |
| 1:C:1333:VAL:CG2  | 1:C:1370:ILE:HG12 | 2.45                     | 0.43              |
| 1:E:459:VAL:CG1   | 1:E:472:ARG:HE    | 2.32                     | 0.43              |
| 1:A:1202:MET:HE2  | 1:A:1204:SER:HB2  | 2.00                     | 0.43              |
| 1:B:1173:LEU:HD11 | 1:B:1420:LYS:CG   | 2.43                     | 0.43              |
| 1:C:1185:MET:HE2  | 1:C:1433:THR:HG23 | 2.01                     | 0.43              |
| 1:D:1186:SER:OG   | 1:D:1190:GLN:HB3  | 2.18                     | 0.43              |
| 1:D:1301:LEU:O    | 1:D:1370:ILE:CG1  | 2.67                     | 0.43              |
| 1:E:1290:ILE:CD1  | 1:E:1308:LYS:HE3  | 2.48                     | 0.43              |
| 1:F:1284:ILE:CD1  | 1:F:1396:PRO:HA   | 2.49                     | 0.43              |
| 1:F:1361:MET:HA   | 1:F:1361:MET:CE   | 2.44                     | 0.43              |
| 1:C:459:VAL:O     | 1:C:463:TYR:HD1   | 2.01                     | 0.43              |
| 1:D:462:LEU:HD23  | 1:D:462:LEU:HA    | 1.83                     | 0.43              |
| 1:D:470:PRO:CG    | 1:D:474:GLU:HG3   | 2.48                     | 0.43              |
| 1:D:1192:LEU:HD11 | 1:D:1434:ARG:HH12 | 1.82                     | 0.43              |
| 1:D:1284:ILE:C    | 1:D:1285:LEU:HD12 | 2.43                     | 0.43              |
| 1:C:449:ILE:CG2   | 1:C:452:ALA:HB2   | 2.49                     | 0.43              |
| 1:E:1193:SER:O    | 1:E:1194:ALA:HB2  | 2.18                     | 0.43              |
| 1:F:1183:LEU:HD12 | 1:F:1193:SER:O    | 2.19                     | 0.43              |
| 1:F:1298:ARG:HH12 | 1:F:1375:THR:CB   | 2.32                     | 0.43              |
| 1:A:449:ILE:CD1   | 1:A:1407:PHE:CE1  | 3.01                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1190:GLN:OE1  | 1:A:1190:GLN:HA   | 2.18                     | 0.43              |
| 1:B:1200:VAL:HB   | 1:B:1275:MET:HG3  | 2.01                     | 0.43              |
| 1:D:1332:GLY:O    | 1:D:1371:GLU:HB2  | 2.19                     | 0.43              |
| 1:E:1307:ILE:HD11 | 1:E:1358:MET:HE1  | 2.01                     | 0.43              |
| 1:E:1399:LEU:HD23 | 1:E:1399:LEU:C    | 2.44                     | 0.43              |
| 1:F:440:ARG:CB    | 1:F:440:ARG:HH21  | 2.31                     | 0.43              |
| 1:A:1255:SER:HB2  | 1:A:1263:ILE:HG22 | 2.01                     | 0.43              |
| 1:A:1298:ARG:HD3  | 1:A:1298:ARG:C    | 2.44                     | 0.43              |
| 1:A:1422:VAL:CG2  | 1:E:1161:LEU:HD22 | 2.48                     | 0.43              |
| 1:B:440:ARG:HB3   | 1:B:442:ARG:HH11  | 1.84                     | 0.43              |
| 1:D:1298:ARG:O    | 1:D:1372:LEU:HB2  | 2.18                     | 0.43              |
| 1:E:427:THR:HG21  | 1:E:487:LEU:CB    | 2.49                     | 0.43              |
| 1:F:456:SER:HA    | 1:F:499:GLU:CG    | 2.48                     | 0.43              |
| 1:F:495:ILE:HG13  | 1:F:496:THR:HG23  | 2.00                     | 0.43              |
| 1:A:1403:TYR:C    | 1:A:1403:TYR:HD1  | 2.26                     | 0.43              |
| 1:B:488:ILE:HD13  | 1:B:505:PHE:HA    | 2.01                     | 0.43              |
| 1:B:1333:VAL:CG1  | 1:B:1344:TYR:CD2  | 3.02                     | 0.43              |
| 1:C:1277:TYR:CE1  | 1:C:1399:LEU:HD12 | 2.54                     | 0.43              |
| 1:C:1408:GLU:HG2  | 1:C:1411:LEU:HD12 | 2.01                     | 0.43              |
| 1:D:1413:TYR:CD1  | 1:D:1413:TYR:C    | 2.97                     | 0.43              |
| 1:E:454:LEU:HB3   | 1:E:457:ASP:CG    | 2.44                     | 0.43              |
| 1:E:1307:ILE:CD1  | 1:E:1358:MET:HE1  | 2.48                     | 0.43              |
| 1:C:430:MET:HB3   | 1:C:437:LEU:HD22  | 2.01                     | 0.42              |
| 1:C:1378:LYS:HG2  | 1:C:1379:LYS:N    | 2.32                     | 0.42              |
| 1:D:1184:LEU:CD2  | 1:D:1192:LEU:HB2  | 2.49                     | 0.42              |
| 1:E:1185:MET:HE2  | 1:E:1433:THR:HG23 | 1.99                     | 0.42              |
| 1:F:1173:LEU:HD11 | 1:F:1420:LYS:HG2  | 2.00                     | 0.42              |
| 1:C:1277:TYR:HE1  | 1:C:1399:LEU:HD12 | 1.84                     | 0.42              |
| 1:D:483:LEU:HD22  | 1:D:503:TYR:CE1   | 2.54                     | 0.42              |
| 1:D:1306:VAL:HG23 | 1:D:1365:GLN:HB2  | 2.01                     | 0.42              |
| 1:E:449:ILE:HG22  | 1:E:450:PRO:HD2   | 2.00                     | 0.42              |
| 1:E:1212:CYS:SG   | 1:E:1267:PRO:HD3  | 2.59                     | 0.42              |
| 1:A:447:ILE:HG23  | 1:A:1414:SER:HB3  | 2.01                     | 0.42              |
| 1:B:1156:PRO:HA   | 1:B:1157:PRO:HD3  | 1.77                     | 0.42              |
| 1:C:1196:VAL:HG23 | 1:C:1283:ILE:HD13 | 2.01                     | 0.42              |
| 1:D:1298:ARG:HE   | 1:D:1375:THR:N    | 2.17                     | 0.42              |
| 1:D:1408:GLU:HG3  | 1:D:1411:LEU:H    | 1.85                     | 0.42              |
| 1:E:427:THR:HG21  | 1:E:487:LEU:HB3   | 2.01                     | 0.42              |
| 1:A:1171:ASN:O    | 1:A:1418:VAL:HG13 | 2.20                     | 0.42              |
| 1:A:1338:MET:CE   | 1:F:491:THR:HB    | 2.49                     | 0.42              |
| 1:A:1345:LYS:CB   | 1:A:1348:GLU:OE2  | 2.68                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1296:VAL:HB   | 1:B:1300:LYS:HB2  | 2.01                     | 0.42              |
| 1:D:478:TYR:CD2   | 1:D:482:LEU:HD11  | 2.55                     | 0.42              |
| 1:E:421:MET:HE2   | 1:E:425:SER:HB3   | 2.01                     | 0.42              |
| 1:F:1159:HIS:ND1  | 1:F:1167:GLY:O    | 2.52                     | 0.42              |
| 1:F:1249:HIS:CE1  | 1:F:1250:GLN:HG2  | 2.54                     | 0.42              |
| 1:A:1414:SER:O    | 1:A:1415:ASP:C    | 2.62                     | 0.42              |
| 1:B:440:ARG:CG    | 1:B:441:ASP:N     | 2.83                     | 0.42              |
| 1:B:1177:VAL:CG2  | 1:B:1424:TYR:HD1  | 2.32                     | 0.42              |
| 1:C:1177:VAL:HB   | 1:C:1424:TYR:HD1  | 1.84                     | 0.42              |
| 1:C:1249:HIS:ND1  | 1:C:1251:CYS:SG   | 2.84                     | 0.42              |
| 1:C:1310:ASN:C    | 1:C:1311:PHE:CD2  | 2.98                     | 0.42              |
| 1:C:1311:PHE:O    | 1:C:1312:LYS:C    | 2.60                     | 0.42              |
| 1:C:1324:ILE:HA   | 1:C:1386:ILE:HG12 | 2.00                     | 0.42              |
| 1:D:1211:GLU:HA   | 1:D:1266:ILE:HD13 | 2.01                     | 0.42              |
| 1:D:1298:ARG:NH1  | 1:D:1375:THR:HG23 | 2.35                     | 0.42              |
| 1:D:1422:VAL:CG1  | 1:D:1423:ARG:N    | 2.80                     | 0.42              |
| 1:E:1251:CYS:SG   | 1:E:1268:PRO:HD3  | 2.60                     | 0.42              |
| 1:E:1252:VAL:HA   | 1:E:1265:PHE:HB3  | 2.01                     | 0.42              |
| 1:E:1273:GLU:OE2  | 1:E:1276:ARG:NH2  | 2.52                     | 0.42              |
| 1:F:443:MET:HE3   | 1:F:448:THR:OG1   | 2.18                     | 0.42              |
| 1:F:463:TYR:HD1   | 1:F:469:PHE:HB3   | 1.85                     | 0.42              |
| 1:A:1289:VAL:C    | 1:A:1290:ILE:HD12 | 2.45                     | 0.42              |
| 1:C:1335:VAL:HG11 | 1:C:1351:ILE:HG21 | 2.01                     | 0.42              |
| 1:D:1171:ASN:OD1  | 1:D:1206:LEU:HA   | 2.20                     | 0.42              |
| 1:D:1217:ASN:CG   | 1:D:1400:LYS:H    | 2.28                     | 0.42              |
| 1:E:450:PRO:HG2   | 1:E:450:PRO:O     | 2.19                     | 0.42              |
| 1:E:1307:ILE:HG21 | 1:E:1388:MET:HE1  | 2.00                     | 0.42              |
| 1:F:463:TYR:HE1   | 1:F:469:PHE:O     | 2.02                     | 0.42              |
| 1:A:1255:SER:HB3  | 1:A:1263:ILE:HA   | 2.02                     | 0.42              |
| 1:B:1312:LYS:HA   | 1:B:1313:PRO:HD3  | 1.93                     | 0.42              |
| 1:C:490:HIS:HA    | 1:C:503:TYR:HD1   | 1.84                     | 0.42              |
| 1:D:1192:LEU:CD1  | 1:D:1434:ARG:HH12 | 2.33                     | 0.42              |
| 1:D:1198:GLY:C    | 1:D:1277:TYR:HE2  | 2.26                     | 0.42              |
| 1:D:1327:PRO:HA   | 1:D:1381:TRP:CE2  | 2.54                     | 0.42              |
| 1:E:1304:LYS:HB3  | 1:E:1304:LYS:HE2  | 1.90                     | 0.42              |
| 1:F:1179:GLU:OE1  | 1:F:1196:VAL:HG11 | 2.20                     | 0.42              |
| 1:A:1290:ILE:N    | 1:A:1290:ILE:CD1  | 2.78                     | 0.42              |
| 1:B:1263:ILE:HD12 | 1:B:1263:ILE:HA   | 1.88                     | 0.42              |
| 1:D:462:LEU:CD1   | 1:D:478:TYR:HD2   | 2.33                     | 0.42              |
| 1:D:1174:PHE:HB2  | 1:D:1203:LYS:HB2  | 2.02                     | 0.42              |
| 1:D:1414:SER:O    | 1:D:1415:ASP:C    | 2.62                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:F:1402:ARG:NH1  | 1:F:1402:ARG:CG   | 2.81                     | 0.42              |
| 1:A:462:LEU:O     | 1:A:466:VAL:CG2   | 2.68                     | 0.42              |
| 1:A:473:ARG:HG2   | 1:A:473:ARG:HH21  | 1.85                     | 0.42              |
| 1:B:1211:GLU:HA   | 1:B:1266:ILE:CD1  | 2.44                     | 0.42              |
| 1:B:1275:MET:HE3  | 1:B:1276:ARG:O    | 2.20                     | 0.42              |
| 1:B:1276:ARG:CG   | 1:B:1277:TYR:N    | 2.76                     | 0.42              |
| 1:C:1201:VAL:CG1  | 1:C:1202:MET:N    | 2.82                     | 0.42              |
| 1:C:1202:MET:CE   | 1:C:1204:SER:HB2  | 2.49                     | 0.42              |
| 1:E:437:LEU:H     | 1:E:461:TRP:CD1   | 2.37                     | 0.42              |
| 1:F:462:LEU:HD23  | 1:F:462:LEU:HA    | 1.77                     | 0.42              |
| 1:B:463:TYR:HD1   | 1:B:469:PHE:HB3   | 1.85                     | 0.42              |
| 1:B:1307:ILE:HD11 | 1:B:1358:MET:HE1  | 2.02                     | 0.42              |
| 1:C:459:VAL:HG11  | 1:C:472:ARG:NH2   | 2.34                     | 0.42              |
| 1:C:463:TYR:HB3   | 1:C:475:ALA:HB2   | 2.01                     | 0.42              |
| 1:F:1184:LEU:HA   | 1:F:1432:GLU:O    | 2.20                     | 0.42              |
| 1:A:1382:ALA:HB1  | 1:A:1383:ARG:HH22 | 1.85                     | 0.41              |
| 1:B:471:GLU:HG3   | 1:B:473:ARG:H     | 1.85                     | 0.41              |
| 1:C:1246:CYS:SG   | 1:C:1248:PHE:CZ   | 3.13                     | 0.41              |
| 1:D:1184:LEU:HD13 | 1:D:1193:SER:HB2  | 2.02                     | 0.41              |
| 1:D:1324:ILE:HA   | 1:D:1325:PRO:HD2  | 1.96                     | 0.41              |
| 1:D:1334:GLN:HG3  | 1:D:1369:GLU:HB3  | 2.02                     | 0.41              |
| 1:E:450:PRO:O     | 1:E:451:ASN:C     | 2.62                     | 0.41              |
| 1:E:1276:ARG:CG   | 1:E:1277:TYR:N    | 2.83                     | 0.41              |
| 1:E:1345:LYS:HD2  | 1:E:1352:VAL:HG21 | 2.02                     | 0.41              |
| 1:A:437:LEU:HD12  | 1:A:438:GLU:N     | 2.35                     | 0.41              |
| 1:B:1174:PHE:O    | 1:B:1175:LEU:HD23 | 2.20                     | 0.41              |
| 1:B:1181:VAL:HG22 | 1:B:1396:PRO:CB   | 2.50                     | 0.41              |
| 1:D:1318:GLN:O    | 1:D:1319:LYS:C    | 2.63                     | 0.41              |
| 1:E:1361:MET:O    | 1:E:1362:LYS:HG3  | 2.20                     | 0.41              |
| 1:F:1392:VAL:HG21 | 1:F:1394:PHE:CE1  | 2.55                     | 0.41              |
| 1:A:459:VAL:O     | 1:A:462:LEU:HB3   | 2.19                     | 0.41              |
| 1:A:1198:GLY:C    | 1:A:1277:TYR:CE2  | 2.98                     | 0.41              |
| 1:B:1249:HIS:HD1  | 1:B:1250:GLN:HG3  | 1.85                     | 0.41              |
| 1:C:1293:VAL:HG21 | 1:C:1383:ARG:NH1  | 2.34                     | 0.41              |
| 1:C:1406:VAL:O    | 1:C:1406:VAL:CG1  | 2.67                     | 0.41              |
| 1:D:1187:PRO:HD3  | 1:D:1434:ARG:HB3  | 2.01                     | 0.41              |
| 1:D:1312:LYS:HA   | 1:D:1313:PRO:HD3  | 1.88                     | 0.41              |
| 1:E:1298:ARG:NE   | 1:E:1374:PRO:HA   | 2.35                     | 0.41              |
| 1:F:440:ARG:HB3   | 1:F:440:ARG:CZ    | 2.50                     | 0.41              |
| 1:F:1318:GLN:O    | 1:F:1319:LYS:C    | 2.63                     | 0.41              |
| 1:F:1342:ALA:HB2  | 1:F:1353:TRP:CD1  | 2.56                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1183:LEU:HD13 | 1:A:1285:LEU:CD2  | 2.50                     | 0.41              |
| 1:B:1287:PHE:HE2  | 1:B:1358:MET:SD   | 2.43                     | 0.41              |
| 1:E:482:LEU:CD2   | 1:E:487:LEU:HD12  | 2.50                     | 0.41              |
| 1:E:489:ARG:NH2   | 1:E:1409:PRO:CG   | 2.84                     | 0.41              |
| 1:E:497:PHE:HD1   | 1:E:503:TYR:OH    | 2.03                     | 0.41              |
| 1:E:1298:ARG:CG   | 1:E:1298:ARG:NH2  | 2.83                     | 0.41              |
| 1:F:1188:GLN:HB2  | 1:F:1190:GLN:HE21 | 1.86                     | 0.41              |
| 1:F:1247:THR:CG2  | 1:F:1276:ARG:HD2  | 2.49                     | 0.41              |
| 1:F:1298:ARG:O    | 1:F:1372:LEU:CD1  | 2.69                     | 0.41              |
| 1:A:1323:ARG:HG3  | 1:A:1323:ARG:NH1  | 2.36                     | 0.41              |
| 1:B:1179:GLU:HB3  | 1:B:1196:VAL:CG1  | 2.50                     | 0.41              |
| 1:D:1181:VAL:HG12 | 1:D:1196:VAL:CG1  | 2.50                     | 0.41              |
| 1:D:1193:SER:O    | 1:D:1194:ALA:HB2  | 2.21                     | 0.41              |
| 1:D:1214:PHE:O    | 1:D:1262:SER:HA   | 2.20                     | 0.41              |
| 1:E:456:SER:HA    | 1:E:499:GLU:HG2   | 2.02                     | 0.41              |
| 1:E:461:TRP:CE3   | 1:E:461:TRP:O     | 2.73                     | 0.41              |
| 1:F:1323:ARG:HB2  | 1:F:1323:ARG:CZ   | 2.50                     | 0.41              |
| 1:A:1292:LEU:HA   | 1:A:1292:LEU:HD12 | 1.66                     | 0.41              |
| 1:B:447:ILE:CG2   | 1:B:448:THR:H     | 2.33                     | 0.41              |
| 1:B:1174:PHE:CD2  | 1:B:1421:TRP:HB2  | 2.55                     | 0.41              |
| 1:B:1425:ILE:CD1  | 1:F:1156:PRO:HG3  | 2.50                     | 0.41              |
| 1:C:447:ILE:HG23  | 1:C:448:THR:H     | 1.84                     | 0.41              |
| 1:F:1178:LEU:HD12 | 1:F:1199:ARG:NH1  | 2.36                     | 0.41              |
| 1:F:1213:LYS:HE2  | 1:F:1403:TYR:OH   | 2.21                     | 0.41              |
| 1:F:1311:PHE:CE1  | 1:F:1360:GLY:CA   | 3.03                     | 0.41              |
| 1:F:1339:LYS:HD3  | 1:F:1364:SER:OG   | 2.21                     | 0.41              |
| 1:A:1171:ASN:ND2  | 1:A:1413:TYR:CZ   | 2.89                     | 0.41              |
| 1:A:1390:PHE:CD1  | 1:A:1428:SER:HB3  | 2.53                     | 0.41              |
| 1:B:447:ILE:CG2   | 1:B:448:THR:N     | 2.83                     | 0.41              |
| 1:C:460:ASP:O     | 1:C:463:TYR:CD1   | 2.73                     | 0.41              |
| 1:D:488:ILE:HD13  | 1:D:488:ILE:HA    | 1.74                     | 0.41              |
| 1:E:492:VAL:CG2   | 1:E:492:VAL:O     | 2.69                     | 0.41              |
| 1:E:1289:VAL:O    | 1:E:1291:PRO:HD3  | 2.21                     | 0.41              |
| 1:E:1402:ARG:NH2  | 1:E:1402:ARG:HG2  | 2.36                     | 0.41              |
| 1:E:1402:ARG:HG2  | 1:E:1402:ARG:HH21 | 1.85                     | 0.41              |
| 1:F:1175:LEU:HD23 | 1:F:1175:LEU:HA   | 1.90                     | 0.41              |
| 1:F:1312:LYS:NZ   | 1:F:1312:LYS:CB   | 2.83                     | 0.41              |
| 1:A:450:PRO:O     | 1:A:451:ASN:C     | 2.62                     | 0.41              |
| 1:A:1183:LEU:HD13 | 1:A:1285:LEU:HD21 | 2.03                     | 0.41              |
| 1:B:456:SER:C     | 1:B:458:VAL:N     | 2.79                     | 0.41              |
| 1:B:482:LEU:HD23  | 1:B:482:LEU:N     | 2.36                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1294:ARG:NH1  | 1:B:1302:GLU:CG   | 2.80                     | 0.41              |
| 1:C:1184:LEU:CB   | 1:C:1193:SER:HB2  | 2.50                     | 0.41              |
| 1:C:1206:LEU:HD13 | 1:C:1406:VAL:HG21 | 2.03                     | 0.41              |
| 1:C:1346:ALA:C    | 1:C:1348:GLU:H    | 2.28                     | 0.41              |
| 1:C:1381:TRP:CZ2  | 1:C:1383:ARG:HG2  | 2.55                     | 0.41              |
| 1:D:1320:ILE:CG2  | 1:D:1388:MET:HE1  | 2.51                     | 0.41              |
| 1:D:1346:ALA:C    | 1:D:1348:GLU:N    | 2.78                     | 0.41              |
| 1:E:1174:PHE:HB2  | 1:E:1203:LYS:HB2  | 2.03                     | 0.41              |
| 1:E:1298:ARG:O    | 1:E:1372:LEU:HD12 | 2.21                     | 0.41              |
| 1:F:447:ILE:H     | 1:F:447:ILE:HG13  | 1.57                     | 0.41              |
| 1:F:450:PRO:O     | 1:F:451:ASN:C     | 2.63                     | 0.41              |
| 1:F:1186:SER:HB3  | 1:F:1192:LEU:HD21 | 2.02                     | 0.41              |
| 1:F:1198:GLY:C    | 1:F:1277:TYR:CE2  | 2.99                     | 0.41              |
| 1:A:1245:ASP:O    | 1:A:1246:CYS:CB   | 2.66                     | 0.41              |
| 1:A:1305:VAL:HG12 | 1:A:1366:ILE:CG2  | 2.42                     | 0.41              |
| 1:A:1416:HIS:ND1  | 1:A:1416:HIS:N    | 2.58                     | 0.41              |
| 1:B:1250:GLN:OE1  | 1:B:1251:CYS:N    | 2.54                     | 0.41              |
| 1:B:1339:LYS:NZ   | 1:B:1363:GLU:O    | 2.54                     | 0.41              |
| 1:B:1353:TRP:CH2  | 1:B:1366:ILE:HB   | 2.56                     | 0.41              |
| 1:B:1380:LYS:H    | 1:B:1380:LYS:HG2  | 1.62                     | 0.41              |
| 1:B:1404:LEU:O    | 1:B:1420:LYS:NZ   | 2.50                     | 0.41              |
| 1:C:434:GLU:HA    | 1:C:434:GLU:OE1   | 2.21                     | 0.41              |
| 1:C:490:HIS:NE2   | 1:C:494:LYS:HD3   | 2.36                     | 0.41              |
| 1:C:1199:ARG:HG3  | 1:C:1273:GLU:HG3  | 2.03                     | 0.41              |
| 1:D:1366:ILE:HG23 | 1:D:1366:ILE:O    | 2.21                     | 0.41              |
| 1:E:462:LEU:CD2   | 1:E:475:ALA:HB1   | 2.51                     | 0.41              |
| 1:E:1310:ASN:C    | 1:E:1311:PHE:CD2  | 2.99                     | 0.41              |
| 1:E:1403:TYR:CE1  | 1:E:1405:LYS:HE3  | 2.55                     | 0.41              |
| 1:F:427:THR:HG21  | 1:F:487:LEU:HB3   | 2.03                     | 0.41              |
| 1:F:433:PRO:HD3   | 1:F:1254:LEU:O    | 2.20                     | 0.41              |
| 1:F:442:ARG:N     | 1:F:442:ARG:CD    | 2.83                     | 0.41              |
| 1:F:442:ARG:HG2   | 1:F:452:ALA:HB3   | 2.03                     | 0.41              |
| 1:F:458:VAL:O     | 1:F:462:LEU:CB    | 2.66                     | 0.41              |
| 1:F:1346:ALA:C    | 1:F:1348:GLU:N    | 2.77                     | 0.41              |
| 1:A:1187:PRO:HD3  | 1:A:1434:ARG:HB2  | 2.00                     | 0.41              |
| 1:A:1298:ARG:HH21 | 1:A:1298:ARG:HG2  | 1.85                     | 0.41              |
| 1:A:1384:PRO:HA   | 1:A:1385:PRO:HD3  | 1.99                     | 0.41              |
| 1:B:1179:GLU:HB2  | 1:B:1396:PRO:HD2  | 2.02                     | 0.41              |
| 1:C:1213:LYS:HE2  | 1:C:1262:SER:OG   | 2.21                     | 0.41              |
| 1:D:1245:ASP:O    | 1:D:1246:CYS:HB3  | 2.21                     | 0.41              |
| 1:E:1296:VAL:O    | 1:E:1300:LYS:HB2  | 2.21                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1216:MET:HE2  | 1:A:1216:MET:HB3  | 1.80                     | 0.40              |
| 1:E:430:MET:H     | 1:E:430:MET:HG3   | 1.70                     | 0.40              |
| 1:E:461:TRP:CD1   | 1:E:465:HIS:CE1   | 3.09                     | 0.40              |
| 1:F:427:THR:OG1   | 1:F:487:LEU:HD13  | 2.21                     | 0.40              |
| 1:B:436:GLY:HA3   | 1:B:465:HIS:HE1   | 1.85                     | 0.40              |
| 1:B:1158:TYR:CE2  | 1:F:1423:ARG:NH2  | 2.90                     | 0.40              |
| 1:B:1170:ARG:CA   | 1:F:1421:TRP:CZ3  | 3.02                     | 0.40              |
| 1:B:1324:ILE:HG12 | 1:B:1386:ILE:HD13 | 2.03                     | 0.40              |
| 1:C:1177:VAL:HG21 | 1:C:1424:TYR:CE1  | 2.56                     | 0.40              |
| 1:C:1318:GLN:O    | 1:C:1319:LYS:C    | 2.63                     | 0.40              |
| 1:D:1399:LEU:C    | 1:D:1399:LEU:HD23 | 2.46                     | 0.40              |
| 1:E:1179:GLU:HB3  | 1:E:1196:VAL:CG1  | 2.51                     | 0.40              |
| 1:F:1174:PHE:CD1  | 1:F:1174:PHE:N    | 2.89                     | 0.40              |
| 1:A:1173:LEU:HD11 | 1:A:1420:LYS:HB3  | 2.03                     | 0.40              |
| 1:B:1289:VAL:C    | 1:B:1290:ILE:HD12 | 2.46                     | 0.40              |
| 1:B:1363:GLU:OE1  | 1:E:445:LEU:HD13  | 2.21                     | 0.40              |
| 1:C:1390:PHE:CD1  | 1:C:1391:GLU:N    | 2.89                     | 0.40              |
| 1:D:1301:LEU:HB2  | 1:D:1370:ILE:HG13 | 2.00                     | 0.40              |
| 1:F:442:ARG:HD3   | 1:F:442:ARG:N     | 2.37                     | 0.40              |
| 1:F:478:TYR:O     | 1:F:482:LEU:HG    | 2.21                     | 0.40              |
| 1:F:1195:HIS:CD2  | 1:F:1278:ARG:NH2  | 2.90                     | 0.40              |
| 1:A:1378:LYS:HE3  | 1:A:1381:TRP:CE2  | 2.53                     | 0.40              |
| 1:B:422:ASP:OD2   | 1:B:424:ALA:HB3   | 2.21                     | 0.40              |
| 1:B:459:VAL:HG21  | 1:B:499:GLU:OE1   | 2.22                     | 0.40              |
| 1:B:488:ILE:HD13  | 1:B:488:ILE:HA    | 1.84                     | 0.40              |
| 1:B:1344:TYR:HE2  | 1:B:1346:ALA:HB2  | 1.81                     | 0.40              |
| 1:B:1384:PRO:HA   | 1:B:1385:PRO:HD3  | 1.98                     | 0.40              |
| 1:B:1403:TYR:CD1  | 1:B:1403:TYR:C    | 3.00                     | 0.40              |
| 1:D:1290:ILE:CB   | 1:D:1306:VAL:HG12 | 2.38                     | 0.40              |
| 1:D:1324:ILE:HG22 | 1:D:1351:ILE:CB   | 2.48                     | 0.40              |
| 1:E:1155:PRO:HA   | 1:E:1156:PRO:HD2  | 1.85                     | 0.40              |
| 1:F:1192:LEU:CD1  | 1:F:1434:ARG:NE   | 2.81                     | 0.40              |
| 1:F:1195:HIS:CD2  | 1:F:1278:ARG:HH21 | 2.39                     | 0.40              |
| 1:A:1183:LEU:HD21 | 1:A:1185:MET:HB2  | 2.02                     | 0.40              |
| 1:A:1325:PRO:HG3  | 1:A:1384:PRO:O    | 2.22                     | 0.40              |
| 1:A:1346:ALA:C    | 1:A:1348:GLU:N    | 2.78                     | 0.40              |
| 1:B:473:ARG:HB2   | 1:B:473:ARG:NH2   | 2.36                     | 0.40              |
| 1:B:1177:VAL:HG21 | 1:B:1424:TYR:CD1  | 2.56                     | 0.40              |
| 1:C:1317:ALA:CB   | 1:C:1392:VAL:HG12 | 2.51                     | 0.40              |
| 1:D:1344:TYR:CE2  | 1:D:1346:ALA:HB2  | 2.56                     | 0.40              |
| 1:E:490:HIS:HA    | 1:E:503:TYR:CD1   | 2.57                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:E:1248:PHE:HE2 | 1:E:1263:ILE:HG21 | 1.86                     | 0.40              |
| 1:F:1294:ARG:CZ  | 1:F:1302:GLU:CG   | 2.99                     | 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     | 345/385 (90%)   | 294 (85%)  | 44 (13%)  | 7 (2%)   | 6           | 32 |
| 1   | B     | 331/385 (86%)   | 284 (86%)  | 40 (12%)  | 7 (2%)   | 5           | 31 |
| 1   | C     | 344/385 (89%)   | 288 (84%)  | 52 (15%)  | 4 (1%)   | 10          | 41 |
| 1   | D     | 326/385 (85%)   | 279 (86%)  | 41 (13%)  | 6 (2%)   | 6           | 34 |
| 1   | E     | 328/385 (85%)   | 282 (86%)  | 39 (12%)  | 7 (2%)   | 5           | 31 |
| 1   | F     | 332/385 (86%)   | 289 (87%)  | 38 (11%)  | 5 (2%)   | 8           | 37 |
| All | All   | 2006/2310 (87%) | 1716 (86%) | 254 (13%) | 36 (2%)  | 6           | 34 |

All (36) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 1251 | CYS  |
| 1   | B     | 493  | ASN  |
| 1   | B     | 1379 | LYS  |
| 1   | C     | 493  | ASN  |
| 1   | E     | 493  | ASN  |
| 1   | E     | 1251 | CYS  |
| 1   | F     | 493  | ASN  |
| 1   | F     | 1190 | GLN  |
| 1   | A     | 493  | ASN  |
| 1   | A     | 1190 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1251 | CYS  |
| 1   | B     | 1194 | ALA  |
| 1   | B     | 1251 | CYS  |
| 1   | B     | 1262 | SER  |
| 1   | C     | 435  | SER  |
| 1   | C     | 1194 | ALA  |
| 1   | D     | 493  | ASN  |
| 1   | D     | 1190 | GLN  |
| 1   | D     | 1194 | ALA  |
| 1   | D     | 1251 | CYS  |
| 1   | E     | 435  | SER  |
| 1   | E     | 1190 | GLN  |
| 1   | F     | 435  | SER  |
| 1   | A     | 1194 | ALA  |
| 1   | B     | 435  | SER  |
| 1   | B     | 1190 | GLN  |
| 1   | E     | 1194 | ALA  |
| 1   | F     | 1251 | CYS  |
| 1   | D     | 1286 | PRO  |
| 1   | A     | 1409 | PRO  |
| 1   | D     | 447  | ILE  |
| 1   | E     | 447  | ILE  |
| 1   | F     | 1409 | PRO  |
| 1   | A     | 447  | ILE  |
| 1   | A     | 470  | PRO  |
| 1   | E     | 470  | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1   | A     | 308/337 (91%) | 257 (83%) | 51 (17%) | 2           | 13 |
| 1   | B     | 298/337 (88%) | 260 (87%) | 38 (13%) | 4           | 21 |
| 1   | C     | 307/337 (91%) | 272 (89%) | 35 (11%) | 5           | 24 |
| 1   | D     | 295/337 (88%) | 253 (86%) | 42 (14%) | 3           | 18 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 1   | E     | 297/337 (88%)   | 267 (90%)  | 30 (10%)  | 7           | 28 |
| 1   | F     | 299/337 (89%)   | 268 (90%)  | 31 (10%)  | 7           | 27 |
| All | All   | 1804/2022 (89%) | 1577 (87%) | 227 (13%) | 4           | 21 |

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

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 427  | THR  |
| 1   | A     | 439  | VAL  |
| 1   | A     | 442  | ARG  |
| 1   | A     | 453  | PHE  |
| 1   | A     | 464  | HIS  |
| 1   | A     | 471  | GLU  |
| 1   | A     | 472  | ARG  |
| 1   | A     | 474  | GLU  |
| 1   | A     | 487  | LEU  |
| 1   | A     | 492  | VAL  |
| 1   | A     | 493  | ASN  |
| 1   | A     | 1157 | PRO  |
| 1   | A     | 1160 | GLU  |
| 1   | A     | 1178 | LEU  |
| 1   | A     | 1181 | VAL  |
| 1   | A     | 1184 | LEU  |
| 1   | A     | 1188 | GLN  |
| 1   | A     | 1191 | VAL  |
| 1   | A     | 1199 | ARG  |
| 1   | A     | 1205 | TYR  |
| 1   | A     | 1211 | GLU  |
| 1   | A     | 1216 | MET  |
| 1   | A     | 1217 | ASN  |
| 1   | A     | 1218 | ASP  |
| 1   | A     | 1241 | ILE  |
| 1   | A     | 1257 | PHE  |
| 1   | A     | 1262 | SER  |
| 1   | A     | 1276 | ARG  |
| 1   | A     | 1277 | TYR  |
| 1   | A     | 1278 | ARG  |
| 1   | A     | 1287 | PHE  |
| 1   | A     | 1290 | ILE  |
| 1   | A     | 1291 | PRO  |
| 1   | A     | 1294 | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1305 | VAL  |
| 1   | A     | 1314 | SER  |
| 1   | A     | 1329 | ASN  |
| 1   | A     | 1339 | LYS  |
| 1   | A     | 1347 | SER  |
| 1   | A     | 1351 | ILE  |
| 1   | A     | 1352 | VAL  |
| 1   | A     | 1355 | ILE  |
| 1   | A     | 1357 | ARG  |
| 1   | A     | 1379 | LYS  |
| 1   | A     | 1383 | ARG  |
| 1   | A     | 1390 | PHE  |
| 1   | A     | 1412 | ASN  |
| 1   | A     | 1414 | SER  |
| 1   | A     | 1416 | HIS  |
| 1   | A     | 1430 | ILE  |
| 1   | A     | 1434 | ARG  |
| 1   | B     | 427  | THR  |
| 1   | B     | 438  | GLU  |
| 1   | B     | 444  | TRP  |
| 1   | B     | 445  | LEU  |
| 1   | B     | 453  | PHE  |
| 1   | B     | 460  | ASP  |
| 1   | B     | 476  | ARG  |
| 1   | B     | 480  | SER  |
| 1   | B     | 1160 | GLU  |
| 1   | B     | 1162 | GLU  |
| 1   | B     | 1186 | SER  |
| 1   | B     | 1197 | SER  |
| 1   | B     | 1216 | MET  |
| 1   | B     | 1246 | CYS  |
| 1   | B     | 1247 | THR  |
| 1   | B     | 1250 | GLN  |
| 1   | B     | 1252 | VAL  |
| 1   | B     | 1253 | ARG  |
| 1   | B     | 1277 | TYR  |
| 1   | B     | 1282 | ASP  |
| 1   | B     | 1286 | PRO  |
| 1   | B     | 1292 | LEU  |
| 1   | B     | 1296 | VAL  |
| 1   | B     | 1300 | LYS  |
| 1   | B     | 1301 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 1304 | LYS  |
| 1   | B     | 1319 | LYS  |
| 1   | B     | 1328 | LEU  |
| 1   | B     | 1333 | VAL  |
| 1   | B     | 1357 | ARG  |
| 1   | B     | 1374 | PRO  |
| 1   | B     | 1380 | LYS  |
| 1   | B     | 1390 | PHE  |
| 1   | B     | 1406 | VAL  |
| 1   | B     | 1413 | TYR  |
| 1   | B     | 1419 | ILE  |
| 1   | B     | 1425 | ILE  |
| 1   | B     | 1432 | GLU  |
| 1   | C     | 421  | MET  |
| 1   | C     | 456  | SER  |
| 1   | C     | 464  | HIS  |
| 1   | C     | 474  | GLU  |
| 1   | C     | 504  | VAL  |
| 1   | C     | 1180 | SER  |
| 1   | C     | 1184 | LEU  |
| 1   | C     | 1191 | VAL  |
| 1   | C     | 1207 | SER  |
| 1   | C     | 1209 | MET  |
| 1   | C     | 1214 | PHE  |
| 1   | C     | 1246 | CYS  |
| 1   | C     | 1255 | SER  |
| 1   | C     | 1264 | SER  |
| 1   | C     | 1277 | TYR  |
| 1   | C     | 1287 | PHE  |
| 1   | C     | 1299 | THR  |
| 1   | C     | 1300 | LYS  |
| 1   | C     | 1302 | GLU  |
| 1   | C     | 1303 | VAL  |
| 1   | C     | 1304 | LYS  |
| 1   | C     | 1305 | VAL  |
| 1   | C     | 1306 | VAL  |
| 1   | C     | 1309 | SER  |
| 1   | C     | 1315 | LEU  |
| 1   | C     | 1325 | PRO  |
| 1   | C     | 1328 | LEU  |
| 1   | C     | 1336 | ILE  |
| 1   | C     | 1356 | LYS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 1357 | ARG  |
| 1   | C     | 1373 | LEU  |
| 1   | C     | 1374 | PRO  |
| 1   | C     | 1410 | LYS  |
| 1   | C     | 1412 | ASN  |
| 1   | C     | 1427 | ARG  |
| 1   | D     | 422  | ASP  |
| 1   | D     | 435  | SER  |
| 1   | D     | 439  | VAL  |
| 1   | D     | 442  | ARG  |
| 1   | D     | 447  | ILE  |
| 1   | D     | 453  | PHE  |
| 1   | D     | 462  | LEU  |
| 1   | D     | 472  | ARG  |
| 1   | D     | 488  | ILE  |
| 1   | D     | 1169 | SER  |
| 1   | D     | 1171 | ASN  |
| 1   | D     | 1177 | VAL  |
| 1   | D     | 1199 | ARG  |
| 1   | D     | 1211 | GLU  |
| 1   | D     | 1212 | CYS  |
| 1   | D     | 1216 | MET  |
| 1   | D     | 1217 | ASN  |
| 1   | D     | 1247 | THR  |
| 1   | D     | 1253 | ARG  |
| 1   | D     | 1277 | TYR  |
| 1   | D     | 1279 | THR  |
| 1   | D     | 1305 | VAL  |
| 1   | D     | 1306 | VAL  |
| 1   | D     | 1307 | ILE  |
| 1   | D     | 1315 | LEU  |
| 1   | D     | 1316 | LEU  |
| 1   | D     | 1322 | VAL  |
| 1   | D     | 1327 | PRO  |
| 1   | D     | 1328 | LEU  |
| 1   | D     | 1329 | ASN  |
| 1   | D     | 1334 | GLN  |
| 1   | D     | 1352 | VAL  |
| 1   | D     | 1355 | ILE  |
| 1   | D     | 1371 | GLU  |
| 1   | D     | 1374 | PRO  |
| 1   | D     | 1383 | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | D     | 1385 | PRO  |
| 1   | D     | 1388 | MET  |
| 1   | D     | 1418 | VAL  |
| 1   | D     | 1420 | LYS  |
| 1   | D     | 1424 | TYR  |
| 1   | D     | 1427 | ARG  |
| 1   | E     | 421  | MET  |
| 1   | E     | 423  | MET  |
| 1   | E     | 426  | VAL  |
| 1   | E     | 445  | LEU  |
| 1   | E     | 450  | PRO  |
| 1   | E     | 457  | ASP  |
| 1   | E     | 464  | HIS  |
| 1   | E     | 465  | HIS  |
| 1   | E     | 487  | LEU  |
| 1   | E     | 492  | VAL  |
| 1   | E     | 496  | THR  |
| 1   | E     | 500  | GLN  |
| 1   | E     | 1209 | MET  |
| 1   | E     | 1211 | GLU  |
| 1   | E     | 1212 | CYS  |
| 1   | E     | 1214 | PHE  |
| 1   | E     | 1277 | TYR  |
| 1   | E     | 1288 | ARG  |
| 1   | E     | 1291 | PRO  |
| 1   | E     | 1292 | LEU  |
| 1   | E     | 1299 | THR  |
| 1   | E     | 1303 | VAL  |
| 1   | E     | 1305 | VAL  |
| 1   | E     | 1316 | LEU  |
| 1   | E     | 1323 | ARG  |
| 1   | E     | 1324 | ILE  |
| 1   | E     | 1355 | ILE  |
| 1   | E     | 1380 | LYS  |
| 1   | E     | 1414 | SER  |
| 1   | E     | 1415 | ASP  |
| 1   | F     | 421  | MET  |
| 1   | F     | 427  | THR  |
| 1   | F     | 447  | ILE  |
| 1   | F     | 448  | THR  |
| 1   | F     | 462  | LEU  |
| 1   | F     | 471  | GLU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | F     | 473  | ARG  |
| 1   | F     | 490  | HIS  |
| 1   | F     | 507  | ASP  |
| 1   | F     | 1159 | HIS  |
| 1   | F     | 1188 | GLN  |
| 1   | F     | 1201 | VAL  |
| 1   | F     | 1214 | PHE  |
| 1   | F     | 1216 | MET  |
| 1   | F     | 1263 | ILE  |
| 1   | F     | 1277 | TYR  |
| 1   | F     | 1279 | THR  |
| 1   | F     | 1301 | LEU  |
| 1   | F     | 1312 | LYS  |
| 1   | F     | 1319 | LYS  |
| 1   | F     | 1321 | GLU  |
| 1   | F     | 1324 | ILE  |
| 1   | F     | 1328 | LEU  |
| 1   | F     | 1339 | LYS  |
| 1   | F     | 1351 | ILE  |
| 1   | F     | 1391 | GLU  |
| 1   | F     | 1393 | PRO  |
| 1   | F     | 1394 | PHE  |
| 1   | F     | 1399 | LEU  |
| 1   | F     | 1404 | LEU  |
| 1   | F     | 1434 | ARG  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 465  | HIS  |
| 1   | A     | 490  | HIS  |
| 1   | A     | 1154 | GLN  |
| 1   | A     | 1171 | ASN  |
| 1   | A     | 1182 | ASN  |
| 1   | A     | 1195 | HIS  |
| 1   | A     | 1250 | GLN  |
| 1   | A     | 1349 | ASN  |
| 1   | A     | 1365 | GLN  |
| 1   | A     | 1389 | ASN  |
| 1   | B     | 451  | ASN  |
| 1   | B     | 1188 | GLN  |
| 1   | B     | 1412 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 451  | ASN  |
| 1   | C     | 465  | HIS  |
| 1   | C     | 1217 | ASN  |
| 1   | C     | 1318 | GLN  |
| 1   | D     | 451  | ASN  |
| 1   | D     | 465  | HIS  |
| 1   | D     | 1217 | ASN  |
| 1   | D     | 1250 | GLN  |
| 1   | D     | 1318 | GLN  |
| 1   | D     | 1329 | ASN  |
| 1   | D     | 1365 | GLN  |
| 1   | D     | 1412 | ASN  |
| 1   | E     | 465  | HIS  |
| 1   | E     | 500  | GLN  |
| 1   | E     | 1190 | GLN  |
| 1   | E     | 1195 | HIS  |
| 1   | E     | 1318 | GLN  |
| 1   | E     | 1365 | GLN  |
| 1   | E     | 1416 | HIS  |
| 1   | F     | 464  | HIS  |
| 1   | F     | 1159 | HIS  |
| 1   | F     | 1188 | GLN  |
| 1   | F     | 1190 | GLN  |
| 1   | F     | 1195 | HIS  |
| 1   | F     | 1217 | ASN  |
| 1   | F     | 1250 | GLN  |
| 1   | F     | 1318 | GLN  |
| 1   | F     | 1412 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | A     | 351/385 (91%)   | 0.28   | 6 (1%) 69 43  | 91, 112, 131, 141     | 0     |
| 1   | B     | 339/385 (88%)   | 0.19   | 2 (0%) 85 65  | 103, 117, 134, 145    | 0     |
| 1   | C     | 350/385 (90%)   | 0.12   | 2 (0%) 85 65  | 99, 119, 132, 147     | 0     |
| 1   | D     | 336/385 (87%)   | 0.31   | 3 (0%) 81 58  | 97, 117, 129, 136     | 0     |
| 1   | E     | 338/385 (87%)   | 0.16   | 1 (0%) 90 76  | 98, 118, 132, 141     | 0     |
| 1   | F     | 340/385 (88%)   | 0.12   | 3 (0%) 81 58  | 100, 120, 133, 140    | 0     |
| All | All   | 2054/2310 (88%) | 0.20   | 17 (0%) 82 60 | 91, 117, 132, 147     | 0     |

All (17) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | F     | 1261 | ARG  | 3.6  |
| 1   | B     | 1435 | CYS  | 3.5  |
| 1   | D     | 421  | MET  | 2.9  |
| 1   | B     | 1374 | PRO  | 2.9  |
| 1   | F     | 1435 | CYS  | 2.7  |
| 1   | E     | 1435 | CYS  | 2.5  |
| 1   | A     | 421  | MET  | 2.4  |
| 1   | A     | 462  | LEU  | 2.3  |
| 1   | F     | 1255 | SER  | 2.2  |
| 1   | C     | 426  | VAL  | 2.2  |
| 1   | D     | 1324 | ILE  | 2.2  |
| 1   | A     | 1377 | ASP  | 2.1  |
| 1   | C     | 510  | GLY  | 2.1  |
| 1   | A     | 1169 | SER  | 2.1  |
| 1   | D     | 1290 | ILE  | 2.1  |
| 1   | A     | 466  | VAL  | 2.1  |
| 1   | A     | 1435 | CYS  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.