



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 28, 2017 – 02:22 PM EDT

PDB ID : 3H3V  
Title : Yeast RNAP II containing poly(A)-signal sequence in the active site  
Authors : Dengl, S.; Cramer, P.  
Deposited on : unknown  
Resolution : 4.00 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

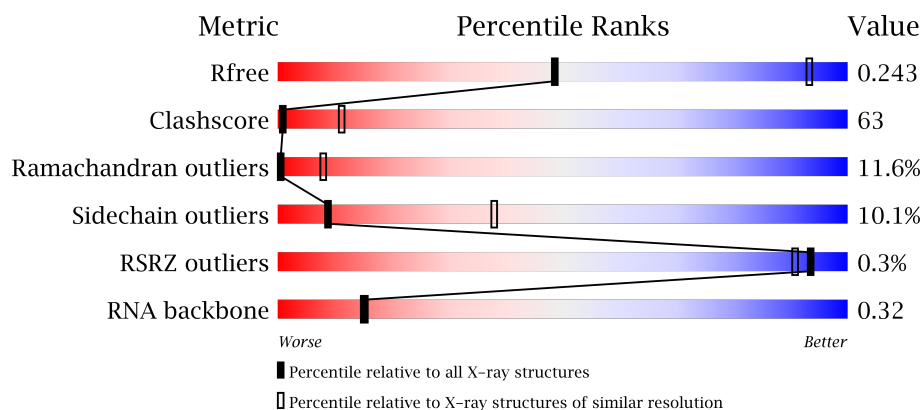
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 Å.

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





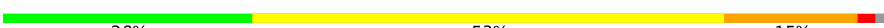


| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 100719                      | 1088 (4.40-3.60)                                      |
| Clashscore            | 112137                      | 1187 (4.40-3.60)                                      |
| Ramachandran outliers | 110173                      | 1139 (4.40-3.60)                                      |
| Sidechain outliers    | 110143                      | 1126 (4.40-3.60)                                      |
| RSRZ outliers         | 101464                      | 1099 (4.40-3.60)                                      |
| RNA backbone          | 2435                        | 1026 (5.04-2.90)                                      |

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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   | B     | 1733   |                  |
| 2   | C     | 1224   |                  |
| 3   | D     | 318    |                  |
| 4   | E     | 221    |                  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 5   | F     | 215    |  |
| 6   | G     | 155    |  |
| 7   | H     | 171    |  |
| 8   | I     | 146    |  |
| 9   | J     | 122    |  |
| 10  | K     | 70     |  |
| 11  | L     | 120    |  |
| 12  | M     | 70     |  |
| 13  | N     | 14     |  |
| 14  | P     | 16     |  |
| 15  | T     | 26     |  |

## 2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 31777 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase II subunit RPB1.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 1   | B     | 1416     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 11140 | 7021 | 1946 | 2111 | 62 |         |         |       |

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 2   | C     | 1108     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 8810  | 5580 | 1541 | 1634 | 55 |         |         |       |

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 3   | D     | 266      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2095  | 1317 | 348 | 417 | 13 |         |         |       |

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4   | E     | 177      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1427  | 882 | 256 | 287 | 2 |         |         |       |

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 5   | F     | 214      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1752  | 1111 | 309 | 321 | 11 |         |         |       |

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | G     | 84       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 679   | 434 | 115 | 127 | 3 |         |         |       |

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7   | H     | 171      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1340  | 861 | 222 | 249 | 8 |         |         |       |

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | I     | 133      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1068  | 673 | 180 | 211 | 4 |         |         |       |

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 9   | J     | 119      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 971   | 596 | 179 | 186 | 10 |         |         |       |

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 10  | K     | 65       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 532   | 339 | 93 | 94 | 6 |         |         |       |

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11  | L     | 114      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 919   | 590 | 156 | 171 | 2 |         |         |       |

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 12  | M     | 46       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 364   | 224 | 72 | 64 | 4 |         |         |       |

- Molecule 13 is a DNA chain called 5'-D(\*AP\*GP\*CP\*TP\*CP\*AP\*AP\*GP\*TP\*AP\*GP\*C  
P\*TP\*GP\*CP\*TP\*TP\*TP\*AP\*TP\*TP\*GP\*CP\*AP\*TP\*T)-3'.

| Mol | Chain | Residues | Atoms |    |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 13  | N     | 7        | Total | C  | N  | O  | P | 11      | 0       | 0     |
|     |       |          | 138   | 67 | 26 | 39 | 6 |         |         |       |

- Molecule 14 is a RNA chain called 5'-D(\*CP\*AP\*GP\*CP\*TP\*AP\*CP\*TP\*TP\*GP\*AP\*GP\*CP\*T)-3'.

| Mol | Chain | Residues | Atoms |    |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 14  | P     | 8        | Total | C  | N  | O  | P | 0       | 0       | 0     |
|     |       |          | 168   | 77 | 33 | 51 | 7 |         |         |       |

- Molecule 15 is a DNA chain called 5'-R(\*UP\*GP\*CP\*AP\*UP\*UP\*UP\*CP\*GP\*CP\*AP\*AP\*UP\*AP\*AP\*A)-3'.

| Mol | Chain | Residues | Atoms |     |    |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|---------|-------|
| 15  | T     | 18       | Total | C   | N  | O   | P  | 8       | 0       | 0     |
|     |       |          | 365   | 177 | 60 | 111 | 17 |         |         |       |

- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 16  | J     | 2        | Total | Zn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 16  | D     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 16  | K     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 16  | B     | 2        | Total | Zn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 16  | C     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 16  | M     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

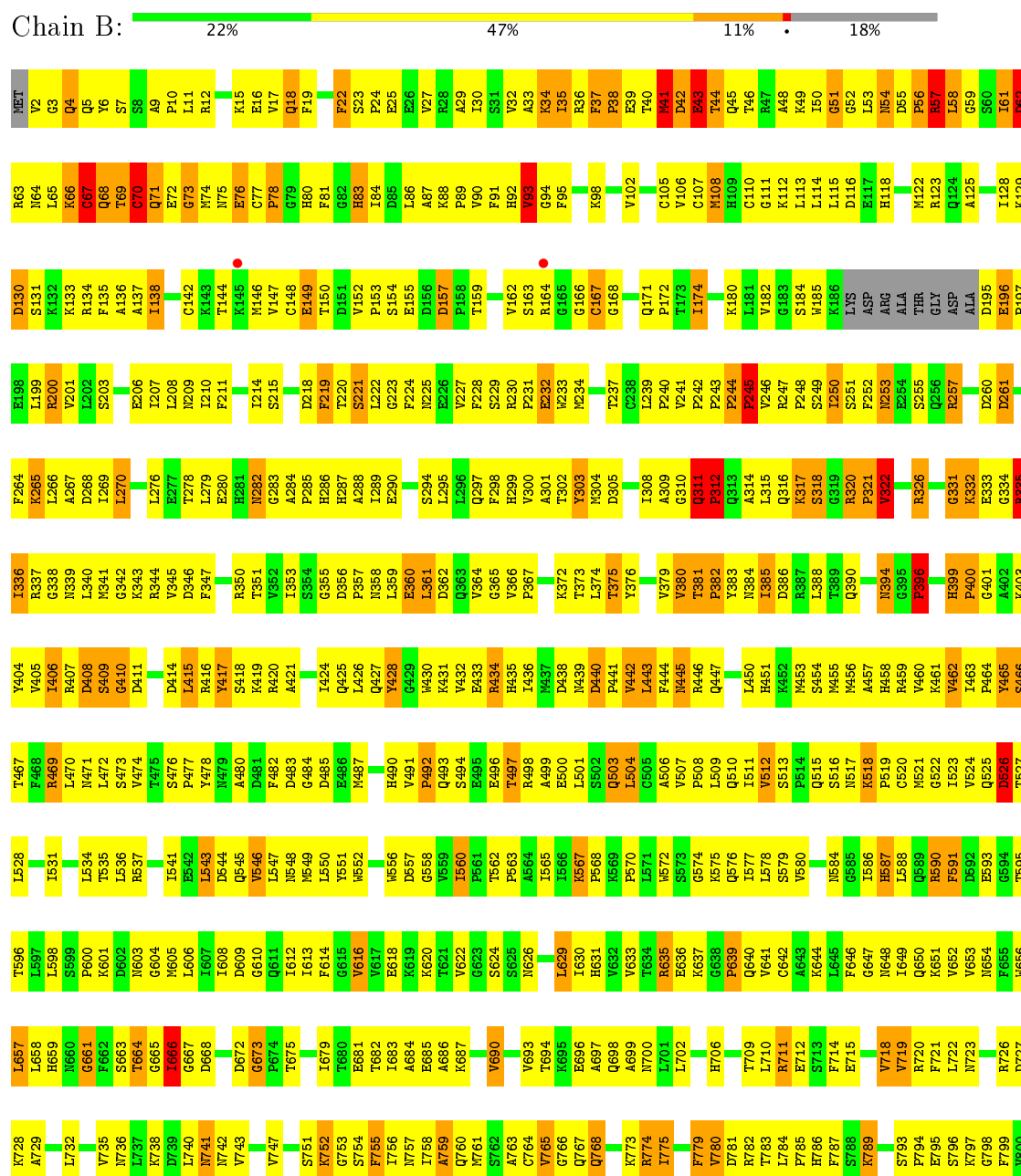
- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 17  | B     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

### 3 Residue-property plots

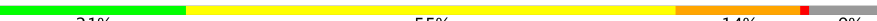
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: DNA-directed RNA polymerase II subunit RPB1



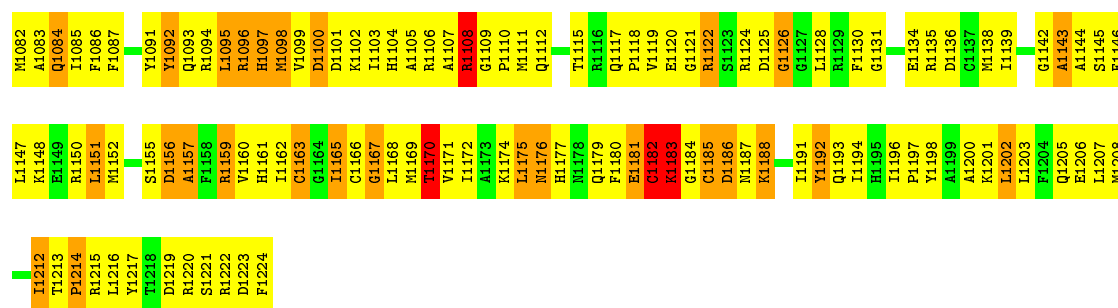
|     |     |     |     |     |       |       |       |       |       |       |       |       |       |      |
|-----|-----|-----|-----|-----|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|
| PRO | SER | SER | PRO | GLY | D1446 | T1385 | E1256 | S1189 | A1126 | M1063 | K1003 | V937  | I867  | E801 |
| SER | PRO | THR | THR | PHE | E1447 | R1386 | M1259 | L1192 | D1127 | V1064 | M1004 | R940  | Y868  | I802 |
| SER | THR | ALA | ALA | THR | S1448 | F1389 | L1260 | L1193 | Q1128 | G1065 | I1006 | R940  | G869  | S803 |
| PRO | PRO | PRO | PRO | TYR | V1450 | M1390 | L1261 | R1194 | Q1130 | V1066 | I1006 | K941  | E870  | T804 |
| THR | THR | THR | THR | GLY | V1451 | D1391 | K1262 | K1131 | Q1131 | L1067 | Q1008 | F942  | D871  | L805 |
| SER | SER | SER | SER | GLY | M1454 | S1392 | I1263 | L1197 | K1132 | A1068 | Q1008 | L943  | G872  | R806 |
| ASN | ASN | ASN | ASN | ALA | P1455 | M1393 | E1265 | D1198 | L1133 | I1072 | A1010 | R944  | M873  | G807 |
| THR | THR | THR | THR | GLY | GLN   | G1395 | M1267 | A1201 | L1134 | E1074 | R1012 | V946  | D874  | L808 |
| PRO | PRO | PRO | PRO | GLY | GLN   | I1397 | L1268 | M1202 | A1137 | P1075 | D1013 | F947  | A876  | T809 |
| THR | THR | THR | THR | ALA | ILE   | M1398 | E1269 | K1205 | I1138 | M1077 | A1015 | V948  | I878  | E812 |
| SER | THR | THR | THR | THR | THR   | R1399 | M1270 | K1206 | E1139 | Q1076 | V1016 | A852  | Q881  | F814 |
| PRO | PRO | PRO | PRO | SER | GLU   | G1400 | L1271 | D1206 | H1140 | M1079 | T1017 | A852  | S882  | F815 |
| SER | PRO | PRO | PRO | SER | ILE   | F1401 | T1272 | L1207 | T1141 | F1018 | L1017 | A852  | S882  | H816 |
| THR | THR | THR | THR | PHE | GLU   | F1402 | T1273 | M1209 | T1142 | M954  | L1018 | A852  | S882  | A817 |
| SER | THR | THR | THR | GLY | GLU   | R1403 | L1274 | M1210 | K1143 | P955  | C1019 | P955  | D884  | M818 |
| PRO | PRO | PRO | PRO | ALA | GLY   | E1404 | G1275 | Q1211 | S1145 | ASN   | C1020 | L956  | T885  | G819 |
| THR | THR | THR | THR | TYR | GLN   | T1405 | V1276 | V1212 | T1146 | PHE   | L1021 | P957  | I886  | G820 |
| SER | THR | THR | THR | GLY | ASP   | V1406 | E1277 | G1213 | T1147 | HIS   | R1023 | N958  | G887  | R821 |
| PRO | PRO | PRO | PRO | GLY | GLY   | E1407 | M1278 | E1214 | I1148 | PHE   | S1024 | I960  | D890  | I825 |
| THR | THR | THR | THR | GLY | GLY   | T1408 | L1279 | R1215 | A1149 | ALA   | R1025 | I960  | D826  | D826 |
| THR | THR | THR | THR | VAL | VAL   | L1409 | E1280 | Q1218 | S1150 | GLY   | L1026 | R962  | R896  | T827 |
| PRO | PRO | PRO | PRO | THR | THR   | E1410 | R1281 | T1219 | I1151 | VAL   | A1027 | I963  | Y897  | A828 |
| SER | PRO | PRO | PRO | SER | PRO   | E1411 | V1282 | I1152 | I1152 | ALA   | T1028 | I964  | R898  | T829 |
| GLY | SER | PRO | PRO | PRO | TYR   | G1412 | M1284 | F1220 | Y1153 | SER   | R1029 | Q965  | R899  | R830 |
| PRO | PRO | PRO | PRO | PHE | ASN   | A1414 | V1284 | K1221 | Y1154 | K1093 | V1031 | D900  | L901  | T831 |
| ALA | ALA | ALA | ALA | GLY | GLU   | S1415 | A1347 | D1223 | D1157 | T1095 | L1032 | L902  | L902  | T834 |
| THR | THR | THR | THR | VAL | SER   | E1416 | E1288 | L1224 | D1157 | Q1033 | E1033 | T903  | T903  | N903 |
| SER | SER | SER | SER | SER | GLY   | E1417 | R1289 | F1225 | P1158 | S1086 | E1034 | T905  | T905  | G835 |
| PRO | PRO | PRO | PRO | SER | LEU   | L1418 | E1290 | V1226 | A1159 | Q1097 | Y1035 | D905  | D905  | Y836 |
| ALA | ALA | ALA | ALA | PRO | VAL   | D1419 | P1291 | I1227 | S1160 | R1036 | L1037 | H906  | H906  | R839 |
| GLN | GLN | GLN | GLN | GLY | ASN   | E1420 | V1292 | M1228 | T1161 | T1038 | T1038 | T907  | T907  | R840 |
| ASP | ASP | ASP | ASP | PHE | ALA   | C1421 | S1293 | S1229 | V1162 | L1101 | K1039 | T976  | T976  | L908 |
| PRO | PRO | PRO | PRO | SER | ASP   | R1422 | P1294 | E1230 | I1163 | K1102 | Q1039 | K977  | K977  | K843 |
| THR | THR | THR | THR | PRO | LEU   | G1423 | T1295 | D1231 | P1164 | E1103 | Q1040 | P978  | P978  | A844 |
| ASP | ASP | ASP | ASP | THR | ASP   | V1424 | G1296 | M1232 | E1165 | L1104 | F1042 | S979  | S979  | L845 |
| VAL | VAL | VAL | VAL | VAL | VAL   | S1425 | E1297 | L1236 | E1167 | L1105 | M1042 | D980  | D980  | E846 |
| LYS | LYS | LYS | LYS | THR | LYS   | E1426 | Y1298 | L1237 | E1170 | N1106 | M1043 | L981  | L981  | D847 |
| THR | THR | THR | THR | THR | ASP   | V1428 | V1299 | I1238 | I1173 | A1108 | V1045 | T982  | T982  | T848 |
| SER | SER | SER | SER | TYR | LEU   | I1429 | K1300 | R1239 | H1173 | K1109 | L1046 | K984  | K984  | M849 |
| PRO | PRO | PRO | PRO | SER | MET   | L1430 | E1301 | C1240 | F1174 | N1110 | S1047 | D985  | D985  | V850 |
| SER | THR | THR | THR | PRO | PHE   | G1431 | P1302 | R1241 | S1175 | M1111 | M1048 | G921  | G921  | H851 |
| PRO | PRO | PRO | PRO | SER | SER   | Q1432 | E1303 | V1242 | S1175 | K1112 | I1049 | D922  | D922  | D853 |
| PRO | PRO | PRO | PRO | PRO | PRO   | M1433 | M1304 | V1243 | L1176 | T1113 | E1050 | L988  | L988  | T855 |
| THR | THR | THR | THR | ALA | LEU   | A1434 | V1305 | ARG   | LEU   | P1114 | A1051 | K924  | K924  | T855 |
| VAL | VAL | VAL | VAL | TYR | VAL   | L1435 | L1306 | PRO   | ASP   | S1115 | Q1052 | L925  | L925  | T856 |
| ASP | ASP | ASP | ASP | SER | ASP   | P1436 | E1307 | PRO   | ASP   | L1116 | F1053 | Q926  | Q926  | R857 |
| PRO | PRO | PRO | PRO | SER | ASP   | I1437 | T1308 | LYS   | GLU   | T1117 | L1054 | V927  | V927  | R858 |
| THR | THR | THR | THR | PRO | SER   | V1374 | D1309 | SER   | GLU   | T1117 | L1054 | V927  | V927  | R858 |
| SER | SER | SER | SER | THR | GLY   | M1375 | V1310 | LEU   | ALA   | T1118 | R1055 | L928  | L928  | S859 |
| PRO | PRO | PRO | PRO | SER | THR   | G1439 | V1311 | ASP   | GLU   | Y1119 | S1056 | L929  | L929  | L860 |
| SER | PRO | PRO | PRO | PRO | ASN   | T1377 | M1312 | ALA   | GLN   | E1120 | V1057 | L997  | L997  | G861 |
| ASP | ASP | ASP | ASP | SER | ASN   | Q1378 | L1313 | GLU   | GLN   | L1121 | V1058 | L998  | L998  | H862 |
| THR | THR | THR | THR | THR | ALA   | F1441 | M1314 | THR   | PHE   | P1122 | H1059 | V999  | V999  | V863 |
| SER | SER | SER | SER | TYR | ALA   | D1442 | S1314 | THR   | ASP   | G1123 | P1060 | R1000 | R1000 | H864 |
| PRO | PRO | PRO | PRO | PRO | MET   | V1443 | E1315 | GLU   | ASP   | H1124 | R1001 | Q935  | Q935  | Q865 |
| ALA | ALA | ALA | ALA | PRO | ALA   | M1444 | V1316 | GLU   | Q1187 | H1124 | R1001 | Q935  | Q935  | Q865 |
| THR | THR | THR | THR | THR | GLY   | I1445 | M1317 | E1255 | Q1188 | A1125 | E1062 | G1002 | G1002 | F866 |

• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

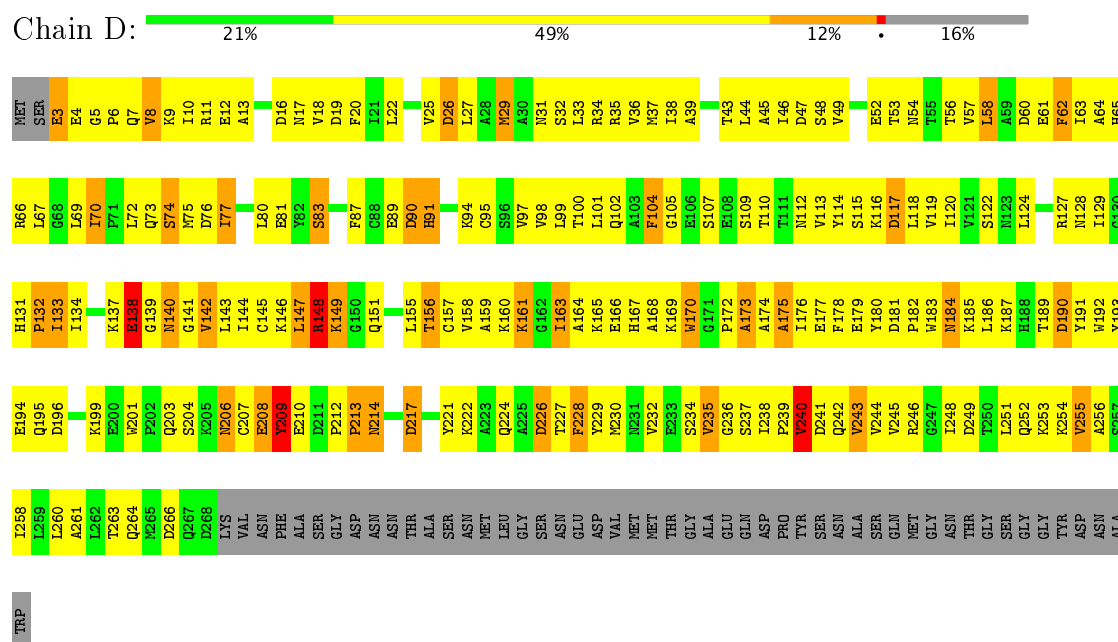
Chain C:  21% 55% 14% 9%



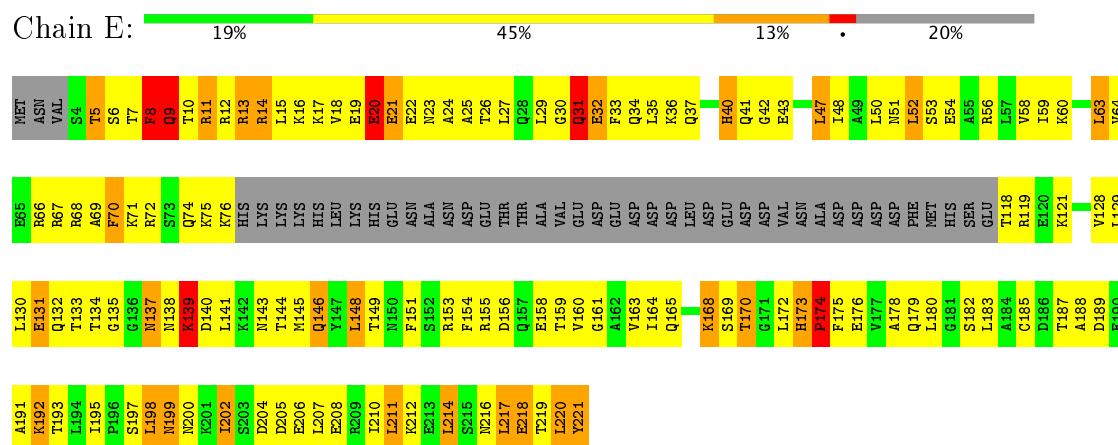




• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

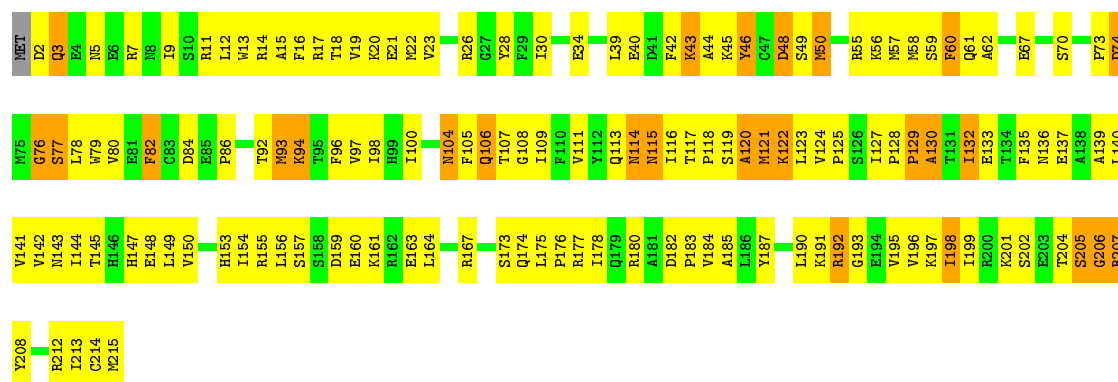


• Molecule 4: DNA-directed RNA polymerase II subunit RPB4

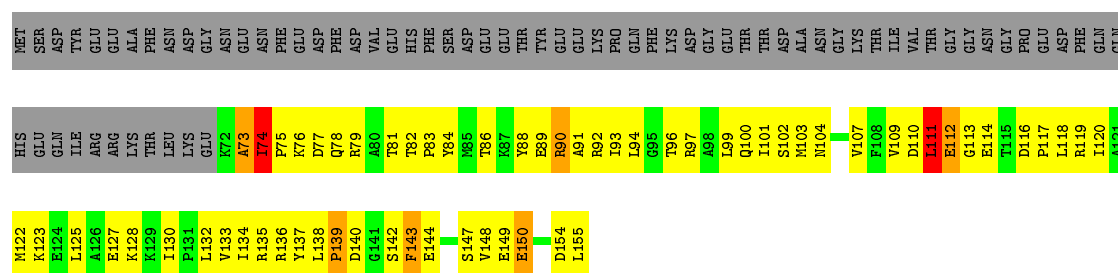


• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

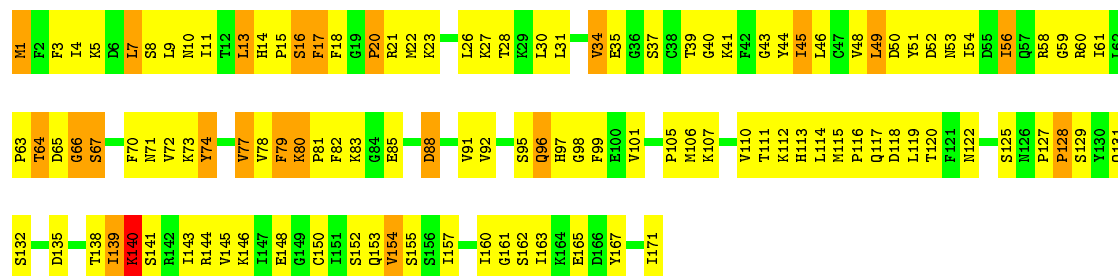




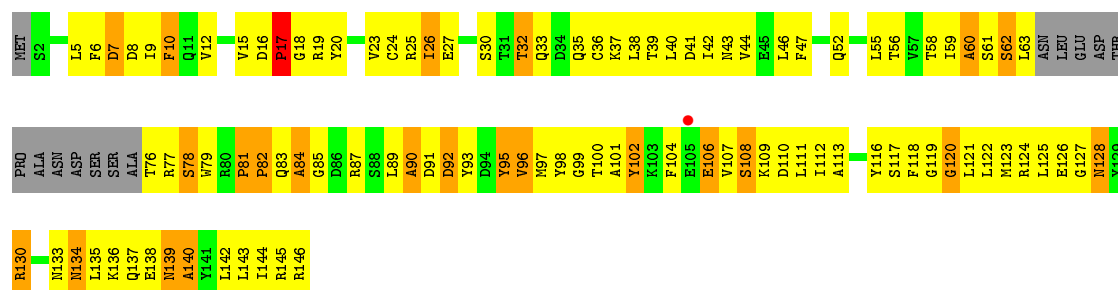
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



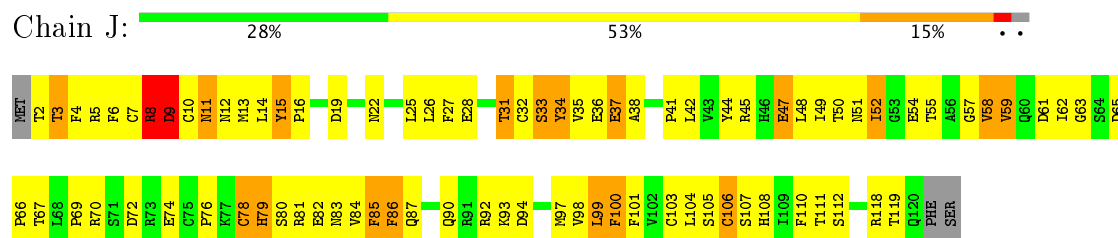
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7



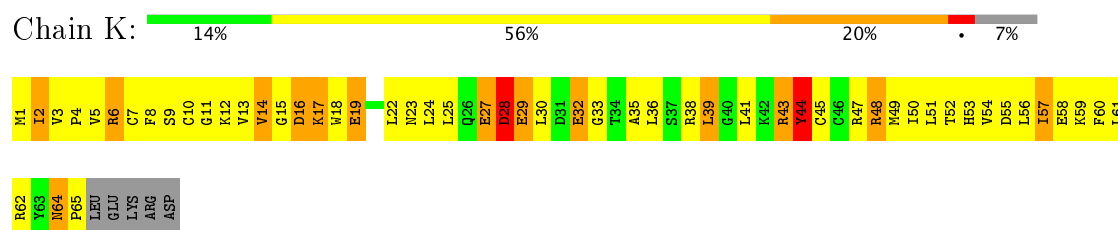
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



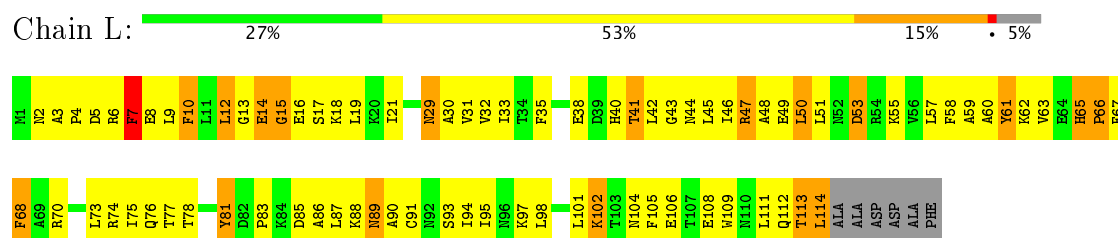
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



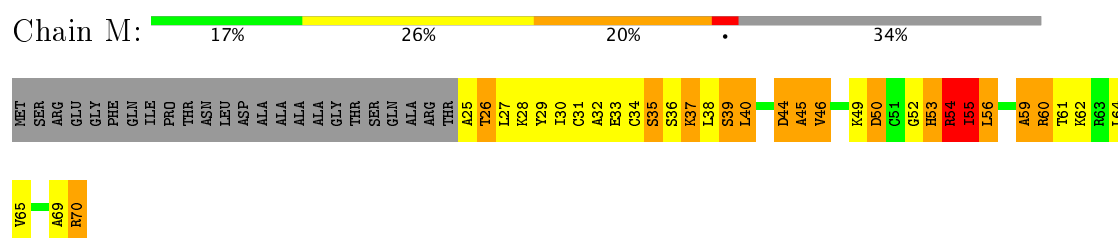
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



- Molecule 11: DNA-directed RNA polymerase II subunit RPB11



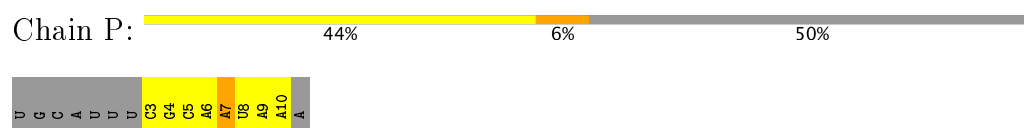
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



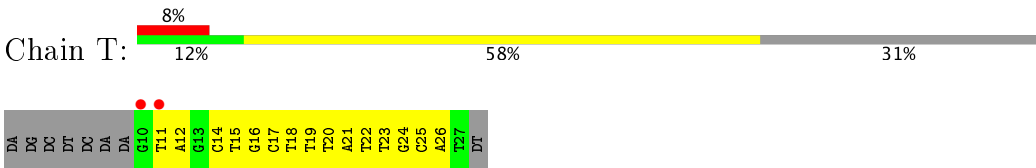
- Molecule 13: 5'-D(\*AP\*GP\*CP\*TP\*CP\*AP\*AP\*GP\*TP\*AP\*GP\*CP\*TP\*GP\*CP\*TP\*TP\*TP\*AP\*TP\*TP\*GP\*CP\*AP\*TP\*T)-3'



- Molecule 14: 5'-D(\*CP\*AP\*GP\*CP\*TP\*AP\*CP\*TP\*TP\*GP\*AP\*GP\*CP\*T)-3'



● Molecule 15: 5'-R(\*UP\*GP\*CP\*AP\*UP\*UP\*UP\*CP\*GP\*CP\*AP\*AP\*UP\*AP\*AP\*A)-3',



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | C 2 2 21  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 222.47Å 391.62Å 284.12Å<br>90.00° 90.00° 90.00°                               | Depositor        |
| Resolution (Å)  | 50.00 – 4.00<br>48.99 – 4.00  | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | (Not available) (50.00-4.00)<br>100.0 (48.99-4.00)                            | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | 0.11  | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.57 (at 4.00Å)   | Xtriage          |
| Refinement program  | CNS 1.2   | Depositor        |
| R, $R_{free}$   | 0.205 , 0.241<br>0.215 , 0.243  | Depositor<br>DCC |
| $R_{free}$ test set   | 8343 reflections (7.99%)  | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 131.8   | Xtriage          |
| Anisotropy  | 0.506   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.27 , 82.8   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$                   | Xtriage          |
| Estimated twinning fraction   | 0.024 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l<br>0.024 for 1/2*h+1/2*k,3/2*h-1/2*k,-l | Xtriage          |
| $F_o, F_c$ correlation  | 0.92  | EDS              |
| Total number of atoms   | 31777   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 138.0   | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.92% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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

| Mol | Chain | Bond lengths |             | Bond angles |                |
|-----|-------|--------------|-------------|-------------|----------------|
|     |       | RMSZ         | # $ Z  > 5$ | RMSZ        | # $ Z  > 5$    |
| 1   | B     | 0.43         | 0/11339     | 0.71        | 4/15334 (0.0%) |
| 2   | C     | 0.43         | 0/8981      | 0.69        | 1/12108 (0.0%) |
| 3   | D     | 0.43         | 0/2133      | 0.71        | 0/2891         |
| 4   | E     | 0.43         | 0/1437      | 0.69        | 0/1925         |
| 5   | F     | 0.42         | 0/1788      | 0.67        | 0/2406         |
| 6   | G     | 0.48         | 0/691       | 0.77        | 0/933          |
| 7   | H     | 0.47         | 0/1368      | 0.73        | 0/1844         |
| 8   | I     | 0.41         | 0/1086      | 0.69        | 0/1470         |
| 9   | J     | 0.40         | 0/989       | 0.66        | 0/1331         |
| 10  | K     | 0.44         | 0/541       | 0.75        | 0/727          |
| 11  | L     | 0.45         | 0/937       | 0.69        | 0/1265         |
| 12  | M     | 0.48         | 0/366       | 0.72        | 0/485          |
| 13  | N     | 0.70         | 0/154       | 0.88        | 0/235          |
| 14  | P     | 0.55         | 0/188       | 0.94        | 0/291          |
| 15  | T     | 0.42         | 0/407       | 0.95        | 0/627          |
| All | All   | 0.44         | 0/32405     | 0.71        | 5/43872 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 10  | K     | 0                   | 1                   |

There are no bond length outliers.

All (5) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | B     | 311 | GLN  | N-CA-C | 5.60 | 126.11      | 111.00   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 1   | B     | 56   | PRO  | N-CA-C | -5.54 | 97.71       | 112.10   |
| 1   | B     | 425  | GLN  | N-CA-C | -5.38 | 96.48       | 111.00   |
| 2   | C     | 1163 | CYS  | N-CA-C | -5.21 | 96.94       | 111.00   |
| 1   | B     | 440  | ASP  | N-CA-C | -5.02 | 97.44       | 111.00   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 10  | K     | 44  | TYR  | Sidechain |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | B     | 11140 | 0        | 11215    | 1481    | 0            |
| 2   | C     | 8810  | 0        | 8847     | 1266    | 0            |
| 3   | D     | 2095  | 0        | 2051     | 295     | 0            |
| 4   | E     | 1427  | 0        | 1451     | 175     | 0            |
| 5   | F     | 1752  | 0        | 1776     | 183     | 0            |
| 6   | G     | 679   | 0        | 701      | 98      | 0            |
| 7   | H     | 1340  | 0        | 1357     | 185     | 0            |
| 8   | I     | 1068  | 0        | 1040     | 166     | 0            |
| 9   | J     | 971   | 0        | 929      | 123     | 0            |
| 10  | K     | 532   | 0        | 542      | 122     | 0            |
| 11  | L     | 919   | 0        | 929      | 135     | 0            |
| 12  | M     | 364   | 0        | 388      | 57      | 0            |
| 13  | N     | 138   | 0        | 80       | 8       | 0            |
| 14  | P     | 168   | 0        | 88       | 15      | 0            |
| 15  | T     | 365   | 0        | 208      | 48      | 0            |
| 16  | B     | 2     | 0        | 0        | 0       | 0            |
| 16  | C     | 1     | 0        | 0        | 0       | 0            |
| 16  | D     | 1     | 0        | 0        | 0       | 0            |
| 16  | J     | 2     | 0        | 0        | 0       | 0            |
| 16  | K     | 1     | 0        | 0        | 0       | 0            |
| 16  | M     | 1     | 0        | 0        | 0       | 0            |
| 17  | B     | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| All | All   | 31777 | 0        | 31602    | 3977    | 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 63.

All (3977) 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) |
|------------------|-------------------|--------------------------|-------------------|
| 15:T:21:DA:C2'   | 15:T:22:DT:H5'    | 1.58                     | 1.32              |
| 15:T:21:DA:H2''  | 15:T:22:DT:C5'    | 1.65                     | 1.25              |
| 15:T:20:DT:C2'   | 15:T:21:DA:H5'    | 1.73                     | 1.18              |
| 11:L:47:ARG:HH11 | 11:L:47:ARG:HB3   | 1.11                     | 1.15              |
| 15:T:20:DT:H2'   | 15:T:21:DA:H5'    | 1.13                     | 1.12              |
| 2:C:1072:MET:HE3 | 2:C:1085:ILE:HB   | 1.28                     | 1.12              |
| 3:D:101:LEU:HD13 | 3:D:118:LEU:HD23  | 1.31                     | 1.10              |
| 2:C:622:LYS:HE2  | 9:J:59:VAL:HG22   | 1.21                     | 1.08              |
| 1:B:590:ARG:HH21 | 1:B:620:LYS:HB3   | 1.10                     | 1.08              |
| 4:E:134:THR:HG22 | 4:E:135:GLY:H     | 1.13                     | 1.08              |
| 1:B:53:LEU:HD23  | 1:B:54:ASN:H      | 1.14                     | 1.07              |
| 1:B:356:ASP:HB2  | 1:B:469:ARG:HH12  | 1.19                     | 1.07              |
| 1:B:981:LEU:HD21 | 1:B:1039:LYS:HA   | 1.35                     | 1.06              |
| 2:C:839:MET:HG3  | 2:C:1010:LEU:HD12 | 1.37                     | 1.06              |
| 1:B:682:THR:HG23 | 1:B:728:LYS:HE3   | 1.30                     | 1.06              |
| 12:M:32:ALA:HB3  | 12:M:55:ILE:HD12  | 1.36                     | 1.06              |
| 2:C:1197:PRO:HG2 | 2:C:1200:ALA:HB2  | 1.38                     | 1.06              |
| 7:H:13:LEU:HD21  | 7:H:17:PHE:HB2    | 1.32                     | 1.06              |
| 1:B:535:THR:HG21 | 1:B:616:VAL:HA    | 1.38                     | 1.05              |
| 8:I:100:THR:HG23 | 8:I:138:GLU:HA    | 1.38                     | 1.03              |
| 2:C:603:LEU:HD12 | 2:C:609:ILE:HG13  | 1.39                     | 1.02              |
| 8:I:59:ILE:HG22  | 8:I:60:ALA:H      | 1.19                     | 1.02              |
| 1:B:1445:ILE:H   | 1:B:1445:ILE:HD12 | 1.20                     | 1.02              |
| 2:C:278:GLN:HG2  | 2:C:279:ASP:H     | 1.24                     | 1.02              |
| 2:C:189:LEU:HA   | 2:C:192:LEU:HD12  | 1.40                     | 1.02              |
| 1:B:443:LEU:HD21 | 1:B:455:MET:HB3   | 1.36                     | 1.01              |
| 4:E:170:THR:HB   | 4:E:172:LEU:HG    | 1.43                     | 1.00              |
| 2:C:516:ASN:HD22 | 2:C:516:ASN:N     | 1.58                     | 1.00              |
| 2:C:577:ALA:HB1  | 2:C:589:VAL:HG11  | 1.41                     | 1.00              |
| 1:B:901:LEU:HB2  | 1:B:926:GLN:HG2   | 1.42                     | 1.00              |
| 1:B:1329:THR:H   | 1:B:1335:ILE:HD11 | 1.27                     | 1.00              |
| 15:T:21:DA:C2'   | 15:T:22:DT:C5'    | 2.30                     | 1.00              |
| 2:C:96:TYR:HB2   | 2:C:129:PHE:HB2   | 1.44                     | 0.99              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:340:LEU:HD13  | 1:B:1429:ILE:HG23 | 1.42                     | 0.99              |
| 6:G:111:LEU:H     | 6:G:111:LEU:HD12  | 1.26                     | 0.99              |
| 3:D:57:VAL:HG11   | 10:K:60:PHE:HB3   | 1.44                     | 0.99              |
| 1:B:1017:LEU:HB2  | 5:F:206:GLY:H     | 1.27                     | 0.99              |
| 1:B:855:THR:HG21  | 1:B:857:ARG:HE    | 1.23                     | 0.99              |
| 1:B:1444:MET:HE1  | 6:G:135:ARG:HB2   | 1.43                     | 0.98              |
| 4:E:12:ARG:HH22   | 4:E:14:ARG:HG3    | 1.27                     | 0.97              |
| 2:C:516:ASN:H     | 2:C:516:ASN:HD22  | 1.12                     | 0.97              |
| 4:E:5:THR:HG22    | 7:H:8:SER:O       | 1.63                     | 0.97              |
| 1:B:446:ARG:HD3   | 1:B:480:ALA:HB2   | 1.46                     | 0.97              |
| 1:B:981:LEU:CD2   | 1:B:1039:LYS:HA   | 1.95                     | 0.96              |
| 2:C:168:GLY:H     | 2:C:450:ALA:HB1   | 1.26                     | 0.96              |
| 1:B:399:HIS:HB3   | 1:B:400:PRO:HD3   | 1.48                     | 0.96              |
| 4:E:185:CYS:HB2   | 4:E:211:LEU:HD21  | 1.45                     | 0.96              |
| 4:E:40:HIS:HB2    | 7:H:73:LYS:HZ2    | 1.30                     | 0.96              |
| 2:C:800:GLN:HG2   | 10:K:52:THR:CG2   | 1.96                     | 0.96              |
| 1:B:768:GLN:HG2   | 1:B:816:HIS:HA    | 1.48                     | 0.96              |
| 1:B:1161:THR:HG22 | 1:B:1163:ILE:H    | 1.30                     | 0.95              |
| 1:B:567:LYS:CD    | 1:B:568:PRO:HD2   | 1.96                     | 0.95              |
| 4:E:14:ARG:HH22   | 4:E:16:LYS:HZ1    | 1.14                     | 0.95              |
| 1:B:40:THR:HG22   | 1:B:41:MET:HG3    | 1.45                     | 0.95              |
| 2:C:121:ASN:HA    | 2:C:207:GLY:HA2   | 1.48                     | 0.95              |
| 5:F:180:ARG:HH21  | 5:F:192:ARG:HB2   | 1.27                     | 0.95              |
| 2:C:728:ARG:HH12  | 2:C:1047:PHE:HB3  | 1.31                     | 0.95              |
| 11:L:49:GLU:HG3   | 11:L:94:ILE:HG12  | 1.44                     | 0.95              |
| 10:K:1:MET:H1     | 10:K:57:ILE:N     | 1.64                     | 0.95              |
| 2:C:999:MET:HG3   | 2:C:1000:PRO:HD2  | 1.49                     | 0.94              |
| 1:B:55:ASP:C      | 1:B:57:ARG:H      | 1.69                     | 0.94              |
| 1:B:567:LYS:CG    | 1:B:568:PRO:HD2   | 1.98                     | 0.94              |
| 1:B:563:PRO:HG3   | 1:B:572:TRP:CZ2   | 2.01                     | 0.94              |
| 3:D:166:GLU:HG3   | 11:L:10:PHE:HZ    | 1.31                     | 0.93              |
| 15:T:25:DC:H42    | 15:T:26:DA:N6     | 1.66                     | 0.93              |
| 2:C:23:ALA:HB1    | 2:C:24:PRO:HD2    | 1.48                     | 0.93              |
| 10:K:12:LYS:O     | 10:K:14:VAL:HG23  | 1.69                     | 0.93              |
| 1:B:1006:ILE:HD11 | 5:F:163:GLU:HG3   | 1.48                     | 0.93              |
| 1:B:1193:LEU:HD22 | 1:B:1260:LEU:HD11 | 1.51                     | 0.93              |
| 12:M:49:LYS:O     | 12:M:50:ASP:HB2   | 1.65                     | 0.93              |
| 1:B:37:PHE:HB2    | 1:B:52:GLY:HA3    | 1.51                     | 0.93              |
| 8:I:23:VAL:HG22   | 8:I:43:ASN:HA     | 1.51                     | 0.93              |
| 1:B:1424:VAL:HG13 | 1:B:1436:ILE:HD11 | 1.52                     | 0.92              |
| 1:B:658:LEU:HD13  | 2:C:831:SER:H     | 1.33                     | 0.92              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:524:VAL:HG12  | 1:B:525:GLN:H     | 1.34                     | 0.92              |
| 1:B:754:SER:H     | 1:B:757:ASN:HD22  | 1.18                     | 0.92              |
| 1:B:1002:GLY:HA3  | 1:B:1007:ILE:HG21 | 1.50                     | 0.91              |
| 7:H:7:LEU:HB2     | 7:H:74:TYR:HE2    | 1.35                     | 0.91              |
| 1:B:1208:THR:HG22 | 1:B:1210:GLY:H    | 1.35                     | 0.91              |
| 1:B:547:LEU:HB3   | 11:L:58:PHE:HE1   | 1.31                     | 0.91              |
| 1:B:41:MET:CB     | 1:B:49:LYS:HA     | 2.01                     | 0.91              |
| 10:K:1:MET:N      | 10:K:57:ILE:H     | 1.68                     | 0.91              |
| 2:C:515:HIS:H     | 2:C:518:HIS:HD2   | 1.13                     | 0.91              |
| 15:T:25:DC:N4     | 15:T:26:DA:H62    | 1.67                     | 0.91              |
| 4:E:40:HIS:HB2    | 7:H:73:LYS:NZ     | 1.86                     | 0.91              |
| 2:C:483:LEU:HD11  | 2:C:491:THR:HG23  | 1.51                     | 0.91              |
| 1:B:225:ASN:HD22  | 1:B:228:PHE:H     | 1.18                     | 0.90              |
| 2:C:806:THR:HG22  | 2:C:808:ALA:H     | 1.37                     | 0.90              |
| 1:B:1160:SER:HA   | 1:B:1170:ILE:HD13 | 1.53                     | 0.90              |
| 11:L:47:ARG:NH1   | 11:L:47:ARG:HB3   | 1.85                     | 0.90              |
| 6:G:90:ARG:HG3    | 6:G:91:ALA:N      | 1.85                     | 0.90              |
| 2:C:821:GLN:HE22  | 2:C:851:PHE:HA    | 1.36                     | 0.90              |
| 4:E:56:ARG:HD3    | 4:E:149:THR:HA    | 1.54                     | 0.90              |
| 1:B:1341:ILE:HG23 | 1:B:1342:GLU:H    | 1.35                     | 0.89              |
| 2:C:1156:ASP:HB3  | 2:C:1198:TYR:H    | 1.37                     | 0.89              |
| 2:C:642:ASP:HA    | 2:C:649:LYS:HA    | 1.51                     | 0.89              |
| 1:B:899:VAL:HG13  | 1:B:908:LEU:HD21  | 1.54                     | 0.89              |
| 1:B:537:ARG:HD2   | 8:I:20:TYR:HE1    | 1.35                     | 0.89              |
| 1:B:265:LYS:HG2   | 1:B:303:TYR:HA    | 1.55                     | 0.89              |
| 1:B:110:CYS:HB3   | 1:B:167:CYS:SG    | 2.13                     | 0.89              |
| 1:B:913:LEU:HD12  | 1:B:914:GLU:H     | 1.38                     | 0.89              |
| 2:C:214:ALA:HB3   | 2:C:498:THR:HA    | 1.52                     | 0.89              |
| 8:I:59:ILE:HG22   | 8:I:60:ALA:N      | 1.86                     | 0.89              |
| 1:B:347:PHE:H     | 2:C:1107:ALA:HA   | 1.38                     | 0.89              |
| 2:C:217:ARG:HE    | 2:C:405:ARG:HB2   | 1.37                     | 0.89              |
| 2:C:810:GLU:HA    | 2:C:815:ARG:HH12  | 1.36                     | 0.88              |
| 6:G:86:THR:OG1    | 6:G:89:GLU:HG3    | 1.74                     | 0.88              |
| 2:C:778:MET:HE2   | 2:C:1094:ARG:HG2  | 1.55                     | 0.88              |
| 5:F:19:VAL:O      | 5:F:23:VAL:HG23   | 1.73                     | 0.88              |
| 1:B:470:LEU:H     | 1:B:470:LEU:HD23  | 1.38                     | 0.88              |
| 1:B:534:LEU:O     | 1:B:574:GLY:HA3   | 1.74                     | 0.88              |
| 2:C:112:LEU:HD21  | 2:C:117:ALA:HB2   | 1.56                     | 0.88              |
| 2:C:46:GLN:HG3    | 2:C:47:GLN:H      | 1.36                     | 0.88              |
| 7:H:91:VAL:HB     | 7:H:139:ILE:O     | 1.72                     | 0.88              |
| 15:T:18:DT:H2''   | 15:T:19:DT:H5'    | 1.56                     | 0.88              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:356:ASP:HB2   | 1:B:469:ARG:NH1   | 1.87                     | 0.88              |
| 1:B:779:PHE:CE1   | 1:B:785:PRO:HD3   | 2.08                     | 0.88              |
| 1:B:590:ARG:HH21  | 1:B:620:LYS:CB    | 1.87                     | 0.88              |
| 1:B:779:PHE:HE1   | 1:B:785:PRO:HD3   | 1.37                     | 0.87              |
| 11:L:12:LEU:H     | 11:L:12:LEU:HD12  | 1.39                     | 0.87              |
| 12:M:27:LEU:HD13  | 12:M:37:LYS:HE2   | 1.56                     | 0.87              |
| 2:C:1159:ARG:HB3  | 2:C:1159:ARG:NH1  | 1.88                     | 0.87              |
| 1:B:1017:LEU:HB3  | 5:F:205:SER:HA    | 1.53                     | 0.87              |
| 1:B:828:ALA:CB    | 2:C:530:GLY:HA2   | 2.04                     | 0.87              |
| 5:F:156:LEU:HD12  | 5:F:195:VAL:HB    | 1.56                     | 0.87              |
| 2:C:737:THR:HG21  | 9:J:66:PRO:HA     | 1.56                     | 0.87              |
| 6:G:82:THR:HG22   | 6:G:84:TYR:H      | 1.36                     | 0.87              |
| 2:C:847:ASP:HB3   | 3:D:167:HIS:NE2   | 1.90                     | 0.87              |
| 2:C:1159:ARG:HH11 | 2:C:1159:ARG:HB3  | 1.38                     | 0.86              |
| 10:K:44:TYR:HA    | 10:K:47:ARG:HB2   | 1.57                     | 0.86              |
| 3:D:6:PRO:HB3     | 3:D:25:VAL:HG12   | 1.55                     | 0.86              |
| 2:C:100:PRO:HD2   | 2:C:180:TYR:HE1   | 1.40                     | 0.86              |
| 8:I:15:VAL:HG22   | 8:I:26:ILE:HD11   | 1.58                     | 0.86              |
| 9:J:111:THR:HG22  | 9:J:112:SER:H     | 1.41                     | 0.86              |
| 2:C:654:ARG:H     | 2:C:657:HIS:HD2   | 1.21                     | 0.86              |
| 1:B:567:LYS:HB3   | 8:I:96:VAL:H      | 1.41                     | 0.86              |
| 1:B:568:PRO:HG2   | 8:I:46:LEU:HD22   | 1.58                     | 0.86              |
| 2:C:393:LYS:HE3   | 2:C:393:LYS:HA    | 1.58                     | 0.85              |
| 1:B:709:THR:HG22  | 1:B:711:ARG:H     | 1.39                     | 0.85              |
| 2:C:387:LEU:O     | 2:C:392:ARG:HB2   | 1.76                     | 0.85              |
| 2:C:1065:GLN:HG3  | 2:C:1067:ARG:H    | 1.39                     | 0.85              |
| 8:I:59:ILE:CG2    | 8:I:60:ALA:H      | 1.89                     | 0.85              |
| 2:C:856:PHE:HD2   | 2:C:967:ARG:HD2   | 1.41                     | 0.85              |
| 4:E:56:ARG:HB2    | 4:E:148:LEU:HD22  | 1.59                     | 0.85              |
| 10:K:57:ILE:HA    | 10:K:60:PHE:HD2   | 1.41                     | 0.85              |
| 3:D:47:ASP:HA     | 12:M:69:ALA:HB3   | 1.57                     | 0.85              |
| 1:B:53:LEU:HD23   | 1:B:54:ASN:N      | 1.92                     | 0.85              |
| 2:C:1180:PHE:HB3  | 2:C:1191:ILE:CD1  | 2.06                     | 0.85              |
| 15:T:20:DT:C2'    | 15:T:21:DA:C5'    | 2.54                     | 0.85              |
| 1:B:321:PRO:O     | 1:B:322:VAL:HB    | 1.75                     | 0.84              |
| 5:F:117:THR:HG22  | 5:F:119:SER:H     | 1.41                     | 0.84              |
| 2:C:549:THR:HG22  | 2:C:550:ASP:H     | 1.41                     | 0.84              |
| 1:B:1094:VAL:HG13 | 1:B:1113:THR:HG21 | 1.58                     | 0.84              |
| 1:B:265:LYS:HA    | 1:B:265:LYS:HE3   | 1.60                     | 0.84              |
| 1:B:901:LEU:H     | 1:B:926:GLN:NE2   | 1.75                     | 0.84              |
| 1:B:172:PRO:HD3   | 1:B:185:TRP:NE1   | 1.93                     | 0.84              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:39:ALA:HA     | 3:D:164:ALA:HB3   | 1.60                     | 0.84              |
| 3:D:45:ALA:HA     | 3:D:72:LEU:HD12   | 1.59                     | 0.84              |
| 4:E:63:LEU:HD12   | 4:E:129:LEU:HG    | 1.58                     | 0.84              |
| 1:B:196:GLU:HG3   | 1:B:197:PRO:HD2   | 1.59                     | 0.84              |
| 2:C:521:LEU:HD22  | 2:C:633:VAL:HG12  | 1.58                     | 0.84              |
| 2:C:1002:THR:HG23 | 2:C:1006:ILE:HG13 | 1.59                     | 0.83              |
| 2:C:261:ARG:NH1   | 2:C:261:ARG:HB3   | 1.93                     | 0.83              |
| 4:E:134:THR:HG22  | 4:E:135:GLY:N     | 1.93                     | 0.83              |
| 1:B:353:ILE:HG21  | 1:B:487:MET:HE3   | 1.59                     | 0.83              |
| 2:C:579:ARG:HB2   | 2:C:586:TRP:NE1   | 1.92                     | 0.83              |
| 7:H:30:LEU:HD13   | 7:H:72:VAL:HG11   | 1.61                     | 0.83              |
| 4:E:47:LEU:HD11   | 7:H:3:PHE:CD2     | 2.13                     | 0.83              |
| 1:B:567:LYS:HD3   | 8:I:95:TYR:CG     | 2.14                     | 0.83              |
| 2:C:210:LYS:HD3   | 2:C:481:GLN:O     | 1.78                     | 0.83              |
| 2:C:825:VAL:HG12  | 2:C:826:ALA:N     | 1.93                     | 0.83              |
| 2:C:770:GLN:OE1   | 2:C:983:ARG:HA    | 1.78                     | 0.83              |
| 9:J:85:PHE:HD2    | 9:J:85:PHE:H      | 1.24                     | 0.83              |
| 1:B:341:MET:CE    | 1:B:843:LYS:HZ1   | 1.90                     | 0.83              |
| 1:B:1341:ILE:HG23 | 1:B:1342:GLU:N    | 1.93                     | 0.83              |
| 2:C:899:ILE:HD11  | 2:C:911:ILE:HA    | 1.59                     | 0.82              |
| 11:L:65:HIS:HD2   | 11:L:67:PHE:H     | 1.25                     | 0.82              |
| 2:C:1072:MET:CE   | 2:C:1085:ILE:HB   | 2.08                     | 0.82              |
| 1:B:598:LEU:HA    | 8:I:122:LEU:HD13  | 1.59                     | 0.82              |
| 1:B:244:PRO:HB2   | 1:B:245:PRO:HD3   | 1.60                     | 0.82              |
| 2:C:773:MET:CE    | 2:C:985:GLY:HA2   | 2.08                     | 0.82              |
| 1:B:679:ILE:HG12  | 1:B:732:LEU:HD12  | 1.62                     | 0.82              |
| 3:D:7:GLN:HG2     | 11:L:104:ASN:HD22 | 1.44                     | 0.82              |
| 2:C:762:ASN:HD21  | 2:C:1024:ALA:HB3  | 1.44                     | 0.82              |
| 6:G:132:LEU:HD11  | 7:H:61:ILE:HD11   | 1.62                     | 0.82              |
| 10:K:48:ARG:HD2   | 10:K:49:MET:N     | 1.95                     | 0.82              |
| 1:B:528:LEU:HD23  | 1:B:751:SER:HB3   | 1.62                     | 0.81              |
| 2:C:953:LEU:HD21  | 2:C:965:LYS:HB2   | 1.62                     | 0.81              |
| 1:B:343:LYS:HZ2   | 2:C:1151:LEU:HB3  | 1.45                     | 0.81              |
| 2:C:520:GLY:H     | 2:C:748:ILE:HG22  | 1.45                     | 0.81              |
| 11:L:113:THR:O    | 11:L:114:LEU:HB2  | 1.79                     | 0.81              |
| 6:G:118:LEU:O     | 6:G:118:LEU:HD12  | 1.79                     | 0.81              |
| 11:L:21:ILE:HG12  | 11:L:33:ILE:HG12  | 1.60                     | 0.81              |
| 1:B:1116:LEU:HB3  | 1:B:1308:THR:HG21 | 1.63                     | 0.81              |
| 2:C:102:VAL:HG21  | 2:C:112:LEU:HD22  | 1.61                     | 0.81              |
| 2:C:359:GLU:O     | 2:C:362:PRO:HD3   | 1.79                     | 0.81              |
| 4:E:47:LEU:HD11   | 7:H:3:PHE:HD2     | 1.42                     | 0.81              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:T:18:DT:C2'    | 15:T:19:DT:H5'    | 2.09                     | 0.81              |
| 1:B:12:ARG:O      | 2:C:1194:ILE:HG22 | 1.81                     | 0.81              |
| 2:C:952:VAL:HG22  | 2:C:966:VAL:HG13  | 1.62                     | 0.81              |
| 8:I:55:LEU:HD22   | 8:I:144:ILE:CG2   | 2.10                     | 0.81              |
| 2:C:579:ARG:HB2   | 2:C:586:TRP:HE1   | 1.43                     | 0.81              |
| 8:I:135:LEU:HD13  | 8:I:137:GLN:HE21  | 1.45                     | 0.81              |
| 1:B:849:MET:CE    | 1:B:1061:GLY:HA2  | 2.09                     | 0.81              |
| 10:K:3:VAL:HG21   | 10:K:18:TRP:HB2   | 1.62                     | 0.81              |
| 10:K:1:MET:H1     | 10:K:57:ILE:H     | 0.86                     | 0.80              |
| 2:C:244:LEU:HD21  | 2:C:366:GLN:NE2   | 1.96                     | 0.80              |
| 3:D:238:ILE:CG2   | 3:D:242:GLN:HB2   | 2.11                     | 0.80              |
| 3:D:46:ILE:HG23   | 3:D:157:CYS:HB3   | 1.63                     | 0.80              |
| 1:B:855:THR:CG2   | 1:B:857:ARG:HE    | 1.94                     | 0.80              |
| 2:C:37:PHE:CE1    | 2:C:41:LYS:HG3    | 2.17                     | 0.80              |
| 7:H:106:MET:HG2   | 7:H:107:LYS:N     | 1.96                     | 0.80              |
| 9:J:50:THR:HG23   | 9:J:52:ILE:HG23   | 1.63                     | 0.80              |
| 2:C:210:LYS:HE2   | 2:C:462:ALA:HA    | 1.62                     | 0.80              |
| 1:B:1148:ILE:HD11 | 1:B:1198:ASP:HA   | 1.64                     | 0.80              |
| 1:B:929:LEU:HD21  | 1:B:983:ILE:HG21  | 1.62                     | 0.80              |
| 1:B:993:LEU:HD23  | 1:B:1022:LEU:HD21 | 1.62                     | 0.80              |
| 1:B:783:THR:HG21  | 1:B:815:PHE:CZ    | 2.16                     | 0.80              |
| 12:M:27:LEU:HB3   | 12:M:37:LYS:HD3   | 1.64                     | 0.80              |
| 1:B:1226:VAL:HG22 | 1:B:1240:CYS:HB3  | 1.62                     | 0.80              |
| 1:B:1343:ALA:HB2  | 5:F:150:VAL:HG22  | 1.63                     | 0.79              |
| 1:B:440:ASP:H     | 1:B:460:VAL:HG12  | 1.47                     | 0.79              |
| 1:B:913:LEU:HD12  | 1:B:914:GLU:N     | 1.96                     | 0.79              |
| 8:I:81:PRO:HB2    | 8:I:82:PRO:HD2    | 1.64                     | 0.79              |
| 15:T:24:DG:H3'    | 15:T:25:DC:H5''   | 1.65                     | 0.79              |
| 1:B:1242:VAL:HG12 | 1:B:1243:VAL:H    | 1.45                     | 0.79              |
| 1:B:743:VAL:O     | 1:B:747:VAL:HG23  | 1.82                     | 0.79              |
| 2:C:1069:PHE:HD1  | 2:C:1069:PHE:H    | 1.27                     | 0.79              |
| 2:C:1085:ILE:N    | 2:C:1085:ILE:HD12 | 1.97                     | 0.79              |
| 2:C:169:ARG:HB2   | 2:C:454:THR:HG23  | 1.65                     | 0.79              |
| 3:D:67:LEU:HD11   | 3:D:155:LEU:HD13  | 1.64                     | 0.79              |
| 5:F:153:HIS:HB3   | 5:F:196:VAL:CG1   | 2.11                     | 0.79              |
| 1:B:849:MET:HE1   | 1:B:1061:GLY:HA2  | 1.65                     | 0.79              |
| 2:C:1147:LEU:O    | 2:C:1151:LEU:HD13 | 1.80                     | 0.79              |
| 3:D:70:ILE:HG12   | 3:D:142:VAL:HG11  | 1.64                     | 0.79              |
| 1:B:1373:ASP:HA   | 1:B:1376:THR:HG22 | 1.65                     | 0.79              |
| 5:F:80:VAL:HG22   | 5:F:109:ILE:HD12  | 1.64                     | 0.79              |
| 7:H:45:ILE:HA     | 7:H:78:VAL:HG12   | 1.64                     | 0.79              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:F:135:PHE:HB3   | 5:F:140:LEU:HD11  | 1.64                     | 0.79              |
| 1:B:973:ILE:HD11  | 1:B:1038:THR:HG23 | 1.64                     | 0.79              |
| 2:C:756:ILE:O     | 2:C:759:PRO:HD3   | 1.83                     | 0.79              |
| 5:F:180:ARG:NH2   | 5:F:192:ARG:HB2   | 1.96                     | 0.79              |
| 2:C:515:HIS:HD2   | 2:C:517:THR:H     | 1.28                     | 0.79              |
| 2:C:593:PRO:HG2   | 2:C:617:ARG:NH2   | 1.97                     | 0.78              |
| 3:D:44:LEU:HB2    | 3:D:77:ILE:HD11   | 1.63                     | 0.78              |
| 5:F:198:ILE:HD11  | 5:F:212:ARG:HG3   | 1.63                     | 0.78              |
| 9:J:93:LYS:HD2    | 9:J:93:LYS:H      | 1.46                     | 0.78              |
| 2:C:847:ASP:HB3   | 3:D:167:HIS:CD2   | 2.17                     | 0.78              |
| 5:F:78:LEU:HD21   | 5:F:80:VAL:HG23   | 1.66                     | 0.78              |
| 1:B:767:GLN:NE2   | 1:B:774:ARG:HB3   | 1.99                     | 0.78              |
| 1:B:180:LYS:NZ    | 1:B:294:SER:HB3   | 1.99                     | 0.78              |
| 2:C:1084:GLN:NE2  | 2:C:1084:GLN:H    | 1.81                     | 0.78              |
| 2:C:167:ILE:HG22  | 2:C:453:ILE:HD11  | 1.64                     | 0.78              |
| 8:I:17:PRO:HB3    | 8:I:24:CYS:SG     | 2.24                     | 0.78              |
| 15:T:21:DA:H2''   | 15:T:22:DT:H5'    | 0.82                     | 0.78              |
| 2:C:800:GLN:HG2   | 10:K:52:THR:HG22  | 1.64                     | 0.78              |
| 4:E:159:THR:O     | 4:E:163:VAL:HG23  | 1.84                     | 0.78              |
| 11:L:47:ARG:HH11  | 11:L:47:ARG:CB    | 1.95                     | 0.78              |
| 2:C:516:ASN:ND2   | 2:C:516:ASN:H     | 1.72                     | 0.78              |
| 3:D:32:SER:O      | 3:D:36:VAL:HG23   | 1.84                     | 0.78              |
| 7:H:14:HIS:CD2    | 7:H:16:SER:HB2    | 2.19                     | 0.78              |
| 1:B:1148:ILE:HG12 | 9:J:49:ILE:HD12   | 1.65                     | 0.78              |
| 1:B:1325:THR:O    | 1:B:1325:THR:HG22 | 1.83                     | 0.78              |
| 1:B:845:LEU:HD22  | 1:B:1374:VAL:HG21 | 1.65                     | 0.78              |
| 1:B:857:ARG:HD3   | 1:B:861:GLY:O     | 1.83                     | 0.78              |
| 2:C:167:ILE:HG22  | 2:C:453:ILE:CD1   | 2.14                     | 0.78              |
| 2:C:25:ILE:HD11   | 2:C:653:VAL:O     | 1.82                     | 0.78              |
| 2:C:29:ASP:HB3    | 2:C:658:ILE:HD13  | 1.65                     | 0.78              |
| 5:F:202:SER:OG    | 5:F:204:THR:HG22  | 1.83                     | 0.78              |
| 8:I:42:ILE:HG23   | 8:I:95:TYR:HE1    | 1.47                     | 0.78              |
| 2:C:329:THR:HA    | 2:C:332:ASP:HB3   | 1.67                     | 0.77              |
| 3:D:43:THR:HG22   | 3:D:44:LEU:H      | 1.47                     | 0.77              |
| 1:B:1193:LEU:HD22 | 1:B:1260:LEU:CD1  | 2.14                     | 0.77              |
| 1:B:608:ILE:HB    | 1:B:613:ILE:HD11  | 1.65                     | 0.77              |
| 3:D:147:LEU:HB2   | 3:D:151:GLN:HB2   | 1.65                     | 0.77              |
| 3:D:196:ASP:HB3   | 3:D:199:LYS:HB2   | 1.65                     | 0.77              |
| 2:C:798:TYR:HE2   | 3:D:62:PHE:CE2    | 2.03                     | 0.77              |
| 2:C:1099:VAL:HG13 | 2:C:1100:ASP:N    | 1.98                     | 0.77              |
| 5:F:94:LYS:NZ     | 5:F:98:ILE:HD11   | 1.99                     | 0.77              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:667:GLY:HA3  | 3:D:192:TRP:CH2   | 2.19                     | 0.77              |
| 1:B:836:TYR:CE2  | 1:B:840:ARG:HD2   | 2.18                     | 0.77              |
| 2:C:830:TYR:CE2  | 2:C:1000:PRO:HD3  | 2.18                     | 0.77              |
| 2:C:1181:GLU:HG3 | 2:C:1188:LYS:HE3  | 1.67                     | 0.77              |
| 4:E:134:THR:CG2  | 4:E:135:GLY:H     | 1.96                     | 0.77              |
| 4:E:202:ILE:HG21 | 4:E:207:LEU:HB2   | 1.66                     | 0.77              |
| 10:K:4:PRO:HD3   | 10:K:53:HIS:CD2   | 2.20                     | 0.77              |
| 3:D:175:ALA:HB2  | 10:K:10:CYS:HB2   | 1.66                     | 0.77              |
| 1:B:885:THR:O    | 1:B:940:ARG:HD2   | 1.83                     | 0.77              |
| 2:C:261:ARG:HB3  | 2:C:261:ARG:HH11  | 1.47                     | 0.77              |
| 2:C:794:ASN:O    | 2:C:795:ILE:HD12  | 1.85                     | 0.77              |
| 3:D:47:ASP:HA    | 12:M:69:ALA:CB    | 2.14                     | 0.77              |
| 7:H:15:PRO:HA    | 7:H:18:PHE:CD1    | 2.20                     | 0.77              |
| 3:D:163:ILE:N    | 3:D:163:ILE:HD13  | 1.98                     | 0.77              |
| 4:E:71:LYS:HG2   | 4:E:74:GLN:HE21   | 1.50                     | 0.77              |
| 7:H:143:ILE:HG22 | 7:H:144:ARG:N     | 2.00                     | 0.77              |
| 7:H:14:HIS:ND1   | 7:H:15:PRO:HD2    | 2.00                     | 0.77              |
| 1:B:524:VAL:HG12 | 1:B:525:GLN:N     | 2.00                     | 0.77              |
| 2:C:828:ALA:HB2  | 2:C:1085:ILE:HG23 | 1.67                     | 0.77              |
| 2:C:589:VAL:HG12 | 2:C:590:HIS:H     | 1.50                     | 0.77              |
| 1:B:763:ALA:O    | 1:B:803:SER:HB3   | 1.84                     | 0.76              |
| 2:C:563:MET:CE   | 2:C:580:VAL:HB    | 2.15                     | 0.76              |
| 2:C:825:VAL:CG1  | 2:C:826:ALA:H     | 1.96                     | 0.76              |
| 5:F:56:LYS:HE3   | 5:F:84:ASP:HB2    | 1.67                     | 0.76              |
| 1:B:1116:LEU:HB3 | 1:B:1308:THR:CG2  | 2.15                     | 0.76              |
| 7:H:115:MET:HB2  | 7:H:116:PRO:HD2   | 1.66                     | 0.76              |
| 14:P:3:C:H2'     | 14:P:4:G:C8       | 2.20                     | 0.76              |
| 1:B:41:MET:N     | 1:B:41:MET:HE3    | 2.00                     | 0.76              |
| 2:C:975:GLN:O    | 2:C:990:ILE:HD12  | 1.85                     | 0.76              |
| 3:D:67:LEU:HD11  | 3:D:155:LEU:CD1   | 2.15                     | 0.76              |
| 9:J:58:VAL:HG13  | 9:J:62:ILE:HD12   | 1.68                     | 0.76              |
| 1:B:1030:ARG:HG3 | 1:B:1034:GLU:OE2  | 1.84                     | 0.76              |
| 6:G:77:ASP:O     | 6:G:78:GLN:HB2    | 1.83                     | 0.76              |
| 1:B:1189:SER:O   | 1:B:1241:ARG:HD3  | 1.86                     | 0.76              |
| 2:C:33:VAL:HG21  | 2:C:638:PHE:HZ    | 1.51                     | 0.76              |
| 6:G:89:GLU:O     | 6:G:93:ILE:HG13   | 1.85                     | 0.76              |
| 1:B:816:HIS:CD2  | 2:C:764:SER:HB2   | 2.21                     | 0.76              |
| 7:H:139:ILE:HG22 | 7:H:140:LYS:H     | 1.50                     | 0.76              |
| 2:C:100:PRO:HD2  | 2:C:180:TYR:CE1   | 2.20                     | 0.76              |
| 2:C:825:VAL:CG1  | 2:C:826:ALA:N     | 2.48                     | 0.76              |
| 2:C:874:PHE:HA   | 2:C:913:GLY:O     | 1.85                     | 0.76              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:66:ARG:NH1    | 10:K:2:ILE:HG21   | 2.01                     | 0.76              |
| 1:B:1015:VAL:HG12 | 1:B:1019:CYS:SG   | 2.25                     | 0.76              |
| 3:D:254:LYS:O     | 3:D:258:ILE:HD13  | 1.85                     | 0.76              |
| 8:I:38:LEU:HD12   | 8:I:124:ARG:O     | 1.86                     | 0.76              |
| 11:L:21:ILE:CG2   | 11:L:31:VAL:HG11  | 2.16                     | 0.76              |
| 1:B:55:ASP:C      | 1:B:57:ARG:N      | 2.37                     | 0.75              |
| 2:C:235:SER:HB3   | 2:C:258:LEU:HG    | 1.68                     | 0.75              |
| 2:C:69:LEU:HD11   | 2:C:425:THR:HG23  | 1.67                     | 0.75              |
| 3:D:133:ILE:HD11  | 3:D:237:SER:HA    | 1.67                     | 0.75              |
| 7:H:4:ILE:HG12    | 7:H:77:VAL:HG23   | 1.66                     | 0.75              |
| 3:D:6:PRO:HB2     | 11:L:101:LEU:HD12 | 1.68                     | 0.75              |
| 3:D:76:ASP:OD2    | 3:D:128:ASN:N     | 2.19                     | 0.75              |
| 13:N:2:DA:H2'     | 13:N:3:DG:C8      | 2.20                     | 0.75              |
| 2:C:217:ARG:HD2   | 2:C:217:ARG:C     | 2.06                     | 0.75              |
| 2:C:603:LEU:HD13  | 2:C:608:ASP:HB2   | 1.68                     | 0.75              |
| 1:B:230:ARG:H     | 1:B:233:TRP:HE3   | 1.28                     | 0.75              |
| 1:B:590:ARG:NH2   | 1:B:620:LYS:HB3   | 1.95                     | 0.75              |
| 2:C:39:ARG:NH2    | 2:C:665:GLU:HG2   | 2.01                     | 0.75              |
| 2:C:879:ARG:NH1   | 2:C:883:LEU:HD13  | 2.00                     | 0.75              |
| 1:B:1143:LEU:O    | 1:B:1146:VAL:HG23 | 1.87                     | 0.75              |
| 1:B:382:PRO:HD3   | 1:B:428:TYR:CE2   | 2.21                     | 0.75              |
| 1:B:668:ASP:HB3   | 1:B:741:ASN:HD21  | 1.52                     | 0.75              |
| 7:H:9:LEU:HD23    | 7:H:30:LEU:HD12   | 1.69                     | 0.75              |
| 1:B:447:GLN:HE22  | 15:T:20:DT:H4'    | 1.52                     | 0.75              |
| 1:B:1424:VAL:HG13 | 1:B:1436:ILE:CD1  | 2.16                     | 0.75              |
| 10:K:14:VAL:HG12  | 10:K:14:VAL:O     | 1.85                     | 0.75              |
| 1:B:1438:THR:HB   | 2:C:1144:ALA:HB3  | 1.66                     | 0.75              |
| 2:C:616:ILE:HD12  | 2:C:616:ILE:N     | 2.00                     | 0.75              |
| 3:D:208:GLU:O     | 3:D:210:GLU:N     | 2.20                     | 0.75              |
| 1:B:1394:THR:HG22 | 1:B:1395:GLY:H    | 1.52                     | 0.74              |
| 2:C:770:GLN:CD    | 2:C:983:ARG:HA    | 2.08                     | 0.74              |
| 1:B:1004:ASN:ND2  | 5:F:167:ARG:HD2   | 2.01                     | 0.74              |
| 1:B:1402:PHE:CE1  | 1:B:1403:GLU:HG3  | 2.21                     | 0.74              |
| 1:B:518:LYS:HE2   | 1:B:624:SER:O     | 1.87                     | 0.74              |
| 2:C:1196:ILE:HD12 | 2:C:1200:ALA:HB3  | 1.68                     | 0.74              |
| 2:C:29:ASP:HB3    | 2:C:658:ILE:CD1   | 2.16                     | 0.74              |
| 1:B:946:VAL:HG13  | 5:F:201:LYS:HB3   | 1.67                     | 0.74              |
| 7:H:44:TYR:HE1    | 7:H:157:ILE:H     | 1.34                     | 0.74              |
| 9:J:14:LEU:HA     | 9:J:28:GLU:O      | 1.86                     | 0.74              |
| 1:B:1208:THR:HB   | 1:B:1211:GLN:HG3  | 1.70                     | 0.74              |
| 7:H:88:ASP:HB3    | 7:H:144:ARG:HA    | 1.68                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:537:ARG:HD2   | 8:I:20:TYR:CE1    | 2.21                     | 0.74              |
| 9:J:51:ASN:O      | 9:J:54:GLU:HG3    | 1.87                     | 0.74              |
| 1:B:567:LYS:HD2   | 1:B:568:PRO:HD2   | 1.66                     | 0.74              |
| 3:D:166:GLU:HG3   | 11:L:10:PHE:CZ    | 2.19                     | 0.74              |
| 9:J:25:LEU:HB3    | 9:J:38:ALA:HB2    | 1.69                     | 0.74              |
| 1:B:1116:LEU:N    | 1:B:1308:THR:HG22 | 2.02                     | 0.74              |
| 3:D:45:ALA:O      | 3:D:159:ALA:HA    | 1.86                     | 0.74              |
| 1:B:353:ILE:HD13  | 1:B:487:MET:HE2   | 1.69                     | 0.74              |
| 2:C:69:LEU:HB3    | 2:C:429:PHE:HE1   | 1.51                     | 0.74              |
| 4:E:144:THR:O     | 4:E:148:LEU:HB2   | 1.87                     | 0.74              |
| 2:C:1007:VAL:HG22 | 2:C:1008:PRO:HD2  | 1.69                     | 0.74              |
| 5:F:23:VAL:HG13   | 5:F:78:LEU:HD13   | 1.68                     | 0.74              |
| 2:C:402:GLY:HA3   | 2:C:695:ALA:HB3   | 1.70                     | 0.74              |
| 5:F:145:THR:HG21  | 5:F:187:TYR:CE2   | 2.23                     | 0.74              |
| 10:K:48:ARG:HE    | 10:K:49:MET:HE2   | 1.53                     | 0.74              |
| 11:L:46:ILE:O     | 11:L:50:LEU:HB2   | 1.87                     | 0.74              |
| 1:B:388:LEU:HD23  | 1:B:432:VAL:HB    | 1.68                     | 0.74              |
| 1:B:4:GLN:O       | 1:B:5:GLN:HB2     | 1.86                     | 0.74              |
| 3:D:38:ILE:HA     | 3:D:173:ALA:HB2   | 1.68                     | 0.74              |
| 7:H:1:MET:SD      | 7:H:79:PHE:HD1    | 2.10                     | 0.74              |
| 1:B:547:LEU:HB3   | 11:L:58:PHE:CE1   | 2.20                     | 0.73              |
| 1:B:741:ASN:HD22  | 1:B:741:ASN:C     | 1.89                     | 0.73              |
| 5:F:16:PHE:CZ     | 5:F:20:LYS:HE2    | 2.23                     | 0.73              |
| 1:B:1394:THR:HG21 | 1:B:1398:MET:SD   | 2.27                     | 0.73              |
| 2:C:731:VAL:HG12  | 2:C:732:SER:H     | 1.53                     | 0.73              |
| 1:B:1329:THR:HG22 | 1:B:1331:SER:H    | 1.53                     | 0.73              |
| 1:B:23:SER:HA     | 1:B:233:TRP:NE1   | 2.03                     | 0.73              |
| 2:C:102:VAL:CG2   | 2:C:112:LEU:HD22  | 2.18                     | 0.73              |
| 2:C:185:THR:O     | 2:C:188:ASP:HB2   | 1.88                     | 0.73              |
| 4:E:12:ARG:NH2    | 4:E:14:ARG:HG3    | 2.00                     | 0.73              |
| 6:G:90:ARG:HD3    | 6:G:155:LEU:HD12  | 1.70                     | 0.73              |
| 1:B:659:HIS:HA    | 2:C:1074:ASN:HD22 | 1.53                     | 0.73              |
| 1:B:541:ILE:HD13  | 1:B:549:MET:CE    | 2.18                     | 0.73              |
| 1:B:682:THR:CG2   | 1:B:728:LYS:HE3   | 2.16                     | 0.73              |
| 2:C:274:PRO:HG2   | 2:C:359:GLU:HB3   | 1.70                     | 0.73              |
| 9:J:82:GLU:O      | 9:J:104:LEU:HG    | 1.88                     | 0.73              |
| 6:G:73:ALA:HA     | 6:G:143:PHE:HE1   | 1.54                     | 0.73              |
| 7:H:139:ILE:HG22  | 7:H:140:LYS:N     | 2.01                     | 0.73              |
| 11:L:65:HIS:CD2   | 11:L:67:PHE:H     | 2.05                     | 0.73              |
| 1:B:41:MET:HB2    | 1:B:49:LYS:HA     | 1.69                     | 0.73              |
| 1:B:903:ASN:HD22  | 1:B:904:THR:N     | 1.87                     | 0.73              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:810:GLU:HA   | 2:C:815:ARG:NH1   | 2.02                     | 0.73              |
| 11:L:49:GLU:HG3  | 11:L:94:ILE:CG1   | 2.19                     | 0.73              |
| 1:B:1114:PRO:HB2 | 1:B:1311:VAL:HG23 | 1.71                     | 0.73              |
| 5:F:94:LYS:HZ3   | 5:F:98:ILE:HD11   | 1.54                     | 0.73              |
| 5:F:78:LEU:HA    | 5:F:107:THR:HB    | 1.71                     | 0.73              |
| 1:B:1028:THR:O   | 1:B:1032:LEU:HD12 | 1.88                     | 0.72              |
| 1:B:722:LEU:HD12 | 1:B:722:LEU:H     | 1.53                     | 0.72              |
| 2:C:758:PHE:HB3  | 2:C:761:HIS:HD2   | 1.53                     | 0.72              |
| 8:I:89:LEU:C     | 8:I:91:ASP:H      | 1.92                     | 0.72              |
| 1:B:1208:THR:O   | 1:B:1212:VAL:HG23 | 1.90                     | 0.72              |
| 1:B:855:THR:HG21 | 1:B:857:ARG:NE    | 2.03                     | 0.72              |
| 8:I:84:ALA:HA    | 8:I:87:ARG:HB2    | 1.70                     | 0.72              |
| 10:K:64:ASN:HB3  | 10:K:65:PRO:CD    | 2.19                     | 0.72              |
| 2:C:902:GLY:O    | 12:M:65:VAL:HG11  | 1.88                     | 0.72              |
| 1:B:339:ASN:HB3  | 2:C:1117:GLN:HE22 | 1.54                     | 0.72              |
| 2:C:378:LEU:O    | 2:C:378:LEU:HD12  | 1.89                     | 0.72              |
| 15:T:20:DT:H2'   | 15:T:21:DA:C5'    | 2.06                     | 0.72              |
| 1:B:90:VAL:CG1   | 1:B:297:GLN:HA    | 2.20                     | 0.72              |
| 1:B:965:GLN:O    | 1:B:968:GLN:HB2   | 1.90                     | 0.72              |
| 2:C:295:GLY:H    | 2:C:298:LEU:HD23  | 1.54                     | 0.72              |
| 6:G:119:ARG:HG3  | 6:G:119:ARG:HH11  | 1.53                     | 0.72              |
| 6:G:76:LYS:C     | 6:G:79:ARG:HD2    | 2.10                     | 0.72              |
| 10:K:1:MET:H3    | 10:K:56:LEU:N     | 1.86                     | 0.72              |
| 1:B:1369:ALA:O   | 1:B:1372:VAL:HG12 | 1.88                     | 0.72              |
| 1:B:269:ILE:HD13 | 1:B:300:VAL:HG22  | 1.71                     | 0.72              |
| 1:B:56:PRO:HD2   | 1:B:58:LEU:HG     | 1.71                     | 0.72              |
| 1:B:709:THR:HB   | 1:B:712:GLU:HG3   | 1.70                     | 0.72              |
| 2:C:642:ASP:HB3  | 2:C:649:LYS:CG    | 2.20                     | 0.72              |
| 3:D:66:ARG:NH2   | 10:K:3:VAL:O      | 2.23                     | 0.72              |
| 8:I:130:ARG:HB3  | 8:I:134:ASN:H     | 1.53                     | 0.72              |
| 1:B:215:SER:HB3  | 1:B:218:ASP:HB2   | 1.69                     | 0.72              |
| 1:B:965:GLN:HA   | 1:B:968:GLN:HG3   | 1.72                     | 0.72              |
| 11:L:53:ASP:OD1  | 11:L:55:LYS:HB2   | 1.90                     | 0.72              |
| 13:N:3:DG:H2''   | 13:N:4:DC:OP2     | 1.88                     | 0.72              |
| 1:B:71:GLN:HE22  | 2:C:1176:ASN:ND2  | 1.88                     | 0.72              |
| 2:C:882:THR:HG22 | 2:C:884:ARG:H     | 1.53                     | 0.72              |
| 7:H:143:ILE:HG22 | 7:H:144:ARG:H     | 1.54                     | 0.72              |
| 11:L:21:ILE:HG23 | 11:L:31:VAL:HG11  | 1.70                     | 0.72              |
| 6:G:109:VAL:HG12 | 6:G:110:ASP:N     | 2.05                     | 0.72              |
| 12:M:53:HIS:HB3  | 12:M:55:ILE:HD13  | 1.71                     | 0.72              |
| 2:C:773:MET:HE2  | 2:C:985:GLY:HA2   | 1.71                     | 0.72              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:865:LYS:NZ   | 2:C:869:SER:HA    | 2.03                     | 0.72              |
| 2:C:798:TYR:CE2  | 3:D:62:PHE:HE2    | 2.08                     | 0.72              |
| 8:I:93:TYR:HB3   | 8:I:144:ILE:O     | 1.89                     | 0.72              |
| 12:M:40:LEU:HD13 | 12:M:44:ASP:HB3   | 1.71                     | 0.72              |
| 1:B:427:GLN:HG3  | 1:B:430:TRP:CE2   | 2.25                     | 0.71              |
| 1:B:41:MET:HB3   | 1:B:49:LYS:HA     | 1.71                     | 0.71              |
| 7:H:79:PHE:HE2   | 7:H:105:PRO:HG2   | 1.54                     | 0.71              |
| 10:K:44:TYR:HD2  | 10:K:44:TYR:H     | 1.36                     | 0.71              |
| 1:B:993:LEU:CD2  | 1:B:1022:LEU:HD21 | 2.20                     | 0.71              |
| 10:K:23:ASN:C    | 10:K:25:LEU:H     | 1.93                     | 0.71              |
| 1:B:639:PRO:HG2  | 1:B:640:GLN:H     | 1.53                     | 0.71              |
| 2:C:910:VAL:HG12 | 2:C:912:ILE:H     | 1.55                     | 0.71              |
| 4:E:128:VAL:O    | 4:E:132:GLN:HG3   | 1.90                     | 0.71              |
| 1:B:1342:GLU:OE2 | 5:F:212:ARG:NH1   | 2.24                     | 0.71              |
| 1:B:586:ILE:HG22 | 1:B:587:HIS:N     | 2.05                     | 0.71              |
| 2:C:351:TYR:O    | 2:C:355:ILE:HG13  | 1.90                     | 0.71              |
| 2:C:642:ASP:HB3  | 2:C:649:LYS:HG3   | 1.72                     | 0.71              |
| 7:H:7:LEU:HD12   | 7:H:74:TYR:OH     | 1.90                     | 0.71              |
| 1:B:567:LYS:CB   | 8:I:95:TYR:HA     | 2.20                     | 0.71              |
| 1:B:1261:LYS:HE3 | 9:J:44:TYR:CD2    | 2.26                     | 0.71              |
| 2:C:819:ALA:HB1  | 2:C:1093:GLN:HE21 | 1.56                     | 0.71              |
| 3:D:238:ILE:HG23 | 3:D:242:GLN:HB2   | 1.71                     | 0.71              |
| 4:E:14:ARG:HH22  | 4:E:16:LYS:NZ     | 1.86                     | 0.71              |
| 5:F:23:VAL:HB    | 5:F:30:ILE:HD11   | 1.71                     | 0.71              |
| 1:B:1017:LEU:CB  | 5:F:205:SER:HA    | 2.19                     | 0.71              |
| 2:C:1201:LYS:HE3 | 2:C:1205:GLN:OE1  | 1.90                     | 0.71              |
| 2:C:175:ARG:HG2  | 2:C:175:ARG:HH11  | 1.56                     | 0.71              |
| 2:C:758:PHE:HB3  | 2:C:761:HIS:CD2   | 2.25                     | 0.71              |
| 8:I:127:GLY:O    | 8:I:128:ASN:HB2   | 1.91                     | 0.71              |
| 1:B:1312:ASN:O   | 1:B:1316:VAL:HG23 | 1.89                     | 0.71              |
| 1:B:866:PHE:C    | 1:B:867:ILE:HD12  | 2.11                     | 0.71              |
| 2:C:1182:CYS:O   | 2:C:1182:CYS:SG   | 2.48                     | 0.71              |
| 2:C:642:ASP:HB3  | 2:C:649:LYS:CD    | 2.20                     | 0.71              |
| 2:C:879:ARG:HH12 | 2:C:883:LEU:HD13  | 1.56                     | 0.71              |
| 1:B:657:LEU:HD12 | 1:B:657:LEU:O     | 1.91                     | 0.71              |
| 1:B:67:CYS:O     | 1:B:70:CYS:HB3    | 1.91                     | 0.71              |
| 1:B:827:THR:HG22 | 1:B:828:ALA:N     | 2.06                     | 0.71              |
| 2:C:69:LEU:HB3   | 2:C:429:PHE:CE1   | 2.25                     | 0.71              |
| 5:F:16:PHE:CE2   | 5:F:20:LYS:HE2    | 2.24                     | 0.71              |
| 7:H:15:PRO:HA    | 7:H:18:PHE:CE1    | 2.26                     | 0.71              |
| 2:C:1187:ASN:O   | 2:C:1188:LYS:HB2  | 1.90                     | 0.70              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:H:80:LYS:N     | 7:H:80:LYS:HD3    | 2.06                     | 0.70              |
| 1:B:567:LYS:HB3  | 8:I:96:VAL:N      | 2.05                     | 0.70              |
| 1:B:1261:LYS:HA  | 1:B:1264:GLU:HB3  | 1.73                     | 0.70              |
| 1:B:483:ASP:HB2  | 2:C:987:LYS:HG3   | 1.73                     | 0.70              |
| 1:B:49:LYS:HZ1   | 1:B:61:ILE:H      | 1.39                     | 0.70              |
| 1:B:710:LEU:HD13 | 9:J:94:ASP:O      | 1.90                     | 0.70              |
| 2:C:168:GLY:N    | 2:C:450:ALA:HB1   | 2.04                     | 0.70              |
| 7:H:7:LEU:HB2    | 7:H:74:TYR:CE2    | 2.24                     | 0.70              |
| 1:B:496:GLU:HG2  | 6:G:99:LEU:HD22   | 1.73                     | 0.70              |
| 1:B:53:LEU:HD22  | 1:B:54:ASN:ND2    | 2.06                     | 0.70              |
| 1:B:92:HIS:O     | 1:B:94:GLY:N      | 2.24                     | 0.70              |
| 2:C:276:ILE:HG22 | 2:C:278:GLN:O     | 1.90                     | 0.70              |
| 3:D:194:GLU:O    | 3:D:195:GLN:HG3   | 1.91                     | 0.70              |
| 2:C:955:THR:CG2  | 2:C:956:THR:N     | 2.54                     | 0.70              |
| 3:D:179:GLU:HG2  | 3:D:180:TYR:N     | 2.07                     | 0.70              |
| 4:E:71:LYS:HG2   | 4:E:74:GLN:NE2    | 2.06                     | 0.70              |
| 8:I:102:TYR:OH   | 8:I:122:LEU:HD22  | 1.91                     | 0.70              |
| 8:I:81:PRO:CB    | 8:I:82:PRO:HD2    | 2.21                     | 0.70              |
| 2:C:190:TYR:CE2  | 10:K:62:ARG:HB3   | 2.26                     | 0.70              |
| 1:B:49:LYS:HZ1   | 1:B:61:ILE:N      | 1.89                     | 0.70              |
| 1:B:728:LYS:O    | 1:B:732:LEU:HG    | 1.91                     | 0.70              |
| 3:D:244:VAL:O    | 3:D:248:ILE:HG13  | 1.90                     | 0.70              |
| 2:C:190:TYR:CD2  | 10:K:62:ARG:HB3   | 2.26                     | 0.70              |
| 15:T:21:DA:H2'   | 15:T:22:DT:C5'    | 2.21                     | 0.70              |
| 1:B:87:ALA:HB3   | 1:B:276:LEU:HD23  | 1.73                     | 0.70              |
| 2:C:102:VAL:HG13 | 2:C:958:GLN:HE21  | 1.56                     | 0.70              |
| 2:C:90:ILE:HD12  | 2:C:432:MET:SD    | 2.32                     | 0.70              |
| 3:D:74:SER:HB3   | 3:D:77:ILE:HG12   | 1.74                     | 0.70              |
| 6:G:111:LEU:H    | 6:G:111:LEU:CD1   | 2.03                     | 0.70              |
| 2:C:313:MET:HE3  | 2:C:386:LEU:HD22  | 1.74                     | 0.70              |
| 2:C:542:MET:CE   | 2:C:743:ILE:HG13  | 2.22                     | 0.70              |
| 9:J:111:THR:HG22 | 9:J:112:SER:N     | 2.06                     | 0.70              |
| 1:B:340:LEU:HD13 | 1:B:1429:ILE:CG2  | 2.20                     | 0.70              |
| 2:C:847:ASP:C    | 2:C:849:GLY:H     | 1.94                     | 0.70              |
| 1:B:351:THR:HB   | 2:C:1103:ILE:HD12 | 1.74                     | 0.70              |
| 1:B:53:LEU:CD2   | 1:B:54:ASN:H      | 2.00                     | 0.70              |
| 1:B:567:LYS:HG3  | 1:B:568:PRO:HD2   | 1.73                     | 0.70              |
| 1:B:886:ILE:HG23 | 1:B:887:GLY:N     | 2.06                     | 0.70              |
| 1:B:886:ILE:HD12 | 1:B:943:LEU:HB3   | 1.72                     | 0.70              |
| 8:I:100:THR:OG1  | 8:I:138:GLU:HG3   | 1.90                     | 0.70              |
| 1:B:105:CYS:O    | 1:B:114:LEU:HG    | 1.92                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1445:ILE:CD1  | 1:B:1445:ILE:H    | 2.00                     | 0.70              |
| 1:B:416:ARG:C     | 1:B:417:TYR:HD2   | 1.95                     | 0.70              |
| 1:B:1208:THR:HG22 | 1:B:1210:GLY:N    | 2.04                     | 0.69              |
| 1:B:382:PRO:HB3   | 1:B:428:TYR:CE2   | 2.26                     | 0.69              |
| 1:B:567:LYS:HD3   | 8:I:95:TYR:CD2    | 2.27                     | 0.69              |
| 1:B:600:PRO:HG2   | 1:B:601:LYS:H     | 1.56                     | 0.69              |
| 1:B:1063:MET:CG   | 1:B:1436:ILE:HG23 | 2.22                     | 0.69              |
| 1:B:915:SER:O     | 1:B:919:ILE:HG13  | 1.91                     | 0.69              |
| 1:B:881:GLN:HE22  | 1:B:960:ILE:H     | 1.39                     | 0.69              |
| 2:C:1122:ARG:HB3  | 15:T:22:DT:OP1    | 1.91                     | 0.69              |
| 2:C:654:ARG:H     | 2:C:657:HIS:CD2   | 2.08                     | 0.69              |
| 3:D:184:ASN:HD21  | 3:D:187:LYS:HA    | 1.56                     | 0.69              |
| 3:D:209:TYR:H     | 3:D:209:TYR:HD1   | 1.40                     | 0.69              |
| 3:D:56:THR:HG22   | 3:D:58:LEU:HD23   | 1.73                     | 0.69              |
| 11:L:45:LEU:HG    | 11:L:94:ILE:HD13  | 1.73                     | 0.69              |
| 1:B:1436:ILE:HD13 | 2:C:1139:ILE:HG23 | 1.73                     | 0.69              |
| 1:B:382:PRO:HB3   | 1:B:428:TYR:HE2   | 1.57                     | 0.69              |
| 1:B:91:PHE:H      | 1:B:297:GLN:HE22  | 1.40                     | 0.69              |
| 2:C:1085:ILE:HD12 | 2:C:1085:ILE:H    | 1.57                     | 0.69              |
| 1:B:853:ASP:O     | 1:B:854:ASN:HB2   | 1.91                     | 0.69              |
| 2:C:52:ASN:OD1    | 2:C:177:LYS:HB2   | 1.92                     | 0.69              |
| 7:H:39:THR:HG22   | 7:H:41:LYS:H      | 1.57                     | 0.69              |
| 11:L:29:ASN:O     | 11:L:76:GLN:HG3   | 1.92                     | 0.69              |
| 5:F:135:PHE:HD2   | 5:F:140:LEU:HD21  | 1.56                     | 0.69              |
| 1:B:49:LYS:NZ     | 1:B:61:ILE:HG13   | 2.07                     | 0.69              |
| 2:C:1007:VAL:CG2  | 2:C:1008:PRO:HD2  | 2.22                     | 0.69              |
| 2:C:378:LEU:O     | 2:C:382:ILE:HG13  | 1.92                     | 0.69              |
| 2:C:916:THR:O     | 2:C:935:ARG:HG2   | 1.92                     | 0.69              |
| 7:H:145:VAL:HG12  | 7:H:146:LYS:N     | 2.08                     | 0.69              |
| 1:B:1445:ILE:HG12 | 7:H:18:PHE:CE2    | 2.27                     | 0.69              |
| 1:B:535:THR:CG2   | 1:B:616:VAL:HA    | 2.20                     | 0.69              |
| 2:C:728:ARG:NH1   | 2:C:1047:PHE:HB3  | 2.07                     | 0.69              |
| 2:C:210:LYS:HD2   | 2:C:480:SER:OG    | 1.91                     | 0.69              |
| 2:C:910:VAL:HG12  | 2:C:911:ILE:N     | 2.07                     | 0.69              |
| 7:H:59:GLY:HA3    | 7:H:70:PHE:CD2    | 2.28                     | 0.69              |
| 11:L:50:LEU:HD11  | 11:L:75:ILE:HD13  | 1.75                     | 0.69              |
| 12:M:32:ALA:HB3   | 12:M:55:ILE:CD1   | 2.18                     | 0.69              |
| 2:C:800:GLN:HG2   | 10:K:52:THR:HG21  | 1.73                     | 0.69              |
| 1:B:738:LYS:HB2   | 1:B:740:LEU:HG    | 1.74                     | 0.69              |
| 1:B:845:LEU:HB3   | 1:B:848:ILE:HD12  | 1.75                     | 0.69              |
| 2:C:1084:GLN:HE21 | 2:C:1084:GLN:H    | 1.40                     | 0.69              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:F:14:ARG:HH21  | 5:F:141:VAL:HG12  | 1.57                     | 0.69              |
| 5:F:22:MET:CE    | 5:F:26:ARG:HE     | 2.06                     | 0.69              |
| 6:G:109:VAL:HG12 | 6:G:110:ASP:H     | 1.57                     | 0.69              |
| 7:H:61:ILE:HG23  | 7:H:66:GLY:O      | 1.93                     | 0.69              |
| 8:I:40:LEU:HD22  | 8:I:123:MET:HE3   | 1.74                     | 0.69              |
| 11:L:58:PHE:HE2  | 11:L:74:ARG:HE    | 1.39                     | 0.69              |
| 2:C:100:PRO:HG3  | 2:C:172:ILE:HD12  | 1.74                     | 0.69              |
| 2:C:906:SER:O    | 2:C:941:LEU:HD23  | 1.93                     | 0.69              |
| 3:D:163:ILE:HD13 | 3:D:163:ILE:H     | 1.55                     | 0.69              |
| 1:B:567:LYS:HB3  | 8:I:95:TYR:HA     | 1.74                     | 0.69              |
| 13:N:2:DA:H2''   | 13:N:3:DG:O5'     | 1.93                     | 0.69              |
| 1:B:1063:MET:SD  | 1:B:1436:ILE:HG23 | 2.33                     | 0.69              |
| 1:B:182:VAL:HG22 | 1:B:201:VAL:HA    | 1.74                     | 0.69              |
| 15:T:25:DC:H42   | 15:T:26:DA:H62    | 1.24                     | 0.69              |
| 1:B:469:ARG:HH11 | 1:B:469:ARG:HB3   | 1.57                     | 0.68              |
| 1:B:844:ALA:O    | 1:B:845:LEU:HD23  | 1.92                     | 0.68              |
| 3:D:241:ASP:O    | 3:D:245:VAL:HG23  | 1.93                     | 0.68              |
| 3:D:69:LEU:HD12  | 3:D:69:LEU:N      | 2.08                     | 0.68              |
| 1:B:86:LEU:HG    | 1:B:237:THR:O     | 1.93                     | 0.68              |
| 1:B:768:GLN:CG   | 1:B:816:HIS:HA    | 2.22                     | 0.68              |
| 2:C:361:LEU:HD21 | 2:C:377:PHE:CD2   | 2.28                     | 0.68              |
| 8:I:24:CYS:HB2   | 8:I:44:VAL:HG21   | 1.75                     | 0.68              |
| 8:I:42:ILE:HG23  | 8:I:95:TYR:CE1    | 2.28                     | 0.68              |
| 1:B:683:ILE:HG21 | 1:B:801:GLU:HG3   | 1.74                     | 0.68              |
| 2:C:174:LEU:HD22 | 2:C:202:TYR:CE1   | 2.29                     | 0.68              |
| 2:C:295:GLY:N    | 2:C:298:LEU:HD23  | 2.09                     | 0.68              |
| 2:C:461:LEU:N    | 2:C:461:LEU:HD12  | 2.08                     | 0.68              |
| 2:C:57:TYR:HD1   | 2:C:57:TYR:N      | 1.92                     | 0.68              |
| 1:B:244:PRO:O    | 1:B:246:VAL:N     | 2.27                     | 0.68              |
| 2:C:539:LEU:H    | 2:C:539:LEU:HD12  | 1.59                     | 0.68              |
| 15:T:21:DA:C2'   | 15:T:22:DT:O5'    | 2.41                     | 0.68              |
| 1:B:637:LYS:HB3  | 1:B:641:VAL:HG11  | 1.75                     | 0.68              |
| 2:C:189:LEU:HD12 | 2:C:196:PRO:HA    | 1.74                     | 0.68              |
| 6:G:111:LEU:HD12 | 6:G:111:LEU:N     | 2.06                     | 0.68              |
| 6:G:82:THR:HG22  | 6:G:84:TYR:N      | 2.08                     | 0.68              |
| 1:B:19:PHE:O     | 1:B:1416:ALA:HA   | 1.94                     | 0.68              |
| 2:C:1095:LEU:H   | 2:C:1095:LEU:HD12 | 1.59                     | 0.68              |
| 1:B:351:THR:HB   | 2:C:1103:ILE:CD1  | 2.24                     | 0.68              |
| 2:C:53:GLN:HG2   | 2:C:547:VAL:CG2   | 2.24                     | 0.68              |
| 2:C:569:TYR:CE1  | 2:C:589:VAL:HG21  | 2.29                     | 0.68              |
| 2:C:570:VAL:HB   | 2:C:573:GLN:HB3   | 1.74                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:579:ARG:HG2   | 2:C:579:ARG:HH11  | 1.58                     | 0.68              |
| 2:C:798:TYR:CE2   | 3:D:62:PHE:CE2    | 2.81                     | 0.68              |
| 5:F:213:ILE:HG12  | 5:F:214:CYS:N     | 2.09                     | 0.68              |
| 1:B:215:SER:HB3   | 1:B:218:ASP:OD2   | 1.94                     | 0.68              |
| 1:B:34:LYS:HG2    | 1:B:36:ARG:NH2    | 2.09                     | 0.68              |
| 1:B:92:HIS:HB3    | 1:B:95:PHE:HB2    | 1.76                     | 0.68              |
| 2:C:243:ALA:CB    | 2:C:251:ILE:HG12  | 2.24                     | 0.68              |
| 2:C:25:ILE:HD12   | 2:C:651:LEU:HD13  | 1.76                     | 0.68              |
| 2:C:651:LEU:HD11  | 2:C:707:PRO:CB    | 2.24                     | 0.68              |
| 5:F:114:ASN:O     | 5:F:115:ASN:HB3   | 1.94                     | 0.68              |
| 12:M:38:LEU:O     | 12:M:39:SER:HB3   | 1.93                     | 0.68              |
| 2:C:361:LEU:HD21  | 2:C:377:PHE:HD2   | 1.58                     | 0.68              |
| 3:D:18:VAL:HG23   | 3:D:240:VAL:HB    | 1.76                     | 0.68              |
| 1:B:1127:ASP:CG   | 1:B:1130:GLN:HB2  | 2.14                     | 0.68              |
| 2:C:1180:PHE:HB3  | 2:C:1191:ILE:HD12 | 1.75                     | 0.68              |
| 2:C:405:ARG:NE    | 2:C:632:ARG:HG3   | 2.09                     | 0.68              |
| 2:C:955:THR:HG22  | 2:C:956:THR:N     | 2.08                     | 0.68              |
| 1:B:1341:ILE:CG2  | 1:B:1342:GLU:H    | 2.06                     | 0.67              |
| 2:C:380:TYR:O     | 2:C:384:ARG:HG2   | 1.95                     | 0.67              |
| 2:C:398:ARG:HH11  | 2:C:398:ARG:HG3   | 1.59                     | 0.67              |
| 2:C:589:VAL:HG12  | 2:C:590:HIS:N     | 2.09                     | 0.67              |
| 3:D:142:VAL:H     | 10:K:16:ASP:HB3   | 1.58                     | 0.67              |
| 3:D:144:ILE:HG22  | 3:D:145:CYS:N     | 2.09                     | 0.67              |
| 2:C:619:ILE:HD12  | 9:J:65:ASP:HB2    | 1.76                     | 0.67              |
| 1:B:1198:ASP:HB3  | 1:B:1201:ALA:HB3  | 1.74                     | 0.67              |
| 1:B:1263:ILE:O    | 1:B:1267:MET:HG3  | 1.94                     | 0.67              |
| 1:B:1373:ASP:O    | 1:B:1376:THR:HG22 | 1.94                     | 0.67              |
| 1:B:93:VAL:HG22   | 1:B:301:ALA:HA    | 1.76                     | 0.67              |
| 1:B:973:ILE:CD1   | 1:B:1038:THR:HG23 | 2.24                     | 0.67              |
| 7:H:9:LEU:HD12    | 7:H:10:ASN:N      | 2.10                     | 0.67              |
| 1:B:446:ARG:HB2   | 1:B:487:MET:SD    | 2.34                     | 0.67              |
| 2:C:622:LYS:HE2   | 9:J:59:VAL:CG2    | 2.13                     | 0.67              |
| 8:I:89:LEU:HB3    | 8:I:91:ASP:OD1    | 1.94                     | 0.67              |
| 10:K:44:TYR:N     | 10:K:44:TYR:HD2   | 1.93                     | 0.67              |
| 1:B:1152:ILE:HG23 | 1:B:1193:LEU:HD13 | 1.76                     | 0.67              |
| 1:B:34:LYS:H      | 1:B:34:LYS:HD3    | 1.59                     | 0.67              |
| 1:B:444:PHE:HB3   | 1:B:458:HIS:CD2   | 2.29                     | 0.67              |
| 2:C:255:GLN:O     | 2:C:271:ALA:HB1   | 1.93                     | 0.67              |
| 1:B:973:ILE:HG21  | 1:B:1036:ARG:O    | 1.95                     | 0.67              |
| 1:B:821:ARG:HD2   | 1:B:825:ILE:HD11  | 1.77                     | 0.67              |
| 2:C:291:ILE:HD11  | 2:C:375:ALA:HB1   | 1.76                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:E:12:ARG:HH22   | 4:E:14:ARG:CG     | 2.02                     | 0.67              |
| 5:F:13:TRP:O      | 5:F:16:PHE:HB3    | 1.95                     | 0.67              |
| 2:C:777:ALA:HA    | 2:C:1095:LEU:HA   | 1.75                     | 0.67              |
| 3:D:34:ARG:HA     | 3:D:37:MET:HE2    | 1.76                     | 0.67              |
| 5:F:182:ASP:HB3   | 5:F:185:ALA:HB2   | 1.75                     | 0.67              |
| 1:B:1227:ILE:HG22 | 1:B:1228:TRP:N    | 2.09                     | 0.67              |
| 1:B:519:PRO:HD3   | 1:B:631:HIS:HD1   | 1.60                     | 0.67              |
| 2:C:185:THR:H     | 2:C:188:ASP:HB2   | 1.60                     | 0.67              |
| 3:D:17:ASN:N      | 3:D:240:VAL:HG11  | 2.10                     | 0.67              |
| 5:F:161:LYS:HD2   | 5:F:195:VAL:HG23  | 1.76                     | 0.67              |
| 5:F:22:MET:HE3    | 5:F:26:ARG:HH21   | 1.58                     | 0.67              |
| 1:B:577:ILE:O     | 1:B:580:VAL:HG23  | 1.94                     | 0.67              |
| 1:B:341:MET:HE2   | 1:B:843:LYS:HZ1   | 1.58                     | 0.67              |
| 2:C:1099:VAL:HG22 | 2:C:1103:ILE:HD13 | 1.74                     | 0.67              |
| 3:D:5:GLY:O       | 3:D:7:GLN:HG3     | 1.95                     | 0.67              |
| 1:B:1211:GLN:O    | 1:B:1214:GLU:HB2  | 1.95                     | 0.67              |
| 1:B:61:ILE:HG22   | 1:B:62:ASP:H      | 1.58                     | 0.67              |
| 2:C:1099:VAL:CG1  | 2:C:1100:ASP:N    | 2.58                     | 0.67              |
| 4:E:153:ARG:HB3   | 4:E:154:PHE:CE1   | 2.30                     | 0.67              |
| 4:E:47:LEU:HD13   | 4:E:48:ILE:N      | 2.10                     | 0.67              |
| 7:H:96:GLN:HG3    | 7:H:97:HIS:CD2    | 2.30                     | 0.67              |
| 2:C:842:ASN:O     | 2:C:846:ILE:HG13  | 1.95                     | 0.67              |
| 5:F:191:LYS:O     | 5:F:193:GLY:N     | 2.27                     | 0.67              |
| 7:H:145:VAL:HG12  | 7:H:146:LYS:H     | 1.60                     | 0.67              |
| 8:I:63:LEU:C      | 8:I:90:ALA:HB3    | 2.16                     | 0.67              |
| 2:C:911:ILE:HD11  | 2:C:941:LEU:HD13  | 1.76                     | 0.66              |
| 3:D:46:ILE:HD12   | 3:D:67:LEU:HB3    | 1.77                     | 0.66              |
| 7:H:111:THR:HG22  | 7:H:113:HIS:H     | 1.59                     | 0.66              |
| 1:B:567:LYS:CD    | 8:I:95:TYR:HA     | 2.25                     | 0.66              |
| 1:B:590:ARG:O     | 1:B:591:PHE:HB2   | 1.93                     | 0.66              |
| 1:B:794:PRO:HG2   | 1:B:795:GLU:OE2   | 1.95                     | 0.66              |
| 5:F:15:ALA:HA     | 5:F:140:LEU:O     | 1.95                     | 0.66              |
| 7:H:51:TYR:O      | 7:H:54:ILE:HG13   | 1.96                     | 0.66              |
| 10:K:36:LEU:HB2   | 10:K:47:ARG:HH12  | 1.59                     | 0.66              |
| 1:B:29:ALA:HB1    | 2:C:1184:GLY:HA3  | 1.77                     | 0.66              |
| 2:C:101:MET:HB3   | 2:C:109:THR:HG22  | 1.76                     | 0.66              |
| 2:C:794:ASN:C     | 2:C:795:ILE:HD12  | 2.15                     | 0.66              |
| 1:B:1325:THR:O    | 5:F:148:GLU:HB2   | 1.95                     | 0.66              |
| 1:B:1445:ILE:N    | 1:B:1445:ILE:HD12 | 2.02                     | 0.66              |
| 1:B:399:HIS:CB    | 1:B:400:PRO:HD3   | 2.24                     | 0.66              |
| 2:C:687:GLU:O     | 2:C:689:LEU:HG    | 1.96                     | 0.66              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:746:SER:HB2  | 2:C:1046:PRO:HG2  | 1.76                     | 0.66              |
| 4:E:170:THR:CB   | 4:E:172:LEU:HG    | 2.22                     | 0.66              |
| 8:I:27:GLU:HG2   | 8:I:39:THR:HG23   | 1.77                     | 0.66              |
| 1:B:765:VAL:HG12 | 1:B:766:GLY:N     | 2.09                     | 0.66              |
| 1:B:903:ASN:HD22 | 1:B:904:THR:H     | 1.41                     | 0.66              |
| 2:C:826:ALA:HB2  | 2:C:1008:PRO:HB3  | 1.77                     | 0.66              |
| 3:D:176:ILE:HG22 | 3:D:177:GLU:N     | 2.09                     | 0.66              |
| 8:I:15:VAL:HG22  | 8:I:26:ILE:CD1    | 2.26                     | 0.66              |
| 1:B:285:PRO:HG2  | 1:B:288:ALA:HB3   | 1.77                     | 0.66              |
| 1:B:56:PRO:O     | 1:B:57:ARG:HD2    | 1.96                     | 0.66              |
| 2:C:243:ALA:HB2  | 2:C:251:ILE:HG12  | 1.78                     | 0.66              |
| 8:I:89:LEU:O     | 8:I:91:ASP:N      | 2.26                     | 0.66              |
| 9:J:7:CYS:HB3    | 9:J:14:LEU:HD21   | 1.77                     | 0.66              |
| 15:T:14:DC:H2"   | 15:T:15:DT:H71    | 1.77                     | 0.66              |
| 1:B:418:SER:O    | 1:B:420:ARG:N     | 2.28                     | 0.66              |
| 1:B:406:ILE:HG13 | 1:B:431:LYS:HB3   | 1.78                     | 0.66              |
| 9:J:80:SER:HB2   | 9:J:103:CYS:SG    | 2.36                     | 0.66              |
| 1:B:852:TYR:CD2  | 1:B:1060:PRO:HB2  | 2.31                     | 0.66              |
| 1:B:690:VAL:HG11 | 1:B:794:PRO:HD3   | 1.78                     | 0.66              |
| 1:B:899:VAL:CG1  | 1:B:908:LEU:HD21  | 2.24                     | 0.66              |
| 2:C:1016:ALA:O   | 2:C:1020:ARG:HG3  | 1.96                     | 0.66              |
| 2:C:792:MET:CE   | 2:C:857:ARG:HH12  | 2.08                     | 0.66              |
| 6:G:97:ARG:O     | 6:G:101:ILE:HG13  | 1.96                     | 0.66              |
| 8:I:98:TYR:HE1   | 8:I:139:ASN:HA    | 1.61                     | 0.66              |
| 1:B:1242:VAL:O   | 1:B:1243:VAL:HB   | 1.96                     | 0.66              |
| 1:B:382:PRO:HD3  | 1:B:428:TYR:CD2   | 2.30                     | 0.66              |
| 1:B:606:LEU:HB3  | 1:B:614:PHE:CE2   | 2.31                     | 0.66              |
| 1:B:70:CYS:O     | 1:B:72:GLU:HG2    | 1.96                     | 0.66              |
| 2:C:1202:LEU:O   | 2:C:1206:GLU:HG3  | 1.95                     | 0.66              |
| 2:C:278:GLN:HG2  | 2:C:279:ASP:N     | 2.05                     | 0.66              |
| 2:C:850:LEU:HD12 | 2:C:851:PHE:N     | 2.11                     | 0.66              |
| 6:G:73:ALA:HA    | 6:G:143:PHE:CE1   | 2.30                     | 0.66              |
| 12:M:40:LEU:HD22 | 12:M:44:ASP:CG    | 2.17                     | 0.66              |
| 12:M:32:ALA:H    | 12:M:55:ILE:HG13  | 1.60                     | 0.66              |
| 1:B:332:LYS:HA   | 1:B:337:ARG:HD2   | 1.78                     | 0.66              |
| 1:B:50:ILE:C     | 1:B:52:GLY:H      | 2.00                     | 0.66              |
| 2:C:1180:PHE:HB3 | 2:C:1191:ILE:HD13 | 1.77                     | 0.66              |
| 2:C:20:ASP:O     | 2:C:22:SER:N      | 2.28                     | 0.66              |
| 3:D:147:LEU:HD23 | 3:D:147:LEU:N     | 2.09                     | 0.66              |
| 4:E:53:SER:H     | 4:E:148:LEU:CD2   | 2.09                     | 0.66              |
| 7:H:117:GLN:C    | 7:H:119:LEU:H     | 1.98                     | 0.66              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:E:40:HIS:CB     | 7:H:73:LYS:NZ    | 2.58                     | 0.66              |
| 8:I:40:LEU:HD13   | 8:I:123:MET:HB2  | 1.78                     | 0.66              |
| 1:B:567:LYS:HD3   | 8:I:95:TYR:HA    | 1.78                     | 0.66              |
| 1:B:441:PRO:HG3   | 1:B:498:ARG:HB2  | 1.77                     | 0.65              |
| 2:C:327:ARG:O     | 2:C:331:LEU:HD13 | 1.95                     | 0.65              |
| 2:C:63:ILE:O      | 2:C:67:SER:HB3   | 1.97                     | 0.65              |
| 2:C:990:ILE:HG22  | 2:C:991:GLY:N    | 2.10                     | 0.65              |
| 1:B:239:LEU:HD12  | 1:B:240:PRO:HD2  | 1.77                     | 0.65              |
| 2:C:1079:LYS:HG2  | 2:C:1080:LYS:H   | 1.61                     | 0.65              |
| 3:D:179:GLU:HG2   | 3:D:180:TYR:H    | 1.61                     | 0.65              |
| 3:D:253:LYS:O     | 3:D:256:ALA:HB3  | 1.96                     | 0.65              |
| 1:B:869:GLY:O     | 5:F:204:THR:HG21 | 1.96                     | 0.65              |
| 1:B:714:PHE:O     | 1:B:718:VAL:HG23 | 1.97                     | 0.65              |
| 1:B:870:GLU:HG2   | 5:F:208:TYR:CG   | 2.31                     | 0.65              |
| 5:F:61:GLN:HB2    | 5:F:79:TRP:HE3   | 1.61                     | 0.65              |
| 1:B:308:ILE:HG22  | 1:B:309:ALA:H    | 1.60                     | 0.65              |
| 1:B:443:LEU:CD2   | 1:B:455:MET:HB3  | 2.20                     | 0.65              |
| 1:B:590:ARG:HB2   | 1:B:590:ARG:HH11 | 1.61                     | 0.65              |
| 1:B:920:LEU:HD23  | 1:B:921:GLY:N    | 2.10                     | 0.65              |
| 3:D:165:LYS:O     | 11:L:6:ARG:NH1   | 2.30                     | 0.65              |
| 3:D:242:GLN:C     | 3:D:244:VAL:H    | 1.99                     | 0.65              |
| 2:C:1001:PHE:CD2  | 3:D:34:ARG:NH2   | 2.65                     | 0.65              |
| 11:L:55:LYS:HD2   | 11:L:81:TYR:CD1  | 2.32                     | 0.65              |
| 1:B:919:ILE:HG21  | 1:B:983:ILE:HD11 | 1.78                     | 0.65              |
| 1:B:298:PHE:CZ    | 1:B:314:ALA:HB2  | 2.32                     | 0.65              |
| 1:B:298:PHE:HZ    | 1:B:314:ALA:HB2  | 1.61                     | 0.65              |
| 1:B:310:GLY:O     | 1:B:312:PRO:HD2  | 1.97                     | 0.65              |
| 1:B:90:VAL:HG11   | 1:B:297:GLN:HA   | 1.79                     | 0.65              |
| 2:C:1160:VAL:HG11 | 2:C:1169:MET:SD  | 2.36                     | 0.65              |
| 2:C:217:ARG:NE    | 2:C:405:ARG:HB2  | 2.10                     | 0.65              |
| 2:C:563:MET:HE1   | 2:C:580:VAL:HB   | 1.77                     | 0.65              |
| 3:D:251:LEU:O     | 3:D:251:LEU:HD12 | 1.95                     | 0.65              |
| 7:H:65:ASP:O      | 7:H:67:SER:N     | 2.29                     | 0.65              |
| 10:K:2:ILE:HG22   | 10:K:3:VAL:O     | 1.96                     | 0.65              |
| 3:D:184:ASN:ND2   | 3:D:187:LYS:HA   | 2.12                     | 0.65              |
| 3:D:43:THR:HG22   | 3:D:44:LEU:N     | 2.12                     | 0.65              |
| 6:G:135:ARG:HG2   | 6:G:137:TYR:CE1  | 2.31                     | 0.65              |
| 1:B:1450:LEU:O    | 1:B:1450:LEU:HG  | 1.96                     | 0.65              |
| 1:B:709:THR:HG22  | 1:B:711:ARG:N    | 2.12                     | 0.65              |
| 2:C:1002:THR:O    | 2:C:1004:GLU:N   | 2.29                     | 0.65              |
| 2:C:1079:LYS:HA   | 3:D:27:LEU:HD21  | 1.79                     | 0.65              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:314:LEU:HD12 | 2:C:314:LEU:H     | 1.61                     | 0.65              |
| 7:H:115:MET:HB3  | 7:H:163:ILE:HD11  | 1.78                     | 0.65              |
| 8:I:139:ASN:O    | 8:I:140:ALA:HB2   | 1.97                     | 0.65              |
| 10:K:5:VAL:HG12  | 10:K:6:ARG:HG3    | 1.77                     | 0.65              |
| 1:B:34:LYS:HG2   | 1:B:36:ARG:HH21   | 1.60                     | 0.65              |
| 1:B:560:ILE:HG13 | 8:I:78:SER:HB2    | 1.78                     | 0.65              |
| 1:B:49:LYS:HE2   | 1:B:61:ILE:HD12   | 1.77                     | 0.65              |
| 2:C:1084:GLN:N   | 2:C:1084:GLN:NE2  | 2.44                     | 0.65              |
| 2:C:1096:ARG:O   | 2:C:1097:HIS:HB2  | 1.97                     | 0.65              |
| 3:D:214:ASN:HB3  | 3:D:217:ASP:OD2   | 1.96                     | 0.65              |
| 8:I:43:ASN:ND2   | 8:I:46:LEU:HD12   | 2.11                     | 0.65              |
| 1:B:1050:GLU:HG2 | 1:B:1051:ALA:N    | 2.12                     | 0.65              |
| 1:B:1411:GLU:HA  | 1:B:1414:ALA:HB3  | 1.78                     | 0.65              |
| 2:C:770:GLN:HG2  | 2:C:983:ARG:O     | 1.97                     | 0.65              |
| 2:C:918:ILE:HD12 | 2:C:935:ARG:NH1   | 2.12                     | 0.65              |
| 2:C:953:LEU:O    | 2:C:953:LEU:HD23  | 1.97                     | 0.65              |
| 1:B:353:ILE:HG21 | 1:B:487:MET:HG3   | 1.78                     | 0.64              |
| 1:B:541:ILE:HD13 | 1:B:549:MET:HE3   | 1.78                     | 0.64              |
| 5:F:17:ARG:O     | 5:F:21:GLU:HG3    | 1.96                     | 0.64              |
| 9:J:26:LEU:HD23  | 9:J:37:GLU:HA     | 1.78                     | 0.64              |
| 1:B:591:PHE:HA   | 1:B:595:THR:HG21  | 1.80                     | 0.64              |
| 2:C:1166:CYS:HB2 | 2:C:1215:ARG:NH1  | 2.12                     | 0.64              |
| 2:C:301:ILE:HG21 | 2:C:314:LEU:HD21  | 1.79                     | 0.64              |
| 2:C:651:LEU:HD11 | 2:C:707:PRO:HB2   | 1.79                     | 0.64              |
| 1:B:305:ASP:OD1  | 1:B:326:ARG:HD2   | 1.98                     | 0.64              |
| 1:B:694:THR:O    | 1:B:698:GLN:HG3   | 1.96                     | 0.64              |
| 1:B:659:HIS:HA   | 2:C:1074:ASN:ND2  | 2.13                     | 0.64              |
| 2:C:210:LYS:HE2  | 2:C:462:ALA:CA    | 2.26                     | 0.64              |
| 2:C:574:SER:HB3  | 2:C:577:ALA:HB2   | 1.79                     | 0.64              |
| 5:F:67:GLU:O     | 5:F:70:SER:HB3    | 1.96                     | 0.64              |
| 7:H:35:GLU:OE2   | 7:H:48:VAL:HG23   | 1.96                     | 0.64              |
| 11:L:57:LEU:HD12 | 11:L:77:THR:O     | 1.97                     | 0.64              |
| 1:B:1289:ARG:HD2 | 1:B:1303:GLU:OE2  | 1.97                     | 0.64              |
| 2:C:496:ARG:O    | 2:C:539:LEU:HD12  | 1.97                     | 0.64              |
| 2:C:880:THR:HG21 | 2:C:934:LYS:HE3   | 1.80                     | 0.64              |
| 1:B:504:LEU:HD11 | 6:G:91:ALA:HB1    | 1.78                     | 0.64              |
| 7:H:110:VAL:HG22 | 7:H:161:GLY:O     | 1.96                     | 0.64              |
| 1:B:1348:LEU:HG  | 1:B:1372:VAL:CG2  | 2.27                     | 0.64              |
| 1:B:320:ARG:NH2  | 14:P:3:C:H1'      | 2.12                     | 0.64              |
| 1:B:343:LYS:NZ   | 2:C:1151:LEU:HB3  | 2.12                     | 0.64              |
| 1:B:896:ARG:NH2  | 1:B:1030:ARG:HH21 | 1.96                     | 0.64              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:960:ILE:O    | 1:B:963:ILE:HG22  | 1.98                     | 0.64              |
| 2:C:57:TYR:CD1   | 2:C:57:TYR:N      | 2.63                     | 0.64              |
| 2:C:953:LEU:CD2  | 2:C:965:LYS:HB2   | 2.28                     | 0.64              |
| 3:D:61:GLU:HA    | 3:D:64:ALA:HB3    | 1.80                     | 0.64              |
| 4:E:180:LEU:HD23 | 4:E:195:ILE:HD12  | 1.77                     | 0.64              |
| 5:F:2:ASP:O      | 5:F:3:GLN:HG2     | 1.98                     | 0.64              |
| 7:H:43:GLY:HA3   | 7:H:80:LYS:HB3    | 1.78                     | 0.64              |
| 1:B:1121:GLU:HG3 | 1:B:1122:PRO:HD2  | 1.78                     | 0.64              |
| 1:B:427:GLN:HG3  | 1:B:430:TRP:CZ2   | 2.32                     | 0.64              |
| 1:B:961:ARG:HH11 | 1:B:961:ARG:HG3   | 1.62                     | 0.64              |
| 3:D:261:ALA:HA   | 3:D:264:GLN:OE1   | 1.98                     | 0.64              |
| 2:C:801:LYS:O    | 10:K:52:THR:CG2   | 2.45                     | 0.64              |
| 2:C:801:LYS:O    | 10:K:52:THR:HG23  | 1.96                     | 0.64              |
| 1:B:834:THR:HG21 | 1:B:1077:THR:HA   | 1.77                     | 0.64              |
| 2:C:1079:LYS:HG2 | 2:C:1080:LYS:N    | 2.13                     | 0.64              |
| 2:C:825:VAL:HG12 | 2:C:826:ALA:H     | 1.58                     | 0.64              |
| 4:E:131:GLU:O    | 4:E:132:GLN:HG2   | 1.97                     | 0.64              |
| 4:E:204:ASP:O    | 4:E:208:GLU:HB2   | 1.98                     | 0.64              |
| 8:I:95:TYR:HE2   | 8:I:97:MET:CG     | 2.11                     | 0.64              |
| 1:B:444:PHE:HB3  | 1:B:458:HIS:HD2   | 1.63                     | 0.64              |
| 1:B:69:THR:O     | 1:B:71:GLN:N      | 2.30                     | 0.64              |
| 2:C:269:ILE:HG21 | 2:C:282:ILE:HD13  | 1.79                     | 0.64              |
| 5:F:23:VAL:O     | 5:F:28:TYR:HB2    | 1.97                     | 0.64              |
| 10:K:35:ALA:O    | 10:K:39:LEU:HD12  | 1.97                     | 0.64              |
| 12:M:39:SER:O    | 12:M:40:LEU:HG    | 1.98                     | 0.64              |
| 1:B:138:ILE:HG21 | 1:B:222:LEU:HD21  | 1.79                     | 0.64              |
| 1:B:768:GLN:HG2  | 1:B:816:HIS:CA    | 2.26                     | 0.64              |
| 2:C:114:PRO:HG3  | 2:C:181:LEU:HD11  | 1.80                     | 0.64              |
| 3:D:248:ILE:HD13 | 11:L:101:LEU:HD23 | 1.80                     | 0.64              |
| 4:E:164:ILE:HG22 | 4:E:168:LYS:HG3   | 1.78                     | 0.64              |
| 1:B:883:LEU:O    | 1:B:886:ILE:HG22  | 1.97                     | 0.64              |
| 2:C:577:ALA:CB   | 2:C:589:VAL:HG11  | 2.20                     | 0.64              |
| 2:C:652:LYS:HB3  | 2:C:689:LEU:HD23  | 1.80                     | 0.64              |
| 2:C:661:LEU:HD23 | 2:C:679:TYR:O     | 1.97                     | 0.64              |
| 2:C:956:THR:CG2  | 2:C:960:GLY:HA2   | 2.28                     | 0.64              |
| 4:E:146:GLN:O    | 4:E:149:THR:HG22  | 1.97                     | 0.64              |
| 10:K:1:MET:N     | 10:K:56:LEU:N     | 2.45                     | 0.64              |
| 1:B:1119:TYR:HA  | 1:B:1305:VAL:HG13 | 1.79                     | 0.63              |
| 1:B:374:LEU:C    | 1:B:436:ILE:HD11  | 2.17                     | 0.63              |
| 1:B:477:PRO:HG2  | 1:B:521:MET:HG2   | 1.80                     | 0.63              |
| 1:B:853:ASP:OD1  | 1:B:855:THR:N     | 2.31                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:1022:THR:O    | 2:C:1022:THR:HG23 | 1.98                     | 0.63              |
| 2:C:113:TYR:HE2   | 2:C:192:LEU:HD22  | 1.63                     | 0.63              |
| 2:C:355:ILE:O     | 2:C:359:GLU:HB2   | 1.98                     | 0.63              |
| 2:C:797:TYR:HB2   | 2:C:852:ARG:O     | 1.98                     | 0.63              |
| 7:H:106:MET:HG2   | 7:H:107:LYS:H     | 1.60                     | 0.63              |
| 1:B:1225:PHE:CZ   | 1:B:1227:ILE:HD11 | 2.33                     | 0.63              |
| 1:B:184:SER:HB3   | 1:B:199:LEU:CD2   | 2.28                     | 0.63              |
| 1:B:675:THR:O     | 1:B:679:ILE:HG13  | 1.97                     | 0.63              |
| 2:C:780:VAL:HG21  | 10:K:56:LEU:HD11  | 1.79                     | 0.63              |
| 1:B:353:ILE:HD13  | 1:B:487:MET:CE    | 2.29                     | 0.63              |
| 1:B:40:THR:HB     | 1:B:41:MET:HE3    | 1.79                     | 0.63              |
| 1:B:883:LEU:HD11  | 1:B:1017:LEU:HD11 | 1.81                     | 0.63              |
| 2:C:65:GLU:OE2    | 2:C:247:GLY:HA2   | 1.95                     | 0.63              |
| 8:I:99:GLY:HA3    | 8:I:118:PHE:HA    | 1.81                     | 0.63              |
| 1:B:40:THR:HB     | 1:B:41:MET:CE     | 2.27                     | 0.63              |
| 2:C:305:VAL:O     | 2:C:305:VAL:HG12  | 1.98                     | 0.63              |
| 2:C:899:ILE:CD1   | 2:C:911:ILE:HA    | 2.27                     | 0.63              |
| 15:T:11:DT:H2"    | 15:T:12:DA:OP2    | 1.99                     | 0.63              |
| 1:B:1120:LEU:H    | 1:B:1120:LEU:HD13 | 1.64                     | 0.63              |
| 1:B:881:GLN:NE2   | 1:B:958:VAL:O     | 2.32                     | 0.63              |
| 2:C:310:MET:O     | 2:C:313:MET:HB2   | 1.99                     | 0.63              |
| 2:C:461:LEU:H     | 2:C:461:LEU:HD12  | 1.64                     | 0.63              |
| 2:C:865:LYS:HB2   | 2:C:961:LEU:HD21  | 1.81                     | 0.63              |
| 6:G:119:ARG:HG3   | 6:G:119:ARG:NH1   | 2.13                     | 0.63              |
| 6:G:73:ALA:O      | 6:G:74:ILE:HG13   | 1.98                     | 0.63              |
| 7:H:15:PRO:HG3    | 7:H:66:GLY:HA3    | 1.79                     | 0.63              |
| 3:D:8:VAL:HG11    | 11:L:105:PHE:HD1  | 1.63                     | 0.63              |
| 1:B:287:HIS:HA    | 1:B:290:GLU:HG2   | 1.81                     | 0.63              |
| 1:B:372:LYS:HA    | 1:B:435:HIS:ND1   | 2.13                     | 0.63              |
| 1:B:901:LEU:O     | 1:B:921:GLY:N     | 2.31                     | 0.63              |
| 1:B:996:ASN:O     | 1:B:998:LEU:N     | 2.29                     | 0.63              |
| 2:C:431:TYR:CD1   | 2:C:447:ALA:HB2   | 2.34                     | 0.63              |
| 2:C:844:SER:HB3   | 2:C:848:ARG:HH12  | 1.64                     | 0.63              |
| 4:E:27:LEU:HD13   | 4:E:173:HIS:HB2   | 1.81                     | 0.63              |
| 10:K:43:ARG:H     | 10:K:43:ARG:HD3   | 1.63                     | 0.63              |
| 1:B:1022:LEU:HD11 | 1:B:1026:LEU:HD12 | 1.81                     | 0.63              |
| 1:B:1042:PHE:CE2  | 1:B:1046:LEU:HD11 | 2.33                     | 0.63              |
| 1:B:107:CYS:HA    | 1:B:171:GLN:OE1   | 1.98                     | 0.63              |
| 2:C:510:LYS:CG    | 2:C:511:PRO:HD3   | 2.28                     | 0.63              |
| 4:E:173:HIS:O     | 4:E:175:PHE:N     | 2.31                     | 0.63              |
| 5:F:13:TRP:CE3    | 5:F:39:LEU:HD13   | 2.34                     | 0.63              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:H:106:MET:CG   | 7:H:107:LYS:N     | 2.60                     | 0.63              |
| 8:I:95:TYR:CE2   | 8:I:97:MET:HG3    | 2.33                     | 0.63              |
| 1:B:185:TRP:CZ3  | 1:B:200:ARG:HG2   | 2.34                     | 0.63              |
| 1:B:399:HIS:HB3  | 1:B:400:PRO:CD    | 2.27                     | 0.63              |
| 1:B:535:THR:HG21 | 1:B:616:VAL:CA    | 2.24                     | 0.63              |
| 1:B:32:VAL:HG21  | 1:B:68:GLN:HE21   | 1.64                     | 0.63              |
| 1:B:751:SER:O    | 1:B:752:LYS:HB2   | 1.96                     | 0.63              |
| 1:B:899:VAL:HB   | 1:B:929:LEU:HD12  | 1.80                     | 0.63              |
| 2:C:1020:ARG:HB2 | 2:C:1022:THR:HG22 | 1.79                     | 0.63              |
| 2:C:105:SER:O    | 2:C:106:ASP:HB2   | 1.98                     | 0.63              |
| 2:C:113:TYR:CE2  | 2:C:192:LEU:HD22  | 2.34                     | 0.63              |
| 3:D:164:ALA:HA   | 3:D:167:HIS:O     | 1.99                     | 0.63              |
| 1:B:134:ARG:HD2  | 1:B:221:SER:O     | 1.99                     | 0.63              |
| 2:C:515:HIS:H    | 2:C:518:HIS:CD2   | 2.05                     | 0.63              |
| 2:C:842:ASN:ND2  | 2:C:845:SER:OG    | 2.31                     | 0.63              |
| 3:D:18:VAL:CG2   | 3:D:240:VAL:HB    | 2.28                     | 0.63              |
| 3:D:45:ALA:HA    | 3:D:72:LEU:CD1    | 2.28                     | 0.63              |
| 4:E:29:LEU:HD13  | 7:H:82:PHE:CZ     | 2.34                     | 0.63              |
| 1:B:1074:GLU:HB3 | 1:B:1075:PRO:HD3  | 1.81                     | 0.62              |
| 1:B:445:ASN:HB2  | 1:B:454:SER:O     | 1.98                     | 0.62              |
| 2:C:334:ILE:O    | 2:C:334:ILE:HG22  | 1.99                     | 0.62              |
| 2:C:580:VAL:HG22 | 2:C:624:LEU:HB3   | 1.81                     | 0.62              |
| 2:C:821:GLN:NE2  | 2:C:851:PHE:HA    | 2.13                     | 0.62              |
| 3:D:8:VAL:HG21   | 11:L:105:PHE:HA   | 1.80                     | 0.62              |
| 7:H:15:PRO:CG    | 7:H:66:GLY:HA3    | 2.29                     | 0.62              |
| 11:L:21:ILE:HG23 | 11:L:31:VAL:CG1   | 2.28                     | 0.62              |
| 11:L:31:VAL:HG12 | 11:L:32:VAL:N     | 2.14                     | 0.62              |
| 1:B:78:PRO:HA    | 2:C:1201:LYS:NZ   | 2.14                     | 0.62              |
| 1:B:902:LEU:HG   | 1:B:926:GLN:HG3   | 1.81                     | 0.62              |
| 1:B:963:ILE:HD11 | 1:B:1048:ASN:CB   | 2.29                     | 0.62              |
| 2:C:192:LEU:O    | 2:C:193:LYS:HB2   | 1.99                     | 0.62              |
| 2:C:37:PHE:HE2   | 2:C:542:MET:HA    | 1.63                     | 0.62              |
| 2:C:880:THR:HB   | 2:C:934:LYS:HD2   | 1.80                     | 0.62              |
| 1:B:41:MET:H     | 1:B:41:MET:HE3    | 1.64                     | 0.62              |
| 1:B:519:PRO:HD3  | 1:B:631:HIS:ND1   | 2.14                     | 0.62              |
| 2:C:193:LYS:NZ   | 12:M:32:ALA:HB1   | 2.15                     | 0.62              |
| 2:C:365:THR:HG23 | 2:C:367:LEU:H     | 1.65                     | 0.62              |
| 2:C:515:HIS:O    | 2:C:518:HIS:HB2   | 2.00                     | 0.62              |
| 2:C:579:ARG:NH1  | 2:C:579:ARG:HG2   | 2.14                     | 0.62              |
| 2:C:850:LEU:HD12 | 2:C:851:PHE:H     | 1.65                     | 0.62              |
| 9:J:50:THR:CG2   | 9:J:52:ILE:HG23   | 2.27                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:K:44:TYR:N     | 10:K:44:TYR:CD2   | 2.64                     | 0.62              |
| 1:B:252:PHE:O     | 1:B:253:ASN:HB2   | 1.98                     | 0.62              |
| 1:B:513:SER:OG    | 1:B:515:GLN:HG2   | 1.99                     | 0.62              |
| 1:B:684:ALA:O     | 1:B:687:LYS:HB2   | 2.00                     | 0.62              |
| 2:C:314:LEU:O     | 2:C:317:CYS:HB3   | 1.98                     | 0.62              |
| 2:C:810:GLU:CA    | 2:C:815:ARG:HH12  | 2.09                     | 0.62              |
| 2:C:843:GLN:O     | 2:C:846:ILE:N     | 2.32                     | 0.62              |
| 4:E:175:PHE:HZ    | 7:H:85:GLU:HG3    | 1.63                     | 0.62              |
| 1:B:719:VAL:HG12  | 1:B:723:ASN:HD21  | 1.65                     | 0.62              |
| 2:C:839:MET:HG3   | 2:C:1010:LEU:CD1  | 2.22                     | 0.62              |
| 3:D:100:THR:HG22  | 3:D:101:LEU:N     | 2.14                     | 0.62              |
| 3:D:235:VAL:HG12  | 10:K:13:VAL:CG2   | 2.29                     | 0.62              |
| 3:D:31:ASN:OD1    | 3:D:34:ARG:HD3    | 1.98                     | 0.62              |
| 6:G:132:LEU:HD11  | 7:H:61:ILE:CD1    | 2.30                     | 0.62              |
| 6:G:75:PRO:HG2    | 6:G:77:ASP:O      | 1.99                     | 0.62              |
| 9:J:35:VAL:HG12   | 9:J:36:GLU:N      | 2.14                     | 0.62              |
| 1:B:1224:LEU:HD11 | 1:B:1240:CYS:HB2  | 1.82                     | 0.62              |
| 1:B:1441:PHE:CZ   | 6:G:89:GLU:HA     | 2.34                     | 0.62              |
| 3:D:36:VAL:HG21   | 3:D:251:LEU:HB2   | 1.80                     | 0.62              |
| 1:B:1325:THR:HG23 | 5:F:148:GLU:N     | 2.14                     | 0.62              |
| 1:B:1029:ARG:HD2  | 1:B:1033:GLN:NE2  | 2.13                     | 0.62              |
| 1:B:1102:LYS:HG2  | 1:B:1106:ASN:HD21 | 1.64                     | 0.62              |
| 1:B:11:LEU:HD12   | 2:C:1193:GLN:O    | 2.00                     | 0.62              |
| 1:B:1349:TYR:CA   | 1:B:1372:VAL:HG21 | 2.29                     | 0.62              |
| 1:B:2:VAL:HG11    | 2:C:1157:ALA:HB1  | 1.82                     | 0.62              |
| 1:B:35:ILE:O      | 1:B:35:ILE:HG22   | 1.99                     | 0.62              |
| 1:B:35:ILE:O      | 1:B:84:ILE:HG13   | 2.00                     | 0.62              |
| 1:B:341:MET:HE1   | 1:B:843:LYS:NZ    | 2.14                     | 0.62              |
| 1:B:863:VAL:HG11  | 1:B:866:PHE:CE2   | 2.34                     | 0.62              |
| 2:C:526:GLU:HG2   | 2:C:538:ASN:HD22  | 1.64                     | 0.62              |
| 2:C:792:MET:HE1   | 2:C:857:ARG:HH12  | 1.63                     | 0.62              |
| 2:C:859:TYR:OH    | 2:C:941:LEU:HD12  | 1.99                     | 0.62              |
| 7:H:122:ASN:HD22  | 7:H:125:SER:HB3   | 1.64                     | 0.62              |
| 8:I:127:GLY:HA3   | 8:I:130:ARG:HH22  | 1.64                     | 0.62              |
| 9:J:8:ARG:O       | 9:J:9:ASP:HB2     | 2.00                     | 0.62              |
| 1:B:222:LEU:O     | 1:B:224:PHE:N     | 2.33                     | 0.62              |
| 1:B:316:GLN:HB2   | 1:B:322:VAL:HG23  | 1.82                     | 0.62              |
| 2:C:115:GLN:HG2   | 2:C:193:LYS:HB2   | 1.81                     | 0.62              |
| 2:C:220:GLY:O     | 2:C:222:ILE:HG13  | 2.00                     | 0.62              |
| 2:C:604:ARG:NH1   | 2:C:691:GLU:OE2   | 2.33                     | 0.62              |
| 3:D:163:ILE:HD11  | 11:L:10:PHE:CE1   | 2.34                     | 0.62              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:110:CYS:SG   | 1:B:111:GLY:N     | 2.72                     | 0.62              |
| 1:B:1430:LEU:O   | 2:C:1196:ILE:HG22 | 2.00                     | 0.62              |
| 1:B:57:ARG:HH11  | 1:B:57:ARG:HG2    | 1.64                     | 0.62              |
| 1:B:809:THR:HG23 | 1:B:812:GLU:OE1   | 2.00                     | 0.62              |
| 2:C:205:ILE:N    | 2:C:205:ILE:HD12  | 2.14                     | 0.62              |
| 2:C:364:ILE:HG12 | 2:C:585:VAL:HG13  | 1.80                     | 0.62              |
| 4:E:30:GLY:O     | 4:E:32:GLU:N      | 2.33                     | 0.62              |
| 7:H:106:MET:CG   | 7:H:107:LYS:H     | 2.12                     | 0.62              |
| 1:B:148:CYS:O    | 1:B:168:GLY:HA2   | 2.00                     | 0.62              |
| 1:B:55:ASP:N     | 1:B:56:PRO:HD3    | 2.15                     | 0.62              |
| 1:B:67:CYS:C     | 1:B:68:GLN:HG3    | 2.21                     | 0.62              |
| 1:B:2:VAL:CG1    | 2:C:1157:ALA:HB1  | 2.29                     | 0.62              |
| 2:C:1181:GLU:CG  | 2:C:1188:LYS:HE3  | 2.30                     | 0.62              |
| 2:C:467:GLY:N    | 2:C:475:SER:HB3   | 2.15                     | 0.62              |
| 2:C:405:ARG:HE   | 2:C:629:ASP:HB3   | 1.64                     | 0.62              |
| 4:E:7:THR:HG21   | 4:E:32:GLU:OE2    | 2.00                     | 0.62              |
| 5:F:153:HIS:HB3  | 5:F:196:VAL:HG11  | 1.82                     | 0.62              |
| 1:B:1153:TYR:CE1 | 9:J:42:LEU:HD13   | 2.35                     | 0.62              |
| 1:B:54:ASN:C     | 1:B:56:PRO:HD3    | 2.20                     | 0.61              |
| 2:C:36:ALA:HA    | 2:C:39:ARG:HD2    | 1.81                     | 0.61              |
| 3:D:148:ARG:HD3  | 3:D:149:LYS:HG3   | 1.82                     | 0.61              |
| 3:D:147:LEU:HD12 | 3:D:151:GLN:O     | 2.00                     | 0.61              |
| 5:F:15:ALA:O     | 5:F:19:VAL:HG23   | 2.00                     | 0.61              |
| 1:B:1074:GLU:HB3 | 1:B:1075:PRO:CD   | 2.29                     | 0.61              |
| 1:B:265:LYS:HD3  | 1:B:302:THR:HG22  | 1.82                     | 0.61              |
| 1:B:180:LYS:HZ2  | 1:B:294:SER:HB3   | 1.66                     | 0.61              |
| 1:B:38:PRO:HA    | 1:B:270:LEU:HD23  | 1.81                     | 0.61              |
| 1:B:50:ILE:O     | 1:B:52:GLY:N      | 2.33                     | 0.61              |
| 2:C:294:ASP:O    | 2:C:296:GLU:N     | 2.29                     | 0.61              |
| 2:C:309:GLN:HG3  | 9:J:52:ILE:HD13   | 1.82                     | 0.61              |
| 2:C:737:THR:CG2  | 9:J:66:PRO:HA     | 2.29                     | 0.61              |
| 2:C:519:TRP:CH2  | 2:C:748:ILE:HD13  | 2.36                     | 0.61              |
| 2:C:792:MET:H    | 2:C:857:ARG:HA    | 1.64                     | 0.61              |
| 4:E:24:ALA:C     | 4:E:26:THR:H      | 2.04                     | 0.61              |
| 4:E:60:LYS:O     | 4:E:64:VAL:HG23   | 1.99                     | 0.61              |
| 9:J:50:THR:HG23  | 9:J:52:ILE:CG2    | 2.30                     | 0.61              |
| 1:B:1155:ASP:OD2 | 1:B:1161:THR:HA   | 1.99                     | 0.61              |
| 1:B:215:SER:HB3  | 1:B:218:ASP:CB    | 2.30                     | 0.61              |
| 2:C:1072:MET:HB2 | 2:C:1085:ILE:HD13 | 1.82                     | 0.61              |
| 2:C:172:ILE:HD13 | 2:C:178:ASN:HD22  | 1.63                     | 0.61              |
| 2:C:583:ASN:OD1  | 2:C:628:THR:HG22  | 2.00                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:J:62:ILE:O      | 9:J:62:ILE:HG12   | 1.99                     | 0.61              |
| 1:B:885:THR:O     | 1:B:885:THR:HG22  | 1.99                     | 0.61              |
| 1:B:899:VAL:HG13  | 1:B:908:LEU:CD2   | 2.30                     | 0.61              |
| 2:C:1169:MET:CE   | 2:C:1201:LYS:HA   | 2.30                     | 0.61              |
| 3:D:31:ASN:O      | 3:D:34:ARG:HB3    | 2.00                     | 0.61              |
| 7:H:7:LEU:HD12    | 7:H:74:TYR:HH     | 1.65                     | 0.61              |
| 7:H:80:LYS:HD3    | 7:H:80:LYS:H      | 1.65                     | 0.61              |
| 1:B:1074:GLU:C    | 1:B:1076:ALA:H    | 2.02                     | 0.61              |
| 1:B:184:SER:HB3   | 1:B:199:LEU:HD23  | 1.82                     | 0.61              |
| 2:C:108:VAL:HG12  | 2:C:109:THR:H     | 1.66                     | 0.61              |
| 2:C:20:ASP:C      | 2:C:22:SER:H      | 2.02                     | 0.61              |
| 2:C:593:PRO:HG2   | 2:C:617:ARG:HH21  | 1.64                     | 0.61              |
| 2:C:778:MET:CE    | 2:C:1094:ARG:HG2  | 2.28                     | 0.61              |
| 2:C:910:VAL:HG12  | 2:C:911:ILE:H     | 1.63                     | 0.61              |
| 10:K:64:ASN:HB3   | 10:K:65:PRO:HD3   | 1.81                     | 0.61              |
| 11:L:61:TYR:CD2   | 11:L:61:TYR:C     | 2.70                     | 0.61              |
| 1:B:1348:LEU:HG   | 1:B:1372:VAL:HG23 | 1.83                     | 0.61              |
| 1:B:18:GLN:HB2    | 2:C:1215:ARG:HB2  | 1.82                     | 0.61              |
| 1:B:88:LYS:HE3    | 1:B:280:GLU:OE2   | 2.00                     | 0.61              |
| 2:C:1012:ILE:HD13 | 2:C:1092:TYR:OH   | 1.99                     | 0.61              |
| 2:C:1182:CYS:O    | 2:C:1183:LYS:O    | 2.19                     | 0.61              |
| 2:C:1196:ILE:HD12 | 2:C:1200:ALA:CB   | 2.30                     | 0.61              |
| 2:C:745:PRO:O     | 2:C:747:MET:N     | 2.34                     | 0.61              |
| 3:D:116:LYS:HD3   | 3:D:140:ASN:HB3   | 1.82                     | 0.61              |
| 4:E:207:LEU:O     | 4:E:211:LEU:HB2   | 2.01                     | 0.61              |
| 9:J:13:MET:CE     | 9:J:14:LEU:H      | 2.13                     | 0.61              |
| 1:B:1315:GLU:C    | 1:B:1317:MET:H    | 2.04                     | 0.61              |
| 1:B:1444:MET:CG   | 7:H:60:ARG:HA     | 2.31                     | 0.61              |
| 2:C:244:LEU:HD11  | 2:C:366:GLN:HE22  | 1.65                     | 0.61              |
| 2:C:390:LEU:O     | 2:C:392:ARG:HG3   | 2.00                     | 0.61              |
| 4:E:33:PHE:CE1    | 7:H:80:LYS:HE3    | 2.36                     | 0.61              |
| 7:H:37:SER:OG     | 7:H:45:ILE:HB     | 2.01                     | 0.61              |
| 1:B:317:LYS:O     | 1:B:318:SER:HB3   | 1.99                     | 0.61              |
| 1:B:417:TYR:N     | 1:B:417:TYR:HD2   | 1.99                     | 0.61              |
| 2:C:287:ARG:HG2   | 2:C:292:ILE:HA    | 1.83                     | 0.61              |
| 3:D:238:ILE:HG22  | 3:D:243:VAL:HG23  | 1.82                     | 0.61              |
| 9:J:13:MET:HE3    | 9:J:14:LEU:H      | 1.65                     | 0.61              |
| 11:L:10:PHE:CD2   | 11:L:10:PHE:N     | 2.68                     | 0.61              |
| 1:B:890:ASP:H     | 1:B:1296:GLY:HA3  | 1.65                     | 0.61              |
| 1:B:152:VAL:HG13  | 1:B:153:PRO:HD2   | 1.82                     | 0.61              |
| 1:B:222:LEU:O     | 1:B:224:PHE:HD1   | 1.83                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:868:MET:O     | 2:C:870:ILE:HG13  | 2.00                     | 0.61              |
| 2:C:884:ARG:HB2   | 2:C:935:ARG:HA    | 1.83                     | 0.61              |
| 2:C:884:ARG:O     | 2:C:936:ASP:HB3   | 1.99                     | 0.61              |
| 7:H:26:LEU:HD11   | 7:H:70:PHE:CD1    | 2.36                     | 0.61              |
| 10:K:8:PHE:H      | 10:K:49:MET:CE    | 2.13                     | 0.61              |
| 1:B:224:PHE:CD2   | 1:B:231:PRO:HG3   | 2.36                     | 0.61              |
| 1:B:266:LEU:HD21  | 1:B:303:TYR:CE1   | 2.36                     | 0.61              |
| 1:B:567:LYS:HD2   | 1:B:568:PRO:CD    | 2.31                     | 0.61              |
| 1:B:57:ARG:NH1    | 1:B:57:ARG:HG2    | 2.15                     | 0.61              |
| 1:B:666:ILE:HD11  | 2:C:1067:ARG:O    | 2.01                     | 0.61              |
| 2:C:44:VAL:CG1    | 2:C:199:MET:HG2   | 2.30                     | 0.61              |
| 2:C:510:LYS:HG3   | 2:C:511:PRO:HD3   | 1.82                     | 0.61              |
| 3:D:22:LEU:HD21   | 3:D:25:VAL:HG11   | 1.81                     | 0.61              |
| 2:C:1079:LYS:CA   | 3:D:27:LEU:HD21   | 2.31                     | 0.61              |
| 7:H:66:GLY:O      | 7:H:67:SER:C      | 2.38                     | 0.61              |
| 8:I:44:VAL:O      | 8:I:44:VAL:HG12   | 2.00                     | 0.61              |
| 9:J:82:GLU:HB3    | 9:J:104:LEU:CD1   | 2.31                     | 0.61              |
| 1:B:1325:THR:HG23 | 5:F:148:GLU:H     | 1.63                     | 0.60              |
| 1:B:1404:GLU:HB2  | 1:B:1408:ILE:HG13 | 1.82                     | 0.60              |
| 1:B:53:LEU:CD2    | 1:B:54:ASN:HD22   | 2.14                     | 0.60              |
| 2:C:288:ALA:HB1   | 2:C:331:LEU:HD12  | 1.83                     | 0.60              |
| 4:E:205:ASP:O     | 4:E:208:GLU:HB3   | 2.00                     | 0.60              |
| 5:F:157:SER:OG    | 5:F:160:GLU:HG3   | 2.01                     | 0.60              |
| 1:B:265:LYS:HG2   | 1:B:303:TYR:CA    | 2.30                     | 0.60              |
| 1:B:806:ARG:HH12  | 2:C:729:ILE:HD11  | 1.66                     | 0.60              |
| 4:E:16:LYS:NZ     | 4:E:16:LYS:HB3    | 2.15                     | 0.60              |
| 4:E:8:PHE:CE2     | 7:H:73:LYS:HD3    | 2.37                     | 0.60              |
| 1:B:364:VAL:HG13  | 1:B:364:VAL:O     | 2.00                     | 0.60              |
| 1:B:446:ARG:CD    | 1:B:480:ALA:HB2   | 2.25                     | 0.60              |
| 1:B:1042:PHE:HE2  | 1:B:1046:LEU:HD11 | 1.66                     | 0.60              |
| 1:B:500:GLU:OE2   | 1:B:1438:THR:HG21 | 2.01                     | 0.60              |
| 1:B:635:ARG:HH11  | 1:B:635:ARG:HA    | 1.64                     | 0.60              |
| 2:C:1220:ARG:NH1  | 2:C:1220:ARG:HB3  | 2.16                     | 0.60              |
| 2:C:603:LEU:HD13  | 2:C:608:ASP:CB    | 2.30                     | 0.60              |
| 2:C:642:ASP:HB3   | 2:C:649:LYS:HD2   | 1.84                     | 0.60              |
| 2:C:735:ALA:O     | 2:C:738:PHE:HE1   | 1.84                     | 0.60              |
| 1:B:92:HIS:O      | 1:B:95:PHE:N      | 2.34                     | 0.60              |
| 1:B:93:VAL:HG13   | 1:B:301:ALA:HB1   | 1.83                     | 0.60              |
| 2:C:758:PHE:HZ    | 2:C:1031:LEU:HD22 | 1.67                     | 0.60              |
| 2:C:493:SER:HA    | 2:C:751:VAL:HG21  | 1.83                     | 0.60              |
| 3:D:39:ALA:CA     | 3:D:164:ALA:HB3   | 2.31                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:E:40:HIS:ND1    | 4:E:41:GLN:HG3    | 2.16                     | 0.60              |
| 6:G:89:GLU:HB3    | 6:G:134:ILE:CD1   | 2.32                     | 0.60              |
| 1:B:1443:VAL:O    | 1:B:1444:MET:HG3  | 2.02                     | 0.60              |
| 1:B:418:SER:C     | 1:B:420:ARG:H     | 2.04                     | 0.60              |
| 1:B:93:VAL:HG21   | 1:B:301:ALA:O     | 2.01                     | 0.60              |
| 2:C:1017:ILE:H    | 2:C:1018:PRO:CD   | 2.15                     | 0.60              |
| 2:C:217:ARG:O     | 2:C:217:ARG:HD2   | 2.00                     | 0.60              |
| 2:C:37:PHE:HE1    | 2:C:41:LYS:HG3    | 1.64                     | 0.60              |
| 2:C:497:ARG:NH2   | 2:C:775:LYS:NZ    | 2.49                     | 0.60              |
| 2:C:745:PRO:C     | 2:C:747:MET:H     | 2.04                     | 0.60              |
| 1:B:1151:GLU:HA   | 9:J:44:TYR:O      | 2.01                     | 0.60              |
| 15:T:15:DT:H2"    | 15:T:16:DG:OP2    | 2.00                     | 0.60              |
| 15:T:24:DG:H5'    | 15:T:25:DC:OP2    | 2.02                     | 0.60              |
| 1:B:341:MET:HE1   | 2:C:1135:ARG:NH1  | 2.16                     | 0.60              |
| 1:B:741:ASN:HD22  | 1:B:742:ASN:N     | 2.00                     | 0.60              |
| 2:C:821:GLN:HE22  | 2:C:851:PHE:CA    | 2.13                     | 0.60              |
| 1:B:1227:ILE:HG22 | 1:B:1228:TRP:H    | 1.66                     | 0.60              |
| 1:B:1329:THR:HG22 | 1:B:1331:SER:N    | 2.17                     | 0.60              |
| 1:B:311:GLN:O     | 1:B:312:PRO:C     | 2.40                     | 0.60              |
| 1:B:647:GLY:O     | 1:B:651:LYS:HG3   | 2.01                     | 0.60              |
| 2:C:878:GLN:HA    | 2:C:885:MET:SD    | 2.42                     | 0.60              |
| 1:B:1001:ARG:O    | 1:B:1002:GLY:O    | 2.19                     | 0.60              |
| 1:B:1101:LEU:HD11 | 1:B:1105:LEU:HD11 | 1.83                     | 0.60              |
| 1:B:350:ARG:HB2   | 2:C:1128:LEU:HD11 | 1.83                     | 0.60              |
| 1:B:871:ASP:OD2   | 1:B:873:MET:HB2   | 2.02                     | 0.60              |
| 2:C:1106:ARG:HD2  | 2:C:1125:ASP:O    | 2.01                     | 0.60              |
| 2:C:117:ALA:HB1   | 2:C:122:LEU:HB2   | 1.84                     | 0.60              |
| 2:C:215:GLN:NE2   | 2:C:215:GLN:HA    | 2.17                     | 0.60              |
| 2:C:879:ARG:HD3   | 2:C:883:LEU:HD22  | 1.84                     | 0.60              |
| 5:F:55:ARG:C      | 5:F:57:MET:H      | 2.05                     | 0.60              |
| 7:H:91:VAL:HG23   | 7:H:141:SER:O     | 2.02                     | 0.60              |
| 1:B:1161:THR:HG22 | 1:B:1163:ILE:HG13 | 1.82                     | 0.60              |
| 2:C:983:ARG:HD2   | 2:C:1091:TYR:HB3  | 1.84                     | 0.60              |
| 2:C:992:ILE:HD11  | 11:L:66:PRO:HB2   | 1.84                     | 0.60              |
| 4:E:145:MET:O     | 4:E:149:THR:HB    | 2.01                     | 0.60              |
| 5:F:48:ASP:CG     | 5:F:49:SER:H      | 2.03                     | 0.60              |
| 9:J:106:CYS:SG    | 9:J:108:HIS:HB2   | 2.42                     | 0.60              |
| 2:C:1181:GLU:HG3  | 2:C:1188:LYS:CE   | 2.32                     | 0.59              |
| 2:C:273:LEU:HD12  | 2:C:276:ILE:HD11  | 1.84                     | 0.59              |
| 2:C:281:PRO:HG2   | 2:C:284:ILE:HG13  | 1.83                     | 0.59              |
| 2:C:562:GLY:O     | 2:C:590:HIS:ND1   | 2.31                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:67:SER:HB2    | 2:C:92:PHE:HD1    | 1.67                     | 0.59              |
| 7:H:1:MET:SD      | 7:H:79:PHE:CD1    | 2.95                     | 0.59              |
| 1:B:339:ASN:HB3   | 2:C:1117:GLN:NE2  | 2.17                     | 0.59              |
| 2:C:496:ARG:HH12  | 2:C:539:LEU:HB2   | 1.66                     | 0.59              |
| 4:E:64:VAL:HG22   | 4:E:129:LEU:HD22  | 1.83                     | 0.59              |
| 8:I:102:TYR:N     | 8:I:102:TYR:CD2   | 2.70                     | 0.59              |
| 1:B:1027:ALA:O    | 1:B:1031:VAL:HG23 | 2.02                     | 0.59              |
| 1:B:1349:TYR:CE1  | 1:B:1368:MET:HE3  | 2.37                     | 0.59              |
| 1:B:567:LYS:HB2   | 1:B:568:PRO:CD    | 2.32                     | 0.59              |
| 1:B:925:LEU:HD13  | 1:B:983:ILE:HD12  | 1.83                     | 0.59              |
| 1:B:986:ILE:HD12  | 1:B:1032:LEU:HD11 | 1.84                     | 0.59              |
| 2:C:980:PHE:HD2   | 2:C:1094:ARG:HA   | 1.67                     | 0.59              |
| 1:B:351:THR:CG2   | 2:C:1103:ILE:HG13 | 2.32                     | 0.59              |
| 2:C:373:ARG:HA    | 2:C:566:LEU:HD23  | 1.84                     | 0.59              |
| 2:C:882:THR:HG22  | 2:C:884:ARG:HB2   | 1.83                     | 0.59              |
| 3:D:138:GLU:N     | 3:D:138:GLU:OE1   | 2.36                     | 0.59              |
| 5:F:118:PRO:O     | 5:F:122:LYS:HG3   | 2.02                     | 0.59              |
| 7:H:23:LYS:HG3    | 7:H:56:ILE:HD13   | 1.85                     | 0.59              |
| 8:I:81:PRO:CB     | 8:I:82:PRO:CD     | 2.80                     | 0.59              |
| 1:B:1129:GLU:HG3  | 1:B:1132:LYS:HD2  | 1.83                     | 0.59              |
| 1:B:1143:LEU:HB2  | 1:B:1271:ILE:HG21 | 1.83                     | 0.59              |
| 1:B:1420:ASP:HB3  | 1:B:1422:ARG:HG3  | 1.83                     | 0.59              |
| 2:C:286:PHE:CD1   | 2:C:297:ILE:HG23  | 2.38                     | 0.59              |
| 2:C:519:TRP:HE1   | 2:C:635:ARG:NH2   | 2.00                     | 0.59              |
| 2:C:847:ASP:C     | 2:C:849:GLY:N     | 2.56                     | 0.59              |
| 2:C:865:LYS:HZ2   | 2:C:869:SER:HA    | 1.65                     | 0.59              |
| 2:C:956:THR:HG23  | 2:C:960:GLY:HA2   | 1.84                     | 0.59              |
| 3:D:112:ASN:HB3   | 3:D:114:TYR:CE1   | 2.38                     | 0.59              |
| 10:K:28:ASP:O     | 10:K:30:LEU:HG    | 2.01                     | 0.59              |
| 1:B:466:SER:HB3   | 11:L:2:ASN:ND2    | 2.17                     | 0.59              |
| 1:B:1076:ALA:HA   | 1:B:1079:MET:CE   | 2.32                     | 0.59              |
| 1:B:358:ASN:C     | 1:B:359:LEU:HD23  | 2.23                     | 0.59              |
| 1:B:445:ASN:HB2   | 1:B:455:MET:HA    | 1.84                     | 0.59              |
| 1:B:511:ILE:HA    | 1:B:521:MET:HE3   | 1.84                     | 0.59              |
| 2:C:600:LEU:O     | 2:C:609:ILE:HD12  | 2.02                     | 0.59              |
| 2:C:782:LEU:HD12  | 2:C:788:ARG:HH11  | 1.66                     | 0.59              |
| 3:D:73:GLN:NE2    | 3:D:75:MET:HB2    | 2.18                     | 0.59              |
| 4:E:54:GLU:O      | 4:E:58:VAL:HG23   | 2.03                     | 0.59              |
| 1:B:1017:LEU:HB2  | 5:F:206:GLY:N     | 2.09                     | 0.59              |
| 1:B:1120:LEU:HD23 | 1:B:1124:HIS:O    | 2.02                     | 0.59              |
| 1:B:629:LEU:HD22  | 1:B:633:VAL:HG23  | 1.83                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:994:GLN:O     | 1:B:996:ASN:N     | 2.35                     | 0.59              |
| 10:K:7:CYS:SG     | 10:K:49:MET:HE3   | 2.42                     | 0.59              |
| 1:B:1193:LEU:HB2  | 1:B:1260:LEU:HD11 | 1.83                     | 0.59              |
| 1:B:1341:ILE:CG2  | 1:B:1342:GLU:N    | 2.63                     | 0.59              |
| 1:B:1420:ASP:O    | 1:B:1421:CYS:HB2  | 2.02                     | 0.59              |
| 1:B:195:ASP:O     | 1:B:196:GLU:HB3   | 2.01                     | 0.59              |
| 1:B:230:ARG:HB2   | 1:B:233:TRP:CE3   | 2.38                     | 0.59              |
| 2:C:982:SER:HB3   | 2:C:1092:TYR:HE2  | 1.66                     | 0.59              |
| 2:C:1099:VAL:CG1  | 2:C:1100:ASP:H    | 2.15                     | 0.59              |
| 2:C:402:GLY:CA    | 2:C:695:ALA:HB3   | 2.32                     | 0.59              |
| 2:C:806:THR:HG23  | 2:C:1046:PRO:HD3  | 1.85                     | 0.59              |
| 7:H:31:LEU:CD2    | 7:H:48:VAL:HG21   | 2.33                     | 0.59              |
| 10:K:16:ASP:OD1   | 10:K:17:LYS:HD2   | 2.02                     | 0.59              |
| 1:B:1041:ALA:O    | 1:B:1045:VAL:HG23 | 2.02                     | 0.59              |
| 1:B:629:LEU:O     | 1:B:633:VAL:HG23  | 2.03                     | 0.59              |
| 2:C:982:SER:HB3   | 2:C:1092:TYR:CE2  | 2.37                     | 0.59              |
| 2:C:610:ASN:HB3   | 2:C:613:VAL:HG23  | 1.84                     | 0.59              |
| 3:D:35:ARG:NH1    | 11:L:41:THR:H     | 1.99                     | 0.59              |
| 4:E:195:ILE:HG22  | 4:E:198:LEU:HG    | 1.84                     | 0.59              |
| 10:K:14:VAL:HG12  | 10:K:50:ILE:HD11  | 1.84                     | 0.59              |
| 1:B:144:THR:O     | 1:B:146:MET:HG3   | 2.03                     | 0.59              |
| 1:B:341:MET:CE    | 1:B:843:LYS:NZ    | 2.66                     | 0.59              |
| 1:B:901:LEU:HG    | 1:B:926:GLN:HE21  | 1.68                     | 0.59              |
| 1:B:979:SER:OG    | 1:B:980:ASP:N     | 2.32                     | 0.59              |
| 2:C:100:PRO:CD    | 2:C:180:TYR:HE1   | 2.12                     | 0.59              |
| 2:C:604:ARG:HA    | 2:C:609:ILE:O     | 2.03                     | 0.59              |
| 1:B:1148:ILE:HG23 | 9:J:49:ILE:HB     | 1.84                     | 0.59              |
| 9:J:69:PRO:HG2    | 9:J:85:PHE:CD2    | 2.38                     | 0.59              |
| 1:B:381:THR:C     | 1:B:383:TYR:H     | 2.06                     | 0.59              |
| 1:B:40:THR:C      | 1:B:41:MET:HG3    | 2.22                     | 0.59              |
| 1:B:477:PRO:CG    | 1:B:521:MET:HG2   | 2.33                     | 0.59              |
| 2:C:563:MET:HE3   | 2:C:580:VAL:HB    | 1.82                     | 0.59              |
| 2:C:797:TYR:OH    | 2:C:971:THR:HG21  | 2.03                     | 0.59              |
| 8:I:98:TYR:CE1    | 8:I:139:ASN:HA    | 2.38                     | 0.59              |
| 11:L:55:LYS:HD2   | 11:L:81:TYR:HD1   | 1.68                     | 0.59              |
| 1:B:1050:GLU:O    | 1:B:1053:PHE:N    | 2.36                     | 0.58              |
| 2:C:1181:GLU:H    | 2:C:1188:LYS:HG2  | 1.69                     | 0.58              |
| 2:C:280:ILE:HB    | 2:C:285:ILE:HD11  | 1.83                     | 0.58              |
| 2:C:331:LEU:O     | 2:C:334:ILE:HB    | 2.03                     | 0.58              |
| 2:C:171:PRO:HD2   | 2:C:457:LEU:HD13  | 1.85                     | 0.58              |
| 6:G:111:LEU:O     | 6:G:113:GLY:N     | 2.36                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:K:22:LEU:O     | 10:K:22:LEU:HD12  | 2.02                     | 0.58              |
| 1:B:679:ILE:HG12  | 1:B:732:LEU:CD1   | 2.33                     | 0.58              |
| 2:C:1167:GLY:HA3  | 2:C:1216:LEU:H    | 1.68                     | 0.58              |
| 2:C:126:SER:OG    | 2:C:172:ILE:HD11  | 2.03                     | 0.58              |
| 2:C:833:TYR:N     | 2:C:833:TYR:HD1   | 2.02                     | 0.58              |
| 2:C:955:THR:CG2   | 2:C:956:THR:H     | 2.14                     | 0.58              |
| 7:H:129:SER:HB3   | 7:H:138:THR:OG1   | 2.03                     | 0.58              |
| 12:M:30:ILE:HG22  | 12:M:31:CYS:N     | 2.17                     | 0.58              |
| 1:B:663:SER:OG    | 1:B:664:THR:N     | 2.36                     | 0.58              |
| 1:B:901:LEU:HD22  | 1:B:919:ILE:HG22  | 1.83                     | 0.58              |
| 1:B:932:GLU:OE1   | 1:B:987:VAL:HG22  | 2.03                     | 0.58              |
| 2:C:102:VAL:HG13  | 2:C:958:GLN:NE2   | 2.18                     | 0.58              |
| 7:H:114:LEU:HG    | 7:H:162:SER:HB3   | 1.84                     | 0.58              |
| 1:B:71:GLN:HG3    | 1:B:72:GLU:N      | 2.19                     | 0.58              |
| 1:B:886:ILE:CG2   | 1:B:887:GLY:N     | 2.66                     | 0.58              |
| 1:B:986:ILE:HG22  | 1:B:987:VAL:N     | 2.18                     | 0.58              |
| 2:C:98:THR:HG23   | 2:C:127:GLY:O     | 2.03                     | 0.58              |
| 2:C:731:VAL:HG12  | 2:C:732:SER:N     | 2.18                     | 0.58              |
| 2:C:885:MET:HA    | 2:C:936:ASP:HB3   | 1.85                     | 0.58              |
| 7:H:138:THR:CG2   | 7:H:139:ILE:HG13  | 2.33                     | 0.58              |
| 8:I:118:PHE:O     | 8:I:120:GLY:N     | 2.35                     | 0.58              |
| 1:B:335:ARG:HH11  | 2:C:1202:LEU:HD13 | 1.66                     | 0.58              |
| 1:B:469:ARG:HB3   | 1:B:469:ARG:NH1   | 2.19                     | 0.58              |
| 1:B:446:ARG:HB2   | 1:B:487:MET:HG2   | 1.86                     | 0.58              |
| 1:B:35:ILE:HB     | 1:B:83:HIS:O      | 2.02                     | 0.58              |
| 2:C:273:LEU:HB2   | 2:C:276:ILE:CD1   | 2.34                     | 0.58              |
| 2:C:701:ILE:HD11  | 2:C:703:ILE:HD11  | 1.84                     | 0.58              |
| 2:C:806:THR:HB    | 2:C:809:MET:HG3   | 1.84                     | 0.58              |
| 2:C:811:TYR:N     | 2:C:811:TYR:CD1   | 2.70                     | 0.58              |
| 2:C:880:THR:O     | 2:C:881:ASN:HB2   | 2.02                     | 0.58              |
| 3:D:98:VAL:HG12   | 3:D:99:LEU:N      | 2.18                     | 0.58              |
| 1:B:49:LYS:HZ1    | 1:B:61:ILE:HG13   | 1.66                     | 0.58              |
| 1:B:947:PHE:HE2   | 1:B:954:TRP:CD2   | 2.22                     | 0.58              |
| 2:C:978:ASP:OD2   | 2:C:1098:MET:HG2  | 2.03                     | 0.58              |
| 2:C:1163:CYS:SG   | 2:C:1165:ILE:HB   | 2.44                     | 0.58              |
| 3:D:98:VAL:HG12   | 3:D:99:LEU:H      | 1.67                     | 0.58              |
| 7:H:45:ILE:HD13   | 7:H:78:VAL:CG1    | 2.34                     | 0.58              |
| 1:B:1299:VAL:HG12 | 1:B:1300:LYS:H    | 1.68                     | 0.58              |
| 1:B:403:LYS:O     | 1:B:415:LEU:HB2   | 2.03                     | 0.58              |
| 1:B:675:THR:OG1   | 1:B:736:ASN:ND2   | 2.37                     | 0.58              |
| 1:B:787:PHE:CE1   | 1:B:796:SER:HA    | 2.38                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:118:ARG:HG2   | 2:C:204:ILE:HD13  | 1.86                     | 0.58              |
| 1:B:41:MET:HB3    | 1:B:50:ILE:H      | 1.69                     | 0.58              |
| 1:B:567:LYS:CB    | 1:B:568:PRO:CD    | 2.81                     | 0.58              |
| 1:B:997:LEU:HD13  | 1:B:1018:PHE:HE2  | 1.69                     | 0.58              |
| 2:C:313:MET:O     | 2:C:316:PRO:HD2   | 2.03                     | 0.58              |
| 2:C:843:GLN:O     | 2:C:846:ILE:HB    | 2.03                     | 0.58              |
| 3:D:172:PRO:O     | 3:D:235:VAL:CG2   | 2.52                     | 0.58              |
| 4:E:14:ARG:NH2    | 4:E:16:LYS:HZ1    | 1.94                     | 0.58              |
| 5:F:127:ILE:HG13  | 5:F:127:ILE:O     | 2.04                     | 0.58              |
| 6:G:75:PRO:C      | 6:G:77:ASP:H      | 2.07                     | 0.58              |
| 1:B:1317:MET:O    | 1:B:1322:ILE:HD11 | 2.03                     | 0.58              |
| 1:B:652:VAL:HG12  | 1:B:653:VAL:N     | 2.18                     | 0.58              |
| 1:B:69:THR:C      | 1:B:71:GLN:H      | 2.07                     | 0.58              |
| 1:B:798:GLY:HA2   | 1:B:815:PHE:HD1   | 1.68                     | 0.58              |
| 1:B:7:SER:HB3     | 2:C:1193:GLN:OE1  | 2.04                     | 0.58              |
| 1:B:84:ILE:HG22   | 1:B:239:LEU:HB3   | 1.85                     | 0.58              |
| 2:C:1172:ILE:HG22 | 2:C:1172:ILE:O    | 2.03                     | 0.58              |
| 2:C:121:ASN:HA    | 2:C:207:GLY:CA    | 2.28                     | 0.58              |
| 2:C:184:ALA:HB1   | 2:C:188:ASP:HB3   | 1.85                     | 0.58              |
| 2:C:398:ARG:HG3   | 2:C:398:ARG:NH1   | 2.18                     | 0.58              |
| 2:C:521:LEU:HB3   | 2:C:633:VAL:HG11  | 1.86                     | 0.58              |
| 2:C:542:MET:HE1   | 2:C:743:ILE:HG13  | 1.86                     | 0.58              |
| 2:C:857:ARG:HD2   | 2:C:945:GLU:OE1   | 2.03                     | 0.58              |
| 4:E:5:THR:HG23    | 7:H:9:LEU:HB2     | 1.86                     | 0.58              |
| 5:F:111:VAL:HG12  | 5:F:137:GLU:HG2   | 1.86                     | 0.58              |
| 6:G:79:ARG:HB3    | 6:G:144:GLU:CD    | 2.23                     | 0.58              |
| 7:H:1:MET:O       | 7:H:3:PHE:CE1     | 2.57                     | 0.58              |
| 11:L:42:LEU:O     | 11:L:46:ILE:HG13  | 2.04                     | 0.58              |
| 1:B:981:LEU:HD23  | 1:B:1039:LYS:HA   | 1.85                     | 0.58              |
| 1:B:1118:VAL:HG23 | 1:B:1306:LEU:HB2  | 1.85                     | 0.58              |
| 1:B:499:ALA:O     | 1:B:503:GLN:HB2   | 2.04                     | 0.58              |
| 1:B:55:ASP:O      | 1:B:55:ASP:CG     | 2.41                     | 0.58              |
| 2:C:310:MET:O     | 2:C:314:LEU:HD12  | 2.04                     | 0.58              |
| 2:C:471:LYS:O     | 2:C:472:ALA:CB    | 2.52                     | 0.58              |
| 3:D:38:ILE:HA     | 3:D:173:ALA:CB    | 2.33                     | 0.58              |
| 1:B:913:LEU:HD23  | 1:B:919:ILE:HD12  | 1.84                     | 0.57              |
| 2:C:244:LEU:O     | 2:C:249:ARG:HG2   | 2.03                     | 0.57              |
| 2:C:862:GLN:HG2   | 2:C:963:PHE:HD1   | 1.69                     | 0.57              |
| 1:B:1436:ILE:O    | 1:B:1437:GLY:C    | 2.43                     | 0.57              |
| 1:B:438:ASP:OD1   | 1:B:461:LYS:HA    | 2.04                     | 0.57              |
| 1:B:584:ASN:HA    | 1:B:609:ASP:O     | 2.04                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:711:ARG:NH2   | 9:J:87:GLN:OE1    | 2.38                     | 0.57              |
| 1:B:63:ARG:HA     | 1:B:74:MET:SD     | 2.44                     | 0.57              |
| 1:B:756:ILE:O     | 1:B:759:ALA:HB3   | 2.04                     | 0.57              |
| 2:C:129:PHE:CE2   | 2:C:166:PHE:HD1   | 2.22                     | 0.57              |
| 2:C:459:TYR:CE1   | 2:C:469:GLN:HG2   | 2.39                     | 0.57              |
| 2:C:56:ASP:HB3    | 2:C:57:TYR:CD1    | 2.38                     | 0.57              |
| 2:C:617:ARG:HA    | 2:C:624:LEU:HD12  | 1.87                     | 0.57              |
| 2:C:63:ILE:HA     | 2:C:421:PHE:CE2   | 2.39                     | 0.57              |
| 3:D:232:VAL:HG21  | 3:D:244:VAL:HG22  | 1.86                     | 0.57              |
| 3:D:6:PRO:CB      | 3:D:25:VAL:HG12   | 2.33                     | 0.57              |
| 7:H:127:PRO:HG3   | 7:H:139:ILE:HD12  | 1.86                     | 0.57              |
| 9:J:99:LEU:N      | 9:J:99:LEU:HD23   | 2.19                     | 0.57              |
| 11:L:18:LYS:NZ    | 11:L:38:GLU:HG2   | 2.19                     | 0.57              |
| 1:B:1057:VAL:HG12 | 1:B:1058:VAL:N    | 2.19                     | 0.57              |
| 1:B:1402:PHE:CD1  | 1:B:1403:GLU:HG3  | 2.38                     | 0.57              |
| 1:B:814:PHE:O     | 1:B:818:MET:HG3   | 2.04                     | 0.57              |
| 4:E:34:GLN:C      | 4:E:36:LYS:H      | 2.07                     | 0.57              |
| 11:L:68:PHE:HD1   | 11:L:70:ARG:NH1   | 2.01                     | 0.57              |
| 1:B:1127:ASP:OD1  | 1:B:1130:GLN:HB2  | 2.04                     | 0.57              |
| 1:B:1205:LYS:O    | 1:B:1207:LEU:HG   | 2.03                     | 0.57              |
| 1:B:1230:GLU:O    | 1:B:1232:ASN:N    | 2.38                     | 0.57              |
| 1:B:1138:ILE:HG21 | 1:B:1316:VAL:HG13 | 1.87                     | 0.57              |
| 1:B:138:ILE:HG21  | 1:B:222:LEU:CD2   | 2.33                     | 0.57              |
| 2:C:1192:TYR:CD1  | 2:C:1192:TYR:N    | 2.73                     | 0.57              |
| 2:C:388:CYS:O     | 2:C:390:LEU:N     | 2.36                     | 0.57              |
| 2:C:446:LEU:HG    | 2:C:446:LEU:O     | 2.03                     | 0.57              |
| 4:E:66:ARG:HD2    | 4:E:133:THR:HB    | 1.84                     | 0.57              |
| 5:F:22:MET:HE2    | 5:F:26:ARG:HE     | 1.70                     | 0.57              |
| 1:B:1373:ASP:HA   | 1:B:1376:THR:CG2  | 2.33                     | 0.57              |
| 1:B:147:VAL:O     | 1:B:149:GLU:HG3   | 2.04                     | 0.57              |
| 1:B:417:TYR:N     | 1:B:417:TYR:CD2   | 2.72                     | 0.57              |
| 1:B:401:GLY:C     | 1:B:435:HIS:CD2   | 2.78                     | 0.57              |
| 2:C:778:MET:HE1   | 2:C:1094:ARG:NE   | 2.19                     | 0.57              |
| 2:C:834:ASN:HB3   | 2:C:840:ILE:HG13  | 1.85                     | 0.57              |
| 2:C:882:THR:CG2   | 2:C:884:ARG:HB2   | 2.35                     | 0.57              |
| 3:D:31:ASN:HA     | 3:D:34:ARG:HB3    | 1.86                     | 0.57              |
| 9:J:119:THR:O     | 9:J:119:THR:HG22  | 2.04                     | 0.57              |
| 9:J:15:TYR:N      | 9:J:15:TYR:CD1    | 2.71                     | 0.57              |
| 1:B:180:LYS:HZ1   | 1:B:294:SER:HB3   | 1.65                     | 0.57              |
| 3:D:43:THR:CG2    | 3:D:44:LEU:H      | 2.10                     | 0.57              |
| 4:E:16:LYS:HG2    | 4:E:18:VAL:HG12   | 1.86                     | 0.57              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:F:178:ILE:HB   | 5:F:212:ARG:HD3   | 1.85                     | 0.57              |
| 4:E:37:GLN:OE1   | 7:H:5:LYS:HD2     | 2.05                     | 0.57              |
| 13:N:2:DA:C2'    | 13:N:3:DG:C8      | 2.88                     | 0.57              |
| 1:B:726:ARG:O    | 1:B:729:ALA:HB3   | 2.04                     | 0.57              |
| 1:B:984:LYS:HG2  | 1:B:988:LEU:HD12  | 1.86                     | 0.57              |
| 2:C:803:LEU:HD12 | 2:C:1032:SER:HB3  | 1.86                     | 0.57              |
| 2:C:1197:PRO:O   | 2:C:1200:ALA:HB3  | 2.04                     | 0.57              |
| 2:C:273:LEU:HD22 | 2:C:360:PHE:HD1   | 1.69                     | 0.57              |
| 2:C:363:HIS:O    | 2:C:364:ILE:HB    | 2.04                     | 0.57              |
| 2:C:361:LEU:HD11 | 2:C:381:MET:HE1   | 1.85                     | 0.57              |
| 1:B:87:ALA:CB    | 1:B:276:LEU:HD23  | 2.35                     | 0.57              |
| 1:B:445:ASN:HA   | 1:B:478:TYR:HE2   | 1.70                     | 0.57              |
| 1:B:35:ILE:HA    | 1:B:52:GLY:O      | 2.04                     | 0.57              |
| 2:C:254:LEU:HD23 | 2:C:381:MET:HE1   | 1.86                     | 0.57              |
| 2:C:582:VAL:HB   | 2:C:587:HIS:CD2   | 2.40                     | 0.57              |
| 7:H:83:LYS:HE2   | 7:H:150:CYS:H     | 1.68                     | 0.57              |
| 10:K:23:ASN:O    | 10:K:25:LEU:N     | 2.38                     | 0.57              |
| 12:M:27:LEU:HB3  | 12:M:37:LYS:CD    | 2.34                     | 0.57              |
| 1:B:320:ARG:HH22 | 14:P:3:C:H1'      | 1.67                     | 0.57              |
| 1:B:1198:ASP:HB3 | 1:B:1201:ALA:CB   | 2.34                     | 0.57              |
| 1:B:567:LYS:HB3  | 8:I:95:TYR:CA     | 2.34                     | 0.57              |
| 2:C:1069:PHE:N   | 2:C:1069:PHE:CD1  | 2.73                     | 0.57              |
| 1:B:667:GLY:HA3  | 3:D:192:TRP:HH2   | 1.69                     | 0.57              |
| 8:I:128:ASN:H    | 8:I:130:ARG:NH2   | 2.02                     | 0.57              |
| 1:B:1276:VAL:HB  | 1:B:1279:ILE:HD12 | 1.86                     | 0.57              |
| 1:B:84:ILE:HD11  | 1:B:270:LEU:HD13  | 1.87                     | 0.57              |
| 1:B:436:ILE:N    | 1:B:436:ILE:HD13  | 2.19                     | 0.57              |
| 1:B:545:GLN:C    | 1:B:547:LEU:N     | 2.56                     | 0.57              |
| 1:B:903:ASN:ND2  | 1:B:904:THR:N     | 2.52                     | 0.57              |
| 1:B:903:ASN:O    | 1:B:907:THR:HB    | 2.05                     | 0.57              |
| 1:B:346:ASP:HB3  | 2:C:1108:ARG:H    | 1.70                     | 0.57              |
| 2:C:176:SER:O    | 2:C:182:SER:HB3   | 2.05                     | 0.57              |
| 3:D:74:SER:HB3   | 3:D:77:ILE:CG1    | 2.34                     | 0.57              |
| 5:F:100:ILE:HG23 | 5:F:105:PHE:CD1   | 2.39                     | 0.57              |
| 7:H:154:VAL:HG12 | 7:H:155:SER:N     | 2.20                     | 0.57              |
| 14:P:5:C:H2'     | 14:P:6:A:C8       | 2.40                     | 0.57              |
| 1:B:1373:ASP:CA  | 1:B:1376:THR:HG22 | 2.34                     | 0.56              |
| 1:B:37:PHE:N     | 1:B:37:PHE:HD1    | 2.03                     | 0.56              |
| 2:C:240:ILE:CG2  | 2:C:254:LEU:HB3   | 2.35                     | 0.56              |
| 2:C:345:LYS:O    | 2:C:347:LYS:HG2   | 2.05                     | 0.56              |
| 2:C:433:GLN:O    | 2:C:434:ARG:HG3   | 2.05                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:J:92:ARG:HG2    | 9:J:94:ASP:OD1    | 2.05                     | 0.56              |
| 14:P:6:A:H2'      | 14:P:7:A:C8       | 2.40                     | 0.56              |
| 1:B:541:ILE:HD13  | 1:B:549:MET:HE1   | 1.87                     | 0.56              |
| 2:C:780:VAL:HG12  | 2:C:782:LEU:O     | 2.05                     | 0.56              |
| 4:E:153:ARG:C     | 4:E:154:PHE:CD1   | 2.78                     | 0.56              |
| 12:M:25:ALA:O     | 12:M:26:THR:HB    | 2.05                     | 0.56              |
| 1:B:1072:ILE:HD11 | 1:B:1368:MET:HA   | 1.86                     | 0.56              |
| 1:B:22:PHE:CD1    | 2:C:1213:THR:HG22 | 2.40                     | 0.56              |
| 1:B:596:THR:C     | 1:B:598:LEU:H     | 2.08                     | 0.56              |
| 1:B:590:ARG:HD3   | 1:B:604:GLY:HA2   | 1.87                     | 0.56              |
| 1:B:881:GLN:NE2   | 1:B:959:ASN:HA    | 2.21                     | 0.56              |
| 1:B:881:GLN:O     | 1:B:953:ASN:HA    | 2.05                     | 0.56              |
| 1:B:901:LEU:HA    | 1:B:907:THR:OG1   | 2.06                     | 0.56              |
| 1:B:90:VAL:HG13   | 1:B:297:GLN:HA    | 1.86                     | 0.56              |
| 2:C:129:PHE:HE2   | 2:C:166:PHE:CD1   | 2.22                     | 0.56              |
| 2:C:129:PHE:HE2   | 2:C:166:PHE:HD1   | 1.54                     | 0.56              |
| 3:D:137:LYS:HB3   | 3:D:138:GLU:OE1   | 2.04                     | 0.56              |
| 3:D:20:PHE:HE1    | 3:D:22:LEU:HB2    | 1.71                     | 0.56              |
| 4:E:64:VAL:O      | 4:E:67:ARG:N      | 2.38                     | 0.56              |
| 7:H:23:LYS:HG3    | 7:H:56:ILE:CD1    | 2.35                     | 0.56              |
| 7:H:13:LEU:O      | 7:H:67:SER:HA     | 2.05                     | 0.56              |
| 1:B:1373:ASP:O    | 1:B:1376:THR:N    | 2.39                     | 0.56              |
| 1:B:401:GLY:C     | 1:B:435:HIS:HD2   | 2.09                     | 0.56              |
| 1:B:719:VAL:CG1   | 1:B:723:ASN:HD21  | 2.18                     | 0.56              |
| 1:B:984:LYS:O     | 1:B:988:LEU:HB2   | 2.06                     | 0.56              |
| 2:C:1002:THR:O    | 2:C:1005:GLY:N    | 2.37                     | 0.56              |
| 2:C:180:TYR:HD1   | 2:C:180:TYR:H     | 1.53                     | 0.56              |
| 3:D:116:LYS:O     | 3:D:118:LEU:N     | 2.37                     | 0.56              |
| 3:D:249:ASP:O     | 3:D:252:GLN:HB3   | 2.05                     | 0.56              |
| 7:H:129:SER:CB    | 7:H:138:THR:OG1   | 2.52                     | 0.56              |
| 7:H:26:LEU:HD12   | 7:H:56:ILE:HG21   | 1.86                     | 0.56              |
| 1:B:1130:GLN:O    | 1:B:1134:ILE:HG13 | 2.04                     | 0.56              |
| 1:B:1334:ASP:C    | 1:B:1336:MET:H    | 2.07                     | 0.56              |
| 1:B:334:GLY:O     | 1:B:336:ILE:N     | 2.39                     | 0.56              |
| 1:B:34:LYS:N      | 1:B:34:LYS:HD3    | 2.20                     | 0.56              |
| 1:B:494:SER:O     | 1:B:497:THR:HB    | 2.05                     | 0.56              |
| 1:B:719:VAL:HG12  | 1:B:723:ASN:ND2   | 2.20                     | 0.56              |
| 1:B:751:SER:O     | 1:B:752:LYS:CB    | 2.53                     | 0.56              |
| 2:C:999:MET:HG2   | 2:C:1007:VAL:HG22 | 1.86                     | 0.56              |
| 2:C:1187:ASN:O    | 2:C:1188:LYS:CB   | 2.54                     | 0.56              |
| 2:C:204:ILE:C     | 2:C:205:ILE:HD12  | 2.25                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:278:GLN:CG    | 2:C:279:ASP:H     | 2.06                     | 0.56              |
| 2:C:838:SER:HA    | 2:C:989:THR:O     | 2.05                     | 0.56              |
| 4:E:198:LEU:O     | 4:E:200:ASN:N     | 2.38                     | 0.56              |
| 5:F:147:HIS:HD2   | 5:F:149:LEU:HB2   | 1.70                     | 0.56              |
| 5:F:5:ASN:O       | 5:F:9:ILE:HG13    | 2.05                     | 0.56              |
| 1:B:1444:MET:HG2  | 7:H:60:ARG:HA     | 1.87                     | 0.56              |
| 8:I:36:CYS:HA     | 8:I:126:GLU:O     | 2.05                     | 0.56              |
| 10:K:14:VAL:CG1   | 10:K:50:ILE:HD11  | 2.36                     | 0.56              |
| 10:K:57:ILE:HA    | 10:K:60:PHE:CD2   | 2.30                     | 0.56              |
| 3:D:258:ILE:HG23  | 11:L:19:LEU:HD11  | 1.88                     | 0.56              |
| 11:L:19:LEU:HD22  | 11:L:33:ILE:CG2   | 2.36                     | 0.56              |
| 1:B:1120:LEU:CD1  | 1:B:1120:LEU:N    | 2.68                     | 0.56              |
| 1:B:211:PHE:HA    | 1:B:214:ILE:HG13  | 1.88                     | 0.56              |
| 1:B:225:ASN:ND2   | 1:B:227:VAL:H     | 2.03                     | 0.56              |
| 1:B:503:GLN:C     | 1:B:504:LEU:HD12  | 2.25                     | 0.56              |
| 1:B:524:VAL:CG1   | 1:B:525:GLN:H     | 2.12                     | 0.56              |
| 1:B:586:ILE:CG2   | 1:B:587:HIS:N     | 2.68                     | 0.56              |
| 2:C:1099:VAL:HG13 | 2:C:1100:ASP:H    | 1.70                     | 0.56              |
| 2:C:496:ARG:NH1   | 2:C:496:ARG:HB3   | 2.20                     | 0.56              |
| 1:B:98:LYS:HE2    | 1:B:224:PHE:CZ    | 2.40                     | 0.56              |
| 2:C:1169:MET:HE1  | 2:C:1201:LYS:HA   | 1.86                     | 0.56              |
| 2:C:459:TYR:CZ    | 2:C:469:GLN:HG2   | 2.41                     | 0.56              |
| 1:B:347:PHE:CE2   | 1:B:375:THR:HG23  | 2.40                     | 0.56              |
| 1:B:37:PHE:N      | 1:B:37:PHE:CD1    | 2.74                     | 0.56              |
| 1:B:382:PRO:CB    | 1:B:428:TYR:HE2   | 2.17                     | 0.56              |
| 2:C:102:VAL:HG23  | 2:C:112:LEU:HB2   | 1.86                     | 0.56              |
| 2:C:212:LEU:HD12  | 2:C:409:ALA:HB1   | 1.87                     | 0.56              |
| 2:C:56:ASP:HB3    | 2:C:57:TYR:HD1    | 1.71                     | 0.56              |
| 2:C:957:ASN:HB3   | 2:C:961:LEU:H     | 1.70                     | 0.56              |
| 4:E:59:ILE:HG21   | 4:E:145:MET:SD    | 2.46                     | 0.56              |
| 5:F:156:LEU:HA    | 5:F:160:GLU:OE1   | 2.04                     | 0.56              |
| 8:I:18:GLY:O      | 8:I:19:ARG:HB2    | 2.05                     | 0.56              |
| 11:L:46:ILE:O     | 11:L:46:ILE:HG22  | 2.06                     | 0.56              |
| 1:B:1114:PRO:HG2  | 1:B:1115:SER:H    | 1.70                     | 0.56              |
| 1:B:1349:TYR:HA   | 1:B:1372:VAL:HG21 | 1.87                     | 0.56              |
| 1:B:18:GLN:NE2    | 1:B:228:PHE:CE1   | 2.74                     | 0.56              |
| 1:B:37:PHE:HB2    | 1:B:52:GLY:CA     | 2.30                     | 0.56              |
| 1:B:527:THR:HG21  | 1:B:650:GLN:HA    | 1.87                     | 0.56              |
| 1:B:693:VAL:HG21  | 1:B:721:PHE:HE1   | 1.70                     | 0.56              |
| 2:C:758:PHE:CE1   | 2:C:1027:ILE:HG22 | 2.41                     | 0.56              |
| 2:C:422:LYS:O     | 2:C:426:LYS:HG2   | 2.05                     | 0.56              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:542:MET:HB3   | 2:C:636:PRO:HD2  | 1.87                     | 0.56              |
| 2:C:616:ILE:HG23  | 2:C:700:SER:OG   | 2.06                     | 0.56              |
| 8:I:100:THR:HG22  | 8:I:101:ALA:N    | 2.21                     | 0.56              |
| 1:B:1076:ALA:HA   | 1:B:1079:MET:HE1 | 1.88                     | 0.56              |
| 2:C:215:GLN:OE1   | 2:C:479:VAL:HG22 | 2.06                     | 0.56              |
| 2:C:411:PRO:O     | 2:C:414:ALA:HB3  | 2.06                     | 0.56              |
| 2:C:521:LEU:HD13  | 2:C:633:VAL:HB   | 1.87                     | 0.56              |
| 3:D:56:THR:CG2    | 3:D:58:LEU:HD23  | 2.36                     | 0.56              |
| 6:G:90:ARG:CG     | 6:G:91:ALA:N     | 2.63                     | 0.56              |
| 1:B:367:PRO:HA    | 1:B:463:ILE:O    | 2.05                     | 0.56              |
| 2:C:221:ASN:N     | 2:C:241:ARG:O    | 2.31                     | 0.56              |
| 5:F:93:MET:SD     | 5:F:97:VAL:HG23  | 2.46                     | 0.56              |
| 7:H:13:LEU:HD12   | 7:H:26:LEU:HD21  | 1.88                     | 0.56              |
| 11:L:109:TRP:O    | 11:L:112:GLN:HB2 | 2.06                     | 0.56              |
| 11:L:58:PHE:HE2   | 11:L:74:ARG:NE   | 2.04                     | 0.56              |
| 1:B:545:GLN:C     | 1:B:547:LEU:H    | 2.09                     | 0.55              |
| 2:C:758:PHE:CE2   | 2:C:1044:ALA:HA  | 2.40                     | 0.55              |
| 1:B:347:PHE:N     | 2:C:1107:ALA:HA  | 2.17                     | 0.55              |
| 2:C:1151:LEU:CD1  | 2:C:1151:LEU:N   | 2.68                     | 0.55              |
| 1:B:78:PRO:HA     | 2:C:1201:LYS:HZ2 | 1.71                     | 0.55              |
| 2:C:423:LYS:HE2   | 2:C:470:LYS:NZ   | 2.21                     | 0.55              |
| 2:C:833:TYR:CD1   | 2:C:833:TYR:N    | 2.70                     | 0.55              |
| 2:C:871:THR:HG22  | 2:C:872:GLU:N    | 2.21                     | 0.55              |
| 2:C:871:THR:HG22  | 2:C:872:GLU:O    | 2.06                     | 0.55              |
| 2:C:906:SER:HA    | 2:C:946:ASN:HB2  | 1.86                     | 0.55              |
| 2:C:956:THR:HG22  | 2:C:957:ASN:O    | 2.07                     | 0.55              |
| 4:E:183:LEU:HD22  | 7:H:144:ARG:NH2  | 2.21                     | 0.55              |
| 1:B:1152:ILE:HG22 | 1:B:1192:LEU:O   | 2.07                     | 0.55              |
| 1:B:230:ARG:N     | 1:B:233:TRP:CE3  | 2.62                     | 0.55              |
| 1:B:441:PRO:CG    | 1:B:498:ARG:HB2  | 2.36                     | 0.55              |
| 1:B:698:GLN:HA    | 9:J:97:MET:O     | 2.06                     | 0.55              |
| 1:B:808:LEU:HD23  | 1:B:813:PHE:HA   | 1.88                     | 0.55              |
| 1:B:857:ARG:NH2   | 6:G:139:PRO:HG3  | 2.21                     | 0.55              |
| 2:C:1047:PHE:CD1  | 2:C:1047:PHE:N   | 2.74                     | 0.55              |
| 2:C:1156:ASP:HB3  | 2:C:1198:TYR:N   | 2.17                     | 0.55              |
| 2:C:311:LEU:O     | 2:C:312:GLU:C    | 2.44                     | 0.55              |
| 1:B:315:LEU:HD12  | 2:C:471:LYS:HB3  | 1.88                     | 0.55              |
| 3:D:254:LYS:C     | 3:D:256:ALA:H    | 2.09                     | 0.55              |
| 3:D:48:SER:HB3    | 3:D:158:VAL:HB   | 1.87                     | 0.55              |
| 7:H:79:PHE:CE2    | 7:H:105:PRO:HG2  | 2.37                     | 0.55              |
| 1:B:1226:VAL:HG22 | 1:B:1240:CYS:CB  | 2.33                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1242:VAL:HG12 | 1:B:1243:VAL:N    | 2.19                     | 0.55              |
| 1:B:1325:THR:O    | 1:B:1325:THR:CG2  | 2.54                     | 0.55              |
| 1:B:224:PHE:CG    | 1:B:231:PRO:HG3   | 2.41                     | 0.55              |
| 1:B:53:LEU:CD2    | 1:B:54:ASN:ND2    | 2.68                     | 0.55              |
| 1:B:666:ILE:HD12  | 1:B:666:ILE:N     | 2.21                     | 0.55              |
| 2:C:38:PHE:CD1    | 2:C:811:TYR:CD2   | 2.94                     | 0.55              |
| 2:C:577:ALA:HB1   | 2:C:589:VAL:CG1   | 2.27                     | 0.55              |
| 4:E:137:ASN:H     | 4:E:137:ASN:ND2   | 2.04                     | 0.55              |
| 5:F:135:PHE:CD2   | 5:F:140:LEU:HD21  | 2.38                     | 0.55              |
| 6:G:82:THR:CG2    | 6:G:84:TYR:H      | 2.16                     | 0.55              |
| 9:J:55:THR:HG22   | 9:J:55:THR:O      | 2.06                     | 0.55              |
| 9:J:59:VAL:C      | 9:J:61:ASP:H      | 2.10                     | 0.55              |
| 1:B:1266:THR:O    | 1:B:1270:ASN:HB2  | 2.06                     | 0.55              |
| 1:B:353:ILE:CG2   | 1:B:487:MET:HE3   | 2.35                     | 0.55              |
| 1:B:541:ILE:HG21  | 1:B:549:MET:CE    | 2.36                     | 0.55              |
| 2:C:757:PRO:HG3   | 2:C:1028:GLU:OE2  | 2.06                     | 0.55              |
| 2:C:418:LYS:HE2   | 2:C:422:LYS:NZ    | 2.21                     | 0.55              |
| 2:C:986:GLN:OE1   | 2:C:986:GLN:HA    | 2.05                     | 0.55              |
| 8:I:59:ILE:O      | 8:I:60:ALA:HB3    | 2.06                     | 0.55              |
| 1:B:1149:ALA:HB2  | 9:J:47:GLU:HA     | 1.88                     | 0.55              |
| 10:K:48:ARG:C     | 10:K:48:ARG:HD2   | 2.27                     | 0.55              |
| 15:T:21:DA:H2'    | 15:T:22:DT:O5'    | 2.03                     | 0.55              |
| 1:B:1210:GLY:O    | 1:B:1214:GLU:HG2  | 2.06                     | 0.55              |
| 1:B:1261:LYS:CA   | 1:B:1264:GLU:HB3  | 2.36                     | 0.55              |
| 1:B:1319:VAL:HG13 | 1:B:1320:PRO:HD2  | 1.88                     | 0.55              |
| 1:B:33:ALA:HB1    | 1:B:56:PRO:HB2    | 1.89                     | 0.55              |
| 2:C:25:ILE:HG22   | 2:C:29:ASP:CB     | 2.36                     | 0.55              |
| 2:C:552:MET:HA    | 2:C:555:ILE:HB    | 1.89                     | 0.55              |
| 2:C:708:GLU:O     | 2:C:710:LEU:N     | 2.39                     | 0.55              |
| 4:E:69:ALA:HA     | 4:E:72:ARG:HG3    | 1.88                     | 0.55              |
| 5:F:153:HIS:CE1   | 5:F:184:VAL:HG11  | 2.41                     | 0.55              |
| 7:H:31:LEU:HD22   | 7:H:48:VAL:HG21   | 1.89                     | 0.55              |
| 8:I:118:PHE:C     | 8:I:120:GLY:H     | 2.10                     | 0.55              |
| 9:J:5:ARG:O       | 9:J:14:LEU:HG     | 2.07                     | 0.55              |
| 10:K:23:ASN:C     | 10:K:25:LEU:N     | 2.60                     | 0.55              |
| 1:B:1280:GLU:O    | 1:B:1282:VAL:HG23 | 2.06                     | 0.55              |
| 1:B:244:PRO:HB2   | 1:B:245:PRO:CD    | 2.32                     | 0.55              |
| 1:B:322:VAL:O     | 1:B:322:VAL:HG12  | 2.07                     | 0.55              |
| 2:C:483:LEU:HD21  | 2:C:491:THR:HG23  | 1.89                     | 0.55              |
| 3:D:182:PRO:HG3   | 3:D:206:ASN:O     | 2.06                     | 0.55              |
| 6:G:130:ILE:O     | 6:G:148:VAL:HG21  | 2.06                     | 0.55              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:1002:GLY:HA3 | 1:B:1007:ILE:CG2  | 2.30                     | 0.55              |
| 1:B:230:ARG:N    | 1:B:233:TRP:HE3   | 2.02                     | 0.55              |
| 1:B:545:GLN:O    | 1:B:547:LEU:N     | 2.40                     | 0.55              |
| 2:C:221:ASN:OD1  | 2:C:242:SER:HA    | 2.06                     | 0.55              |
| 2:C:315:LYS:N    | 2:C:316:PRO:HD2   | 2.21                     | 0.55              |
| 2:C:273:LEU:HD22 | 2:C:360:PHE:CD1   | 2.42                     | 0.55              |
| 2:C:51:PHE:CD2   | 2:C:173:MET:HB3   | 2.41                     | 0.55              |
| 5:F:147:HIS:CD2  | 5:F:149:LEU:H     | 2.25                     | 0.55              |
| 7:H:153:GLN:HG3  | 7:H:154:VAL:HG23  | 1.87                     | 0.55              |
| 1:B:1351:GLU:O   | 1:B:1355:VAL:HG23 | 2.07                     | 0.55              |
| 1:B:61:ILE:HG22  | 1:B:62:ASP:N      | 2.22                     | 0.55              |
| 2:C:1008:PRO:HB2 | 2:C:1010:LEU:O    | 2.07                     | 0.55              |
| 2:C:508:LEU:O    | 2:C:509:ALA:HB3   | 2.07                     | 0.55              |
| 2:C:583:ASN:HD21 | 2:C:628:THR:CG2   | 2.20                     | 0.55              |
| 2:C:637:LEU:HD21 | 2:C:742:GLU:OE2   | 2.07                     | 0.55              |
| 2:C:520:GLY:N    | 2:C:748:ILE:HG22  | 2.19                     | 0.55              |
| 2:C:973:ILE:HG23 | 2:C:974:PRO:HD2   | 1.88                     | 0.55              |
| 5:F:78:LEU:HD21  | 5:F:80:VAL:CG2    | 2.37                     | 0.55              |
| 1:B:1149:ALA:CB  | 9:J:47:GLU:HA     | 2.36                     | 0.55              |
| 1:B:150:THR:HG23 | 1:B:166:GLY:HA2   | 1.89                     | 0.55              |
| 1:B:608:ILE:C    | 1:B:610:GLY:H     | 2.10                     | 0.55              |
| 2:C:60:GLN:HE22  | 2:C:94:LYS:HA     | 1.72                     | 0.55              |
| 3:D:80:LEU:HD22  | 3:D:129:ILE:HD13  | 1.88                     | 0.55              |
| 5:F:43:LYS:O     | 5:F:45:LYS:N      | 2.40                     | 0.55              |
| 7:H:143:ILE:CG2  | 7:H:144:ARG:H     | 2.20                     | 0.55              |
| 7:H:81:PRO:HG3   | 7:H:106:MET:SD    | 2.46                     | 0.55              |
| 8:I:130:ARG:HA   | 8:I:133:ASN:HB2   | 1.89                     | 0.55              |
| 8:I:139:ASN:O    | 8:I:140:ALA:CB    | 2.55                     | 0.55              |
| 10:K:8:PHE:H     | 10:K:49:MET:HE1   | 1.70                     | 0.55              |
| 11:L:93:SER:O    | 11:L:97:LYS:HG3   | 2.06                     | 0.55              |
| 1:B:407:ARG:HG2  | 1:B:430:TRP:CZ2   | 2.41                     | 0.55              |
| 1:B:682:THR:HG23 | 1:B:728:LYS:CE    | 2.22                     | 0.55              |
| 1:B:828:ALA:HB3  | 2:C:530:GLY:HA2   | 1.87                     | 0.55              |
| 2:C:654:ARG:N    | 2:C:657:HIS:HD2   | 1.96                     | 0.55              |
| 3:D:11:ARG:HD3   | 3:D:209:TYR:OH    | 2.07                     | 0.55              |
| 4:E:35:LEU:HA    | 4:E:47:LEU:HB2    | 1.89                     | 0.55              |
| 5:F:121:MET:O    | 5:F:124:VAL:HG23  | 2.07                     | 0.55              |
| 1:B:185:TRP:HZ3  | 1:B:200:ARG:HG2   | 1.71                     | 0.54              |
| 1:B:586:ILE:HG22 | 1:B:587:HIS:H     | 1.69                     | 0.54              |
| 2:C:1103:ILE:O   | 2:C:1122:ARG:NH1  | 2.40                     | 0.54              |
| 2:C:423:LYS:HE2  | 2:C:470:LYS:HZ1   | 1.72                     | 0.54              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:843:GLN:O    | 2:C:844:SER:C     | 2.45                     | 0.54              |
| 3:D:212:PRO:HB3  | 3:D:213:PRO:HD2   | 1.89                     | 0.54              |
| 4:E:5:THR:CG2    | 7:H:9:LEU:HB2     | 2.36                     | 0.54              |
| 5:F:157:SER:C    | 5:F:159:ASP:H     | 2.09                     | 0.54              |
| 5:F:78:LEU:C     | 5:F:78:LEU:HD23   | 2.28                     | 0.54              |
| 1:B:503:GLN:HE21 | 6:G:90:ARG:HH21   | 1.54                     | 0.54              |
| 1:B:172:PRO:HB3  | 1:B:185:TRP:CD2   | 2.42                     | 0.54              |
| 1:B:206:GLU:O    | 1:B:210:ILE:HG13  | 2.07                     | 0.54              |
| 1:B:29:ALA:HB1   | 2:C:1184:GLY:CA   | 2.36                     | 0.54              |
| 1:B:709:THR:HG22 | 1:B:710:LEU:N     | 2.22                     | 0.54              |
| 1:B:827:THR:CG2  | 1:B:828:ALA:N     | 2.70                     | 0.54              |
| 1:B:87:ALA:HB3   | 1:B:276:LEU:CD2   | 2.37                     | 0.54              |
| 2:C:361:LEU:HD21 | 2:C:377:PHE:HB3   | 1.88                     | 0.54              |
| 3:D:46:ILE:CG2   | 3:D:157:CYS:HB3   | 2.35                     | 0.54              |
| 3:D:44:LEU:HG    | 3:D:159:ALA:HB1   | 1.88                     | 0.54              |
| 3:D:173:ALA:O    | 3:D:174:ALA:HB3   | 2.06                     | 0.54              |
| 3:D:34:ARG:O     | 3:D:38:ILE:HG13   | 2.07                     | 0.54              |
| 7:H:3:PHE:CD1    | 7:H:80:LYS:NZ     | 2.75                     | 0.54              |
| 8:I:107:VAL:O    | 8:I:108:SER:O     | 2.25                     | 0.54              |
| 1:B:54:ASN:HD21  | 1:B:247:ARG:HH12  | 1.55                     | 0.54              |
| 1:B:374:LEU:CB   | 1:B:436:ILE:HD11  | 2.37                     | 0.54              |
| 1:B:829:VAL:C    | 1:B:831:THR:H     | 2.10                     | 0.54              |
| 2:C:485:ARG:NH2  | 2:C:782:LEU:HD11  | 2.22                     | 0.54              |
| 2:C:942:ARG:O    | 2:C:944:THR:N     | 2.41                     | 0.54              |
| 5:F:22:MET:HE3   | 5:F:26:ARG:HE     | 1.71                     | 0.54              |
| 6:G:89:GLU:OE2   | 6:G:134:ILE:HG21  | 2.07                     | 0.54              |
| 12:M:38:LEU:CD1  | 12:M:49:LYS:HG2   | 2.38                     | 0.54              |
| 1:B:172:PRO:HD3  | 1:B:185:TRP:CE2   | 2.43                     | 0.54              |
| 1:B:347:PHE:HE2  | 1:B:375:THR:HG23  | 1.73                     | 0.54              |
| 1:B:356:ASP:CB   | 1:B:469:ARG:HH12  | 2.08                     | 0.54              |
| 1:B:498:ARG:HA   | 1:B:501:LEU:HD12  | 1.88                     | 0.54              |
| 1:B:765:VAL:HG23 | 1:B:802:ASN:O     | 2.07                     | 0.54              |
| 1:B:896:ARG:NH2  | 1:B:1030:ARG:NH2  | 2.56                     | 0.54              |
| 2:C:1095:LEU:N   | 2:C:1095:LEU:HD12 | 2.22                     | 0.54              |
| 2:C:542:MET:HE2  | 2:C:743:ILE:HG13  | 1.89                     | 0.54              |
| 4:E:53:SER:H     | 4:E:148:LEU:HD21  | 1.72                     | 0.54              |
| 5:F:93:MET:HE3   | 5:F:123:LEU:HB2   | 1.87                     | 0.54              |
| 8:I:40:LEU:HD22  | 8:I:123:MET:CE    | 2.37                     | 0.54              |
| 8:I:135:LEU:HD13 | 8:I:137:GLN:NE2   | 2.19                     | 0.54              |
| 9:J:35:VAL:HG12  | 9:J:36:GLU:H      | 1.73                     | 0.54              |
| 11:L:19:LEU:HD21 | 11:L:35:PHE:CE2   | 2.42                     | 0.54              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 15:T:19:DT:H2'    | 15:T:20:DT:C6    | 2.42                     | 0.54              |
| 1:B:1213:GLY:O    | 1:B:1214:GLU:C   | 2.45                     | 0.54              |
| 1:B:1394:THR:HG22 | 1:B:1395:GLY:N   | 2.21                     | 0.54              |
| 1:B:353:ILE:CD1   | 1:B:487:MET:HE2  | 2.36                     | 0.54              |
| 1:B:69:THR:C      | 1:B:71:GLN:N     | 2.61                     | 0.54              |
| 1:B:18:GLN:CB     | 2:C:1215:ARG:HB2 | 2.37                     | 0.54              |
| 2:C:312:GLU:O     | 2:C:315:LYS:HB2  | 2.07                     | 0.54              |
| 2:C:240:ILE:HG21  | 2:C:381:MET:HE1  | 1.89                     | 0.54              |
| 2:C:693:ILE:HD11  | 2:C:740:HIS:CD2  | 2.43                     | 0.54              |
| 2:C:984:HIS:NE2   | 2:C:1025:HIS:HA  | 2.23                     | 0.54              |
| 3:D:174:ALA:O     | 3:D:175:ALA:HB2  | 2.08                     | 0.54              |
| 4:E:160:VAL:O     | 4:E:164:ILE:HG13 | 2.06                     | 0.54              |
| 6:G:86:THR:HG23   | 6:G:89:GLU:OE1   | 2.08                     | 0.54              |
| 9:J:34:TYR:CD2    | 9:J:35:VAL:N     | 2.75                     | 0.54              |
| 1:B:1144:LYS:HD2  | 1:B:1268:LEU:O   | 2.08                     | 0.54              |
| 1:B:1308:THR:HG23 | 1:B:1309:ASP:N   | 2.21                     | 0.54              |
| 1:B:149:GLU:HB2   | 1:B:164:ARG:HH21 | 1.72                     | 0.54              |
| 1:B:500:GLU:OE2   | 2:C:1145:SER:HB2 | 2.06                     | 0.54              |
| 1:B:853:ASP:OD1   | 1:B:855:THR:HG22 | 2.08                     | 0.54              |
| 2:C:1001:PHE:CZ   | 2:C:1073:TYR:HB2 | 2.42                     | 0.54              |
| 2:C:314:LEU:O     | 2:C:318:VAL:HG23 | 2.08                     | 0.54              |
| 2:C:449:ASN:C     | 2:C:451:LYS:H    | 2.10                     | 0.54              |
| 2:C:642:ASP:CB    | 2:C:649:LYS:HG3  | 2.38                     | 0.54              |
| 3:D:255:VAL:HG12  | 11:L:91:CYS:HB3  | 1.90                     | 0.54              |
| 3:D:175:ALA:HB3   | 10:K:43:ARG:HH22 | 1.71                     | 0.54              |
| 1:B:472:LEU:HD11  | 2:C:835:GLN:NE2  | 2.22                     | 0.54              |
| 1:B:809:THR:H     | 1:B:812:GLU:HB2  | 1.71                     | 0.54              |
| 1:B:91:PHE:N      | 1:B:297:GLN:HE22 | 2.04                     | 0.54              |
| 1:B:901:LEU:H     | 1:B:926:GLN:CD   | 2.10                     | 0.54              |
| 2:C:1001:PHE:CE2  | 3:D:34:ARG:CZ    | 2.91                     | 0.54              |
| 2:C:1084:GLN:OE1  | 3:D:189:THR:HG22 | 2.08                     | 0.54              |
| 2:C:393:LYS:CE    | 2:C:393:LYS:HA   | 2.35                     | 0.54              |
| 2:C:247:GLY:H     | 2:C:418:LYS:HZ1  | 1.54                     | 0.54              |
| 3:D:35:ARG:HA     | 3:D:38:ILE:HD12  | 1.89                     | 0.54              |
| 4:E:118:THR:HB    | 4:E:121:LYS:CB   | 2.38                     | 0.54              |
| 4:E:141:LEU:HD12  | 4:E:141:LEU:O    | 2.07                     | 0.54              |
| 4:E:207:LEU:HD12  | 4:E:207:LEU:O    | 2.08                     | 0.54              |
| 6:G:116:ASP:O     | 6:G:120:ILE:HG13 | 2.07                     | 0.54              |
| 7:H:14:HIS:CD2    | 7:H:16:SER:CB    | 2.91                     | 0.54              |
| 9:J:93:LYS:CD     | 9:J:93:LYS:H     | 2.18                     | 0.54              |
| 15:T:25:DC:N4     | 15:T:26:DA:N6    | 2.34                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:367:PRO:HB3   | 1:B:466:SER:HA    | 1.89                     | 0.54              |
| 1:B:471:ASN:OD1   | 1:B:472:LEU:N     | 2.41                     | 0.54              |
| 1:B:639:PRO:HG2   | 1:B:640:GLN:N     | 2.22                     | 0.54              |
| 1:B:834:THR:HG21  | 1:B:1077:THR:CA   | 2.38                     | 0.54              |
| 1:B:977:LYS:HB3   | 1:B:978:PRO:HD2   | 1.89                     | 0.54              |
| 2:C:1183:LYS:O    | 2:C:1183:LYS:HE3  | 2.06                     | 0.54              |
| 2:C:357:GLN:O     | 2:C:366:GLN:HA    | 2.08                     | 0.54              |
| 2:C:601:ARG:O     | 2:C:605:ARG:HG3   | 2.08                     | 0.54              |
| 2:C:651:LEU:HD11  | 2:C:707:PRO:HB3   | 1.89                     | 0.54              |
| 5:F:213:ILE:HG12  | 5:F:214:CYS:H     | 1.69                     | 0.54              |
| 1:B:1152:ILE:HD11 | 9:J:44:TYR:HD2    | 1.73                     | 0.54              |
| 1:B:17:VAL:HG23   | 1:B:1421:CYS:SG   | 2.48                     | 0.54              |
| 1:B:251:SER:HA    | 1:B:257:ARG:O     | 2.08                     | 0.54              |
| 1:B:35:ILE:HD13   | 1:B:241:VAL:HG11  | 1.88                     | 0.54              |
| 1:B:443:LEU:HD12  | 2:C:1146:PHE:CE2  | 2.42                     | 0.54              |
| 1:B:485:ASP:OD1   | 14:P:10:A:H4'     | 2.08                     | 0.54              |
| 1:B:827:THR:O     | 1:B:831:THR:HB    | 2.08                     | 0.54              |
| 2:C:762:ASN:ND2   | 2:C:1024:ALA:HB3  | 2.18                     | 0.54              |
| 2:C:25:ILE:HD12   | 2:C:651:LEU:CD1   | 2.36                     | 0.54              |
| 2:C:274:PRO:O     | 2:C:275:TYR:HB2   | 2.07                     | 0.54              |
| 2:C:365:THR:HG21  | 2:C:370:PHE:CD1   | 2.43                     | 0.54              |
| 2:C:642:ASP:CA    | 2:C:649:LYS:HG3   | 2.38                     | 0.54              |
| 2:C:745:PRO:C     | 2:C:747:MET:N     | 2.60                     | 0.54              |
| 5:F:14:ARG:HH21   | 5:F:141:VAL:CG1   | 2.21                     | 0.54              |
| 7:H:44:TYR:CD2    | 7:H:105:PRO:HB2   | 2.43                     | 0.54              |
| 8:I:59:ILE:CG2    | 8:I:60:ALA:N      | 2.56                     | 0.54              |
| 1:B:1022:LEU:CD1  | 1:B:1026:LEU:HD12 | 2.38                     | 0.54              |
| 1:B:115:LEU:HD12  | 1:B:142:CYS:HB3   | 1.89                     | 0.54              |
| 1:B:1349:TYR:HE1  | 1:B:1368:MET:HE3  | 1.73                     | 0.54              |
| 1:B:834:THR:HG21  | 1:B:1077:THR:OG1  | 2.08                     | 0.54              |
| 2:C:1015:HIS:O    | 2:C:1018:PRO:HD2  | 2.08                     | 0.54              |
| 1:B:490:HIS:HB3   | 2:C:1150:ARG:NH1  | 2.22                     | 0.54              |
| 2:C:1180:PHE:O    | 2:C:1181:GLU:O    | 2.26                     | 0.54              |
| 3:D:246:ARG:HA    | 3:D:249:ASP:HB3   | 1.89                     | 0.54              |
| 1:B:1324:PRO:HB2  | 5:F:142:VAL:HG11  | 1.88                     | 0.54              |
| 1:B:1343:ALA:HB2  | 5:F:150:VAL:CG2   | 2.35                     | 0.54              |
| 1:B:1152:ILE:HG13 | 9:J:44:TYR:HB3    | 1.90                     | 0.54              |
| 11:L:18:LYS:HZ2   | 11:L:38:GLU:HG2   | 1.71                     | 0.54              |
| 11:L:48:ALA:O     | 11:L:51:LEU:N     | 2.39                     | 0.54              |
| 1:B:1254:ALA:O    | 1:B:1255:GLU:HB2  | 2.07                     | 0.53              |
| 1:B:1329:THR:CG2  | 1:B:1331:SER:HB3  | 2.38                     | 0.53              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:101:MET:HA    | 2:C:112:LEU:H    | 1.73                     | 0.53              |
| 2:C:288:ALA:CB    | 2:C:331:LEU:HD12 | 2.38                     | 0.53              |
| 2:C:653:VAL:HA    | 2:C:689:LEU:HD22 | 1.89                     | 0.53              |
| 1:B:1001:ARG:NE   | 6:G:83:PRO:HD3   | 2.23                     | 0.53              |
| 8:I:15:VAL:HA     | 8:I:26:ILE:HG12  | 1.90                     | 0.53              |
| 1:B:152:VAL:CG1   | 1:B:153:PRO:HD2  | 2.38                     | 0.53              |
| 1:B:709:THR:HB    | 1:B:712:GLU:H    | 1.73                     | 0.53              |
| 1:B:858:ASN:HD22  | 1:B:858:ASN:C    | 2.11                     | 0.53              |
| 2:C:117:ALA:CB    | 2:C:122:LEU:HB2  | 2.38                     | 0.53              |
| 2:C:642:ASP:CA    | 2:C:649:LYS:HA   | 2.29                     | 0.53              |
| 3:D:52:GLU:HA     | 12:M:64:LEU:HD22 | 1.90                     | 0.53              |
| 11:L:40:HIS:O     | 11:L:43:GLY:N    | 2.41                     | 0.53              |
| 11:L:58:PHE:CD1   | 11:L:59:ALA:N    | 2.76                     | 0.53              |
| 1:B:1264:GLU:HG3  | 1:B:1265:ASN:N   | 2.22                     | 0.53              |
| 1:B:1118:VAL:CG2  | 1:B:1306:LEU:HB2 | 2.38                     | 0.53              |
| 1:B:524:VAL:CG1   | 1:B:525:GLN:N    | 2.71                     | 0.53              |
| 1:B:606:LEU:HB3   | 1:B:614:PHE:CD2  | 2.44                     | 0.53              |
| 1:B:896:ARG:HD3   | 1:B:897:TYR:CE1  | 2.44                     | 0.53              |
| 2:C:100:PRO:HD3   | 2:C:172:ILE:CD1  | 2.38                     | 0.53              |
| 2:C:112:LEU:HD12  | 2:C:113:TYR:H    | 1.72                     | 0.53              |
| 2:C:23:ALA:HB1    | 2:C:24:PRO:CD    | 2.29                     | 0.53              |
| 2:C:365:THR:HG23  | 2:C:367:LEU:N    | 2.23                     | 0.53              |
| 2:C:400:HIS:O     | 2:C:402:GLY:N    | 2.41                     | 0.53              |
| 2:C:498:THR:CG2   | 2:C:537:LYS:HB2  | 2.38                     | 0.53              |
| 2:C:653:VAL:HG22  | 2:C:689:LEU:HB3  | 1.90                     | 0.53              |
| 2:C:707:PRO:HG2   | 2:C:708:GLU:H    | 1.72                     | 0.53              |
| 1:B:526:ASP:HB2   | 2:C:835:GLN:OE1  | 2.07                     | 0.53              |
| 3:D:69:LEU:HD12   | 3:D:69:LEU:H     | 1.73                     | 0.53              |
| 4:E:154:PHE:CE2   | 4:E:163:VAL:HG21 | 2.43                     | 0.53              |
| 5:F:156:LEU:HD12  | 5:F:195:VAL:CB   | 2.32                     | 0.53              |
| 5:F:192:ARG:O     | 5:F:192:ARG:HG2  | 2.07                     | 0.53              |
| 8:I:32:THR:HG22   | 8:I:33:GLN:OE1   | 2.07                     | 0.53              |
| 9:J:76:PRO:HD2    | 9:J:108:HIS:HD2  | 1.73                     | 0.53              |
| 9:J:111:THR:CG2   | 9:J:112:SER:H    | 2.18                     | 0.53              |
| 15:T:18:DT:OP2    | 15:T:18:DT:C7    | 2.57                     | 0.53              |
| 15:T:24:DG:C2     | 15:T:25:DC:H1'   | 2.43                     | 0.53              |
| 1:B:416:ARG:HG3   | 1:B:417:TYR:CE2  | 2.44                     | 0.53              |
| 1:B:365:GLY:HA3   | 1:B:463:ILE:HD13 | 1.91                     | 0.53              |
| 2:C:807:ARG:HG2   | 2:C:1045:SER:OG  | 2.08                     | 0.53              |
| 2:C:1115:THR:HG22 | 2:C:1117:GLN:HG3 | 1.91                     | 0.53              |
| 2:C:1183:LYS:C    | 2:C:1185:CYS:H   | 2.12                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:233:PRO:HG2   | 2:C:234:ILE:HD13  | 1.90                     | 0.53              |
| 2:C:273:LEU:O     | 2:C:276:ILE:HB    | 2.07                     | 0.53              |
| 2:C:308:TRP:HZ3   | 9:J:45:ARG:HB3    | 1.72                     | 0.53              |
| 2:C:165:VAL:HG11  | 2:C:448:ILE:HD13  | 1.91                     | 0.53              |
| 2:C:46:GLN:HG3    | 2:C:47:GLN:N      | 2.14                     | 0.53              |
| 2:C:483:LEU:CD1   | 2:C:491:THR:HG23  | 2.31                     | 0.53              |
| 2:C:53:GLN:HG2    | 2:C:547:VAL:HG21  | 1.90                     | 0.53              |
| 3:D:65:HIS:CE1    | 3:D:69:LEU:HD11   | 2.42                     | 0.53              |
| 6:G:76:LYS:O      | 6:G:79:ARG:HD2    | 2.08                     | 0.53              |
| 11:L:65:HIS:C     | 11:L:65:HIS:CD2   | 2.82                     | 0.53              |
| 11:L:68:PHE:CD1   | 11:L:70:ARG:NH1   | 2.76                     | 0.53              |
| 1:B:10:PRO:HD2    | 2:C:1191:ILE:O    | 2.09                     | 0.53              |
| 1:B:1431:GLY:HA3  | 2:C:1152:MET:HE2  | 1.91                     | 0.53              |
| 1:B:215:SER:HB3   | 1:B:218:ASP:CG    | 2.29                     | 0.53              |
| 1:B:332:LYS:H     | 1:B:337:ARG:HB3   | 1.74                     | 0.53              |
| 1:B:32:VAL:O      | 1:B:57:ARG:HD3    | 2.09                     | 0.53              |
| 1:B:760:GLN:HG2   | 1:B:765:VAL:HA    | 1.89                     | 0.53              |
| 2:C:1110:PRO:HG3  | 2:C:1124:ARG:O    | 2.08                     | 0.53              |
| 2:C:431:TYR:CG    | 2:C:447:ALA:HB2   | 2.42                     | 0.53              |
| 2:C:516:ASN:ND2   | 2:C:516:ASN:N     | 2.30                     | 0.53              |
| 2:C:642:ASP:C     | 2:C:644:GLU:H     | 2.11                     | 0.53              |
| 2:C:1006:ILE:HD13 | 10:K:44:TYR:HE2   | 1.74                     | 0.53              |
| 1:B:547:LEU:HD13  | 11:L:58:PHE:HD1   | 1.74                     | 0.53              |
| 12:M:49:LYS:O     | 12:M:50:ASP:CB    | 2.47                     | 0.53              |
| 1:B:1370:LEU:O    | 1:B:1373:ASP:HB2  | 2.09                     | 0.53              |
| 1:B:399:HIS:CB    | 1:B:400:PRO:CD    | 2.86                     | 0.53              |
| 1:B:53:LEU:CD2    | 1:B:54:ASN:N      | 2.68                     | 0.53              |
| 1:B:62:ASP:HB3    | 1:B:64:ASN:ND2    | 2.23                     | 0.53              |
| 3:D:183:TRP:CZ2   | 3:D:207:CYS:HB3   | 2.44                     | 0.53              |
| 7:H:49:LEU:HD21   | 7:H:77:VAL:HB     | 1.89                     | 0.53              |
| 15:T:20:DT:C3'    | 15:T:21:DA:H5'    | 2.34                     | 0.53              |
| 1:B:1197:LEU:HD11 | 1:B:1238:ILE:HD11 | 1.90                     | 0.53              |
| 1:B:382:PRO:CD    | 1:B:428:TYR:CE2   | 2.89                     | 0.53              |
| 1:B:401:GLY:CA    | 1:B:435:HIS:HD2   | 2.22                     | 0.53              |
| 1:B:814:PHE:O     | 1:B:817:ALA:HB3   | 2.09                     | 0.53              |
| 1:B:947:PHE:CD1   | 1:B:947:PHE:N     | 2.76                     | 0.53              |
| 1:B:30:ILE:HG23   | 2:C:1170:THR:HG23 | 1.91                     | 0.53              |
| 2:C:233:PRO:HG2   | 2:C:234:ILE:CD1   | 2.38                     | 0.53              |
| 2:C:224:GLN:O     | 2:C:238:ALA:HA    | 2.08                     | 0.53              |
| 2:C:309:GLN:O     | 2:C:312:GLU:HB3   | 2.08                     | 0.53              |
| 2:C:510:LYS:CB    | 2:C:511:PRO:HD3   | 2.39                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:98:VAL:HG23   | 3:D:122:SER:HB3   | 1.90                     | 0.53              |
| 4:E:216:ASN:O     | 4:E:218:GLU:N     | 2.42                     | 0.53              |
| 8:I:106:GLU:HG2   | 8:I:112:ILE:HG12  | 1.91                     | 0.53              |
| 8:I:47:PHE:CD2    | 8:I:95:TYR:HD1    | 2.27                     | 0.53              |
| 8:I:81:PRO:HB2    | 8:I:82:PRO:CD     | 2.36                     | 0.53              |
| 8:I:89:LEU:C      | 8:I:91:ASP:N      | 2.60                     | 0.53              |
| 11:L:19:LEU:HD21  | 11:L:35:PHE:CD2   | 2.42                     | 0.53              |
| 12:M:34:CYS:O     | 12:M:36:SER:N     | 2.41                     | 0.53              |
| 1:B:963:ILE:HD11  | 1:B:1048:ASN:HB2  | 1.89                     | 0.53              |
| 1:B:711:ARG:O     | 1:B:714:PHE:HB3   | 2.08                     | 0.53              |
| 1:B:75:ASN:O      | 1:B:76:GLU:CB     | 2.57                     | 0.53              |
| 1:B:783:THR:HG22  | 1:B:784:LEU:CD2   | 2.38                     | 0.53              |
| 2:C:1147:LEU:HD23 | 2:C:1148:LYS:N    | 2.24                     | 0.53              |
| 2:C:114:PRO:HD3   | 2:C:124:TYR:CE1   | 2.44                     | 0.53              |
| 2:C:292:ILE:HG23  | 2:C:325:GLN:O     | 2.08                     | 0.53              |
| 2:C:637:LEU:HD22  | 2:C:741:CYS:O     | 2.09                     | 0.53              |
| 2:C:990:ILE:CG2   | 2:C:991:GLY:N     | 2.71                     | 0.53              |
| 3:D:134:ILE:HG23  | 3:D:141:GLY:H     | 1.74                     | 0.53              |
| 6:G:110:ASP:O     | 6:G:112:GLU:N     | 2.42                     | 0.53              |
| 1:B:1152:ILE:CG1  | 9:J:44:TYR:HB3    | 2.39                     | 0.53              |
| 9:J:74:GLU:HB2    | 9:J:79:HIS:HA     | 1.89                     | 0.53              |
| 10:K:3:VAL:CG2    | 10:K:18:TRP:HB2   | 2.34                     | 0.53              |
| 1:B:1106:ASN:O    | 1:B:1107:VAL:HB   | 2.09                     | 0.53              |
| 1:B:1224:LEU:HD12 | 1:B:1241:ARG:O    | 2.08                     | 0.53              |
| 1:B:1308:THR:HG23 | 1:B:1310:GLY:H    | 1.74                     | 0.53              |
| 1:B:1316:VAL:HG12 | 1:B:1316:VAL:O    | 2.09                     | 0.53              |
| 1:B:1438:THR:HB   | 2:C:1144:ALA:CB   | 2.36                     | 0.53              |
| 1:B:1454:MET:HG3  | 1:B:1454:MET:O    | 2.09                     | 0.53              |
| 1:B:504:LEU:HD11  | 6:G:91:ALA:CB     | 2.38                     | 0.53              |
| 1:B:668:ASP:OD1   | 1:B:741:ASN:ND2   | 2.42                     | 0.53              |
| 2:C:1106:ARG:HD3  | 2:C:1126:GLY:O    | 2.09                     | 0.53              |
| 2:C:1162:ILE:HD11 | 2:C:1194:ILE:HD13 | 1.90                     | 0.53              |
| 2:C:96:TYR:N      | 2:C:129:PHE:O     | 2.30                     | 0.53              |
| 2:C:203:PHE:HB3   | 2:C:205:ILE:HD11  | 1.91                     | 0.53              |
| 2:C:370:PHE:HD2   | 2:C:373:ARG:CD    | 2.22                     | 0.53              |
| 2:C:613:VAL:HG13  | 2:C:627:PHE:O     | 2.08                     | 0.53              |
| 2:C:889:THR:HG22  | 2:C:891:ASP:H     | 1.74                     | 0.53              |
| 4:E:66:ARG:O      | 4:E:70:PHE:HB2    | 2.08                     | 0.53              |
| 6:G:93:ILE:HD13   | 6:G:148:VAL:HG12  | 1.91                     | 0.53              |
| 8:I:25:ARG:HA     | 8:I:41:ASP:HA     | 1.90                     | 0.53              |
| 1:B:1152:ILE:HD11 | 9:J:44:TYR:HB3    | 1.90                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1323:ASP:O    | 1:B:1325:THR:N    | 2.38                     | 0.53              |
| 1:B:34:LYS:CG     | 1:B:36:ARG:HH21   | 2.22                     | 0.53              |
| 1:B:416:ARG:C     | 1:B:417:TYR:CD2   | 2.80                     | 0.53              |
| 1:B:527:THR:CG2   | 1:B:650:GLN:HA    | 2.39                     | 0.53              |
| 1:B:548:ASN:HA    | 11:L:60:ALA:HB1   | 1.91                     | 0.53              |
| 2:C:430:ARG:O     | 2:C:434:ARG:HD2   | 2.08                     | 0.53              |
| 2:C:750:GLY:O     | 2:C:751:VAL:C     | 2.46                     | 0.53              |
| 4:E:185:CYS:HB2   | 4:E:211:LEU:CD2   | 2.29                     | 0.53              |
| 7:H:27:LYS:O      | 7:H:30:LEU:N      | 2.41                     | 0.53              |
| 8:I:55:LEU:HD22   | 8:I:144:ILE:HG21  | 1.90                     | 0.53              |
| 1:B:1443:VAL:HG23 | 1:B:1443:VAL:O    | 2.09                     | 0.52              |
| 1:B:249:SER:O     | 1:B:250:ILE:HG13  | 2.09                     | 0.52              |
| 1:B:416:ARG:HG3   | 1:B:417:TYR:CD2   | 2.44                     | 0.52              |
| 1:B:470:LEU:H     | 1:B:470:LEU:CD2   | 2.17                     | 0.52              |
| 1:B:551:TYR:CE2   | 11:L:62:LYS:HE2   | 2.44                     | 0.52              |
| 1:B:774:ARG:NH2   | 1:B:797:LYS:HB2   | 2.24                     | 0.52              |
| 2:C:1177:HIS:CB   | 2:C:1179:GLN:HE21 | 2.21                     | 0.52              |
| 2:C:117:ALA:HA    | 2:C:122:LEU:HD12  | 1.90                     | 0.52              |
| 2:C:999:MET:HG3   | 2:C:1000:PRO:CD   | 2.33                     | 0.52              |
| 3:D:208:GLU:C     | 3:D:210:GLU:H     | 2.13                     | 0.52              |
| 4:E:217:LEU:O     | 4:E:219:THR:N     | 2.41                     | 0.52              |
| 1:B:1239:ARG:HB3  | 1:B:1239:ARG:HH11 | 1.74                     | 0.52              |
| 1:B:1323:ASP:C    | 1:B:1325:THR:H    | 2.12                     | 0.52              |
| 1:B:1348:LEU:O    | 1:B:1352:VAL:HG23 | 2.08                     | 0.52              |
| 1:B:54:ASN:ND2    | 1:B:247:ARG:HH12  | 2.07                     | 0.52              |
| 1:B:593:GLU:C     | 1:B:595:THR:H     | 2.12                     | 0.52              |
| 1:B:528:LEU:CD2   | 1:B:751:SER:HB3   | 2.38                     | 0.52              |
| 1:B:860:LEU:CD1   | 1:B:1393:ASN:HD22 | 2.22                     | 0.52              |
| 2:C:827:ILE:HG12  | 2:C:1012:ILE:HG13 | 1.91                     | 0.52              |
| 2:C:44:VAL:HG11   | 2:C:199:MET:HG2   | 1.91                     | 0.52              |
| 2:C:304:ASP:OD1   | 2:C:306:ASN:HB2   | 2.09                     | 0.52              |
| 2:C:212:LEU:HD21  | 2:C:461:LEU:HG    | 1.90                     | 0.52              |
| 2:C:582:VAL:HG23  | 2:C:626:ILE:HB    | 1.91                     | 0.52              |
| 2:C:732:SER:HB2   | 2:C:734:HIS:CD2   | 2.44                     | 0.52              |
| 2:C:758:PHE:CZ    | 2:C:1044:ALA:HA   | 2.44                     | 0.52              |
| 2:C:844:SER:HB3   | 2:C:848:ARG:NH1   | 2.24                     | 0.52              |
| 2:C:955:THR:HG22  | 2:C:956:THR:O     | 2.09                     | 0.52              |
| 3:D:239:PRO:HB2   | 3:D:241:ASP:OD1   | 2.09                     | 0.52              |
| 3:D:255:VAL:O     | 3:D:255:VAL:HG12  | 2.09                     | 0.52              |
| 5:F:108:GLY:HA3   | 5:F:132:ILE:HG22  | 1.90                     | 0.52              |
| 7:H:79:PHE:CE2    | 7:H:105:PRO:CG    | 2.93                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:L:17:SER:O     | 11:L:18:LYS:C     | 2.45                     | 0.52              |
| 1:B:1313:LEU:HD23 | 1:B:1338:VAL:HG21 | 1.91                     | 0.52              |
| 1:B:388:LEU:CD2   | 1:B:432:VAL:HB    | 2.37                     | 0.52              |
| 1:B:442:VAL:O     | 1:B:457:ALA:HA    | 2.10                     | 0.52              |
| 1:B:883:LEU:CD2   | 1:B:1021:LEU:HB2  | 2.40                     | 0.52              |
| 2:C:1174:LYS:O    | 2:C:1176:ASN:N    | 2.42                     | 0.52              |
| 2:C:90:ILE:HG23   | 2:C:133:LYS:O     | 2.09                     | 0.52              |
| 2:C:44:VAL:O      | 2:C:45:SER:C      | 2.48                     | 0.52              |
| 2:C:899:ILE:HG22  | 2:C:903:VAL:HG21  | 1.91                     | 0.52              |
| 2:C:95:ILE:HG13   | 2:C:129:PHE:O     | 2.08                     | 0.52              |
| 8:I:26:ILE:HG23   | 8:I:27:GLU:N      | 2.24                     | 0.52              |
| 1:B:1193:LEU:CD2  | 1:B:1260:LEU:HD11 | 2.32                     | 0.52              |
| 1:B:1427:ASN:O    | 1:B:1431:GLY:N    | 2.41                     | 0.52              |
| 1:B:172:PRO:HG3   | 1:B:185:TRP:CZ2   | 2.45                     | 0.52              |
| 1:B:399:HIS:O     | 1:B:401:GLY:N     | 2.43                     | 0.52              |
| 1:B:541:ILE:HG22  | 1:B:546:VAL:HG23  | 1.90                     | 0.52              |
| 2:C:1001:PHE:CE1  | 2:C:1073:TYR:HB2  | 2.45                     | 0.52              |
| 1:B:1428:VAL:HG22 | 2:C:1151:LEU:HD21 | 1.90                     | 0.52              |
| 2:C:298:LEU:N     | 2:C:298:LEU:HD22  | 2.24                     | 0.52              |
| 3:D:7:GLN:HG2     | 11:L:104:ASN:ND2  | 2.19                     | 0.52              |
| 4:E:192:LYS:HD2   | 4:E:199:ASN:HA    | 1.91                     | 0.52              |
| 6:G:79:ARG:HB3    | 6:G:144:GLU:OE1   | 2.09                     | 0.52              |
| 1:B:332:LYS:CA    | 1:B:337:ARG:HD2   | 2.39                     | 0.52              |
| 1:B:556:TRP:CE3   | 1:B:558:GLY:HA2   | 2.45                     | 0.52              |
| 2:C:1106:ARG:HG3  | 2:C:1107:ALA:N    | 2.23                     | 0.52              |
| 2:C:1120:GLU:HG2  | 2:C:1121:GLY:N    | 2.23                     | 0.52              |
| 2:C:240:ILE:HG22  | 2:C:254:LEU:HB3   | 1.91                     | 0.52              |
| 2:C:34:ILE:HD13   | 2:C:747:MET:HE2   | 1.91                     | 0.52              |
| 2:C:825:VAL:HG13  | 2:C:826:ALA:H     | 1.73                     | 0.52              |
| 2:C:995:ARG:NH1   | 3:D:165:LYS:HA    | 2.25                     | 0.52              |
| 3:D:18:VAL:HG12   | 3:D:18:VAL:O      | 2.09                     | 0.52              |
| 1:B:1289:ARG:NH1  | 1:B:1326:ARG:NH1  | 2.58                     | 0.52              |
| 1:B:1364:ASN:O    | 1:B:1366:ARG:HG3  | 2.10                     | 0.52              |
| 1:B:747:VAL:HG21  | 1:B:758:ILE:HD11  | 1.91                     | 0.52              |
| 2:C:510:LYS:HG3   | 2:C:511:PRO:CD    | 2.38                     | 0.52              |
| 2:C:525:ALA:O     | 2:C:768:THR:HG23  | 2.09                     | 0.52              |
| 2:C:916:THR:HB    | 2:C:935:ARG:HD2   | 1.90                     | 0.52              |
| 3:D:116:LYS:HG3   | 3:D:117:ASP:N     | 2.24                     | 0.52              |
| 7:H:125:SER:OG    | 7:H:128:PRO:HA    | 2.09                     | 0.52              |
| 4:E:141:LEU:HD22  | 7:H:46:LEU:O      | 2.09                     | 0.52              |
| 7:H:98:GLY:HA3    | 7:H:110:VAL:O     | 2.09                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:568:PRO:CG    | 8:I:46:LEU:HD22   | 2.37                     | 0.52              |
| 11:L:55:LYS:HB3   | 11:L:81:TYR:CE1   | 2.45                     | 0.52              |
| 1:B:1004:ASN:OD1  | 1:B:1005:GLU:N    | 2.42                     | 0.52              |
| 1:B:1341:ILE:HD12 | 1:B:1379:GLY:O    | 2.10                     | 0.52              |
| 1:B:560:ILE:CG1   | 8:I:78:SER:HB2    | 2.39                     | 0.52              |
| 1:B:798:GLY:HA2   | 1:B:815:PHE:CD1   | 2.45                     | 0.52              |
| 1:B:947:PHE:CE2   | 1:B:954:TRP:CE2   | 2.98                     | 0.52              |
| 2:C:245:GLU:O     | 2:C:246:LYS:HG3   | 2.09                     | 0.52              |
| 8:I:40:LEU:CD1    | 8:I:123:MET:HB2   | 2.40                     | 0.52              |
| 12:M:28:LYS:O     | 12:M:29:TYR:HD2   | 1.93                     | 0.52              |
| 1:B:1006:ILE:O    | 1:B:1009:ASN:HB2  | 2.09                     | 0.52              |
| 1:B:107:CYS:HA    | 1:B:171:GLN:CD    | 2.30                     | 0.52              |
| 1:B:34:LYS:HB2    | 1:B:36:ARG:HH21   | 1.75                     | 0.52              |
| 1:B:476:SER:N     | 1:B:477:PRO:CD    | 2.73                     | 0.52              |
| 1:B:556:TRP:CZ3   | 1:B:558:GLY:HA2   | 2.45                     | 0.52              |
| 2:C:1097:HIS:N    | 2:C:1098:MET:HE2  | 2.25                     | 0.52              |
| 2:C:467:GLY:N     | 2:C:475:SER:CB    | 2.72                     | 0.52              |
| 3:D:31:ASN:O      | 3:D:32:SER:C      | 2.48                     | 0.52              |
| 3:D:69:LEU:O      | 10:K:6:ARG:HD2    | 2.10                     | 0.52              |
| 12:M:55:ILE:O     | 12:M:56:LEU:HB2   | 2.07                     | 0.52              |
| 1:B:853:ASP:O     | 1:B:1000:LEU:HD21 | 2.10                     | 0.52              |
| 1:B:1018:PHE:O    | 1:B:1021:LEU:HB3  | 2.10                     | 0.52              |
| 1:B:1107:VAL:HG12 | 1:B:1107:VAL:O    | 2.10                     | 0.52              |
| 1:B:1381:LEU:HD23 | 1:B:1381:LEU:N    | 2.25                     | 0.52              |
| 1:B:466:SER:CB    | 11:L:2:ASN:HD22   | 2.22                     | 0.52              |
| 1:B:710:LEU:HD12  | 1:B:710:LEU:H     | 1.75                     | 0.52              |
| 1:B:863:VAL:HG11  | 1:B:866:PHE:CD2   | 2.45                     | 0.52              |
| 2:C:100:PRO:CG    | 2:C:172:ILE:HD12  | 2.39                     | 0.52              |
| 2:C:115:GLN:HB2   | 2:C:194:GLU:HG2   | 1.92                     | 0.52              |
| 2:C:332:ASP:C     | 2:C:334:ILE:H     | 2.13                     | 0.52              |
| 2:C:248:SER:H     | 2:C:418:LYS:NZ    | 2.08                     | 0.52              |
| 2:C:745:PRO:O     | 2:C:748:ILE:HG12  | 2.10                     | 0.52              |
| 2:C:976:ILE:O     | 2:C:990:ILE:HB    | 2.10                     | 0.52              |
| 4:E:130:LEU:O     | 4:E:132:GLN:N     | 2.32                     | 0.52              |
| 5:F:190:LEU:O     | 5:F:191:LYS:HG2   | 2.10                     | 0.52              |
| 6:G:116:ASP:HB3   | 6:G:119:ARG:HB2   | 1.91                     | 0.52              |
| 6:G:75:PRO:C      | 6:G:77:ASP:N      | 2.63                     | 0.52              |
| 9:J:2:THR:O       | 9:J:3:THR:C       | 2.48                     | 0.52              |
| 11:L:55:LYS:HB3   | 11:L:81:TYR:CD1   | 2.44                     | 0.52              |
| 1:B:547:LEU:HD22  | 11:L:58:PHE:CD1   | 2.45                     | 0.52              |
| 1:B:1332:PHE:CE1  | 1:B:1348:LEU:HD13 | 2.45                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:219:PHE:CE2   | 1:B:231:PRO:HD2   | 2.45                     | 0.52              |
| 1:B:522:GLY:HA2   | 1:B:630:ILE:CD1   | 2.39                     | 0.52              |
| 1:B:91:PHE:HB2    | 1:B:297:GLN:HE22  | 1.75                     | 0.52              |
| 2:C:642:ASP:O     | 2:C:644:GLU:N     | 2.40                     | 0.52              |
| 2:C:637:LEU:HD11  | 2:C:703:ILE:HD13  | 1.91                     | 0.52              |
| 3:D:18:VAL:O      | 3:D:20:PHE:HD2    | 1.93                     | 0.52              |
| 3:D:203:GLN:HG2   | 3:D:207:CYS:SG    | 2.50                     | 0.52              |
| 4:E:16:LYS:HZ3    | 4:E:16:LYS:HB3    | 1.74                     | 0.52              |
| 5:F:55:ARG:C      | 5:F:57:MET:N      | 2.63                     | 0.52              |
| 2:C:294:ASP:HB2   | 9:J:12:ASN:HA     | 1.91                     | 0.52              |
| 10:K:53:HIS:HE1   | 10:K:55:ASP:OD1   | 1.94                     | 0.52              |
| 1:B:1437:GLY:O    | 1:B:1439:GLY:N    | 2.43                     | 0.51              |
| 1:B:466:SER:O     | 1:B:467:THR:HG23  | 2.10                     | 0.51              |
| 1:B:498:ARG:HG3   | 1:B:499:ALA:H     | 1.75                     | 0.51              |
| 1:B:590:ARG:CD    | 1:B:604:GLY:HA2   | 2.39                     | 0.51              |
| 1:B:606:LEU:HD11  | 1:B:608:ILE:HG13  | 1.92                     | 0.51              |
| 2:C:1085:ILE:CD1  | 2:C:1085:ILE:H    | 2.22                     | 0.51              |
| 3:D:112:ASN:CB    | 3:D:114:TYR:CE1   | 2.93                     | 0.51              |
| 7:H:143:ILE:CG2   | 7:H:144:ARG:N     | 2.69                     | 0.51              |
| 1:B:247:ARG:HH11  | 1:B:247:ARG:HG3   | 1.75                     | 0.51              |
| 1:B:250:ILE:O     | 1:B:250:ILE:HG22  | 2.10                     | 0.51              |
| 1:B:355:GLY:N     | 1:B:482:PHE:CZ    | 2.78                     | 0.51              |
| 1:B:50:ILE:C      | 1:B:52:GLY:N      | 2.64                     | 0.51              |
| 1:B:947:PHE:CD2   | 1:B:954:TRP:CE2   | 2.98                     | 0.51              |
| 2:C:1010:LEU:O    | 2:C:1011:ILE:CG1  | 2.58                     | 0.51              |
| 2:C:172:ILE:CD1   | 2:C:178:ASN:HD22  | 2.23                     | 0.51              |
| 2:C:298:LEU:CD2   | 2:C:298:LEU:H     | 2.22                     | 0.51              |
| 2:C:364:ILE:HG22  | 2:C:365:THR:N     | 2.25                     | 0.51              |
| 2:C:579:ARG:CB    | 2:C:586:TRP:HE1   | 2.18                     | 0.51              |
| 1:B:482:PHE:CE1   | 2:C:836:GLU:HB2   | 2.45                     | 0.51              |
| 3:D:176:ILE:CG2   | 3:D:177:GLU:N     | 2.72                     | 0.51              |
| 5:F:154:ILE:O     | 5:F:196:VAL:HA    | 2.11                     | 0.51              |
| 1:B:1152:ILE:HD11 | 9:J:44:TYR:CD2    | 2.46                     | 0.51              |
| 1:B:1063:MET:SD   | 1:B:1436:ILE:HG12 | 2.50                     | 0.51              |
| 1:B:116:ASP:C     | 1:B:118:HIS:H     | 2.13                     | 0.51              |
| 1:B:1114:PRO:HB2  | 1:B:1311:VAL:CG2  | 2.39                     | 0.51              |
| 1:B:108:MET:HB3   | 1:B:210:ILE:HD13  | 1.91                     | 0.51              |
| 1:B:24:PRO:HD2    | 1:B:233:TRP:HE1   | 1.74                     | 0.51              |
| 1:B:458:HIS:CE1   | 1:B:507:VAL:HG21  | 2.45                     | 0.51              |
| 1:B:6:TYR:CD1     | 1:B:7:SER:N       | 2.78                     | 0.51              |
| 1:B:951:GLU:HB3   | 1:B:954:TRP:HZ2   | 1.74                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:425:THR:HA   | 2:C:428:ILE:HD12  | 1.91                     | 0.51              |
| 2:C:654:ARG:HG3  | 2:C:654:ARG:HH11  | 1.76                     | 0.51              |
| 2:C:810:GLU:HB2  | 2:C:815:ARG:HH22  | 1.76                     | 0.51              |
| 4:E:16:LYS:CG    | 4:E:18:VAL:HG12   | 2.40                     | 0.51              |
| 1:B:1006:ILE:CD1 | 5:F:163:GLU:HG3   | 2.31                     | 0.51              |
| 4:E:40:HIS:CB    | 7:H:73:LYS:HZ2    | 2.10                     | 0.51              |
| 1:B:1138:ILE:CG2 | 1:B:1316:VAL:HG13 | 2.40                     | 0.51              |
| 1:B:34:LYS:CB    | 1:B:36:ARG:HH21   | 2.23                     | 0.51              |
| 1:B:821:ARG:HB2  | 1:B:821:ARG:NH1   | 2.25                     | 0.51              |
| 2:C:203:PHE:N    | 2:C:203:PHE:CD1   | 2.79                     | 0.51              |
| 2:C:324:ILE:CG2  | 2:C:325:GLN:N     | 2.73                     | 0.51              |
| 2:C:549:THR:HG22 | 2:C:550:ASP:N     | 2.19                     | 0.51              |
| 2:C:583:ASN:HD21 | 2:C:628:THR:HG22  | 1.74                     | 0.51              |
| 8:I:143:LEU:N    | 8:I:143:LEU:HD12  | 2.26                     | 0.51              |
| 9:J:13:MET:O     | 9:J:14:LEU:HD23   | 2.11                     | 0.51              |
| 1:B:1019:CYS:O   | 1:B:1022:LEU:N    | 2.44                     | 0.51              |
| 1:B:1336:MET:HE3 | 1:B:1381:LEU:HG   | 1.93                     | 0.51              |
| 1:B:586:ILE:CG2  | 1:B:587:HIS:H     | 2.23                     | 0.51              |
| 1:B:853:ASP:C    | 1:B:853:ASP:OD1   | 2.49                     | 0.51              |
| 2:C:63:ILE:HA    | 2:C:421:PHE:HE2   | 1.76                     | 0.51              |
| 2:C:603:LEU:CD1  | 2:C:609:ILE:HG13  | 2.27                     | 0.51              |
| 3:D:242:GLN:C    | 3:D:244:VAL:N     | 2.63                     | 0.51              |
| 3:D:56:THR:HG21  | 3:D:145:CYS:SG    | 2.50                     | 0.51              |
| 9:J:101:PHE:HB2  | 9:J:110:PHE:CE2   | 2.45                     | 0.51              |
| 11:L:10:PHE:HD2  | 11:L:10:PHE:N     | 2.09                     | 0.51              |
| 1:B:852:TYR:CE2  | 1:B:1060:PRO:HB2  | 2.45                     | 0.51              |
| 1:B:526:ASP:OD1  | 2:C:1013:ASN:ND2  | 2.42                     | 0.51              |
| 2:C:547:VAL:HG12 | 2:C:612:GLU:OE2   | 2.11                     | 0.51              |
| 2:C:614:SER:OG   | 2:C:627:PHE:HB2   | 2.10                     | 0.51              |
| 2:C:806:THR:HG21 | 2:C:808:ALA:HB3   | 1.91                     | 0.51              |
| 4:E:29:LEU:HD22  | 7:H:82:PHE:CE2    | 2.46                     | 0.51              |
| 7:H:112:LYS:NZ   | 7:H:120:THR:HA    | 2.26                     | 0.51              |
| 2:C:848:ARG:HD2  | 10:K:8:PHE:O      | 2.11                     | 0.51              |
| 1:B:1121:GLU:CG  | 1:B:1122:PRO:HD2  | 2.40                     | 0.51              |
| 1:B:248:PRO:O    | 1:B:260:ASP:HB2   | 2.09                     | 0.51              |
| 1:B:358:ASN:O    | 1:B:359:LEU:HD23  | 2.11                     | 0.51              |
| 1:B:476:SER:N    | 1:B:477:PRO:HD3   | 2.26                     | 0.51              |
| 1:B:54:ASN:HD22  | 1:B:54:ASN:N      | 2.08                     | 0.51              |
| 1:B:779:PHE:O    | 1:B:780:VAL:C     | 2.49                     | 0.51              |
| 1:B:848:ILE:HA   | 1:B:857:ARG:O     | 2.11                     | 0.51              |
| 2:C:185:THR:O    | 2:C:186:GLU:C     | 2.49                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:708:GLU:HG3  | 2:C:709:ASP:H    | 1.75                     | 0.51              |
| 2:C:752:ALA:O    | 2:C:755:ILE:HG13 | 2.11                     | 0.51              |
| 3:D:232:VAL:HG11 | 3:D:244:VAL:HG22 | 1.92                     | 0.51              |
| 4:E:172:LEU:HB3  | 4:E:176:GLU:OE1  | 2.11                     | 0.51              |
| 4:E:216:ASN:C    | 4:E:218:GLU:N    | 2.64                     | 0.51              |
| 5:F:182:ASP:O    | 5:F:185:ALA:HB3  | 2.10                     | 0.51              |
| 5:F:23:VAL:HB    | 5:F:30:ILE:CD1   | 2.39                     | 0.51              |
| 7:H:14:HIS:HD2   | 7:H:16:SER:HB2   | 1.70                     | 0.51              |
| 1:B:268:ASP:HB3  | 1:B:299:HIS:ND1  | 2.26                     | 0.51              |
| 1:B:453:MET:HB3  | 1:B:456:MET:HE2  | 1.93                     | 0.51              |
| 1:B:351:THR:HG22 | 2:C:1103:ILE:HA  | 1.92                     | 0.51              |
| 2:C:244:LEU:HD21 | 2:C:366:GLN:HE21 | 1.71                     | 0.51              |
| 2:C:284:ILE:HD13 | 2:C:333:PHE:HD2  | 1.76                     | 0.51              |
| 2:C:582:VAL:HA   | 2:C:626:ILE:O    | 2.10                     | 0.51              |
| 2:C:840:ILE:CG2  | 2:C:994:TYR:HD1  | 2.24                     | 0.51              |
| 4:E:220:LEU:O    | 4:E:221:TYR:HD1  | 1.93                     | 0.51              |
| 5:F:96:PHE:CE1   | 5:F:100:ILE:HD11 | 2.46                     | 0.51              |
| 7:H:132:SER:HB3  | 7:H:135:ASP:HB2  | 1.92                     | 0.51              |
| 9:J:82:GLU:HB3   | 9:J:104:LEU:HG   | 1.93                     | 0.51              |
| 1:B:709:THR:HG23 | 9:J:94:ASP:HA    | 1.91                     | 0.51              |
| 11:L:57:LEU:H    | 11:L:77:THR:HA   | 1.75                     | 0.51              |
| 1:B:1121:GLU:HB3 | 1:B:1124:HIS:HD2 | 1.75                     | 0.51              |
| 1:B:882:SER:HA   | 1:B:952:ALA:O    | 2.11                     | 0.51              |
| 2:C:1032:SER:O   | 2:C:1036:ALA:HB2 | 2.11                     | 0.51              |
| 2:C:165:VAL:O    | 2:C:167:ILE:HD12 | 2.11                     | 0.51              |
| 2:C:498:THR:HG22 | 2:C:537:LYS:H    | 1.75                     | 0.51              |
| 2:C:834:ASN:HA   | 2:C:838:SER:O    | 2.09                     | 0.51              |
| 6:G:103:MET:HE1  | 7:H:65:ASP:HA    | 1.92                     | 0.51              |
| 9:J:55:THR:HG22  | 9:J:58:VAL:HG21  | 1.93                     | 0.51              |
| 12:M:31:CYS:HA   | 12:M:56:LEU:HD23 | 1.92                     | 0.51              |
| 1:B:1350:LYS:O   | 1:B:1354:ASN:ND2 | 2.44                     | 0.51              |
| 1:B:102:VAL:HG11 | 1:B:211:PHE:CE2  | 2.46                     | 0.51              |
| 1:B:958:VAL:HG12 | 1:B:960:ILE:HG13 | 1.92                     | 0.51              |
| 2:C:273:LEU:HB2  | 2:C:276:ILE:HG13 | 1.93                     | 0.51              |
| 2:C:345:LYS:HG3  | 2:C:348:ARG:HH21 | 1.75                     | 0.51              |
| 2:C:471:LYS:O    | 2:C:472:ALA:HB2  | 2.10                     | 0.51              |
| 4:E:11:ARG:HD3   | 4:E:12:ARG:N     | 2.26                     | 0.51              |
| 4:E:51:ASN:O     | 4:E:54:GLU:HB3   | 2.11                     | 0.51              |
| 1:B:1342:GLU:OE2 | 5:F:198:ILE:HD13 | 2.11                     | 0.51              |
| 9:J:45:ARG:HE    | 9:J:47:GLU:HG3   | 1.75                     | 0.51              |
| 3:D:235:VAL:HG12 | 10:K:13:VAL:HG22 | 1.93                     | 0.51              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:1299:VAL:HG12 | 1:B:1300:LYS:N   | 2.25                     | 0.50              |
| 1:B:639:PRO:CG    | 1:B:640:GLN:H    | 2.21                     | 0.50              |
| 1:B:875:ALA:O     | 1:B:878:ILE:HG13 | 2.10                     | 0.50              |
| 1:B:898:ARG:HB2   | 1:B:933:TYR:HE1  | 1.76                     | 0.50              |
| 2:C:758:PHE:CE1   | 2:C:1027:ILE:CG2 | 2.94                     | 0.50              |
| 2:C:167:ILE:HG22  | 2:C:453:ILE:HD12 | 1.91                     | 0.50              |
| 2:C:29:ASP:CB     | 2:C:658:ILE:HD13 | 2.39                     | 0.50              |
| 2:C:911:ILE:O     | 2:C:911:ILE:HG22 | 2.10                     | 0.50              |
| 3:D:99:LEU:O      | 3:D:156:THR:HA   | 2.11                     | 0.50              |
| 3:D:70:ILE:HG22   | 3:D:70:ILE:O     | 2.10                     | 0.50              |
| 5:F:153:HIS:HB3   | 5:F:196:VAL:HG13 | 1.88                     | 0.50              |
| 7:H:117:GLN:O     | 7:H:119:LEU:N    | 2.45                     | 0.50              |
| 1:B:942:PHE:C     | 1:B:942:PHE:CD2  | 2.84                     | 0.50              |
| 2:C:1160:VAL:HG12 | 2:C:1161:HIS:N   | 2.26                     | 0.50              |
| 2:C:126:SER:O     | 2:C:169:ARG:HA   | 2.11                     | 0.50              |
| 2:C:820:GLY:C     | 2:C:821:GLN:HG3  | 2.31                     | 0.50              |
| 2:C:911:ILE:HD11  | 2:C:941:LEU:CD1  | 2.41                     | 0.50              |
| 2:C:948:ILE:HG22  | 2:C:949:VAL:O    | 2.11                     | 0.50              |
| 3:D:77:ILE:HG23   | 3:D:161:LYS:HE3  | 1.93                     | 0.50              |
| 3:D:204:SER:O     | 3:D:207:CYS:SG   | 2.68                     | 0.50              |
| 3:D:63:ILE:HA     | 3:D:66:ARG:HG3   | 1.94                     | 0.50              |
| 8:I:42:ILE:O      | 8:I:44:VAL:HG23  | 2.11                     | 0.50              |
| 12:M:55:ILE:O     | 12:M:56:LEU:CB   | 2.59                     | 0.50              |
| 1:B:1015:VAL:CG1  | 1:B:1019:CYS:SG  | 2.98                     | 0.50              |
| 1:B:1094:VAL:HG13 | 1:B:1113:THR:CG2 | 2.36                     | 0.50              |
| 1:B:268:ASP:HB3   | 1:B:299:HIS:CE1  | 2.47                     | 0.50              |
| 1:B:357:PRO:HD2   | 2:C:833:TYR:CE1  | 2.47                     | 0.50              |
| 1:B:528:LEU:O     | 1:B:531:ILE:HG22 | 2.12                     | 0.50              |
| 1:B:608:ILE:HG13  | 1:B:613:ILE:HD12 | 1.94                     | 0.50              |
| 1:B:754:SER:O     | 1:B:755:PHE:C    | 2.49                     | 0.50              |
| 1:B:665:GLY:HA3   | 2:C:1086:PHE:CD1 | 2.46                     | 0.50              |
| 2:C:1212:ILE:O    | 2:C:1214:PRO:HD3 | 2.11                     | 0.50              |
| 2:C:865:LYS:HZ3   | 2:C:869:SER:HA   | 1.74                     | 0.50              |
| 2:C:861:ASP:OD1   | 2:C:914:LYS:HD2  | 2.11                     | 0.50              |
| 3:D:213:PRO:O     | 3:D:214:ASN:CB   | 2.59                     | 0.50              |
| 3:D:243:VAL:O     | 3:D:243:VAL:HG12 | 2.11                     | 0.50              |
| 5:F:182:ASP:HB3   | 5:F:185:ALA:CB   | 2.41                     | 0.50              |
| 1:B:537:ARG:HH22  | 8:I:122:LEU:CD1  | 2.24                     | 0.50              |
| 11:L:73:LEU:CD2   | 11:L:75:ILE:HD11 | 2.40                     | 0.50              |
| 11:L:6:ARG:O      | 11:L:9:LEU:HG    | 2.11                     | 0.50              |
| 12:M:30:ILE:O     | 12:M:56:LEU:HA   | 2.11                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:M:52:GLY:O     | 12:M:54:ARG:N     | 2.44                     | 0.50              |
| 1:B:997:LEU:HD13  | 1:B:1018:PHE:CE2  | 2.46                     | 0.50              |
| 1:B:1332:PHE:N    | 1:B:1332:PHE:CD2  | 2.80                     | 0.50              |
| 1:B:1445:ILE:HD11 | 7:H:61:ILE:HG12   | 1.93                     | 0.50              |
| 1:B:42:ASP:O      | 1:B:44:THR:N      | 2.41                     | 0.50              |
| 1:B:362:ASP:OD2   | 1:B:459:ARG:HD3   | 2.11                     | 0.50              |
| 1:B:598:LEU:HD22  | 8:I:25:ARG:NH1    | 2.27                     | 0.50              |
| 1:B:635:ARG:HA    | 1:B:635:ARG:NH1   | 2.25                     | 0.50              |
| 2:C:1034:VAL:HG12 | 2:C:1035:ALA:N    | 2.25                     | 0.50              |
| 2:C:1069:PHE:HA   | 2:C:1085:ILE:O    | 2.11                     | 0.50              |
| 2:C:409:ALA:O     | 2:C:413:LEU:HG    | 2.11                     | 0.50              |
| 3:D:213:PRO:HG2   | 3:D:214:ASN:H     | 1.77                     | 0.50              |
| 4:E:10:THR:O      | 4:E:10:THR:HG22   | 2.12                     | 0.50              |
| 6:G:88:TYR:N      | 6:G:88:TYR:CD1    | 2.79                     | 0.50              |
| 7:H:49:LEU:HD23   | 7:H:49:LEU:N      | 2.25                     | 0.50              |
| 7:H:63:PRO:O      | 7:H:64:THR:CB     | 2.59                     | 0.50              |
| 8:I:130:ARG:HB3   | 8:I:133:ASN:HB2   | 1.93                     | 0.50              |
| 3:D:22:LEU:HD11   | 11:L:101:LEU:HD11 | 1.94                     | 0.50              |
| 11:L:68:PHE:N     | 11:L:68:PHE:CD2   | 2.76                     | 0.50              |
| 11:L:6:ARG:O      | 11:L:8:GLU:N      | 2.45                     | 0.50              |
| 1:B:1063:MET:HG3  | 2:C:1139:ILE:O    | 2.12                     | 0.50              |
| 1:B:1317:MET:HE2  | 1:B:1327:ILE:HG21 | 1.94                     | 0.50              |
| 1:B:568:PRO:HB2   | 3:D:221:TYR:CZ    | 2.46                     | 0.50              |
| 1:B:622:VAL:O     | 1:B:622:VAL:HG13  | 2.11                     | 0.50              |
| 2:C:1095:LEU:H    | 2:C:1095:LEU:CD1  | 2.21                     | 0.50              |
| 8:I:127:GLY:O     | 8:I:128:ASN:CB    | 2.58                     | 0.50              |
| 8:I:35:GLN:O      | 8:I:37:LYS:HG3    | 2.12                     | 0.50              |
| 13:N:1:DC:H2''    | 13:N:2:DA:O5'     | 2.12                     | 0.50              |
| 1:B:1153:TYR:HB2  | 1:B:1192:LEU:HD23 | 1.93                     | 0.50              |
| 1:B:637:LYS:O     | 1:B:641:VAL:HG21  | 2.12                     | 0.50              |
| 1:B:942:PHE:HD2   | 1:B:942:PHE:C     | 2.15                     | 0.50              |
| 2:C:1010:LEU:O    | 2:C:1011:ILE:HG13 | 2.11                     | 0.50              |
| 2:C:910:VAL:CG1   | 2:C:911:ILE:N     | 2.75                     | 0.50              |
| 3:D:191:TYR:HD2   | 3:D:201:TRP:CD1   | 2.29                     | 0.50              |
| 5:F:176:PRO:O     | 5:F:212:ARG:HA    | 2.12                     | 0.50              |
| 7:H:115:MET:HB2   | 7:H:116:PRO:CD    | 2.37                     | 0.50              |
| 1:B:1015:VAL:O    | 1:B:1017:LEU:N    | 2.45                     | 0.50              |
| 1:B:1329:THR:HG22 | 1:B:1331:SER:HB3  | 1.93                     | 0.50              |
| 1:B:91:PHE:H      | 1:B:297:GLN:NE2   | 2.07                     | 0.50              |
| 1:B:86:LEU:HD21   | 1:B:239:LEU:HB2   | 1.93                     | 0.50              |
| 1:B:901:LEU:HB2   | 1:B:926:GLN:CG    | 2.28                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:992:ASP:O    | 1:B:993:LEU:C     | 2.49                     | 0.50              |
| 2:C:1196:ILE:HB  | 2:C:1197:PRO:HD2  | 1.94                     | 0.50              |
| 2:C:236:HIS:CE1  | 2:C:389:ALA:HA    | 2.47                     | 0.50              |
| 2:C:265:SER:O    | 2:C:266:ALA:HB3   | 2.11                     | 0.50              |
| 2:C:461:LEU:H    | 2:C:461:LEU:CD1   | 2.25                     | 0.50              |
| 2:C:508:LEU:HG   | 2:C:509:ALA:N     | 2.27                     | 0.50              |
| 2:C:58:THR:O     | 2:C:62:ILE:HG13   | 2.11                     | 0.50              |
| 2:C:945:GLU:O    | 2:C:946:ASN:HB3   | 2.10                     | 0.50              |
| 3:D:228:PHE:N    | 3:D:228:PHE:CD1   | 2.80                     | 0.50              |
| 4:E:161:GLY:O    | 4:E:165:GLN:HG3   | 2.11                     | 0.50              |
| 5:F:145:THR:HG21 | 5:F:187:TYR:CD2   | 2.46                     | 0.50              |
| 8:I:95:TYR:CE2   | 8:I:97:MET:CG     | 2.92                     | 0.50              |
| 12:M:38:LEU:O    | 12:M:39:SER:CB    | 2.58                     | 0.50              |
| 1:B:1008:GLN:O   | 1:B:1011:GLN:HB3  | 2.11                     | 0.50              |
| 1:B:1334:ASP:O   | 1:B:1336:MET:N    | 2.45                     | 0.50              |
| 1:B:498:ARG:HG3  | 1:B:499:ALA:N     | 2.26                     | 0.50              |
| 1:B:596:THR:C    | 1:B:598:LEU:N     | 2.63                     | 0.50              |
| 2:C:1004:GLU:HB2 | 2:C:1006:ILE:HG12 | 1.94                     | 0.50              |
| 2:C:1079:LYS:CG  | 2:C:1080:LYS:H    | 2.22                     | 0.50              |
| 2:C:118:ARG:HD3  | 2:C:204:ILE:CD1   | 2.41                     | 0.50              |
| 2:C:247:GLY:O    | 2:C:248:SER:HB3   | 2.11                     | 0.50              |
| 2:C:656:GLY:O    | 2:C:657:HIS:C     | 2.50                     | 0.50              |
| 2:C:846:ILE:HG23 | 2:C:974:PRO:HG2   | 1.93                     | 0.50              |
| 5:F:108:GLY:HA3  | 5:F:132:ILE:CG2   | 2.42                     | 0.50              |
| 8:I:59:ILE:O     | 8:I:60:ALA:CB     | 2.59                     | 0.50              |
| 9:J:82:GLU:OE2   | 9:J:104:LEU:HD12  | 2.11                     | 0.50              |
| 9:J:82:GLU:HB3   | 9:J:104:LEU:HD12  | 1.94                     | 0.50              |
| 1:B:1187:GLN:HG3 | 1:B:1188:GLN:HG3  | 1.94                     | 0.50              |
| 1:B:1451:VAL:O   | 1:B:1454:MET:HG2  | 2.12                     | 0.50              |
| 1:B:260:ASP:OD1  | 1:B:261:ASP:N     | 2.45                     | 0.50              |
| 1:B:300:VAL:O    | 1:B:300:VAL:HG12  | 2.12                     | 0.50              |
| 2:C:1008:PRO:HD3 | 2:C:1087:PHE:HE1  | 1.76                     | 0.50              |
| 2:C:1072:MET:HE1 | 2:C:1087:PHE:HD1  | 1.76                     | 0.50              |
| 2:C:189:LEU:O    | 2:C:192:LEU:N     | 2.36                     | 0.50              |
| 2:C:281:PRO:O    | 2:C:283:VAL:N     | 2.45                     | 0.50              |
| 2:C:611:PRO:HG2  | 2:C:685:LEU:HD21  | 1.92                     | 0.50              |
| 2:C:873:THR:CG2  | 2:C:874:PHE:N     | 2.75                     | 0.50              |
| 2:C:955:THR:HG23 | 2:C:956:THR:H     | 1.76                     | 0.50              |
| 4:E:176:GLU:HG2  | 4:E:197:SER:OG    | 2.11                     | 0.50              |
| 4:E:51:ASN:OD1   | 4:E:51:ASN:O      | 2.30                     | 0.50              |
| 6:G:75:PRO:HG3   | 6:G:78:GLN:OE1    | 2.12                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:G:77:ASP:OD1    | 6:G:78:GLN:N      | 2.45                     | 0.50              |
| 7:H:52:ASP:C      | 7:H:53:ASN:HD22   | 2.14                     | 0.50              |
| 14:P:8:U:H2'      | 14:P:9:A:C8       | 2.47                     | 0.50              |
| 1:B:1100:ARG:NH2  | 1:B:1351:GLU:HG2  | 2.27                     | 0.49              |
| 1:B:1371:LEU:O    | 1:B:1375:MET:HG3  | 2.12                     | 0.49              |
| 1:B:1397:LEU:O    | 1:B:1400:CYS:HB3  | 2.12                     | 0.49              |
| 1:B:1418:LEU:HD12 | 1:B:1419:ASP:N    | 2.27                     | 0.49              |
| 1:B:409:SER:O     | 1:B:411:ASP:N     | 2.45                     | 0.49              |
| 1:B:546:VAL:HG21  | 1:B:572:TRP:CE3   | 2.46                     | 0.49              |
| 1:B:886:ILE:CG2   | 1:B:887:GLY:H     | 2.25                     | 0.49              |
| 2:C:185:THR:N     | 2:C:188:ASP:HB2   | 2.26                     | 0.49              |
| 2:C:601:ARG:HD3   | 2:C:605:ARG:HH21  | 1.77                     | 0.49              |
| 4:E:144:THR:HG21  | 7:H:46:LEU:HD13   | 1.94                     | 0.49              |
| 5:F:163:GLU:O     | 5:F:164:LEU:C     | 2.49                     | 0.49              |
| 1:B:852:TYR:CD1   | 6:G:136:ARG:HB3   | 2.47                     | 0.49              |
| 11:L:7:PHE:HA     | 11:L:10:PHE:CE2   | 2.47                     | 0.49              |
| 15:T:18:DT:O5'    | 15:T:18:DT:H6     | 1.94                     | 0.49              |
| 1:B:1254:ALA:O    | 1:B:1255:GLU:CB   | 2.60                     | 0.49              |
| 1:B:1389:PHE:CD1  | 1:B:1390:ASN:N    | 2.80                     | 0.49              |
| 1:B:373:THR:HG21  | 2:C:1105:ALA:CB   | 2.42                     | 0.49              |
| 1:B:50:ILE:HG22   | 1:B:52:GLY:H      | 1.77                     | 0.49              |
| 1:B:722:LEU:N     | 1:B:722:LEU:HD12  | 2.26                     | 0.49              |
| 1:B:344:ARG:HD2   | 2:C:1118:PRO:O    | 2.11                     | 0.49              |
| 2:C:234:ILE:HG21  | 2:C:237:VAL:HG23  | 1.94                     | 0.49              |
| 2:C:401:PHE:HD2   | 2:C:521:LEU:HD12  | 1.77                     | 0.49              |
| 2:C:704:ALA:HB2   | 2:C:738:PHE:CD2   | 2.47                     | 0.49              |
| 2:C:981:ALA:HB2   | 2:C:987:LYS:HA    | 1.94                     | 0.49              |
| 3:D:128:ASN:O     | 3:D:129:ILE:HG13  | 2.11                     | 0.49              |
| 6:G:93:ILE:HD11   | 6:G:134:ILE:HD11  | 1.95                     | 0.49              |
| 8:I:8:ASP:HB3     | 8:I:10:PHE:CE1    | 2.47                     | 0.49              |
| 1:B:896:ARG:HH22  | 1:B:1030:ARG:HH21 | 1.59                     | 0.49              |
| 1:B:1198:ASP:O    | 1:B:1202:MET:HG2  | 2.13                     | 0.49              |
| 1:B:588:LEU:O     | 1:B:606:LEU:HA    | 2.12                     | 0.49              |
| 1:B:896:ARG:HD3   | 1:B:897:TYR:HE1   | 1.77                     | 0.49              |
| 1:B:946:VAL:HB    | 1:B:947:PHE:HD1   | 1.76                     | 0.49              |
| 2:C:35:SER:O      | 2:C:39:ARG:HG3    | 2.12                     | 0.49              |
| 2:C:570:VAL:CB    | 2:C:573:GLN:HB3   | 2.41                     | 0.49              |
| 2:C:785:TYR:CD1   | 2:C:785:TYR:C     | 2.86                     | 0.49              |
| 2:C:806:THR:CG2   | 2:C:808:ALA:HB3   | 2.42                     | 0.49              |
| 3:D:254:LYS:C     | 3:D:256:ALA:N     | 2.65                     | 0.49              |
| 8:I:5:LEU:HD12    | 8:I:60:ALA:HA     | 1.94                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 9:J:106:CYS:O    | 9:J:107:SER:HB2   | 2.11                     | 0.49              |
| 1:B:1377:THR:O   | 1:B:1379:GLY:N    | 2.45                     | 0.49              |
| 1:B:134:ARG:O    | 1:B:138:ILE:HG13  | 2.12                     | 0.49              |
| 1:B:1441:PHE:CE2 | 6:G:89:GLU:HG2    | 2.48                     | 0.49              |
| 1:B:396:PRO:HG3  | 1:B:416:ARG:HB3   | 1.95                     | 0.49              |
| 1:B:347:PHE:CE2  | 1:B:493:GLN:OE1   | 2.64                     | 0.49              |
| 1:B:32:VAL:HG21  | 1:B:68:GLN:NE2    | 2.25                     | 0.49              |
| 1:B:68:GLN:C     | 1:B:70:CYS:H      | 2.15                     | 0.49              |
| 2:C:1110:PRO:O   | 2:C:1119:VAL:HG13 | 2.11                     | 0.49              |
| 1:B:12:ARG:CZ    | 2:C:1192:TYR:HE2  | 2.25                     | 0.49              |
| 2:C:203:PHE:HD1  | 2:C:203:PHE:N     | 2.11                     | 0.49              |
| 2:C:385:LEU:HD23 | 2:C:386:LEU:HD23  | 1.94                     | 0.49              |
| 2:C:388:CYS:O    | 2:C:391:ASP:N     | 2.45                     | 0.49              |
| 2:C:638:PHE:HB3  | 2:C:651:LEU:HD22  | 1.94                     | 0.49              |
| 3:D:254:LYS:O    | 3:D:256:ALA:N     | 2.45                     | 0.49              |
| 5:F:61:GLN:HB2   | 5:F:79:TRP:CE3    | 2.44                     | 0.49              |
| 6:G:143:PHE:CD1  | 6:G:143:PHE:C     | 2.86                     | 0.49              |
| 8:I:101:ALA:HB2  | 8:I:116:TYR:CE1   | 2.47                     | 0.49              |
| 10:K:27:GLU:C    | 10:K:29:GLU:H     | 2.16                     | 0.49              |
| 2:C:798:TYR:CD1  | 10:K:4:PRO:HB3    | 2.48                     | 0.49              |
| 11:L:61:TYR:O    | 11:L:62:LYS:HB3   | 2.12                     | 0.49              |
| 11:L:90:ALA:O    | 11:L:94:ILE:HG13  | 2.12                     | 0.49              |
| 1:B:225:ASN:HD22 | 1:B:228:PHE:N     | 1.97                     | 0.49              |
| 1:B:360:GLU:O    | 1:B:361:LEU:C     | 2.51                     | 0.49              |
| 1:B:446:ARG:HB2  | 1:B:487:MET:CG    | 2.42                     | 0.49              |
| 1:B:608:ILE:C    | 1:B:610:GLY:N     | 2.65                     | 0.49              |
| 1:B:872:GLY:C    | 1:B:1058:VAL:HG23 | 2.33                     | 0.49              |
| 2:C:412:LEU:HB3  | 2:C:466:TRP:CZ2   | 2.47                     | 0.49              |
| 2:C:401:PHE:CD2  | 2:C:521:LEU:HD12  | 2.48                     | 0.49              |
| 2:C:785:TYR:CD1  | 2:C:786:ASN:N     | 2.80                     | 0.49              |
| 2:C:861:ASP:OD1  | 2:C:862:GLN:N     | 2.45                     | 0.49              |
| 2:C:859:TYR:CZ   | 2:C:941:LEU:HD12  | 2.47                     | 0.49              |
| 4:E:51:ASN:O     | 4:E:52:LEU:O      | 2.31                     | 0.49              |
| 5:F:124:VAL:N    | 5:F:125:PRO:HD2   | 2.28                     | 0.49              |
| 5:F:16:PHE:O     | 5:F:19:VAL:N      | 2.45                     | 0.49              |
| 5:F:46:TYR:CD2   | 5:F:58:MET:HG2    | 2.47                     | 0.49              |
| 5:F:50:MET:HG3   | 5:F:50:MET:O      | 2.12                     | 0.49              |
| 8:I:6:PHE:O      | 8:I:58:THR:HA     | 2.12                     | 0.49              |
| 9:J:11:ASN:C     | 9:J:12:ASN:HD22   | 2.15                     | 0.49              |
| 9:J:69:PRO:HG2   | 9:J:85:PHE:CE2    | 2.47                     | 0.49              |
| 12:M:61:THR:HG22 | 12:M:62:LYS:N     | 2.27                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1161:THR:CG2  | 1:B:1163:ILE:HG13 | 2.42                     | 0.49              |
| 1:B:1116:LEU:HB3  | 1:B:1308:THR:HG22 | 1.95                     | 0.49              |
| 1:B:1344:GLY:O    | 1:B:1345:ARG:C    | 2.51                     | 0.49              |
| 1:B:278:THR:O     | 1:B:278:THR:HG22  | 2.12                     | 0.49              |
| 2:C:108:VAL:HG12  | 2:C:109:THR:N     | 2.25                     | 0.49              |
| 2:C:531:GLN:HG3   | 2:C:532:ALA:H     | 1.76                     | 0.49              |
| 2:C:526:GLU:HB2   | 2:C:771:SER:HB3   | 1.94                     | 0.49              |
| 4:E:195:ILE:HG22  | 4:E:195:ILE:O     | 2.13                     | 0.49              |
| 5:F:23:VAL:HG13   | 5:F:78:LEU:CD1    | 2.39                     | 0.49              |
| 8:I:138:GLU:HG2   | 8:I:139:ASN:N     | 2.28                     | 0.49              |
| 15:T:18:DT:C2'    | 15:T:19:DT:C5'    | 2.88                     | 0.49              |
| 1:B:1423:GLY:O    | 1:B:1426:GLU:HB2  | 2.13                     | 0.49              |
| 1:B:244:PRO:CB    | 1:B:245:PRO:CD    | 2.91                     | 0.49              |
| 1:B:408:ASP:O     | 1:B:410:GLY:N     | 2.38                     | 0.49              |
| 1:B:963:ILE:HD11  | 1:B:1048:ASN:HB3  | 1.93                     | 0.49              |
| 2:C:1072:MET:CE   | 2:C:1087:PHE:HD1  | 2.25                     | 0.49              |
| 2:C:1166:CYS:O    | 2:C:1168:LEU:N    | 2.45                     | 0.49              |
| 2:C:1201:LYS:CG   | 2:C:1202:LEU:N    | 2.75                     | 0.49              |
| 2:C:175:ARG:HG2   | 2:C:175:ARG:NH1   | 2.27                     | 0.49              |
| 2:C:44:VAL:HG13   | 2:C:199:MET:HG2   | 1.94                     | 0.49              |
| 2:C:483:LEU:HD11  | 2:C:491:THR:CG2   | 2.33                     | 0.49              |
| 2:C:60:GLN:NE2    | 2:C:94:LYS:HA     | 2.28                     | 0.49              |
| 2:C:798:TYR:HE2   | 3:D:62:PHE:CZ     | 2.30                     | 0.49              |
| 2:C:975:GLN:HG2   | 2:C:976:ILE:N     | 2.28                     | 0.49              |
| 5:F:117:THR:HG22  | 5:F:119:SER:N     | 2.21                     | 0.49              |
| 5:F:135:PHE:CB    | 5:F:140:LEU:HD11  | 2.40                     | 0.49              |
| 11:L:12:LEU:HD12  | 11:L:12:LEU:N     | 2.20                     | 0.49              |
| 11:L:67:PHE:C     | 11:L:68:PHE:HD2   | 2.16                     | 0.49              |
| 12:M:44:ASP:O     | 12:M:45:ALA:HB3   | 2.11                     | 0.49              |
| 1:B:1305:VAL:HG12 | 1:B:1306:LEU:N    | 2.27                     | 0.49              |
| 1:B:356:ASP:OD1   | 1:B:358:ASN:HB2   | 2.13                     | 0.49              |
| 1:B:44:THR:O      | 1:B:44:THR:HG22   | 2.12                     | 0.49              |
| 1:B:567:LYS:CG    | 1:B:568:PRO:CD    | 2.80                     | 0.49              |
| 1:B:590:ARG:NH2   | 1:B:620:LYS:C     | 2.66                     | 0.49              |
| 1:B:586:ILE:HB    | 1:B:610:GLY:HA2   | 1.95                     | 0.49              |
| 1:B:901:LEU:N     | 1:B:926:GLN:NE2   | 2.55                     | 0.49              |
| 2:C:1135:ARG:O    | 2:C:1136:ASP:C    | 2.50                     | 0.49              |
| 2:C:864:LYS:N     | 2:C:872:GLU:OE1   | 2.40                     | 0.49              |
| 1:B:667:GLY:CA    | 3:D:192:TRP:CH2   | 2.95                     | 0.49              |
| 3:D:133:ILE:HD13  | 3:D:236:GLY:C     | 2.32                     | 0.49              |
| 4:E:12:ARG:HH12   | 4:E:14:ARG:HG3    | 1.78                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:E:24:ALA:O     | 4:E:26:THR:N      | 2.36                     | 0.49              |
| 4:E:33:PHE:CE2   | 7:H:80:LYS:NZ     | 2.73                     | 0.49              |
| 5:F:128:PRO:HA   | 5:F:129:PRO:C     | 2.32                     | 0.49              |
| 5:F:106:GLN:HA   | 5:F:130:ALA:HA    | 1.95                     | 0.49              |
| 8:I:82:PRO:C     | 8:I:84:ALA:H      | 2.16                     | 0.49              |
| 1:B:852:TYR:CD2  | 1:B:1060:PRO:CB   | 2.96                     | 0.49              |
| 1:B:162:VAL:HG12 | 1:B:163:SER:N     | 2.27                     | 0.49              |
| 1:B:457:ALA:HB3  | 1:B:506:ALA:HA    | 1.94                     | 0.49              |
| 1:B:738:LYS:HD2  | 1:B:740:LEU:HD21  | 1.95                     | 0.49              |
| 2:C:1017:ILE:N   | 2:C:1018:PRO:CD   | 2.76                     | 0.49              |
| 2:C:203:PHE:HB3  | 2:C:205:ILE:CD1   | 2.43                     | 0.49              |
| 2:C:254:LEU:CD2  | 2:C:361:LEU:HD13  | 2.43                     | 0.49              |
| 2:C:446:LEU:O    | 2:C:447:ALA:HB3   | 2.13                     | 0.49              |
| 3:D:114:TYR:HB3  | 3:D:140:ASN:O     | 2.13                     | 0.49              |
| 3:D:99:LEU:HA    | 3:D:119:VAL:O     | 2.12                     | 0.49              |
| 6:G:76:LYS:HE3   | 6:G:150:GLU:OE2   | 2.12                     | 0.49              |
| 1:B:1444:MET:HG3 | 7:H:60:ARG:HA     | 1.94                     | 0.49              |
| 1:B:598:LEU:HD23 | 8:I:122:LEU:HD12  | 1.95                     | 0.49              |
| 1:B:1323:ASP:OD1 | 1:B:1326:ARG:HG3  | 2.13                     | 0.49              |
| 1:B:1335:ILE:O   | 1:B:1335:ILE:CG2  | 2.61                     | 0.49              |
| 1:B:24:PRO:HG2   | 1:B:25:GLU:OE1    | 2.12                     | 0.49              |
| 1:B:537:ARG:HH12 | 8:I:122:LEU:HG    | 1.77                     | 0.49              |
| 1:B:613:ILE:O    | 1:B:614:PHE:HB3   | 2.12                     | 0.49              |
| 1:B:341:MET:HE1  | 1:B:843:LYS:HZ1   | 1.65                     | 0.49              |
| 1:B:954:TRP:HB3  | 1:B:955:PRO:HD2   | 1.95                     | 0.49              |
| 2:C:1181:GLU:O   | 2:C:1182:CYS:CB   | 2.60                     | 0.49              |
| 2:C:199:MET:N    | 2:C:199:MET:SD    | 2.86                     | 0.49              |
| 2:C:792:MET:HE2  | 2:C:857:ARG:NH1   | 2.28                     | 0.49              |
| 4:E:34:GLN:C     | 4:E:36:LYS:N      | 2.65                     | 0.49              |
| 8:I:26:ILE:CG2   | 8:I:27:GLU:N      | 2.76                     | 0.49              |
| 9:J:105:SER:O    | 9:J:106:CYS:HB2   | 2.12                     | 0.49              |
| 11:L:40:HIS:O    | 11:L:41:THR:C     | 2.51                     | 0.49              |
| 1:B:1380:GLY:C   | 1:B:1381:LEU:HD23 | 2.33                     | 0.48              |
| 1:B:1389:PHE:CG  | 1:B:1390:ASN:N    | 2.81                     | 0.48              |
| 1:B:34:LYS:N     | 1:B:34:LYS:CD     | 2.76                     | 0.48              |
| 1:B:374:LEU:HB2  | 1:B:436:ILE:HD11  | 1.95                     | 0.48              |
| 1:B:53:LEU:O     | 1:B:54:ASN:O      | 2.31                     | 0.48              |
| 2:C:243:ALA:HB1  | 2:C:251:ILE:HG12  | 1.93                     | 0.48              |
| 2:C:288:ALA:HA   | 2:C:331:LEU:HD12  | 1.94                     | 0.48              |
| 3:D:16:ASP:C     | 3:D:240:VAL:HG11  | 2.33                     | 0.48              |
| 3:D:26:ASP:O     | 3:D:27:LEU:C      | 2.50                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:E:64:VAL:HA     | 4:E:129:LEU:HD11  | 1.95                     | 0.48              |
| 7:H:9:LEU:HD12    | 7:H:10:ASN:H      | 1.76                     | 0.48              |
| 8:I:56:THR:HB     | 8:I:145:ARG:HG2   | 1.95                     | 0.48              |
| 10:K:5:VAL:O      | 10:K:6:ARG:O      | 2.31                     | 0.48              |
| 3:D:10:ILE:HD12   | 11:L:108:GLU:O    | 2.13                     | 0.48              |
| 1:B:1146:VAL:HG11 | 1:B:1202:MET:SD   | 2.53                     | 0.48              |
| 1:B:135:PHE:CD1   | 1:B:222:LEU:HD22  | 2.48                     | 0.48              |
| 1:B:40:THR:HG22   | 1:B:41:MET:CG     | 2.31                     | 0.48              |
| 1:B:971:PHE:HE2   | 1:B:1040:GLN:HG2  | 1.78                     | 0.48              |
| 2:C:1098:MET:H    | 2:C:1098:MET:HE3  | 1.78                     | 0.48              |
| 2:C:114:PRO:HG2   | 2:C:115:GLN:H     | 1.77                     | 0.48              |
| 2:C:1162:ILE:HD11 | 2:C:1194:ILE:CD1  | 2.43                     | 0.48              |
| 2:C:324:ILE:HG12  | 2:C:329:THR:HG22  | 1.95                     | 0.48              |
| 2:C:351:TYR:CD2   | 2:C:355:ILE:HD11  | 2.49                     | 0.48              |
| 2:C:30:SER:HB3    | 2:C:743:ILE:O     | 2.13                     | 0.48              |
| 3:D:100:THR:HG21  | 3:D:102:GLN:HE21  | 1.78                     | 0.48              |
| 4:E:23:ASN:O      | 7:H:83:LYS:HB2    | 2.14                     | 0.48              |
| 5:F:157:SER:OG    | 5:F:159:ASP:HB2   | 2.14                     | 0.48              |
| 7:H:117:GLN:C     | 7:H:119:LEU:N     | 2.66                     | 0.48              |
| 9:J:101:PHE:HB2   | 9:J:110:PHE:CZ    | 2.47                     | 0.48              |
| 9:J:85:PHE:CD2    | 9:J:85:PHE:N      | 2.72                     | 0.48              |
| 9:J:99:LEU:O      | 9:J:111:THR:HG23  | 2.13                     | 0.48              |
| 11:L:13:GLY:O     | 11:L:14:GLU:C     | 2.51                     | 0.48              |
| 11:L:50:LEU:HD11  | 11:L:75:ILE:CD1   | 2.42                     | 0.48              |
| 1:B:1333:ILE:O    | 1:B:1333:ILE:HD13 | 2.13                     | 0.48              |
| 1:B:90:VAL:HG12   | 1:B:297:GLN:NE2   | 2.28                     | 0.48              |
| 2:C:1010:LEU:C    | 2:C:1011:ILE:HG13 | 2.34                     | 0.48              |
| 2:C:361:LEU:N     | 2:C:362:PRO:CD    | 2.76                     | 0.48              |
| 2:C:363:HIS:O     | 2:C:365:THR:N     | 2.41                     | 0.48              |
| 2:C:554:ILE:O     | 2:C:558:LEU:HG    | 2.13                     | 0.48              |
| 2:C:847:ASP:O     | 2:C:849:GLY:N     | 2.46                     | 0.48              |
| 3:D:44:LEU:CG     | 3:D:159:ALA:HB1   | 2.43                     | 0.48              |
| 4:E:14:ARG:NH2    | 4:E:16:LYS:NZ     | 2.59                     | 0.48              |
| 4:E:41:GLN:HB2    | 4:E:43:GLU:HG3    | 1.94                     | 0.48              |
| 8:I:123:MET:HE3   | 8:I:142:LEU:HD21  | 1.94                     | 0.48              |
| 10:K:64:ASN:CB    | 10:K:65:PRO:CD    | 2.89                     | 0.48              |
| 1:B:1006:ILE:HD12 | 5:F:167:ARG:CG    | 2.44                     | 0.48              |
| 1:B:137:ALA:O     | 1:B:138:ILE:C     | 2.51                     | 0.48              |
| 1:B:366:VAL:HG21  | 1:B:460:VAL:HG23  | 1.96                     | 0.48              |
| 1:B:598:LEU:HA    | 8:I:122:LEU:CD1   | 2.38                     | 0.48              |
| 1:B:35:ILE:HG22   | 1:B:84:ILE:HD12   | 1.95                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:1138:MET:HE2  | 2:C:1143:ALA:HB3  | 1.96                     | 0.48              |
| 2:C:1183:LYS:HE3  | 2:C:1183:LYS:N    | 2.29                     | 0.48              |
| 2:C:259:TYR:HB2   | 2:C:268:THR:HG23  | 1.96                     | 0.48              |
| 2:C:288:ALA:CA    | 2:C:331:LEU:HD12  | 2.43                     | 0.48              |
| 2:C:459:TYR:CD1   | 2:C:469:GLN:NE2   | 2.81                     | 0.48              |
| 2:C:658:ILE:HG22  | 2:C:659:ALA:N     | 2.27                     | 0.48              |
| 2:C:779:GLY:O     | 2:C:795:ILE:HA    | 2.13                     | 0.48              |
| 2:C:802:PRO:HG2   | 2:C:805:THR:HG22  | 1.95                     | 0.48              |
| 3:D:43:THR:O      | 3:D:77:ILE:HG13   | 2.12                     | 0.48              |
| 4:E:189:ASP:HB3   | 7:H:167:TYR:OH    | 2.13                     | 0.48              |
| 8:I:58:THR:HB     | 8:I:143:LEU:HD13  | 1.94                     | 0.48              |
| 10:K:16:ASP:OD1   | 10:K:17:LYS:CD    | 2.62                     | 0.48              |
| 11:L:60:ALA:O     | 11:L:73:LEU:HD12  | 2.14                     | 0.48              |
| 15:T:18:DT:OP2    | 15:T:18:DT:H73    | 2.14                     | 0.48              |
| 1:B:1011:GLN:HE21 | 1:B:1015:VAL:HG21 | 1.77                     | 0.48              |
| 1:B:129:LYS:O     | 1:B:130:ASP:HB2   | 2.14                     | 0.48              |
| 1:B:279:LEU:HB3   | 1:B:289:ILE:HD11  | 1.95                     | 0.48              |
| 1:B:305:ASP:CG    | 1:B:326:ARG:HD2   | 2.33                     | 0.48              |
| 1:B:332:LYS:O     | 1:B:333:GLU:HB2   | 2.13                     | 0.48              |
| 1:B:513:SER:HB2   | 1:B:520:CYS:HB3   | 1.95                     | 0.48              |
| 1:B:650:GLN:HB3   | 1:B:654:ASN:ND2   | 2.28                     | 0.48              |
| 1:B:942:PHE:HD2   | 1:B:942:PHE:O     | 1.96                     | 0.48              |
| 2:C:1085:ILE:HG22 | 2:C:1086:PHE:N    | 2.28                     | 0.48              |
| 2:C:1151:LEU:N    | 2:C:1151:LEU:HD12 | 2.28                     | 0.48              |
| 2:C:180:TYR:N     | 2:C:180:TYR:CD1   | 2.81                     | 0.48              |
| 2:C:797:TYR:HE1   | 2:C:854:LEU:HD23  | 1.78                     | 0.48              |
| 2:C:890:TYR:O     | 2:C:893:LEU:HB2   | 2.13                     | 0.48              |
| 3:D:73:GLN:HE21   | 3:D:75:MET:N      | 2.10                     | 0.48              |
| 7:H:139:ILE:CG2   | 7:H:140:LYS:H     | 2.16                     | 0.48              |
| 1:B:698:GLN:NE2   | 9:J:99:LEU:HD21   | 2.28                     | 0.48              |
| 1:B:1030:ARG:NH1  | 1:B:1035:TYR:OH   | 2.46                     | 0.48              |
| 1:B:1227:ILE:CG2  | 1:B:1228:TRP:N    | 2.77                     | 0.48              |
| 1:B:302:THR:O     | 1:B:304:MET:N     | 2.47                     | 0.48              |
| 1:B:390:GLN:HE21  | 1:B:394:ASN:HD21  | 1.62                     | 0.48              |
| 1:B:718:VAL:O     | 1:B:722:LEU:HD12  | 2.13                     | 0.48              |
| 2:C:744:HIS:ND1   | 2:C:745:PRO:HD2   | 2.29                     | 0.48              |
| 2:C:773:MET:HA    | 2:C:776:GLN:HE21  | 1.78                     | 0.48              |
| 2:C:843:GLN:N     | 2:C:994:TYR:O     | 2.31                     | 0.48              |
| 5:F:136:ASN:HB3   | 5:F:139:ALA:HB3   | 1.95                     | 0.48              |
| 6:G:75:PRO:HG2    | 6:G:78:GLN:HB2    | 1.96                     | 0.48              |
| 1:B:1152:ILE:CD1  | 9:J:44:TYR:HB3    | 2.44                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:J:69:PRO:HB2    | 9:J:85:PHE:CE2    | 2.49                     | 0.48              |
| 10:K:35:ALA:C     | 10:K:39:LEU:HD12  | 2.33                     | 0.48              |
| 1:B:491:VAL:HG12  | 1:B:492:PRO:O     | 2.14                     | 0.48              |
| 1:B:836:TYR:CZ    | 1:B:840:ARG:HD2   | 2.48                     | 0.48              |
| 1:B:912:LEU:O     | 1:B:978:PRO:HA    | 2.14                     | 0.48              |
| 2:C:1079:LYS:CG   | 2:C:1080:LYS:N    | 2.75                     | 0.48              |
| 2:C:486:TYR:N     | 2:C:486:TYR:CD2   | 2.80                     | 0.48              |
| 2:C:508:LEU:O     | 2:C:509:ALA:CB    | 2.62                     | 0.48              |
| 4:E:71:LYS:HA     | 4:E:74:GLN:HG3    | 1.96                     | 0.48              |
| 1:B:1443:VAL:HG23 | 7:H:61:ILE:HB     | 1.96                     | 0.48              |
| 8:I:104:PHE:CE2   | 8:I:136:LYS:HG2   | 2.49                     | 0.48              |
| 10:K:3:VAL:CG1    | 10:K:15:GLY:HA2   | 2.43                     | 0.48              |
| 10:K:4:PRO:HD3    | 10:K:53:HIS:HD2   | 1.76                     | 0.48              |
| 1:B:1220:PHE:O    | 1:B:1221:LYS:HB2  | 2.14                     | 0.48              |
| 1:B:1155:ASP:HB3  | 1:B:1241:ARG:HH21 | 1.79                     | 0.48              |
| 1:B:1334:ASP:C    | 1:B:1336:MET:N    | 2.67                     | 0.48              |
| 1:B:1450:LEU:O    | 1:B:1450:LEU:CG   | 2.60                     | 0.48              |
| 1:B:298:PHE:O     | 1:B:301:ALA:HB3   | 2.12                     | 0.48              |
| 1:B:826:ASP:O     | 1:B:827:THR:C     | 2.52                     | 0.48              |
| 1:B:88:LYS:HB3    | 1:B:89:PRO:HD2    | 1.95                     | 0.48              |
| 2:C:1044:ALA:O    | 2:C:1045:SER:O    | 2.31                     | 0.48              |
| 2:C:834:ASN:ND2   | 2:C:1013:ASN:HA   | 2.29                     | 0.48              |
| 6:G:96:THR:O      | 6:G:100:GLN:HG3   | 2.14                     | 0.48              |
| 8:I:102:TYR:H     | 8:I:102:TYR:HD2   | 1.57                     | 0.48              |
| 8:I:130:ARG:HB3   | 8:I:133:ASN:CB    | 2.44                     | 0.48              |
| 2:C:1006:ILE:HG23 | 10:K:43:ARG:HG3   | 1.96                     | 0.48              |
| 11:L:47:ARG:C     | 11:L:47:ARG:HD2   | 2.34                     | 0.48              |
| 1:B:114:LEU:O     | 1:B:115:LEU:HG    | 2.13                     | 0.48              |
| 1:B:1276:VAL:HB   | 1:B:1279:ILE:CD1  | 2.43                     | 0.48              |
| 1:B:351:THR:HG21  | 2:C:1103:ILE:HG13 | 1.95                     | 0.48              |
| 1:B:567:LYS:CB    | 1:B:568:PRO:HD2   | 2.41                     | 0.48              |
| 1:B:826:ASP:O     | 1:B:830:LYS:N     | 2.32                     | 0.48              |
| 1:B:858:ASN:ND2   | 1:B:860:LEU:H     | 2.12                     | 0.48              |
| 1:B:923:LEU:O     | 1:B:927:VAL:HG23  | 2.14                     | 0.48              |
| 2:C:1005:GLY:O    | 2:C:1006:ILE:C    | 2.51                     | 0.48              |
| 2:C:479:VAL:HG12  | 2:C:480:SER:N     | 2.29                     | 0.48              |
| 2:C:637:LEU:O     | 2:C:690:VAL:HG13  | 2.14                     | 0.48              |
| 3:D:148:ARG:CD    | 3:D:149:LYS:H     | 2.27                     | 0.48              |
| 3:D:18:VAL:O      | 3:D:19:ASP:C      | 2.52                     | 0.48              |
| 3:D:133:ILE:CD1   | 3:D:237:SER:N     | 2.77                     | 0.48              |
| 5:F:173:SER:O     | 5:F:175:LEU:N     | 2.46                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:H:10:ASN:OD1   | 7:H:71:ASN:HA     | 2.12                     | 0.48              |
| 7:H:13:LEU:HD23  | 7:H:14:HIS:N      | 2.28                     | 0.48              |
| 8:I:10:PHE:CD1   | 8:I:10:PHE:N      | 2.82                     | 0.48              |
| 9:J:78:CYS:SG    | 9:J:106:CYS:HB2   | 2.54                     | 0.48              |
| 9:J:58:VAL:HG13  | 9:J:62:ILE:CD1    | 2.41                     | 0.48              |
| 3:D:235:VAL:HG12 | 10:K:13:VAL:HG23  | 1.96                     | 0.48              |
| 11:L:2:ASN:O     | 11:L:3:ALA:C      | 2.53                     | 0.48              |
| 3:D:35:ARG:NH1   | 11:L:40:HIS:HB2   | 2.28                     | 0.48              |
| 2:C:193:LYS:HZ2  | 12:M:32:ALA:HB1   | 1.78                     | 0.48              |
| 1:B:1140:HIS:HA  | 1:B:1274:ARG:O    | 2.14                     | 0.48              |
| 1:B:1120:LEU:CD1 | 1:B:1304:TRP:O    | 2.61                     | 0.48              |
| 1:B:1332:PHE:H   | 1:B:1332:PHE:HD2  | 1.62                     | 0.48              |
| 1:B:504:LEU:N    | 1:B:504:LEU:HD12  | 2.29                     | 0.48              |
| 1:B:512:VAL:HA   | 1:B:519:PRO:HA    | 1.95                     | 0.48              |
| 1:B:774:ARG:NH1  | 1:B:797:LYS:HG3   | 2.28                     | 0.48              |
| 1:B:490:HIS:ND1  | 2:C:1150:ARG:NH1  | 2.62                     | 0.48              |
| 2:C:1215:ARG:C   | 2:C:1216:LEU:HD23 | 2.35                     | 0.48              |
| 2:C:368:GLU:O    | 2:C:370:PHE:N     | 2.42                     | 0.48              |
| 3:D:161:LYS:O    | 3:D:170:TRP:NE1   | 2.47                     | 0.48              |
| 3:D:22:LEU:HD13  | 3:D:230:MET:HE1   | 1.95                     | 0.48              |
| 3:D:232:VAL:HG11 | 3:D:244:VAL:CG2   | 2.44                     | 0.48              |
| 1:B:870:GLU:HB2  | 5:F:204:THR:HG21  | 1.96                     | 0.48              |
| 7:H:140:LYS:H    | 7:H:140:LYS:HG2   | 1.38                     | 0.48              |
| 11:L:30:ALA:HB2  | 11:L:76:GLN:HG3   | 1.95                     | 0.48              |
| 2:C:852:ARG:NH2  | 12:M:70:ARG:OXT   | 2.26                     | 0.48              |
| 1:B:12:ARG:NH2   | 2:C:1192:TYR:HE2  | 2.12                     | 0.47              |
| 1:B:317:LYS:O    | 1:B:318:SER:CB    | 2.62                     | 0.47              |
| 1:B:384:ASN:C    | 1:B:386:ASP:N     | 2.66                     | 0.47              |
| 1:B:722:LEU:HD23 | 1:B:799:PHE:CD1   | 2.49                     | 0.47              |
| 2:C:258:LEU:HG   | 2:C:258:LEU:O     | 2.14                     | 0.47              |
| 2:C:291:ILE:HD13 | 2:C:300:HIS:CD2   | 2.49                     | 0.47              |
| 2:C:562:GLY:HA3  | 2:C:590:HIS:CE1   | 2.49                     | 0.47              |
| 2:C:604:ARG:HB2  | 2:C:609:ILE:HB    | 1.95                     | 0.47              |
| 2:C:687:GLU:O    | 2:C:688:GLY:C     | 2.52                     | 0.47              |
| 2:C:773:MET:HE1  | 2:C:985:GLY:HA2   | 1.94                     | 0.47              |
| 5:F:77:SER:O     | 5:F:105:PHE:HB3   | 2.14                     | 0.47              |
| 5:F:93:MET:SD    | 5:F:97:VAL:CG2    | 3.02                     | 0.47              |
| 7:H:39:THR:O     | 7:H:43:GLY:N      | 2.43                     | 0.47              |
| 7:H:43:GLY:HA2   | 7:H:157:ILE:HD11  | 1.96                     | 0.47              |
| 8:I:116:TYR:HB2  | 8:I:123:MET:HB3   | 1.96                     | 0.47              |
| 3:D:221:TYR:CD2  | 8:I:46:LEU:HD23   | 2.48                     | 0.47              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:355:GLY:N     | 1:B:482:PHE:CE1  | 2.81                     | 0.47              |
| 1:B:54:ASN:HD21   | 1:B:247:ARG:NH1  | 2.11                     | 0.47              |
| 1:B:784:LEU:HD11  | 1:B:815:PHE:CE2  | 2.48                     | 0.47              |
| 2:C:1002:THR:HG23 | 2:C:1006:ILE:O   | 2.14                     | 0.47              |
| 2:C:1034:VAL:O    | 2:C:1036:ALA:N   | 2.47                     | 0.47              |
| 2:C:367:LEU:HD12  | 2:C:370:PHE:CZ   | 2.48                     | 0.47              |
| 2:C:405:ARG:HD2   | 2:C:631:GLY:HA3  | 1.96                     | 0.47              |
| 2:C:45:SER:O      | 2:C:48:LEU:N     | 2.47                     | 0.47              |
| 2:C:591:ARG:O     | 2:C:593:PRO:HD3  | 2.14                     | 0.47              |
| 3:D:143:LEU:HD21  | 3:D:146:LYS:HE2  | 1.96                     | 0.47              |
| 3:D:172:PRO:O     | 3:D:235:VAL:HG22 | 2.12                     | 0.47              |
| 3:D:83:SER:OG     | 3:D:160:LYS:HD3  | 2.14                     | 0.47              |
| 6:G:103:MET:HE3   | 7:H:66:GLY:N     | 2.30                     | 0.47              |
| 1:B:548:ASN:OD1   | 11:L:60:ALA:HB1  | 2.13                     | 0.47              |
| 14:P:8:U:O2'      | 14:P:9:A:H5'     | 2.13                     | 0.47              |
| 1:B:1242:VAL:O    | 1:B:1243:VAL:CB  | 2.60                     | 0.47              |
| 1:B:50:ILE:HG22   | 1:B:52:GLY:N     | 2.28                     | 0.47              |
| 1:B:629:LEU:HD22  | 1:B:633:VAL:CG2  | 2.44                     | 0.47              |
| 1:B:784:LEU:HD21  | 1:B:815:PHE:HE2  | 1.80                     | 0.47              |
| 1:B:78:PRO:CA     | 2:C:1201:LYS:HZ2 | 2.27                     | 0.47              |
| 2:C:1004:GLU:OE2  | 2:C:1064:TYR:CE2 | 2.67                     | 0.47              |
| 4:E:118:THR:HB    | 4:E:121:LYS:HB3  | 1.94                     | 0.47              |
| 5:F:124:VAL:CG1   | 5:F:132:ILE:HG13 | 2.44                     | 0.47              |
| 5:F:42:PHE:CE1    | 5:F:58:MET:HE3   | 2.49                     | 0.47              |
| 6:G:135:ARG:CZ    | 6:G:143:PHE:CE2  | 2.97                     | 0.47              |
| 7:H:145:VAL:CG1   | 7:H:146:LYS:N    | 2.76                     | 0.47              |
| 8:I:40:LEU:HD12   | 8:I:122:LEU:O    | 2.14                     | 0.47              |
| 10:K:19:GLU:O     | 10:K:23:ASN:HB2  | 2.14                     | 0.47              |
| 11:L:108:GLU:O    | 11:L:112:GLN:HG2 | 2.15                     | 0.47              |
| 3:D:252:GLN:HG3   | 11:L:95:ILE:HG23 | 1.96                     | 0.47              |
| 1:B:116:ASP:C     | 1:B:118:HIS:N    | 2.68                     | 0.47              |
| 1:B:1224:LEU:HD12 | 1:B:1225:PHE:N   | 2.29                     | 0.47              |
| 1:B:184:SER:CB    | 1:B:199:LEU:HD23 | 2.44                     | 0.47              |
| 1:B:441:PRO:HD2   | 1:B:498:ARG:CZ   | 2.44                     | 0.47              |
| 1:B:796:SER:C     | 1:B:798:GLY:H    | 2.18                     | 0.47              |
| 2:C:1081:LEU:O    | 2:C:1083:ALA:N   | 2.48                     | 0.47              |
| 2:C:273:LEU:HG    | 2:C:276:ILE:HD12 | 1.95                     | 0.47              |
| 2:C:298:LEU:CD2   | 2:C:298:LEU:N    | 2.77                     | 0.47              |
| 2:C:600:LEU:HD13  | 2:C:626:ILE:HD11 | 1.96                     | 0.47              |
| 2:C:628:THR:O     | 2:C:628:THR:HG23 | 2.13                     | 0.47              |
| 1:B:816:HIS:CD2   | 2:C:764:SER:H    | 2.32                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:792:MET:CE   | 2:C:857:ARG:NH1   | 2.76                     | 0.47              |
| 2:C:811:TYR:H    | 2:C:811:TYR:HD1   | 1.61                     | 0.47              |
| 2:C:908:GLU:O    | 2:C:909:ASP:O     | 2.33                     | 0.47              |
| 5:F:43:LYS:C     | 5:F:45:LYS:H      | 2.18                     | 0.47              |
| 7:H:91:VAL:HG22  | 7:H:101:VAL:HG22  | 1.97                     | 0.47              |
| 8:I:109:LYS:HB2  | 8:I:111:LEU:HD12  | 1.96                     | 0.47              |
| 10:K:2:ILE:HG12  | 10:K:57:ILE:HD12  | 1.95                     | 0.47              |
| 12:M:53:HIS:O    | 12:M:55:ILE:HG12  | 2.15                     | 0.47              |
| 1:B:381:THR:O    | 1:B:383:TYR:N     | 2.48                     | 0.47              |
| 1:B:43:GLU:O     | 1:B:44:THR:HB     | 2.13                     | 0.47              |
| 1:B:535:THR:HG23 | 1:B:575:LYS:HG2   | 1.95                     | 0.47              |
| 1:B:919:ILE:HG23 | 1:B:925:LEU:HD12  | 1.97                     | 0.47              |
| 1:B:455:MET:HE3  | 2:C:1134:GLU:HG3  | 1.97                     | 0.47              |
| 2:C:284:ILE:HD13 | 2:C:333:PHE:CD2   | 2.49                     | 0.47              |
| 2:C:792:MET:HA   | 2:C:856:PHE:O     | 2.14                     | 0.47              |
| 2:C:996:ARG:NH1  | 3:D:38:ILE:HG23   | 2.30                     | 0.47              |
| 3:D:77:ILE:HA    | 3:D:129:ILE:HD11  | 1.97                     | 0.47              |
| 3:D:142:VAL:H    | 10:K:16:ASP:CB    | 2.27                     | 0.47              |
| 3:D:148:ARG:CG   | 3:D:149:LYS:H     | 2.28                     | 0.47              |
| 1:B:667:GLY:CA   | 3:D:192:TRP:HH2   | 2.27                     | 0.47              |
| 3:D:69:LEU:CD1   | 3:D:69:LEU:N      | 2.77                     | 0.47              |
| 4:E:56:ARG:CD    | 4:E:149:THR:HA    | 2.36                     | 0.47              |
| 1:B:789:LYS:HE3  | 9:J:67:THR:OG1    | 2.14                     | 0.47              |
| 9:J:4:PHE:HE1    | 9:J:6:PHE:HE2     | 1.63                     | 0.47              |
| 10:K:56:LEU:O    | 10:K:59:LYS:N     | 2.48                     | 0.47              |
| 1:B:1048:ASN:O   | 1:B:1049:ILE:C    | 2.52                     | 0.47              |
| 1:B:1097:GLY:O   | 1:B:1100:ARG:HB3  | 2.14                     | 0.47              |
| 1:B:1335:ILE:O   | 1:B:1335:ILE:HG22 | 2.14                     | 0.47              |
| 1:B:1336:MET:HE2 | 1:B:1381:LEU:HD23 | 1.97                     | 0.47              |
| 1:B:295:LEU:O    | 1:B:298:PHE:HB3   | 2.15                     | 0.47              |
| 1:B:753:GLY:HA2  | 1:B:757:ASN:ND2   | 2.30                     | 0.47              |
| 1:B:898:ARG:HB2  | 1:B:933:TYR:CE1   | 2.49                     | 0.47              |
| 1:B:959:ASN:OD1  | 1:B:961:ARG:HB3   | 2.14                     | 0.47              |
| 1:B:335:ARG:NH1  | 2:C:1202:LEU:HD13 | 2.29                     | 0.47              |
| 1:B:15:LYS:HG3   | 2:C:1219:ASP:HA   | 1.97                     | 0.47              |
| 2:C:473:MET:C    | 2:C:475:SER:H     | 2.18                     | 0.47              |
| 2:C:980:PHE:CA   | 2:C:1095:LEU:HD11 | 2.44                     | 0.47              |
| 3:D:44:LEU:HA    | 3:D:160:LYS:O     | 2.13                     | 0.47              |
| 2:C:1079:LYS:N   | 3:D:27:LEU:HD21   | 2.30                     | 0.47              |
| 4:E:210:ILE:O    | 4:E:214:LEU:HD23  | 2.14                     | 0.47              |
| 4:E:47:LEU:HD11  | 7:H:3:PHE:CE2     | 2.49                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:G:130:ILE:O     | 6:G:148:VAL:CG2   | 2.62                     | 0.47              |
| 7:H:30:LEU:HD13   | 7:H:72:VAL:CG1    | 2.39                     | 0.47              |
| 8:I:102:TYR:N     | 8:I:102:TYR:HD2   | 2.09                     | 0.47              |
| 8:I:128:ASN:O     | 8:I:128:ASN:OD1   | 2.32                     | 0.47              |
| 8:I:84:ALA:CA     | 8:I:87:ARG:HB2    | 2.40                     | 0.47              |
| 1:B:567:LYS:CB    | 8:I:96:VAL:H      | 2.20                     | 0.47              |
| 3:D:114:TYR:HE2   | 10:K:19:GLU:OE2   | 1.97                     | 0.47              |
| 11:L:63:VAL:HG23  | 11:L:63:VAL:O     | 2.14                     | 0.47              |
| 10:K:65:PRO:HG3   | 12:M:32:ALA:O     | 2.14                     | 0.47              |
| 1:B:1317:MET:CE   | 1:B:1327:ILE:HG21 | 2.44                     | 0.47              |
| 1:B:1329:THR:O    | 1:B:1331:SER:N    | 2.48                     | 0.47              |
| 1:B:1345:ARG:HD2  | 1:B:1373:ASP:OD1  | 2.13                     | 0.47              |
| 1:B:1402:PHE:O    | 1:B:1403:GLU:HB2  | 2.14                     | 0.47              |
| 1:B:1410:PHE:HA   | 2:C:1212:ILE:CD1  | 2.45                     | 0.47              |
| 1:B:331:GLY:O     | 1:B:332:LYS:O     | 2.33                     | 0.47              |
| 1:B:49:LYS:NZ     | 1:B:61:ILE:H      | 2.11                     | 0.47              |
| 1:B:63:ARG:HG2    | 1:B:74:MET:SD     | 2.54                     | 0.47              |
| 1:B:951:GLU:HB3   | 1:B:954:TRP:CZ2   | 2.49                     | 0.47              |
| 1:B:961:ARG:NH1   | 1:B:961:ARG:HG3   | 2.28                     | 0.47              |
| 2:C:980:PHE:CD2   | 2:C:1094:ARG:HA   | 2.50                     | 0.47              |
| 2:C:776:GLN:O     | 2:C:1095:LEU:HA   | 2.14                     | 0.47              |
| 2:C:284:ILE:HG23  | 2:C:324:ILE:CD1   | 2.44                     | 0.47              |
| 2:C:373:ARG:HD2   | 2:C:567:GLU:OE2   | 2.14                     | 0.47              |
| 2:C:483:LEU:HD21  | 2:C:491:THR:CG2   | 2.45                     | 0.47              |
| 2:C:530:GLY:O     | 2:C:533:CYS:HB2   | 2.15                     | 0.47              |
| 2:C:782:LEU:HB3   | 2:C:784:ASN:OD1   | 2.15                     | 0.47              |
| 2:C:897:GLY:O     | 2:C:898:LEU:HD23  | 2.15                     | 0.47              |
| 3:D:186:LEU:HD12  | 3:D:186:LEU:N     | 2.30                     | 0.47              |
| 3:D:89:GLU:O      | 3:D:90:ASP:HB3    | 2.15                     | 0.47              |
| 4:E:27:LEU:CD1    | 4:E:173:HIS:HB2   | 2.43                     | 0.47              |
| 8:I:113:ALA:HB2   | 8:I:126:GLU:HG3   | 1.97                     | 0.47              |
| 1:B:1161:THR:HG22 | 1:B:1162:VAL:N    | 2.29                     | 0.47              |
| 1:B:243:PRO:HB2   | 1:B:244:PRO:HD2   | 1.97                     | 0.47              |
| 1:B:537:ARG:NH1   | 8:I:120:GLY:O     | 2.48                     | 0.47              |
| 1:B:781:ASP:O     | 1:B:789:LYS:HA    | 2.14                     | 0.47              |
| 2:C:230:ALA:N     | 2:C:231:PRO:HD2   | 2.29                     | 0.47              |
| 2:C:461:LEU:N     | 2:C:461:LEU:CD1   | 2.77                     | 0.47              |
| 2:C:611:PRO:O     | 2:C:692:TYR:HB2   | 2.14                     | 0.47              |
| 2:C:797:TYR:O     | 2:C:799:PRO:HD3   | 2.14                     | 0.47              |
| 3:D:77:ILE:HD13   | 3:D:77:ILE:HA     | 1.68                     | 0.47              |
| 5:F:111:VAL:CG1   | 5:F:137:GLU:HG2   | 2.45                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:F:11:ARG:HH21   | 5:F:141:VAL:HG21  | 1.79                     | 0.47              |
| 5:F:26:ARG:HH22   | 5:F:133:GLU:CD    | 2.17                     | 0.47              |
| 8:I:40:LEU:HD23   | 8:I:42:ILE:HD11   | 1.97                     | 0.47              |
| 12:M:30:ILE:HG22  | 12:M:31:CYS:H     | 1.79                     | 0.47              |
| 12:M:36:SER:O     | 12:M:37:LYS:O     | 2.33                     | 0.47              |
| 1:B:1340:GLY:HA2  | 5:F:183:PRO:HD2   | 1.96                     | 0.47              |
| 1:B:297:GLN:O     | 1:B:301:ALA:HB2   | 2.14                     | 0.47              |
| 1:B:367:PRO:HB3   | 1:B:465:TYR:O     | 2.15                     | 0.47              |
| 2:C:1125:ASP:O    | 2:C:1126:GLY:O    | 2.33                     | 0.47              |
| 2:C:1161:HIS:NE2  | 2:C:1175:LEU:HD21 | 2.29                     | 0.47              |
| 2:C:581:PHE:HA    | 2:C:585:VAL:O     | 2.15                     | 0.47              |
| 2:C:882:THR:HG21  | 2:C:935:ARG:CA    | 2.45                     | 0.47              |
| 2:C:941:LEU:HD21  | 2:C:946:ASN:HA    | 1.97                     | 0.47              |
| 3:D:181:ASP:OD1   | 3:D:185:LYS:HB2   | 2.15                     | 0.47              |
| 6:G:109:VAL:HG11  | 6:G:127:GLU:OE2   | 2.14                     | 0.47              |
| 7:H:51:TYR:C      | 7:H:51:TYR:CD2    | 2.88                     | 0.47              |
| 7:H:59:GLY:HA3    | 7:H:70:PHE:CE2    | 2.50                     | 0.47              |
| 11:L:73:LEU:HD21  | 11:L:75:ILE:HD11  | 1.96                     | 0.47              |
| 1:B:115:LEU:CD1   | 1:B:142:CYS:HB3   | 2.45                     | 0.47              |
| 1:B:1239:ARG:HB3  | 1:B:1239:ARG:NH1  | 2.30                     | 0.47              |
| 1:B:1377:THR:HA   | 5:F:212:ARG:HH21  | 1.79                     | 0.47              |
| 1:B:1446:ASP:O    | 1:B:1447:GLU:C    | 2.53                     | 0.47              |
| 1:B:492:PRO:O     | 1:B:493:GLN:NE2   | 2.47                     | 0.47              |
| 1:B:774:ARG:O     | 1:B:775:ILE:C     | 2.52                     | 0.47              |
| 1:B:780:VAL:HG23  | 2:C:699:GLU:OE1   | 2.14                     | 0.47              |
| 2:C:370:PHE:HD2   | 2:C:373:ARG:HD2   | 1.79                     | 0.47              |
| 3:D:113:VAL:O     | 3:D:144:ILE:N     | 2.48                     | 0.47              |
| 7:H:27:LYS:HD3    | 7:H:51:TYR:CE2    | 2.50                     | 0.47              |
| 7:H:88:ASP:N      | 7:H:88:ASP:OD2    | 2.40                     | 0.47              |
| 10:K:36:LEU:CB    | 10:K:47:ARG:HH12  | 2.27                     | 0.47              |
| 1:B:1315:GLU:C    | 1:B:1317:MET:N    | 2.67                     | 0.47              |
| 1:B:1364:ASN:O    | 1:B:1365:TYR:C    | 2.53                     | 0.47              |
| 1:B:1376:THR:HG23 | 1:B:1377:THR:N    | 2.29                     | 0.47              |
| 1:B:547:LEU:HD13  | 11:L:58:PHE:CD1   | 2.50                     | 0.47              |
| 1:B:665:GLY:O     | 1:B:667:GLY:N     | 2.48                     | 0.47              |
| 1:B:821:ARG:HH11  | 1:B:821:ARG:HB2   | 1.80                     | 0.47              |
| 2:C:1115:THR:O    | 2:C:1115:THR:HG22 | 2.13                     | 0.47              |
| 2:C:129:PHE:HD2   | 2:C:166:PHE:HA    | 1.79                     | 0.47              |
| 2:C:376:PHE:CZ    | 2:C:569:TYR:HB3   | 2.50                     | 0.47              |
| 2:C:313:MET:CE    | 2:C:386:LEU:HD22  | 2.42                     | 0.47              |
| 2:C:430:ARG:HB3   | 2:C:434:ARG:CZ    | 2.45                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:582:VAL:CG2   | 2:C:626:ILE:HB    | 2.45                     | 0.47              |
| 2:C:899:ILE:HG22  | 2:C:903:VAL:CG2   | 2.45                     | 0.47              |
| 5:F:136:ASN:HB3   | 5:F:139:ALA:CB    | 2.45                     | 0.47              |
| 7:H:138:THR:HG23  | 7:H:139:ILE:HG13  | 1.97                     | 0.47              |
| 7:H:153:GLN:O     | 7:H:154:VAL:C     | 2.53                     | 0.47              |
| 7:H:34:VAL:HG11   | 7:H:74:TYR:OH     | 2.14                     | 0.47              |
| 7:H:80:LYS:O      | 7:H:80:LYS:HG2    | 2.15                     | 0.47              |
| 9:J:100:PHE:CD1   | 9:J:100:PHE:N     | 2.83                     | 0.47              |
| 15:T:18:DT:H2'    | 15:T:19:DT:H5'    | 1.95                     | 0.47              |
| 1:B:1036:ARG:HG2  | 1:B:1036:ARG:HH11 | 1.80                     | 0.46              |
| 1:B:255:SER:OG    | 2:C:918:ILE:HG21  | 2.15                     | 0.46              |
| 1:B:264:PHE:O     | 1:B:267:ALA:HB3   | 2.14                     | 0.46              |
| 1:B:418:SER:C     | 1:B:420:ARG:N     | 2.67                     | 0.46              |
| 1:B:965:GLN:HA    | 1:B:968:GLN:CG    | 2.44                     | 0.46              |
| 2:C:1138:MET:CE   | 2:C:1143:ALA:HB3  | 2.45                     | 0.46              |
| 2:C:254:LEU:HD23  | 2:C:381:MET:CE    | 2.44                     | 0.46              |
| 2:C:324:ILE:HG22  | 2:C:325:GLN:N     | 2.29                     | 0.46              |
| 2:C:596:LEU:O     | 2:C:599:THR:HB    | 2.15                     | 0.46              |
| 2:C:882:THR:O     | 2:C:884:ARG:N     | 2.48                     | 0.46              |
| 4:E:214:LEU:C     | 4:E:216:ASN:H     | 2.18                     | 0.46              |
| 4:E:6:SER:OG      | 4:E:7:THR:N       | 2.47                     | 0.46              |
| 5:F:177:ARG:HD3   | 5:F:215:MET:CG    | 2.44                     | 0.46              |
| 5:F:39:LEU:O      | 5:F:43:LYS:HG3    | 2.14                     | 0.46              |
| 8:I:127:GLY:CA    | 8:I:130:ARG:HH22  | 2.28                     | 0.46              |
| 11:L:77:THR:HG23  | 11:L:83:PRO:HB3   | 1.97                     | 0.46              |
| 1:B:208:LEU:HD23  | 1:B:208:LEU:C     | 2.36                     | 0.46              |
| 1:B:346:ASP:HB3   | 2:C:1108:ARG:N    | 2.30                     | 0.46              |
| 2:C:1183:LYS:HA   | 2:C:1186:ASP:HA   | 1.97                     | 0.46              |
| 2:C:386:LEU:C     | 2:C:388:CYS:N     | 2.68                     | 0.46              |
| 2:C:467:GLY:CA    | 2:C:475:SER:HB3   | 2.44                     | 0.46              |
| 2:C:753:ALA:HA    | 2:C:756:ILE:HD12  | 1.97                     | 0.46              |
| 2:C:903:VAL:HG12  | 2:C:904:ARG:N     | 2.29                     | 0.46              |
| 3:D:124:LEU:O     | 3:D:127:ARG:HG2   | 2.16                     | 0.46              |
| 3:D:191:TYR:HB3   | 3:D:201:TRP:CD1   | 2.50                     | 0.46              |
| 4:E:51:ASN:HB3    | 4:E:178:ALA:HA    | 1.98                     | 0.46              |
| 6:G:99:LEU:O      | 6:G:102:SER:OG    | 2.29                     | 0.46              |
| 7:H:21:ARG:HA     | 7:H:21:ARG:HD3    | 1.68                     | 0.46              |
| 2:C:308:TRP:CZ3   | 9:J:45:ARG:HB3    | 2.49                     | 0.46              |
| 15:T:14:DC:C2'    | 15:T:15:DT:H71    | 2.43                     | 0.46              |
| 1:B:1385:THR:HG22 | 1:B:1386:ARG:H    | 1.79                     | 0.46              |
| 1:B:23:SER:HA     | 1:B:233:TRP:CD1   | 2.51                     | 0.46              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:399:HIS:CE1   | 1:B:462:VAL:HG11 | 2.49                     | 0.46              |
| 1:B:591:PHE:HA    | 1:B:595:THR:OG1  | 2.15                     | 0.46              |
| 1:B:61:ILE:O      | 1:B:63:ARG:N     | 2.49                     | 0.46              |
| 1:B:793:SER:HB2   | 1:B:794:PRO:HD2  | 1.97                     | 0.46              |
| 2:C:1151:LEU:CD1  | 2:C:1151:LEU:H   | 2.28                     | 0.46              |
| 2:C:1159:ARG:HD3  | 2:C:1193:GLN:HB2 | 1.96                     | 0.46              |
| 2:C:493:SER:N     | 2:C:751:VAL:HG11 | 2.30                     | 0.46              |
| 2:C:825:VAL:O     | 2:C:826:ALA:HB2  | 2.14                     | 0.46              |
| 2:C:865:LYS:HE2   | 2:C:871:THR:OG1  | 2.15                     | 0.46              |
| 3:D:132:PRO:O     | 3:D:133:ILE:C    | 2.54                     | 0.46              |
| 3:D:133:ILE:HD11  | 3:D:237:SER:CA   | 2.42                     | 0.46              |
| 3:D:45:ALA:CA     | 3:D:72:LEU:HD12  | 2.37                     | 0.46              |
| 4:E:59:ILE:O      | 4:E:60:LYS:C     | 2.51                     | 0.46              |
| 7:H:145:VAL:CG1   | 7:H:146:LYS:H    | 2.27                     | 0.46              |
| 8:I:91:ASP:C      | 8:I:93:TYR:H     | 2.18                     | 0.46              |
| 11:L:42:LEU:HD21  | 11:L:46:ILE:HD11 | 1.97                     | 0.46              |
| 12:M:27:LEU:HD23  | 12:M:27:LEU:H    | 1.79                     | 0.46              |
| 3:D:47:ASP:CA     | 12:M:69:ALA:CB   | 2.91                     | 0.46              |
| 1:B:1074:GLU:C    | 1:B:1076:ALA:N   | 2.68                     | 0.46              |
| 1:B:1173:HIS:C    | 1:B:1174:PHE:HD1 | 2.17                     | 0.46              |
| 1:B:1385:THR:HG22 | 1:B:1386:ARG:N   | 2.30                     | 0.46              |
| 1:B:1418:LEU:HD12 | 1:B:1419:ASP:H   | 1.79                     | 0.46              |
| 1:B:22:PHE:CE2    | 1:B:30:ILE:HD12  | 2.50                     | 0.46              |
| 1:B:51:GLY:HA2    | 1:B:56:PRO:HA    | 1.97                     | 0.46              |
| 1:B:591:PHE:CD2   | 1:B:595:THR:HB   | 2.50                     | 0.46              |
| 2:C:171:PRO:HD2   | 2:C:457:LEU:CD1  | 2.46                     | 0.46              |
| 2:C:47:GLN:HB3    | 2:C:173:MET:HE1  | 1.98                     | 0.46              |
| 1:B:828:ALA:HB1   | 2:C:530:GLY:HA2  | 1.91                     | 0.46              |
| 3:D:234:SER:OG    | 3:D:235:VAL:N    | 2.48                     | 0.46              |
| 4:E:118:THR:HG22  | 4:E:118:THR:O    | 2.15                     | 0.46              |
| 7:H:138:THR:HG22  | 7:H:139:ILE:HG13 | 1.96                     | 0.46              |
| 10:K:36:LEU:HD22  | 10:K:41:LEU:HD12 | 1.96                     | 0.46              |
| 10:K:48:ARG:CD    | 10:K:49:MET:N    | 2.75                     | 0.46              |
| 11:L:19:LEU:HD22  | 11:L:33:ILE:HG21 | 1.98                     | 0.46              |
| 1:B:1164:PRO:HG2  | 1:B:1165:GLU:H   | 1.80                     | 0.46              |
| 1:B:445:ASN:HA    | 1:B:478:TYR:CE2  | 2.49                     | 0.46              |
| 1:B:500:GLU:O     | 1:B:504:LEU:HD13 | 2.15                     | 0.46              |
| 1:B:710:LEU:HD12  | 1:B:710:LEU:N    | 2.30                     | 0.46              |
| 1:B:868:TYR:C     | 1:B:868:TYR:CD1  | 2.85                     | 0.46              |
| 1:B:886:ILE:HB    | 1:B:943:LEU:HD12 | 1.98                     | 0.46              |
| 2:C:1006:ILE:HD13 | 10:K:44:TYR:CE2  | 2.51                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:276:ILE:O     | 2:C:276:ILE:HG22  | 2.15                     | 0.46              |
| 2:C:498:THR:HG22  | 2:C:537:LYS:HB2   | 1.96                     | 0.46              |
| 2:C:579:ARG:NH1   | 2:C:622:LYS:O     | 2.49                     | 0.46              |
| 2:C:755:ILE:H     | 2:C:755:ILE:HG13  | 1.50                     | 0.46              |
| 1:B:807:GLY:HA2   | 2:C:760:ASP:O     | 2.15                     | 0.46              |
| 4:E:12:ARG:HH21   | 4:E:12:ARG:HG3    | 1.80                     | 0.46              |
| 4:E:20:GLU:O      | 4:E:21:GLU:O      | 2.32                     | 0.46              |
| 5:F:147:HIS:HD2   | 5:F:149:LEU:H     | 1.62                     | 0.46              |
| 1:B:1006:ILE:HD12 | 5:F:167:ARG:HG3   | 1.98                     | 0.46              |
| 8:I:145:ARG:HG3   | 8:I:146:ARG:HG3   | 1.97                     | 0.46              |
| 10:K:9:SER:HB2    | 10:K:45:CYS:HB2   | 1.97                     | 0.46              |
| 1:B:1102:LYS:O    | 1:B:1106:ASN:ND2  | 2.49                     | 0.46              |
| 1:B:1215:ARG:NH1  | 1:B:1272:THR:O    | 2.49                     | 0.46              |
| 1:B:1330:ASN:O    | 1:B:1332:PHE:N    | 2.48                     | 0.46              |
| 1:B:442:VAL:HG12  | 1:B:490:HIS:O     | 2.14                     | 0.46              |
| 1:B:563:PRO:HG3   | 1:B:572:TRP:CE2   | 2.49                     | 0.46              |
| 1:B:51:GLY:O      | 1:B:56:PRO:HB3    | 2.16                     | 0.46              |
| 1:B:639:PRO:CG    | 1:B:640:GLN:N     | 2.79                     | 0.46              |
| 1:B:71:GLN:CG     | 1:B:72:GLU:N      | 2.77                     | 0.46              |
| 1:B:867:ILE:N     | 1:B:867:ILE:HD12  | 2.31                     | 0.46              |
| 2:C:803:LEU:CD1   | 2:C:1032:SER:HB3  | 2.46                     | 0.46              |
| 2:C:1174:LYS:O    | 2:C:1175:LEU:C    | 2.54                     | 0.46              |
| 2:C:1197:PRO:HG2  | 2:C:1200:ALA:CB   | 2.27                     | 0.46              |
| 2:C:299:GLU:HB3   | 2:C:571:PRO:HG3   | 1.97                     | 0.46              |
| 2:C:388:CYS:C     | 2:C:390:LEU:H     | 2.19                     | 0.46              |
| 2:C:557:PHE:C     | 2:C:557:PHE:CD2   | 2.89                     | 0.46              |
| 2:C:570:VAL:CG2   | 2:C:573:GLN:HB3   | 2.46                     | 0.46              |
| 2:C:615:MET:C     | 2:C:616:ILE:HD12  | 2.36                     | 0.46              |
| 2:C:873:THR:HG22  | 2:C:874:PHE:N     | 2.31                     | 0.46              |
| 2:C:910:VAL:CG1   | 2:C:911:ILE:H     | 2.27                     | 0.46              |
| 5:F:11:ARG:C      | 5:F:13:TRP:N      | 2.69                     | 0.46              |
| 6:G:109:VAL:CG1   | 6:G:110:ASP:N     | 2.74                     | 0.46              |
| 10:K:57:ILE:HG12  | 10:K:61:LEU:HD11  | 1.96                     | 0.46              |
| 12:M:70:ARG:HH11  | 12:M:70:ARG:HG2   | 1.80                     | 0.46              |
| 1:B:1411:GLU:O    | 1:B:1411:GLU:HG2  | 2.15                     | 0.46              |
| 1:B:1424:VAL:HG11 | 2:C:1139:ILE:HD13 | 1.97                     | 0.46              |
| 1:B:157:ASP:C     | 1:B:159:THR:H     | 2.18                     | 0.46              |
| 1:B:23:SER:O      | 1:B:27:VAL:HG23   | 2.16                     | 0.46              |
| 1:B:709:THR:CB    | 1:B:712:GLU:HG3   | 2.42                     | 0.46              |
| 1:B:77:CYS:C      | 1:B:78:PRO:O      | 2.51                     | 0.46              |
| 1:B:886:ILE:HD12  | 1:B:943:LEU:CB    | 2.42                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:933:TYR:O    | 1:B:937:VAL:HG23  | 2.15                     | 0.46              |
| 1:B:947:PHE:HD1  | 1:B:947:PHE:N     | 2.13                     | 0.46              |
| 2:C:1002:THR:CG2 | 2:C:1006:ILE:HG13 | 2.37                     | 0.46              |
| 2:C:758:PHE:CZ   | 2:C:1031:LEU:HD22 | 2.48                     | 0.46              |
| 3:D:115:SER:HB3  | 3:D:142:VAL:HB    | 1.98                     | 0.46              |
| 3:D:229:TYR:N    | 3:D:229:TYR:CD1   | 2.84                     | 0.46              |
| 3:D:6:PRO:HG2    | 11:L:101:LEU:HB2  | 1.98                     | 0.46              |
| 5:F:116:ILE:HG22 | 5:F:120:ALA:HB3   | 1.97                     | 0.46              |
| 6:G:94:LEU:HD21  | 6:G:122:MET:HA    | 1.98                     | 0.46              |
| 8:I:58:THR:HG22  | 8:I:59:ILE:H      | 1.81                     | 0.46              |
| 1:B:1403:GLU:O   | 15:T:16:DG:OP1    | 2.33                     | 0.46              |
| 1:B:203:SER:O    | 1:B:206:GLU:HB3   | 2.15                     | 0.46              |
| 1:B:84:ILE:HD11  | 1:B:270:LEU:HD22  | 1.97                     | 0.46              |
| 1:B:90:VAL:HG13  | 1:B:297:GLN:CD    | 2.36                     | 0.46              |
| 1:B:403:LYS:O    | 1:B:404:TYR:CD2   | 2.68                     | 0.46              |
| 1:B:438:ASP:O    | 1:B:439:ASN:HB2   | 2.15                     | 0.46              |
| 1:B:572:TRP:HA   | 1:B:576:GLN:OE1   | 2.16                     | 0.46              |
| 1:B:650:GLN:HB3  | 1:B:654:ASN:HD21  | 1.81                     | 0.46              |
| 1:B:72:GLU:O     | 1:B:73:GLY:O      | 2.34                     | 0.46              |
| 2:C:1098:MET:H   | 2:C:1098:MET:CE   | 2.27                     | 0.46              |
| 2:C:1099:VAL:O   | 2:C:1101:ASP:N    | 2.49                     | 0.46              |
| 2:C:244:LEU:HD13 | 2:C:247:GLY:O     | 2.15                     | 0.46              |
| 2:C:361:LEU:HD11 | 2:C:381:MET:CE    | 2.44                     | 0.46              |
| 2:C:240:ILE:HD13 | 2:C:377:PHE:HE2   | 1.81                     | 0.46              |
| 2:C:557:PHE:O    | 2:C:557:PHE:CD2   | 2.69                     | 0.46              |
| 2:C:654:ARG:O    | 2:C:656:GLY:N     | 2.48                     | 0.46              |
| 2:C:807:ARG:NH1  | 2:C:807:ARG:HB3   | 2.30                     | 0.46              |
| 2:C:879:ARG:NH1  | 2:C:883:LEU:HD22  | 2.30                     | 0.46              |
| 3:D:163:ILE:N    | 3:D:163:ILE:CD1   | 2.68                     | 0.46              |
| 3:D:191:TYR:CD2  | 3:D:201:TRP:CD1   | 3.04                     | 0.46              |
| 3:D:221:TYR:CE1  | 3:D:222:LYS:HG3   | 2.51                     | 0.46              |
| 3:D:252:GLN:CG   | 11:L:95:ILE:HG23  | 2.46                     | 0.46              |
| 4:E:64:VAL:CG2   | 4:E:129:LEU:HD22  | 2.46                     | 0.46              |
| 5:F:144:ILE:HG13 | 5:F:145:THR:N     | 2.29                     | 0.46              |
| 5:F:60:PHE:C     | 5:F:60:PHE:CD2    | 2.88                     | 0.46              |
| 9:J:72:ASP:HA    | 9:J:81:ARG:O      | 2.15                     | 0.46              |
| 14:P:3:C:H42     | 15:T:26:DA:N6     | 2.13                     | 0.46              |
| 1:B:106:VAL:HG12 | 1:B:107:CYS:N     | 2.30                     | 0.46              |
| 1:B:591:PHE:HA   | 1:B:595:THR:CG2   | 2.45                     | 0.46              |
| 1:B:578:LEU:HD23 | 1:B:612:ILE:CD1   | 2.46                     | 0.46              |
| 1:B:590:ARG:NH2  | 1:B:620:LYS:CB    | 2.65                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:877:HIS:ND1  | 1:B:1056:SER:HA  | 2.31                     | 0.46              |
| 1:B:897:TYR:N    | 1:B:897:TYR:CD1  | 2.84                     | 0.46              |
| 2:C:1214:PRO:HG2 | 2:C:1214:PRO:O   | 2.16                     | 0.46              |
| 2:C:172:ILE:HG22 | 2:C:173:MET:N    | 2.31                     | 0.46              |
| 2:C:56:ASP:CB    | 2:C:57:TYR:HD1   | 2.28                     | 0.46              |
| 2:C:583:ASN:ND2  | 2:C:628:THR:HG22 | 2.30                     | 0.46              |
| 5:F:202:SER:HG   | 5:F:204:THR:HG22 | 1.80                     | 0.46              |
| 1:B:172:PRO:HA   | 1:B:184:SER:O    | 2.16                     | 0.46              |
| 1:B:843:LYS:HA   | 1:B:846:GLU:HG3  | 1.98                     | 0.46              |
| 2:C:746:SER:CB   | 2:C:1046:PRO:HG2 | 2.45                     | 0.46              |
| 2:C:216:GLU:HA   | 2:C:406:LEU:HD23 | 1.97                     | 0.46              |
| 2:C:276:ILE:HD13 | 2:C:280:ILE:HD11 | 1.98                     | 0.46              |
| 2:C:29:ASP:O     | 2:C:30:SER:C     | 2.54                     | 0.46              |
| 2:C:329:THR:O    | 2:C:329:THR:HG22 | 2.16                     | 0.46              |
| 2:C:33:VAL:HG21  | 2:C:638:PHE:CZ   | 2.40                     | 0.46              |
| 2:C:637:LEU:HD22 | 2:C:742:GLU:HA   | 1.97                     | 0.46              |
| 2:C:840:ILE:HB   | 2:C:1011:ILE:HB  | 1.98                     | 0.46              |
| 2:C:841:MET:O    | 2:C:993:THR:HA   | 2.16                     | 0.46              |
| 4:E:137:ASN:HD22 | 4:E:138:ASN:N    | 2.14                     | 0.46              |
| 5:F:157:SER:C    | 5:F:159:ASP:N    | 2.69                     | 0.46              |
| 8:I:7:ASP:O      | 8:I:8:ASP:HB2    | 2.15                     | 0.46              |
| 10:K:14:VAL:CG1  | 10:K:14:VAL:O    | 2.58                     | 0.46              |
| 11:L:86:ALA:HA   | 11:L:89:ASN:ND2  | 2.31                     | 0.46              |
| 15:T:22:DT:C2'   | 15:T:23:DT:O5'   | 2.64                     | 0.46              |
| 1:B:1280:GLU:O   | 1:B:1281:ARG:C   | 2.54                     | 0.45              |
| 1:B:18:GLN:HB3   | 2:C:1215:ARG:HG3 | 1.97                     | 0.45              |
| 1:B:445:ASN:CB   | 1:B:455:MET:HG2  | 2.46                     | 0.45              |
| 1:B:546:VAL:O    | 1:B:550:LEU:HG   | 2.16                     | 0.45              |
| 1:B:857:ARG:NH1  | 6:G:139:PRO:HB2  | 2.31                     | 0.45              |
| 2:C:1166:CYS:O   | 2:C:1166:CYS:SG  | 2.73                     | 0.45              |
| 2:C:423:LYS:CE   | 2:C:470:LYS:HZ1  | 2.30                     | 0.45              |
| 2:C:363:HIS:HD2  | 2:C:585:VAL:HG22 | 1.81                     | 0.45              |
| 2:C:878:GLN:O    | 2:C:879:ARG:C    | 2.54                     | 0.45              |
| 3:D:147:LEU:CD2  | 3:D:147:LEU:N    | 2.79                     | 0.45              |
| 2:C:847:ASP:CB   | 3:D:167:HIS:CD2  | 2.95                     | 0.45              |
| 3:D:238:ILE:HG21 | 3:D:242:GLN:HB2  | 1.95                     | 0.45              |
| 4:E:24:ALA:C     | 4:E:26:THR:N     | 2.69                     | 0.45              |
| 4:E:8:PHE:O      | 4:E:9:GLN:HB2    | 2.14                     | 0.45              |
| 8:I:83:GLN:C     | 8:I:85:GLY:H     | 2.19                     | 0.45              |
| 12:M:28:LYS:HB3  | 12:M:39:SER:HA   | 1.97                     | 0.45              |
| 15:T:11:DT:H1'   | 15:T:12:DA:H5'   | 1.97                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:266:LEU:HD21  | 1:B:303:TYR:CZ    | 2.51                     | 0.45              |
| 1:B:427:GLN:HB2   | 1:B:430:TRP:CD1   | 2.51                     | 0.45              |
| 2:C:1000:PRO:O    | 2:C:1007:VAL:HG23 | 2.16                     | 0.45              |
| 1:B:350:ARG:CB    | 2:C:1128:LEU:HD11 | 2.46                     | 0.45              |
| 2:C:195:CYS:SG    | 2:C:196:PRO:HD2   | 2.56                     | 0.45              |
| 2:C:367:LEU:HD12  | 2:C:370:PHE:CE1   | 2.51                     | 0.45              |
| 2:C:388:CYS:C     | 2:C:390:LEU:N     | 2.70                     | 0.45              |
| 2:C:544:CYS:HB3   | 2:C:634:TYR:CE1   | 2.51                     | 0.45              |
| 2:C:885:MET:HA    | 2:C:936:ASP:CB    | 2.46                     | 0.45              |
| 3:D:69:LEU:CD1    | 3:D:69:LEU:H      | 2.30                     | 0.45              |
| 4:E:59:ILE:O      | 4:E:63:LEU:HB2    | 2.16                     | 0.45              |
| 6:G:138:LEU:HB2   | 6:G:142:SER:O     | 2.15                     | 0.45              |
| 6:G:75:PRO:O      | 6:G:77:ASP:O      | 2.34                     | 0.45              |
| 7:H:95:SER:C      | 7:H:97:HIS:H      | 2.19                     | 0.45              |
| 8:I:62:SER:OG     | 8:I:63:LEU:N      | 2.48                     | 0.45              |
| 1:B:709:THR:HG21  | 9:J:93:LYS:O      | 2.16                     | 0.45              |
| 3:D:35:ARG:HH11   | 11:L:41:THR:N     | 2.14                     | 0.45              |
| 1:B:1147:THR:HA   | 1:B:1197:LEU:HD23 | 1.98                     | 0.45              |
| 1:B:343:LYS:HB3   | 2:C:1117:GLN:OE1  | 2.17                     | 0.45              |
| 1:B:630:ILE:HD13  | 1:B:646:PHE:CZ    | 2.51                     | 0.45              |
| 2:C:1034:VAL:HG21 | 2:C:1055:ILE:HG23 | 1.98                     | 0.45              |
| 2:C:1106:ARG:NH2  | 2:C:1109:GLY:H    | 2.14                     | 0.45              |
| 1:B:782:ARG:NH2   | 2:C:699:GLU:O     | 2.45                     | 0.45              |
| 3:D:100:THR:HG22  | 3:D:101:LEU:H     | 1.80                     | 0.45              |
| 3:D:101:LEU:HD13  | 3:D:118:LEU:CD2   | 2.23                     | 0.45              |
| 3:D:133:ILE:HD13  | 3:D:237:SER:N     | 2.32                     | 0.45              |
| 3:D:91:HIS:CD2    | 3:D:91:HIS:O      | 2.69                     | 0.45              |
| 5:F:124:VAL:HG13  | 5:F:132:ILE:HG13  | 1.98                     | 0.45              |
| 6:G:135:ARG:HD3   | 6:G:143:PHE:CE2   | 2.50                     | 0.45              |
| 8:I:82:PRO:O      | 8:I:84:ALA:N      | 2.36                     | 0.45              |
| 8:I:84:ALA:HA     | 8:I:87:ARG:HD2    | 1.98                     | 0.45              |
| 13:N:6:DA:C2      | 15:T:12:DA:C2     | 3.04                     | 0.45              |
| 1:B:1220:PHE:CE2  | 1:B:1263:ILE:HG23 | 2.51                     | 0.45              |
| 1:B:414:ASP:OD1   | 1:B:416:ARG:CG    | 2.65                     | 0.45              |
| 1:B:434:ARG:HD2   | 1:B:435:HIS:O     | 2.16                     | 0.45              |
| 2:C:33:VAL:O      | 2:C:36:ALA:HB3    | 2.15                     | 0.45              |
| 2:C:542:MET:HG2   | 2:C:747:MET:HB3   | 1.98                     | 0.45              |
| 2:C:560:GLU:O     | 2:C:561:TRP:CD1   | 2.70                     | 0.45              |
| 2:C:731:VAL:CG1   | 2:C:732:SER:H     | 2.23                     | 0.45              |
| 3:D:11:ARG:HD3    | 3:D:209:TYR:CZ    | 2.51                     | 0.45              |
| 2:C:996:ARG:HH21  | 3:D:175:ALA:HA    | 1.81                     | 0.45              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:E:176:GLU:O     | 4:E:179:GLN:N    | 2.49                     | 0.45              |
| 5:F:13:TRP:CZ3    | 5:F:39:LEU:HB2   | 2.51                     | 0.45              |
| 7:H:22:MET:O      | 7:H:23:LYS:C     | 2.54                     | 0.45              |
| 9:J:32:CYS:SG     | 9:J:33:SER:N     | 2.86                     | 0.45              |
| 1:B:1159:ARG:O    | 1:B:1160:SER:HB3 | 2.16                     | 0.45              |
| 1:B:219:PHE:CD2   | 1:B:231:PRO:HD2  | 2.51                     | 0.45              |
| 1:B:320:ARG:HA    | 1:B:321:PRO:HD3  | 1.87                     | 0.45              |
| 1:B:522:GLY:HA2   | 1:B:630:ILE:HD13 | 1.98                     | 0.45              |
| 1:B:578:LEU:HD23  | 1:B:612:ILE:HD11 | 1.99                     | 0.45              |
| 1:B:696:GLU:OE2   | 1:B:702:LEU:HD21 | 2.17                     | 0.45              |
| 2:C:1107:ALA:O    | 2:C:1108:ARG:O   | 2.35                     | 0.45              |
| 2:C:54:PHE:HE1    | 2:C:414:ALA:HA   | 1.81                     | 0.45              |
| 2:C:859:TYR:OH    | 2:C:941:LEU:CD1  | 2.65                     | 0.45              |
| 3:D:8:VAL:HG21    | 11:L:105:PHE:CA  | 2.46                     | 0.45              |
| 5:F:156:LEU:HD12  | 5:F:195:VAL:CG1  | 2.46                     | 0.45              |
| 5:F:207:ARG:HH11  | 5:F:207:ARG:CB   | 2.29                     | 0.45              |
| 5:F:34:GLU:O      | 5:F:34:GLU:HG2   | 2.16                     | 0.45              |
| 7:H:91:VAL:HA     | 7:H:101:VAL:HA   | 1.98                     | 0.45              |
| 8:I:76:THR:O      | 8:I:76:THR:HG22  | 2.15                     | 0.45              |
| 1:B:1403:GLU:OE2  | 15:T:16:DG:H4'   | 2.16                     | 0.45              |
| 1:B:1170:ILE:HG13 | 1:B:1170:ILE:H   | 1.49                     | 0.45              |
| 1:B:302:THR:HA    | 1:B:305:ASP:O    | 2.17                     | 0.45              |
| 1:B:482:PHE:C     | 1:B:484:GLY:H    | 2.20                     | 0.45              |
| 1:B:511:ILE:O     | 1:B:519:PRO:HA   | 2.17                     | 0.45              |
| 1:B:699:ALA:O     | 1:B:700:ASN:CB   | 2.65                     | 0.45              |
| 1:B:878:ILE:HG22  | 1:B:956:LEU:N    | 2.32                     | 0.45              |
| 2:C:1039:GLY:O    | 10:K:32:GLU:HB2  | 2.15                     | 0.45              |
| 2:C:1099:VAL:C    | 2:C:1101:ASP:H   | 2.19                     | 0.45              |
| 2:C:1111:MET:SD   | 2:C:1118:PRO:HA  | 2.56                     | 0.45              |
| 2:C:995:ARG:HH11  | 3:D:165:LYS:HA   | 1.82                     | 0.45              |
| 4:E:140:ASP:O     | 4:E:143:ASN:N    | 2.49                     | 0.45              |
| 9:J:86:PHE:CE1    | 9:J:100:PHE:HB2  | 2.52                     | 0.45              |
| 9:J:8:ARG:HG3     | 9:J:34:TYR:CE1   | 2.52                     | 0.45              |
| 1:B:1154:TYR:N    | 9:J:41:PRO:O     | 2.49                     | 0.45              |
| 9:J:4:PHE:C       | 9:J:4:PHE:CD1    | 2.90                     | 0.45              |
| 9:J:55:THR:HG23   | 9:J:86:PHE:CZ    | 2.52                     | 0.45              |
| 1:B:1209:MET:SD   | 1:B:1236:LEU:HB3 | 2.57                     | 0.45              |
| 1:B:332:LYS:HB2   | 1:B:337:ARG:NH1  | 2.32                     | 0.45              |
| 1:B:38:PRO:HG2    | 1:B:39:GLU:N     | 2.31                     | 0.45              |
| 1:B:606:LEU:CB    | 1:B:614:PHE:CE2  | 3.00                     | 0.45              |
| 1:B:697:ALA:HB2   | 1:B:702:LEU:HD12 | 1.99                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:510:LYS:CB    | 2:C:511:PRO:CD    | 2.94                     | 0.45              |
| 2:C:683:SER:O     | 2:C:685:LEU:N     | 2.50                     | 0.45              |
| 3:D:183:TRP:O     | 3:D:185:LYS:N     | 2.50                     | 0.45              |
| 3:D:226:ASP:O     | 3:D:227:THR:HB    | 2.17                     | 0.45              |
| 4:E:52:LEU:HB2    | 4:E:182:SER:HB3   | 1.98                     | 0.45              |
| 4:E:68:ARG:O      | 4:E:72:ARG:HG3    | 2.16                     | 0.45              |
| 7:H:1:MET:SD      | 7:H:1:MET:C       | 2.95                     | 0.45              |
| 7:H:45:ILE:O      | 7:H:45:ILE:HG22   | 2.17                     | 0.45              |
| 9:J:54:GLU:OE2    | 9:J:118:ARG:NH1   | 2.49                     | 0.45              |
| 2:C:110:HIS:CD2   | 12:M:54:ARG:HH22  | 2.35                     | 0.45              |
| 1:B:130:ASP:H     | 1:B:134:ARG:HH21  | 1.64                     | 0.45              |
| 1:B:1411:GLU:HA   | 1:B:1414:ALA:CB   | 2.46                     | 0.45              |
| 1:B:24:PRO:HD2    | 1:B:233:TRP:NE1   | 2.32                     | 0.45              |
| 1:B:390:GLN:HE21  | 1:B:394:ASN:ND2   | 2.15                     | 0.45              |
| 1:B:470:LEU:HD13  | 1:B:487:MET:HE1   | 1.99                     | 0.45              |
| 1:B:898:ARG:HD3   | 1:B:933:TYR:CD1   | 2.52                     | 0.45              |
| 2:C:983:ARG:CD    | 2:C:1091:TYR:HB3  | 2.47                     | 0.45              |
| 2:C:1146:PHE:CZ   | 2:C:1150:ARG:HD2  | 2.52                     | 0.45              |
| 2:C:118:ARG:HD3   | 2:C:204:ILE:HD13  | 1.99                     | 0.45              |
| 2:C:205:ILE:N     | 2:C:205:ILE:CD1   | 2.79                     | 0.45              |
| 2:C:400:HIS:ND1   | 2:C:400:HIS:O     | 2.48                     | 0.45              |
| 2:C:53:GLN:HG2    | 2:C:547:VAL:HG22  | 1.95                     | 0.45              |
| 2:C:616:ILE:HG13  | 2:C:697:GLU:HG2   | 1.98                     | 0.45              |
| 3:D:10:ILE:CG2    | 3:D:13:ALA:HB2    | 2.46                     | 0.45              |
| 3:D:3:GLU:OE1     | 3:D:4:GLU:HB2     | 2.17                     | 0.45              |
| 3:D:8:VAL:HG11    | 11:L:105:PHE:CD1  | 2.48                     | 0.45              |
| 4:E:51:ASN:O      | 4:E:52:LEU:C      | 2.54                     | 0.45              |
| 5:F:113:GLN:HA    | 5:F:137:GLU:HG3   | 1.99                     | 0.45              |
| 5:F:48:ASP:CG     | 5:F:49:SER:N      | 2.70                     | 0.45              |
| 6:G:120:ILE:O     | 6:G:123:LYS:HB3   | 2.17                     | 0.45              |
| 9:J:101:PHE:CD1   | 9:J:101:PHE:N     | 2.84                     | 0.45              |
| 11:L:42:LEU:HD21  | 11:L:46:ILE:CD1   | 2.46                     | 0.45              |
| 12:M:38:LEU:HD11  | 12:M:49:LYS:HE2   | 1.98                     | 0.45              |
| 1:B:1120:LEU:HD21 | 1:B:1304:TRP:O    | 2.17                     | 0.45              |
| 1:B:1444:MET:HE3  | 1:B:1444:MET:HB2  | 1.86                     | 0.45              |
| 1:B:344:ARG:HG2   | 1:B:344:ARG:HH11  | 1.81                     | 0.45              |
| 1:B:500:GLU:OE1   | 2:C:1143:ALA:C    | 2.55                     | 0.45              |
| 1:B:836:TYR:CD2   | 1:B:840:ARG:HD2   | 2.50                     | 0.45              |
| 1:B:873:MET:HG2   | 1:B:957:PRO:HB3   | 1.99                     | 0.45              |
| 2:C:100:PRO:HD3   | 2:C:172:ILE:HD12  | 1.99                     | 0.45              |
| 2:C:1151:LEU:H    | 2:C:1151:LEU:HD13 | 1.81                     | 0.45              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:81:PHE:CE1    | 2:C:1208:MET:HE2 | 2.51                     | 0.45              |
| 2:C:224:GLN:HA    | 2:C:396:ASP:OD2  | 2.17                     | 0.45              |
| 2:C:247:GLY:N     | 2:C:418:LYS:HZ1  | 2.14                     | 0.45              |
| 2:C:467:GLY:H     | 2:C:475:SER:CB   | 2.30                     | 0.45              |
| 2:C:487:THR:O     | 2:C:490:SER:HB3  | 2.17                     | 0.45              |
| 2:C:65:GLU:HG3    | 2:C:66:ASP:OD1   | 2.17                     | 0.45              |
| 2:C:635:ARG:NH2   | 2:C:742:GLU:OE2  | 2.48                     | 0.45              |
| 2:C:952:VAL:HG13  | 2:C:966:VAL:HG22 | 1.97                     | 0.45              |
| 3:D:67:LEU:CD1    | 3:D:155:LEU:HD13 | 2.42                     | 0.45              |
| 3:D:169:LYS:NZ    | 12:M:69:ALA:HB3  | 2.32                     | 0.45              |
| 4:E:216:ASN:O     | 4:E:217:LEU:C    | 2.54                     | 0.45              |
| 4:E:35:LEU:CD2    | 4:E:173:HIS:HB3  | 2.46                     | 0.45              |
| 5:F:154:ILE:HG22  | 5:F:155:ARG:N    | 2.30                     | 0.45              |
| 5:F:161:LYS:HD2   | 5:F:195:VAL:CG2  | 2.46                     | 0.45              |
| 5:F:197:LYS:HE2   | 5:F:199:ILE:HD11 | 1.98                     | 0.45              |
| 6:G:125:LEU:O     | 6:G:125:LEU:HG   | 2.16                     | 0.45              |
| 8:I:58:THR:HG22   | 8:I:59:ILE:N     | 2.31                     | 0.45              |
| 9:J:34:TYR:O      | 9:J:35:VAL:CG2   | 2.65                     | 0.45              |
| 10:K:16:ASP:O     | 10:K:18:TRP:N    | 2.49                     | 0.45              |
| 10:K:36:LEU:HD11  | 10:K:51:LEU:HB2  | 1.98                     | 0.45              |
| 10:K:57:ILE:CA    | 10:K:60:PHE:HD2  | 2.22                     | 0.45              |
| 1:B:1120:LEU:HD11 | 1:B:1304:TRP:O   | 2.17                     | 0.45              |
| 1:B:1434:ALA:O    | 1:B:1436:ILE:N   | 2.50                     | 0.45              |
| 1:B:207:ILE:O     | 1:B:211:PHE:HD1  | 2.00                     | 0.45              |
| 1:B:366:VAL:CG2   | 1:B:460:VAL:HG23 | 2.47                     | 0.45              |
| 1:B:921:GLY:O     | 1:B:922:ASP:C    | 2.55                     | 0.45              |
| 1:B:946:VAL:HB    | 1:B:947:PHE:CD1  | 2.52                     | 0.45              |
| 2:C:1163:CYS:HB3  | 2:C:1166:CYS:O   | 2.17                     | 0.45              |
| 2:C:281:PRO:HD2   | 2:C:284:ILE:HD12 | 1.98                     | 0.45              |
| 2:C:294:ASP:C     | 2:C:296:GLU:H    | 2.17                     | 0.45              |
| 2:C:360:PHE:HD2   | 2:C:374:LYS:HD3  | 1.82                     | 0.45              |
| 3:D:258:ILE:N     | 3:D:258:ILE:HD12 | 2.32                     | 0.45              |
| 3:D:70:ILE:HD11   | 3:D:144:ILE:CG1  | 2.47                     | 0.45              |
| 5:F:124:VAL:N     | 5:F:125:PRO:CD   | 2.80                     | 0.45              |
| 7:H:119:LEU:HD12  | 7:H:131:GLN:C    | 2.37                     | 0.45              |
| 10:K:1:MET:N      | 10:K:55:ASP:C    | 2.70                     | 0.45              |
| 1:B:1155:ASP:OD2  | 1:B:1162:VAL:N   | 2.49                     | 0.44              |
| 1:B:1120:LEU:CD2  | 1:B:1304:TRP:O   | 2.65                     | 0.44              |
| 1:B:24:PRO:HB3    | 1:B:237:THR:HB   | 1.99                     | 0.44              |
| 1:B:338:GLY:O     | 1:B:342:GLY:O    | 2.35                     | 0.44              |
| 1:B:497:THR:HG22  | 1:B:498:ARG:N    | 2.32                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:544:ASP:CG   | 1:B:545:GLN:N    | 2.70                     | 0.44              |
| 2:C:1096:ARG:O   | 2:C:1097:HIS:CB  | 2.62                     | 0.44              |
| 2:C:977:GLY:HA3  | 2:C:1099:VAL:HB  | 2.00                     | 0.44              |
| 2:C:644:GLU:C    | 2:C:646:LEU:H    | 2.21                     | 0.44              |
| 2:C:707:PRO:O    | 2:C:711:GLU:HG2  | 2.17                     | 0.44              |
| 1:B:358:ASN:ND2  | 2:C:833:TYR:OH   | 2.50                     | 0.44              |
| 2:C:935:ARG:HG3  | 2:C:935:ARG:O    | 2.18                     | 0.44              |
| 3:D:34:ARG:HA    | 3:D:37:MET:CE    | 2.46                     | 0.44              |
| 4:E:40:HIS:C     | 4:E:42:GLY:H     | 2.20                     | 0.44              |
| 7:H:15:PRO:HG2   | 7:H:66:GLY:HA3   | 1.99                     | 0.44              |
| 1:B:567:LYS:HE3  | 8:I:46:LEU:HB3   | 1.98                     | 0.44              |
| 8:I:98:TYR:CD1   | 8:I:99:GLY:N     | 2.85                     | 0.44              |
| 1:B:218:ASP:O    | 1:B:219:PHE:C    | 2.55                     | 0.44              |
| 1:B:497:THR:O    | 1:B:500:GLU:N    | 2.42                     | 0.44              |
| 1:B:541:ILE:HD12 | 1:B:577:ILE:HD11 | 1.99                     | 0.44              |
| 1:B:899:VAL:CB   | 1:B:929:LEU:HD12 | 2.45                     | 0.44              |
| 2:C:253:THR:HG22 | 2:C:254:LEU:N    | 2.33                     | 0.44              |
| 2:C:254:LEU:HD22 | 2:C:361:LEU:HD13 | 1.99                     | 0.44              |
| 2:C:35:SER:HA    | 2:C:811:TYR:HE2  | 1.81                     | 0.44              |
| 2:C:34:ILE:O     | 2:C:37:PHE:N     | 2.51                     | 0.44              |
| 2:C:449:ASN:O    | 2:C:451:LYS:N    | 2.50                     | 0.44              |
| 2:C:45:SER:O     | 2:C:46:GLN:C     | 2.54                     | 0.44              |
| 5:F:23:VAL:HG12  | 5:F:28:TYR:HB2   | 1.99                     | 0.44              |
| 7:H:27:LYS:O     | 7:H:30:LEU:HB3   | 2.18                     | 0.44              |
| 4:E:138:ASN:ND2  | 7:H:35:GLU:HB3   | 2.32                     | 0.44              |
| 1:B:567:LYS:CG   | 8:I:95:TYR:HA    | 2.48                     | 0.44              |
| 9:J:15:TYR:HD1   | 9:J:15:TYR:N     | 2.13                     | 0.44              |
| 10:K:56:LEU:O    | 10:K:57:ILE:C    | 2.54                     | 0.44              |
| 10:K:57:ILE:HG12 | 10:K:61:LEU:CD1  | 2.48                     | 0.44              |
| 1:B:1189:SER:OG  | 1:B:1256:GLU:OE1 | 2.22                     | 0.44              |
| 1:B:1343:ALA:O   | 1:B:1346:ALA:HB3 | 2.18                     | 0.44              |
| 1:B:372:LYS:HA   | 1:B:435:HIS:HD1  | 1.82                     | 0.44              |
| 1:B:375:THR:OG1  | 1:B:376:TYR:N    | 2.49                     | 0.44              |
| 1:B:380:VAL:HG23 | 1:B:430:TRP:O    | 2.17                     | 0.44              |
| 1:B:709:THR:CG2  | 1:B:711:ARG:HB2  | 2.46                     | 0.44              |
| 1:B:940:ARG:HH11 | 1:B:940:ARG:HG2  | 1.82                     | 0.44              |
| 2:C:102:VAL:O    | 2:C:104:GLU:HG2  | 2.17                     | 0.44              |
| 2:C:129:PHE:CD2  | 2:C:166:PHE:HA   | 2.52                     | 0.44              |
| 2:C:51:PHE:CZ    | 2:C:172:ILE:HA   | 2.53                     | 0.44              |
| 2:C:25:ILE:HG23  | 2:C:658:ILE:HD12 | 2.00                     | 0.44              |
| 2:C:361:LEU:HG   | 2:C:363:HIS:CE1  | 2.52                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:362:PRO:C    | 2:C:363:HIS:O    | 2.55                     | 0.44              |
| 2:C:529:GLU:OE1  | 2:C:769:TYR:CE2  | 2.71                     | 0.44              |
| 2:C:683:SER:C    | 2:C:685:LEU:N    | 2.70                     | 0.44              |
| 2:C:842:ASN:ND2  | 2:C:845:SER:CB   | 2.80                     | 0.44              |
| 2:C:841:MET:SD   | 2:C:846:ILE:HD11 | 2.57                     | 0.44              |
| 2:C:843:GLN:HB3  | 2:C:994:TYR:O    | 2.18                     | 0.44              |
| 1:B:1441:PHE:HZ  | 6:G:89:GLU:HA    | 1.79                     | 0.44              |
| 11:L:68:PHE:N    | 11:L:68:PHE:HD2  | 2.15                     | 0.44              |
| 15:T:24:DG:H2'   | 15:T:25:DC:O4'   | 2.17                     | 0.44              |
| 1:B:108:MET:HA   | 1:B:210:ILE:HG23 | 1.99                     | 0.44              |
| 1:B:1423:GLY:HA3 | 1:B:1426:GLU:HG2 | 1.98                     | 0.44              |
| 1:B:241:VAL:HA   | 1:B:242:PRO:HD2  | 1.88                     | 0.44              |
| 1:B:269:ILE:CG2  | 1:B:300:VAL:HG22 | 2.47                     | 0.44              |
| 1:B:546:VAL:HG12 | 1:B:546:VAL:O    | 2.16                     | 0.44              |
| 1:B:49:LYS:NZ    | 1:B:61:ILE:N     | 2.63                     | 0.44              |
| 1:B:709:THR:HG21 | 1:B:711:ARG:HB2  | 1.99                     | 0.44              |
| 1:B:808:LEU:HD23 | 1:B:813:PHE:N    | 2.33                     | 0.44              |
| 2:C:1076:HIS:CD2 | 11:L:40:HIS:CE1  | 3.05                     | 0.44              |
| 2:C:31:TRP:CZ3   | 2:C:34:ILE:HD12  | 2.53                     | 0.44              |
| 2:C:167:ILE:CG2  | 2:C:453:ILE:HD11 | 2.42                     | 0.44              |
| 2:C:570:VAL:HB   | 2:C:573:GLN:CB   | 2.47                     | 0.44              |
| 2:C:658:ILE:HG22 | 2:C:662:MET:HE2  | 1.98                     | 0.44              |
| 2:C:906:SER:O    | 2:C:907:GLY:O    | 2.35                     | 0.44              |
| 2:C:1065:GLN:HB2 | 3:D:201:TRP:CZ3  | 2.53                     | 0.44              |
| 5:F:182:ASP:OD1  | 5:F:183:PRO:HD2  | 2.17                     | 0.44              |
| 8:I:8:ASP:C      | 8:I:9:ILE:HG13   | 2.38                     | 0.44              |
| 9:J:16:PRO:HB3   | 9:J:27:PHE:CE2   | 2.52                     | 0.44              |
| 10:K:57:ILE:HG23 | 10:K:58:GLU:N    | 2.33                     | 0.44              |
| 12:M:34:CYS:SG   | 12:M:34:CYS:O    | 2.74                     | 0.44              |
| 14:P:6:A:C4      | 14:P:7:A:C8      | 3.06                     | 0.44              |
| 14:P:8:U:H2'     | 14:P:9:A:H8      | 1.83                     | 0.44              |
| 1:B:1126:ALA:O   | 1:B:1128:GLN:N   | 2.47                     | 0.44              |
| 1:B:1437:GLY:O   | 1:B:1438:THR:C   | 2.54                     | 0.44              |
| 1:B:123:ARG:NH2  | 1:B:155:GLU:HG2  | 2.33                     | 0.44              |
| 1:B:241:VAL:HG13 | 1:B:266:LEU:HD13 | 1.98                     | 0.44              |
| 1:B:601:LYS:HB2  | 1:B:603:ASN:ND2  | 2.33                     | 0.44              |
| 1:B:626:ASN:O    | 1:B:631:HIS:CD2  | 2.71                     | 0.44              |
| 2:C:418:LYS:HE2  | 2:C:422:LYS:HZ1  | 1.82                     | 0.44              |
| 2:C:806:THR:C    | 2:C:808:ALA:N    | 2.71                     | 0.44              |
| 2:C:838:SER:CA   | 2:C:989:THR:O    | 2.66                     | 0.44              |
| 2:C:899:ILE:HD11 | 2:C:911:ILE:HG12 | 2.00                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:66:ARG:CZ     | 10:K:2:ILE:HG21   | 2.47                     | 0.44              |
| 8:I:93:TYR:N      | 8:I:93:TYR:CD1    | 2.85                     | 0.44              |
| 15:T:21:DA:H2'    | 15:T:22:DT:C6     | 2.53                     | 0.44              |
| 1:B:1118:VAL:HG12 | 1:B:1327:ILE:HG13 | 1.98                     | 0.44              |
| 1:B:1272:THR:C    | 1:B:1273:LEU:HD12 | 2.38                     | 0.44              |
| 1:B:1447:GLU:OE2  | 7:H:23:LYS:HB2    | 2.17                     | 0.44              |
| 1:B:648:ASN:O     | 1:B:649:ILE:C     | 2.54                     | 0.44              |
| 1:B:886:ILE:HG23  | 1:B:887:GLY:H     | 1.78                     | 0.44              |
| 2:C:1004:GLU:OE2  | 2:C:1064:TYR:HE2  | 2.01                     | 0.44              |
| 2:C:1162:ILE:HG23 | 2:C:1168:LEU:O    | 2.18                     | 0.44              |
| 1:B:16:GLU:CD     | 2:C:1220:ARG:HA   | 2.38                     | 0.44              |
| 2:C:683:SER:C     | 2:C:685:LEU:H     | 2.20                     | 0.44              |
| 2:C:684:LEU:O     | 2:C:689:LEU:HB2   | 2.17                     | 0.44              |
| 2:C:636:PRO:O     | 2:C:743:ILE:HD11  | 2.17                     | 0.44              |
| 2:C:753:ALA:HA    | 2:C:756:ILE:CD1   | 2.48                     | 0.44              |
| 3:D:67:LEU:HD13   | 3:D:157:CYS:SG    | 2.57                     | 0.44              |
| 1:B:227:VAL:HG12  | 4:E:15:LEU:HD23   | 1.98                     | 0.44              |
| 5:F:12:LEU:HD22   | 5:F:55:ARG:CZ     | 2.48                     | 0.44              |
| 9:J:83:ASN:OD1    | 9:J:103:CYS:HA    | 2.16                     | 0.44              |
| 10:K:30:LEU:HD11  | 10:K:38:ARG:HH12  | 1.82                     | 0.44              |
| 11:L:33:ILE:HD13  | 11:L:87:LEU:HD22  | 1.99                     | 0.44              |
| 14:P:6:A:H2'      | 14:P:7:A:O4'      | 2.17                     | 0.44              |
| 1:B:1224:LEU:HG   | 1:B:1226:VAL:HG23 | 2.00                     | 0.44              |
| 1:B:1287:TYR:O    | 1:B:1302:PRO:HA   | 2.18                     | 0.44              |
| 1:B:230:ARG:O     | 1:B:231:PRO:C     | 2.55                     | 0.44              |
| 1:B:22:PHE:HD2    | 1:B:27:VAL:HG22   | 1.83                     | 0.44              |
| 1:B:765:VAL:HG12  | 1:B:766:GLY:H     | 1.81                     | 0.44              |
| 2:C:378:LEU:C     | 2:C:378:LEU:HD12  | 2.38                     | 0.44              |
| 2:C:681:TRP:O     | 2:C:684:LEU:N     | 2.51                     | 0.44              |
| 2:C:984:HIS:CD2   | 2:C:1025:HIS:HA   | 2.52                     | 0.44              |
| 3:D:101:LEU:C     | 3:D:102:GLN:HG3   | 2.38                     | 0.44              |
| 3:D:155:LEU:HB3   | 3:D:156:THR:H     | 1.46                     | 0.44              |
| 5:F:78:LEU:CD2    | 5:F:80:VAL:HG23   | 2.43                     | 0.44              |
| 11:L:85:ASP:O     | 11:L:88:LYS:HB2   | 2.17                     | 0.44              |
| 11:L:87:LEU:O     | 11:L:90:ALA:HB3   | 2.18                     | 0.44              |
| 1:B:1051:ALA:O    | 1:B:1055:ARG:HG3  | 2.18                     | 0.44              |
| 1:B:1104:ILE:C    | 1:B:1106:ASN:N    | 2.71                     | 0.44              |
| 1:B:1118:VAL:HG23 | 1:B:1118:VAL:O    | 2.17                     | 0.44              |
| 1:B:22:PHE:CD2    | 1:B:27:VAL:HG22   | 2.53                     | 0.44              |
| 1:B:516:SER:O     | 1:B:517:ASN:C     | 2.55                     | 0.44              |
| 1:B:867:ILE:HG22  | 1:B:872:GLY:N     | 2.33                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:185:THR:H     | 2:C:188:ASP:CB    | 2.29                     | 0.44              |
| 2:C:282:ILE:CD1   | 2:C:382:ILE:HG21  | 2.48                     | 0.44              |
| 2:C:425:THR:O     | 2:C:428:ILE:HB    | 2.18                     | 0.44              |
| 2:C:880:THR:CB    | 2:C:934:LYS:HD2   | 2.46                     | 0.44              |
| 2:C:882:THR:HB    | 2:C:934:LYS:O     | 2.17                     | 0.44              |
| 7:H:18:PHE:HA     | 7:H:22:MET:CE     | 2.48                     | 0.44              |
| 7:H:88:ASP:HB3    | 7:H:144:ARG:CA    | 2.42                     | 0.44              |
| 11:L:68:PHE:HB3   | 11:L:70:ARG:NH1   | 2.32                     | 0.44              |
| 1:B:1215:ARG:HA   | 1:B:1215:ARG:HD2  | 1.86                     | 0.44              |
| 1:B:1239:ARG:HH22 | 1:B:1241:ARG:HH22 | 1.65                     | 0.44              |
| 1:B:1349:TYR:HB2  | 1:B:1372:VAL:HG21 | 1.98                     | 0.44              |
| 1:B:243:PRO:CB    | 1:B:244:PRO:HD2   | 2.46                     | 0.44              |
| 1:B:409:SER:O     | 1:B:410:GLY:C     | 2.56                     | 0.44              |
| 1:B:507:VAL:N     | 1:B:508:PRO:CD    | 2.81                     | 0.44              |
| 1:B:577:ILE:C     | 1:B:579:SER:N     | 2.69                     | 0.44              |
| 2:C:1165:ILE:O    | 2:C:1217:TYR:CE1  | 2.71                     | 0.44              |
| 1:B:18:GLN:O      | 2:C:1215:ARG:HG2  | 2.18                     | 0.44              |
| 2:C:303:TYR:O     | 2:C:304:ASP:HB2   | 2.18                     | 0.44              |
| 2:C:361:LEU:HG    | 2:C:363:HIS:HE1   | 1.82                     | 0.44              |
| 2:C:881:ASN:O     | 2:C:883:LEU:HG    | 2.18                     | 0.44              |
| 2:C:913:GLY:HA2   | 2:C:938:SER:OG    | 2.18                     | 0.44              |
| 4:E:208:GLU:O     | 4:E:212:LYS:HG3   | 2.18                     | 0.44              |
| 4:E:40:HIS:CE1    | 4:E:41:GLN:HG3    | 2.53                     | 0.44              |
| 5:F:175:LEU:HD23  | 5:F:175:LEU:HA    | 1.78                     | 0.44              |
| 7:H:3:PHE:N       | 7:H:3:PHE:CD1     | 2.85                     | 0.44              |
| 10:K:53:HIS:C     | 10:K:53:HIS:ND1   | 2.71                     | 0.44              |
| 1:B:108:MET:SD    | 1:B:108:MET:N     | 2.91                     | 0.43              |
| 1:B:239:LEU:HA    | 1:B:240:PRO:HD2   | 1.90                     | 0.43              |
| 1:B:92:HIS:O      | 1:B:93:VAL:C      | 2.56                     | 0.43              |
| 1:B:466:SER:O     | 2:C:1103:ILE:HD11 | 2.18                     | 0.43              |
| 2:C:255:GLN:O     | 2:C:271:ALA:CB    | 2.66                     | 0.43              |
| 2:C:293:PRO:HD2   | 2:C:296:GLU:OE1   | 2.18                     | 0.43              |
| 2:C:39:ARG:NH2    | 2:C:665:GLU:CG    | 2.77                     | 0.43              |
| 2:C:465:ASN:HD22  | 2:C:465:ASN:N     | 2.15                     | 0.43              |
| 3:D:83:SER:OG     | 3:D:160:LYS:HB3   | 2.17                     | 0.43              |
| 4:E:29:LEU:N      | 4:E:29:LEU:HD23   | 2.32                     | 0.43              |
| 1:B:1346:ALA:CB   | 5:F:149:LEU:HD12  | 2.48                     | 0.43              |
| 7:H:91:VAL:HG12   | 7:H:92:VAL:N      | 2.32                     | 0.43              |
| 8:I:130:ARG:CB    | 8:I:134:ASN:H     | 2.25                     | 0.43              |
| 8:I:55:LEU:HD22   | 8:I:144:ILE:HG23  | 1.96                     | 0.43              |
| 10:K:1:MET:N      | 10:K:57:ILE:HG22  | 2.33                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:K:64:ASN:HD22  | 10:K:65:PRO:HD3   | 1.83                     | 0.43              |
| 1:B:1138:ILE:O    | 1:B:1275:GLY:HA3  | 2.19                     | 0.43              |
| 1:B:1156:PRO:O    | 1:B:1158:PRO:HD3  | 2.18                     | 0.43              |
| 1:B:367:PRO:CB    | 1:B:466:SER:HA    | 2.48                     | 0.43              |
| 1:B:668:ASP:HB3   | 1:B:741:ASN:ND2   | 2.27                     | 0.43              |
| 1:B:858:ASN:C     | 1:B:858:ASN:ND2   | 2.71                     | 0.43              |
| 2:C:1072:MET:HE3  | 2:C:1085:ILE:CB   | 2.21                     | 0.43              |
| 1:B:351:THR:HG22  | 2:C:1103:ILE:HG13 | 2.00                     | 0.43              |
| 2:C:1142:GLY:O    | 2:C:1144:ALA:N    | 2.51                     | 0.43              |
| 1:B:2:VAL:HG13    | 2:C:1157:ALA:HB1  | 2.00                     | 0.43              |
| 2:C:234:ILE:N     | 2:C:234:ILE:HD12  | 2.34                     | 0.43              |
| 2:C:289:LEU:HD22  | 2:C:371:GLU:O     | 2.17                     | 0.43              |
| 2:C:582:VAL:HB    | 2:C:587:HIS:HD2   | 1.82                     | 0.43              |
| 2:C:616:ILE:N     | 2:C:616:ILE:CD1   | 2.70                     | 0.43              |
| 3:D:44:LEU:HD23   | 3:D:72:LEU:HD12   | 2.00                     | 0.43              |
| 4:E:156:ASP:HB2   | 4:E:159:THR:HG23  | 2.01                     | 0.43              |
| 5:F:18:THR:O      | 5:F:19:VAL:C      | 2.57                     | 0.43              |
| 8:I:56:THR:O      | 8:I:144:ILE:HA    | 2.18                     | 0.43              |
| 10:K:1:MET:H2     | 10:K:55:ASP:HA    | 1.82                     | 0.43              |
| 10:K:3:VAL:HA     | 10:K:53:HIS:CD2   | 2.53                     | 0.43              |
| 1:B:552:TRP:HE1   | 11:L:62:LYS:HB2   | 1.83                     | 0.43              |
| 1:B:1114:PRO:HG2  | 1:B:1115:SER:N    | 2.33                     | 0.43              |
| 1:B:414:ASP:C     | 1:B:414:ASP:OD1   | 2.57                     | 0.43              |
| 1:B:43:GLU:HG3    | 1:B:46:THR:O      | 2.18                     | 0.43              |
| 2:C:1007:VAL:HG22 | 2:C:1008:PRO:CD   | 2.43                     | 0.43              |
| 2:C:1065:GLN:NE2  | 2:C:1066:SER:H    | 2.16                     | 0.43              |
| 2:C:1165:ILE:O    | 2:C:1217:TYR:HE1  | 2.00                     | 0.43              |
| 2:C:329:THR:CA    | 2:C:332:ASP:HB3   | 2.44                     | 0.43              |
| 2:C:390:LEU:O     | 2:C:391:ASP:C     | 2.56                     | 0.43              |
| 2:C:488:TYR:CG    | 2:C:817:LEU:HD12  | 2.53                     | 0.43              |
| 2:C:653:VAL:CG2   | 2:C:689:LEU:HB3   | 2.48                     | 0.43              |
| 2:C:860:MET:HG2   | 2:C:861:ASP:N     | 2.32                     | 0.43              |
| 2:C:757:PRO:HD3   | 2:C:983:ARG:NH2   | 2.33                     | 0.43              |
| 4:E:156:ASP:C     | 4:E:158:GLU:H     | 2.21                     | 0.43              |
| 5:F:124:VAL:HB    | 5:F:125:PRO:HD3   | 2.00                     | 0.43              |
| 5:F:20:LYS:HZ3    | 5:F:60:PHE:HE1    | 1.63                     | 0.43              |
| 6:G:138:LEU:O     | 6:G:140:ASP:N     | 2.50                     | 0.43              |
| 6:G:76:LYS:NZ     | 7:H:58:ARG:HH22   | 2.16                     | 0.43              |
| 7:H:39:THR:HG22   | 7:H:40:GLY:N      | 2.33                     | 0.43              |
| 9:J:82:GLU:HB3    | 9:J:104:LEU:CG    | 2.47                     | 0.43              |
| 11:L:7:PHE:C      | 11:L:7:PHE:CD1    | 2.91                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1142:THR:O    | 1:B:1143:LEU:C    | 2.56                     | 0.43              |
| 1:B:297:GLN:O     | 1:B:297:GLN:HG3   | 2.18                     | 0.43              |
| 1:B:353:ILE:HG21  | 1:B:487:MET:CG    | 2.48                     | 0.43              |
| 1:B:38:PRO:HG2    | 1:B:39:GLU:H      | 1.83                     | 0.43              |
| 1:B:808:LEU:CD2   | 1:B:813:PHE:HA    | 2.47                     | 0.43              |
| 2:C:234:ILE:HG21  | 2:C:237:VAL:CG2   | 2.48                     | 0.43              |
| 2:C:31:TRP:O      | 2:C:32:ALA:C      | 2.57                     | 0.43              |
| 2:C:519:TRP:CD1   | 2:C:519:TRP:C     | 2.91                     | 0.43              |
| 2:C:637:LEU:CD2   | 2:C:742:GLU:HA    | 2.48                     | 0.43              |
| 5:F:113:GLN:HG2   | 5:F:137:GLU:OE1   | 2.18                     | 0.43              |
| 5:F:153:HIS:ND1   | 5:F:184:VAL:HG11  | 2.33                     | 0.43              |
| 8:I:95:TYR:HB3    | 8:I:144:ILE:HB    | 1.99                     | 0.43              |
| 8:I:84:ALA:O      | 8:I:89:LEU:HD21   | 2.18                     | 0.43              |
| 10:K:3:VAL:HG11   | 10:K:14:VAL:O     | 2.18                     | 0.43              |
| 10:K:52:THR:O     | 10:K:53:HIS:C     | 2.57                     | 0.43              |
| 2:C:1076:HIS:CD2  | 11:L:40:HIS:NE2   | 2.85                     | 0.43              |
| 15:T:24:DG:H3'    | 15:T:25:DC:C5'    | 2.43                     | 0.43              |
| 1:B:1039:LYS:HE3  | 1:B:1043:ASP:OD2  | 2.18                     | 0.43              |
| 1:B:1226:VAL:HG13 | 1:B:1239:ARG:O    | 2.18                     | 0.43              |
| 1:B:196:GLU:HG3   | 1:B:197:PRO:CD    | 2.41                     | 0.43              |
| 1:B:54:ASN:H      | 1:B:54:ASN:HD22   | 1.66                     | 0.43              |
| 1:B:605:MET:HE1   | 1:B:612:ILE:HG23  | 1.99                     | 0.43              |
| 1:B:982:THR:O     | 1:B:985:ASP:HB2   | 2.19                     | 0.43              |
| 2:C:1035:ALA:HB1  | 2:C:1040:ASN:O    | 2.17                     | 0.43              |
| 1:B:443:LEU:HD12  | 2:C:1146:PHE:CZ   | 2.54                     | 0.43              |
| 2:C:229:ALA:HB1   | 2:C:231:PRO:HD2   | 2.01                     | 0.43              |
| 2:C:496:ARG:HH11  | 2:C:496:ARG:HB3   | 1.81                     | 0.43              |
| 1:B:786:HIS:HE1   | 2:C:519:TRP:CZ2   | 2.36                     | 0.43              |
| 2:C:908:GLU:O     | 2:C:909:ASP:C     | 2.56                     | 0.43              |
| 3:D:142:VAL:O     | 3:D:142:VAL:HG12  | 2.19                     | 0.43              |
| 3:D:236:GLY:O     | 3:D:237:SER:C     | 2.57                     | 0.43              |
| 3:D:97:VAL:HB     | 3:D:159:ALA:HB3   | 2.00                     | 0.43              |
| 4:E:206:GLU:C     | 4:E:208:GLU:N     | 2.70                     | 0.43              |
| 4:E:175:PHE:CZ    | 7:H:85:GLU:HG3    | 2.48                     | 0.43              |
| 9:J:74:GLU:HB2    | 9:J:79:HIS:CA     | 2.48                     | 0.43              |
| 1:B:1026:LEU:HA   | 1:B:1026:LEU:HD23 | 1.76                     | 0.43              |
| 1:B:1127:ASP:HB3  | 1:B:1130:GLN:HB3  | 2.01                     | 0.43              |
| 1:B:113:LEU:HG    | 1:B:218:ASP:OD1   | 2.19                     | 0.43              |
| 1:B:1227:ILE:CG2  | 1:B:1228:TRP:H    | 2.30                     | 0.43              |
| 1:B:1377:THR:OG1  | 1:B:1378:GLN:N    | 2.47                     | 0.43              |
| 1:B:83:HIS:HA     | 1:B:239:LEU:O     | 2.18                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:244:PRO:CB   | 1:B:245:PRO:HD3   | 2.37                     | 0.43              |
| 1:B:269:ILE:HG23 | 1:B:300:VAL:CG2   | 2.48                     | 0.43              |
| 1:B:463:ILE:HD12 | 1:B:469:ARG:CD    | 2.48                     | 0.43              |
| 2:C:1102:LYS:C   | 2:C:1122:ARG:NH1  | 2.72                     | 0.43              |
| 2:C:273:LEU:CG   | 2:C:276:ILE:HD12  | 2.48                     | 0.43              |
| 2:C:281:PRO:C    | 2:C:283:VAL:N     | 2.72                     | 0.43              |
| 2:C:31:TRP:CE3   | 2:C:34:ILE:HD12   | 2.54                     | 0.43              |
| 2:C:383:ASN:ND2  | 2:C:387:LEU:HD22  | 2.34                     | 0.43              |
| 2:C:806:THR:CG2  | 2:C:808:ALA:H     | 2.20                     | 0.43              |
| 3:D:174:ALA:O    | 3:D:175:ALA:CB    | 2.67                     | 0.43              |
| 4:E:187:THR:HG22 | 4:E:188:ALA:H     | 1.84                     | 0.43              |
| 4:E:31:GLN:C     | 4:E:33:PHE:H      | 2.22                     | 0.43              |
| 7:H:1:MET:O      | 7:H:3:PHE:HE1     | 2.00                     | 0.43              |
| 7:H:35:GLU:CG    | 7:H:48:VAL:HG23   | 2.48                     | 0.43              |
| 7:H:99:PHE:HZ    | 7:H:163:ILE:HD13  | 1.83                     | 0.43              |
| 8:I:93:TYR:HB3   | 8:I:144:ILE:C     | 2.39                     | 0.43              |
| 10:K:43:ARG:HG2  | 10:K:45:CYS:SG    | 2.59                     | 0.43              |
| 11:L:59:ALA:HA   | 11:L:74:ARG:O     | 2.18                     | 0.43              |
| 1:B:1377:THR:O   | 1:B:1378:GLN:C    | 2.57                     | 0.43              |
| 1:B:16:GLU:HB3   | 1:B:1418:LEU:HD11 | 1.99                     | 0.43              |
| 1:B:207:ILE:HG23 | 1:B:211:PHE:CE1   | 2.53                     | 0.43              |
| 1:B:722:LEU:H    | 1:B:722:LEU:CD1   | 2.28                     | 0.43              |
| 1:B:971:PHE:CE2  | 1:B:1040:GLN:HG2  | 2.54                     | 0.43              |
| 1:B:345:VAL:CG1  | 2:C:1130:PHE:HB2  | 2.49                     | 0.43              |
| 2:C:1183:LYS:CE  | 2:C:1183:LYS:N    | 2.82                     | 0.43              |
| 2:C:1200:ALA:O   | 2:C:1201:LYS:C    | 2.57                     | 0.43              |
| 2:C:314:LEU:N    | 2:C:314:LEU:HD12  | 2.31                     | 0.43              |
| 2:C:459:TYR:HE2  | 2:C:465:ASN:HB2   | 1.83                     | 0.43              |
| 2:C:866:TYR:N    | 2:C:866:TYR:CD1   | 2.87                     | 0.43              |
| 2:C:956:THR:HG22 | 2:C:957:ASN:N     | 2.34                     | 0.43              |
| 2:C:55:VAL:HG13  | 2:C:97:VAL:HG21   | 2.00                     | 0.43              |
| 3:D:53:THR:HG22  | 3:D:54:ASN:N      | 2.34                     | 0.43              |
| 4:E:63:LEU:HB3   | 4:E:129:LEU:HD21  | 2.00                     | 0.43              |
| 4:E:153:ARG:HB3  | 4:E:154:PHE:CD1   | 2.53                     | 0.43              |
| 5:F:124:VAL:HG13 | 5:F:132:ILE:CG1   | 2.48                     | 0.43              |
| 5:F:46:TYR:N     | 5:F:46:TYR:CD1    | 2.87                     | 0.43              |
| 1:B:1055:ARG:NE  | 6:G:154:ASP:OD1   | 2.47                     | 0.43              |
| 7:H:1:MET:HE3    | 7:H:81:PRO:HA     | 2.01                     | 0.43              |
| 7:H:20:PRO:CD    | 7:H:21:ARG:H      | 2.32                     | 0.43              |
| 10:K:58:GLU:HA   | 10:K:61:LEU:HD12  | 1.99                     | 0.43              |
| 3:D:29:MET:CE    | 11:L:98:LEU:HG    | 2.48                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:M:27:LEU:N     | 12:M:27:LEU:HD23  | 2.34                     | 0.43              |
| 12:M:52:GLY:O     | 12:M:53:HIS:C     | 2.56                     | 0.43              |
| 1:B:1021:LEU:O    | 1:B:1024:SER:HB3  | 2.19                     | 0.43              |
| 1:B:122:MET:O     | 1:B:125:ALA:HB3   | 2.19                     | 0.43              |
| 1:B:230:ARG:HB3   | 1:B:232:GLU:HG2   | 1.99                     | 0.43              |
| 2:C:1034:VAL:O    | 2:C:1037:LEU:N    | 2.51                     | 0.43              |
| 2:C:1215:ARG:O    | 2:C:1216:LEU:HD23 | 2.18                     | 0.43              |
| 2:C:1219:ASP:O    | 2:C:1219:ASP:OD1  | 2.36                     | 0.43              |
| 2:C:247:GLY:H     | 2:C:418:LYS:NZ    | 2.17                     | 0.43              |
| 2:C:281:PRO:HB2   | 2:C:283:VAL:HG23  | 2.00                     | 0.43              |
| 2:C:510:LYS:HB2   | 2:C:511:PRO:HD3   | 2.01                     | 0.43              |
| 2:C:798:TYR:CE1   | 10:K:4:PRO:HB3    | 2.54                     | 0.43              |
| 3:D:31:ASN:O      | 3:D:35:ARG:HG3    | 2.17                     | 0.43              |
| 3:D:91:HIS:HD2    | 3:D:91:HIS:O      | 2.01                     | 0.43              |
| 6:G:118:LEU:O     | 6:G:122:MET:HG3   | 2.17                     | 0.43              |
| 8:I:30:SER:HB3    | 8:I:36:CYS:HB3    | 2.00                     | 0.43              |
| 1:B:1283:VAL:HG12 | 1:B:1284:MET:N    | 2.32                     | 0.43              |
| 1:B:1291:VAL:HG13 | 1:B:1292:PRO:N    | 2.33                     | 0.43              |
| 1:B:146:MET:HB3   | 1:B:171:GLN:O     | 2.18                     | 0.43              |
| 1:B:229:SER:HB3   | 1:B:1413:GLY:O    | 2.18                     | 0.43              |
| 1:B:741:ASN:C     | 1:B:741:ASN:ND2   | 2.62                     | 0.43              |
| 1:B:884:ASP:C     | 1:B:886:ILE:H     | 2.22                     | 0.43              |
| 1:B:997:LEU:N     | 1:B:997:LEU:HD23  | 2.34                     | 0.43              |
| 1:B:9:ALA:HB1     | 1:B:10:PRO:HD2    | 2.00                     | 0.43              |
| 2:C:125:SER:CB    | 2:C:171:PRO:HA    | 2.49                     | 0.43              |
| 2:C:48:LEU:O      | 2:C:49:ASP:C      | 2.57                     | 0.43              |
| 2:C:531:GLN:HG3   | 2:C:532:ALA:N     | 2.34                     | 0.43              |
| 2:C:641:GLU:C     | 2:C:643:ASP:H     | 2.21                     | 0.43              |
| 1:B:658:LEU:CD1   | 2:C:830:TYR:CD1   | 3.02                     | 0.43              |
| 2:C:882:THR:HG1   | 2:C:933:SER:N     | 2.17                     | 0.43              |
| 3:D:10:ILE:CD1    | 11:L:109:TRP:HA   | 2.49                     | 0.43              |
| 5:F:79:TRP:CD1    | 5:F:96:PHE:HE1    | 2.37                     | 0.43              |
| 5:F:94:LYS:O      | 5:F:98:ILE:HG13   | 2.19                     | 0.43              |
| 9:J:7:CYS:HB2     | 9:J:34:TYR:CG     | 2.54                     | 0.43              |
| 9:J:58:VAL:O      | 9:J:58:VAL:HG12   | 2.19                     | 0.43              |
| 1:B:850:VAL:HG12  | 1:B:1060:PRO:HA   | 2.01                     | 0.43              |
| 1:B:1167:GLU:O    | 1:B:1170:ILE:HG13 | 2.19                     | 0.43              |
| 1:B:1313:LEU:O    | 1:B:1315:GLU:N    | 2.52                     | 0.43              |
| 1:B:265:LYS:HD3   | 1:B:302:THR:CG2   | 2.48                     | 0.43              |
| 1:B:381:THR:C     | 1:B:383:TYR:N     | 2.71                     | 0.43              |
| 1:B:80:HIS:N      | 1:B:243:PRO:HG3   | 2.33                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:853:ASP:CG   | 1:B:855:THR:HG22 | 2.38                     | 0.43              |
| 1:B:946:VAL:HG22 | 5:F:201:LYS:HD2  | 2.00                     | 0.43              |
| 2:C:1033:LYS:NZ  | 2:C:1070:GLU:OE1 | 2.50                     | 0.43              |
| 2:C:347:LYS:O    | 2:C:350:GLN:HB3  | 2.18                     | 0.43              |
| 2:C:531:GLN:CG   | 2:C:532:ALA:H    | 2.31                     | 0.43              |
| 2:C:882:THR:HB   | 2:C:934:LYS:C    | 2.39                     | 0.43              |
| 2:C:948:ILE:O    | 2:C:968:VAL:HG13 | 2.19                     | 0.43              |
| 3:D:100:THR:CG2  | 3:D:102:GLN:HE21 | 2.32                     | 0.43              |
| 3:D:100:THR:HG21 | 3:D:102:GLN:NE2  | 2.34                     | 0.43              |
| 3:D:208:GLU:C    | 3:D:210:GLU:N    | 2.71                     | 0.43              |
| 4:E:34:GLN:O     | 4:E:47:LEU:HD23  | 2.18                     | 0.43              |
| 5:F:82:PHE:CD1   | 5:F:82:PHE:N     | 2.87                     | 0.43              |
| 6:G:147:SER:O    | 6:G:148:VAL:C    | 2.57                     | 0.43              |
| 7:H:1:MET:O      | 7:H:1:MET:CE     | 2.67                     | 0.43              |
| 7:H:80:LYS:HE2   | 7:H:82:PHE:CE1   | 2.54                     | 0.43              |
| 8:I:113:ALA:HA   | 8:I:125:LEU:O    | 2.19                     | 0.43              |
| 8:I:15:VAL:CG2   | 8:I:26:ILE:HD11  | 2.37                     | 0.43              |
| 9:J:105:SER:O    | 9:J:106:CYS:CB   | 2.66                     | 0.43              |
| 9:J:26:LEU:HD22  | 9:J:35:VAL:HG12  | 2.01                     | 0.43              |
| 9:J:54:GLU:OE2   | 9:J:118:ARG:CZ   | 2.67                     | 0.43              |
| 1:B:133:LYS:O    | 1:B:136:ALA:HB3  | 2.19                     | 0.42              |
| 1:B:1368:MET:O   | 1:B:1372:VAL:HB  | 2.18                     | 0.42              |
| 1:B:345:VAL:HG11 | 2:C:1130:PHE:HB2 | 2.00                     | 0.42              |
| 1:B:40:THR:HB    | 1:B:41:MET:HE2   | 1.99                     | 0.42              |
| 1:B:465:TYR:CZ   | 11:L:4:PRO:HD2   | 2.54                     | 0.42              |
| 1:B:774:ARG:HB2  | 1:B:797:LYS:HB3  | 2.01                     | 0.42              |
| 1:B:853:ASP:OD1  | 1:B:855:THR:CB   | 2.67                     | 0.42              |
| 2:C:1003:ALA:HA  | 3:D:178:PHE:O    | 2.18                     | 0.42              |
| 2:C:308:TRP:CD1  | 2:C:308:TRP:N    | 2.86                     | 0.42              |
| 2:C:498:THR:HG22 | 2:C:537:LYS:O    | 2.18                     | 0.42              |
| 2:C:657:HIS:O    | 2:C:660:LYS:HB3  | 2.19                     | 0.42              |
| 2:C:680:THR:HB   | 2:C:681:TRP:H    | 1.55                     | 0.42              |
| 2:C:792:MET:HG3  | 2:C:855:PHE:CE1  | 2.54                     | 0.42              |
| 3:D:44:LEU:HD21  | 3:D:159:ALA:HB1  | 2.01                     | 0.42              |
| 6:G:116:ASP:HB3  | 6:G:119:ARG:CB   | 2.49                     | 0.42              |
| 6:G:88:TYR:HD1   | 6:G:88:TYR:H     | 1.66                     | 0.42              |
| 7:H:15:PRO:O     | 7:H:16:SER:C     | 2.57                     | 0.42              |
| 8:I:116:TYR:HE2  | 8:I:140:ALA:HB3  | 1.84                     | 0.42              |
| 9:J:90:GLN:HE21  | 9:J:92:ARG:HD2   | 1.82                     | 0.42              |
| 1:B:1007:ILE:O   | 1:B:1010:ALA:N   | 2.52                     | 0.42              |
| 1:B:1265:ASN:C   | 1:B:1267:MET:N   | 2.71                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:208:LEU:HD23  | 1:B:209:ASN:N     | 2.34                     | 0.42              |
| 1:B:247:ARG:NH1   | 1:B:247:ARG:HG3   | 2.35                     | 0.42              |
| 1:B:380:VAL:CG1   | 1:B:385:ILE:HG12  | 2.49                     | 0.42              |
| 2:C:1027:ILE:C    | 2:C:1029:CYS:N    | 2.72                     | 0.42              |
| 2:C:1102:LYS:O    | 2:C:1103:ILE:C    | 2.58                     | 0.42              |
| 2:C:1160:VAL:CG1  | 2:C:1161:HIS:N    | 2.82                     | 0.42              |
| 1:B:30:ILE:HD11   | 2:C:1168:LEU:CD1  | 2.49                     | 0.42              |
| 2:C:1177:HIS:HB2  | 2:C:1179:GLN:HE21 | 1.84                     | 0.42              |
| 1:B:1409:LEU:HD13 | 2:C:1207:LEU:HD21 | 2.01                     | 0.42              |
| 2:C:303:TYR:HH    | 2:C:586:TRP:HH2   | 1.65                     | 0.42              |
| 2:C:37:PHE:CD1    | 2:C:41:LYS:HG3    | 2.53                     | 0.42              |
| 2:C:487:THR:CG2   | 2:C:488:TYR:N     | 2.82                     | 0.42              |
| 2:C:553:PRO:O     | 2:C:557:PHE:HB2   | 2.18                     | 0.42              |
| 2:C:599:THR:O     | 2:C:603:LEU:HB2   | 2.19                     | 0.42              |
| 2:C:801:LYS:O     | 10:K:52:THR:HG21  | 2.17                     | 0.42              |
| 2:C:893:LEU:HD22  | 2:C:897:GLY:C     | 2.39                     | 0.42              |
| 2:C:95:ILE:HG13   | 2:C:130:VAL:HG22  | 2.01                     | 0.42              |
| 3:D:101:LEU:HD12  | 3:D:101:LEU:HA    | 1.88                     | 0.42              |
| 4:E:30:GLY:O      | 4:E:31:GLN:C      | 2.57                     | 0.42              |
| 8:I:118:PHE:C     | 8:I:120:GLY:N     | 2.73                     | 0.42              |
| 11:L:31:VAL:CG1   | 11:L:32:VAL:N     | 2.81                     | 0.42              |
| 1:B:1215:ARG:HH11 | 1:B:1215:ARG:HG2  | 1.82                     | 0.42              |
| 1:B:1064:VAL:HG12 | 1:B:1370:LEU:HD22 | 2.01                     | 0.42              |
| 1:B:1437:GLY:HA3  | 6:G:88:TYR:CD2    | 2.53                     | 0.42              |
| 1:B:269:ILE:HD11  | 1:B:300:VAL:HA    | 2.00                     | 0.42              |
| 1:B:269:ILE:HG12  | 1:B:299:HIS:HB3   | 2.01                     | 0.42              |
| 1:B:497:THR:O     | 1:B:498:ARG:C     | 2.57                     | 0.42              |
| 1:B:590:ARG:HH11  | 1:B:590:ARG:CB    | 2.30                     | 0.42              |
| 1:B:658:LEU:HD11  | 2:C:830:TYR:CE1   | 2.55                     | 0.42              |
| 1:B:715:GLU:O     | 1:B:718:VAL:HB    | 2.19                     | 0.42              |
| 1:B:787:PHE:HE1   | 1:B:796:SER:HA    | 1.82                     | 0.42              |
| 1:B:898:ARG:HA    | 1:B:933:TYR:CD1   | 2.55                     | 0.42              |
| 2:C:1084:GLN:N    | 2:C:1084:GLN:HE21 | 2.09                     | 0.42              |
| 2:C:424:LEU:O     | 2:C:428:ILE:HG13  | 2.19                     | 0.42              |
| 2:C:528:PRO:HG3   | 2:C:536:VAL:HB    | 2.01                     | 0.42              |
| 2:C:659:ALA:HA    | 2:C:662:MET:HE2   | 2.00                     | 0.42              |
| 2:C:662:MET:HA    | 2:C:665:GLU:HB2   | 2.01                     | 0.42              |
| 3:D:107:SER:C     | 3:D:109:SER:H     | 2.23                     | 0.42              |
| 3:D:99:LEU:HD23   | 3:D:120:ILE:HA    | 2.00                     | 0.42              |
| 3:D:242:GLN:O     | 3:D:244:VAL:N     | 2.53                     | 0.42              |
| 4:E:160:VAL:O     | 4:E:160:VAL:HG12  | 2.20                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:H:44:TYR:HD2    | 7:H:105:PRO:HB2   | 1.85                     | 0.42              |
| 8:I:117:SER:HA    | 8:I:121:LEU:O     | 2.19                     | 0.42              |
| 2:C:1039:GLY:HA2  | 10:K:51:LEU:HD21  | 2.01                     | 0.42              |
| 3:D:35:ARG:HH11   | 11:L:41:THR:H     | 1.62                     | 0.42              |
| 12:M:59:ALA:O     | 12:M:60:ARG:O     | 2.38                     | 0.42              |
| 15:T:18:DT:OP2    | 15:T:18:DT:H72    | 2.19                     | 0.42              |
| 1:B:1005:GLU:O    | 1:B:1006:ILE:C    | 2.58                     | 0.42              |
| 1:B:1011:GLN:NE2  | 1:B:1015:VAL:HG21 | 2.34                     | 0.42              |
| 1:B:1398:MET:C    | 1:B:1400:CYS:N    | 2.73                     | 0.42              |
| 1:B:1063:MET:HG3  | 1:B:1436:ILE:HG23 | 2.01                     | 0.42              |
| 1:B:364:VAL:CG1   | 1:B:364:VAL:O     | 2.68                     | 0.42              |
| 1:B:761:MET:HA    | 1:B:804:TYR:HB2   | 2.00                     | 0.42              |
| 1:B:864:ILE:O     | 1:B:865:GLN:HG2   | 2.20                     | 0.42              |
| 2:C:1017:ILE:H    | 2:C:1018:PRO:HD2  | 1.84                     | 0.42              |
| 2:C:1034:VAL:C    | 2:C:1036:ALA:N    | 2.72                     | 0.42              |
| 2:C:185:THR:O     | 2:C:188:ASP:N     | 2.52                     | 0.42              |
| 2:C:698:GLU:O     | 2:C:701:ILE:HG12  | 2.20                     | 0.42              |
| 2:C:119:LEU:HD23  | 2:C:789:MET:HB2   | 2.02                     | 0.42              |
| 2:C:861:ASP:CG    | 2:C:914:LYS:HD2   | 2.38                     | 0.42              |
| 2:C:948:ILE:HD12  | 2:C:969:ARG:NH1   | 2.34                     | 0.42              |
| 3:D:186:LEU:HD21  | 3:D:224:GLN:C     | 2.40                     | 0.42              |
| 3:D:44:LEU:CD2    | 3:D:159:ALA:HB1   | 2.49                     | 0.42              |
| 5:F:160:GLU:O     | 5:F:163:GLU:HB3   | 2.19                     | 0.42              |
| 8:I:15:VAL:HG13   | 8:I:26:ILE:HG13   | 2.01                     | 0.42              |
| 1:B:567:LYS:NZ    | 8:I:47:PHE:HB3    | 2.34                     | 0.42              |
| 9:J:70:ARG:NH1    | 9:J:84:VAL:HB     | 2.35                     | 0.42              |
| 1:B:1017:LEU:O    | 1:B:1018:PHE:C    | 2.57                     | 0.42              |
| 1:B:1040:GLN:O    | 1:B:1041:ALA:C    | 2.58                     | 0.42              |
| 1:B:1214:GLU:O    | 1:B:1218:GLN:HG2  | 2.19                     | 0.42              |
| 1:B:1279:ILE:HG23 | 1:B:1308:THR:OG1  | 2.20                     | 0.42              |
| 1:B:420:ARG:O     | 1:B:421:ALA:C     | 2.58                     | 0.42              |
| 1:B:427:GLN:HB2   | 1:B:430:TRP:CG    | 2.54                     | 0.42              |
| 1:B:404:TYR:HB2   | 1:B:433:GLU:HB2   | 2.00                     | 0.42              |
| 1:B:44:THR:O      | 1:B:45:GLN:HB2    | 2.18                     | 0.42              |
| 1:B:543:LEU:O     | 1:B:544:ASP:C     | 2.57                     | 0.42              |
| 1:B:546:VAL:HG21  | 1:B:572:TRP:HB2   | 2.01                     | 0.42              |
| 1:B:557:ASP:N     | 1:B:557:ASP:OD1   | 2.52                     | 0.42              |
| 1:B:565:ILE:O     | 1:B:570:PRO:HA    | 2.19                     | 0.42              |
| 1:B:606:LEU:HG    | 1:B:613:ILE:HB    | 2.00                     | 0.42              |
| 1:B:786:HIS:O     | 1:B:787:PHE:HD2   | 2.01                     | 0.42              |
| 1:B:820:GLY:O     | 1:B:821:ARG:C     | 2.57                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:858:ASN:HD22  | 1:B:858:ASN:H    | 1.68                     | 0.42              |
| 2:C:286:PHE:HE1   | 2:C:301:ILE:HD11 | 1.84                     | 0.42              |
| 2:C:401:PHE:C     | 2:C:403:LYS:H    | 2.23                     | 0.42              |
| 2:C:487:THR:HG22  | 2:C:488:TYR:N    | 2.34                     | 0.42              |
| 2:C:566:LEU:HD22  | 2:C:586:TRP:HB3  | 2.01                     | 0.42              |
| 2:C:638:PHE:HB2   | 2:C:741:CYS:HB3  | 2.01                     | 0.42              |
| 2:C:496:ARG:HD3   | 2:C:751:VAL:HG22 | 2.01                     | 0.42              |
| 2:C:799:PRO:HB3   | 2:C:818:PRO:HG2  | 2.00                     | 0.42              |
| 3:D:33:LEU:O      | 3:D:34:ARG:C     | 2.57                     | 0.42              |
| 4:E:17:LYS:O      | 4:E:17:LYS:HD3   | 2.19                     | 0.42              |
| 4:E:66:ARG:HG3    | 7:H:51:TYR:CD1   | 2.55                     | 0.42              |
| 8:I:130:ARG:CA    | 8:I:133:ASN:HB2  | 2.50                     | 0.42              |
| 9:J:19:ASP:OD1    | 9:J:22:ASN:HB2   | 2.19                     | 0.42              |
| 10:K:51:LEU:O     | 10:K:51:LEU:HD12 | 2.18                     | 0.42              |
| 10:K:53:HIS:CE1   | 10:K:55:ASP:OD1  | 2.72                     | 0.42              |
| 11:L:29:ASN:O     | 11:L:30:ALA:HB2  | 2.20                     | 0.42              |
| 1:B:1259:MET:O    | 1:B:1261:LYS:N   | 2.49                     | 0.42              |
| 1:B:1293:SER:OG   | 1:B:1295:THR:CG2 | 2.67                     | 0.42              |
| 1:B:1116:LEU:HB2  | 1:B:1329:THR:OG1 | 2.20                     | 0.42              |
| 1:B:399:HIS:CG    | 1:B:400:PRO:N    | 2.85                     | 0.42              |
| 1:B:773:LYS:HG3   | 1:B:773:LYS:H    | 1.58                     | 0.42              |
| 1:B:808:LEU:HD23  | 1:B:812:GLU:C    | 2.39                     | 0.42              |
| 1:B:858:ASN:ND2   | 1:B:858:ASN:H    | 2.17                     | 0.42              |
| 1:B:885:THR:O     | 1:B:885:THR:CG2  | 2.66                     | 0.42              |
| 1:B:666:ILE:HD11  | 2:C:1086:PHE:HE1 | 1.85                     | 0.42              |
| 2:C:120:ARG:HB2   | 2:C:122:LEU:HG   | 2.00                     | 0.42              |
| 3:D:167:HIS:CD2   | 3:D:168:ALA:H    | 2.37                     | 0.42              |
| 3:D:189:THR:HG22  | 3:D:190:ASP:N    | 2.34                     | 0.42              |
| 2:C:997:GLU:HB3   | 3:D:35:ARG:NH2   | 2.34                     | 0.42              |
| 5:F:177:ARG:HD3   | 5:F:215:MET:HG2  | 2.02                     | 0.42              |
| 5:F:61:GLN:HG2    | 5:F:62:ALA:N     | 2.35                     | 0.42              |
| 6:G:92:ARG:O      | 6:G:93:ILE:C     | 2.56                     | 0.42              |
| 8:I:96:VAL:HG13   | 8:I:143:LEU:HG   | 2.01                     | 0.42              |
| 9:J:69:PRO:HB2    | 9:J:85:PHE:HE2   | 1.84                     | 0.42              |
| 12:M:46:VAL:O     | 12:M:46:VAL:HG12 | 2.19                     | 0.42              |
| 13:N:5:DT:H2"     | 13:N:6:DA:C8     | 2.54                     | 0.42              |
| 1:B:1111:MET:HG3  | 1:B:1113:THR:O   | 2.19                     | 0.42              |
| 1:B:1239:ARG:HH22 | 1:B:1241:ARG:NH2 | 2.16                     | 0.42              |
| 1:B:241:VAL:O     | 1:B:241:VAL:HG12 | 2.19                     | 0.42              |
| 1:B:382:PRO:CD    | 1:B:428:TYR:HE2  | 2.32                     | 0.42              |
| 1:B:471:ASN:O     | 1:B:474:VAL:HG12 | 2.19                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:873:MET:HG3   | 1:B:1056:SER:O    | 2.20                     | 0.42              |
| 2:C:1130:PHE:CD2  | 2:C:1130:PHE:O    | 2.73                     | 0.42              |
| 1:B:658:LEU:CD1   | 2:C:831:SER:H     | 2.19                     | 0.42              |
| 3:D:6:PRO:CG      | 11:L:101:LEU:HB2  | 2.49                     | 0.42              |
| 4:E:18:VAL:O      | 4:E:18:VAL:HG13   | 2.19                     | 0.42              |
| 5:F:22:MET:HE3    | 5:F:26:ARG:NH2    | 2.30                     | 0.42              |
| 7:H:106:MET:HB3   | 7:H:106:MET:HE2   | 1.72                     | 0.42              |
| 8:I:100:THR:HA    | 8:I:138:GLU:O     | 2.20                     | 0.42              |
| 11:L:42:LEU:CD2   | 11:L:46:ILE:CD1   | 2.98                     | 0.42              |
| 11:L:5:ASP:O      | 11:L:6:ARG:C      | 2.57                     | 0.42              |
| 1:B:1277:GLU:O    | 1:B:1278:ASN:HB2  | 2.20                     | 0.42              |
| 1:B:56:PRO:O      | 1:B:57:ARG:CG     | 2.68                     | 0.42              |
| 1:B:681:GLU:HA    | 1:B:684:ALA:HB3   | 2.01                     | 0.42              |
| 2:C:1066:SER:O    | 2:C:1067:ARG:HD3  | 2.18                     | 0.42              |
| 2:C:1159:ARG:HH11 | 2:C:1159:ARG:CB   | 2.21                     | 0.42              |
| 2:C:205:ILE:O     | 2:C:206:ASN:C     | 2.57                     | 0.42              |
| 2:C:272:THR:OG1   | 2:C:279:ASP:OD1   | 2.37                     | 0.42              |
| 2:C:30:SER:O      | 2:C:33:VAL:HG23   | 2.20                     | 0.42              |
| 2:C:401:PHE:O     | 2:C:404:LYS:N     | 2.45                     | 0.42              |
| 2:C:578:THR:HG23  | 2:C:622:LYS:C     | 2.40                     | 0.42              |
| 2:C:653:VAL:CA    | 2:C:689:LEU:HD22  | 2.49                     | 0.42              |
| 2:C:880:THR:HG22  | 2:C:880:THR:O     | 2.20                     | 0.42              |
| 2:C:899:ILE:HD11  | 2:C:911:ILE:CA    | 2.42                     | 0.42              |
| 2:C:997:GLU:N     | 2:C:997:GLU:OE2   | 2.51                     | 0.42              |
| 3:D:49:VAL:CG1    | 3:D:155:LEU:HD22  | 2.50                     | 0.42              |
| 8:I:116:TYR:O     | 8:I:122:LEU:HA    | 2.19                     | 0.42              |
| 10:K:57:ILE:O     | 10:K:60:PHE:HB2   | 2.20                     | 0.42              |
| 1:B:108:MET:HA    | 1:B:210:ILE:CG2   | 2.50                     | 0.42              |
| 1:B:1194:ARG:HH11 | 1:B:1194:ARG:HG2  | 1.83                     | 0.42              |
| 1:B:1266:THR:HA   | 1:B:1270:ASN:HD22 | 1.84                     | 0.42              |
| 1:B:1346:ALA:HB3  | 5:F:149:LEU:HD12  | 2.02                     | 0.42              |
| 1:B:17:VAL:HA     | 2:C:1215:ARG:O    | 2.20                     | 0.42              |
| 1:B:350:ARG:HH11  | 1:B:350:ARG:HG3   | 1.84                     | 0.42              |
| 1:B:373:THR:HG21  | 2:C:1105:ALA:HB3  | 2.01                     | 0.42              |
| 1:B:578:LEU:HG    | 1:B:578:LEU:O     | 2.19                     | 0.42              |
| 1:B:808:LEU:HG    | 1:B:812:GLU:HB3   | 2.02                     | 0.42              |
| 1:B:818:MET:H     | 1:B:818:MET:HG3   | 1.70                     | 0.42              |
| 1:B:898:ARG:HA    | 1:B:933:TYR:HD1   | 1.85                     | 0.42              |
| 2:C:1182:CYS:O    | 2:C:1183:LYS:C    | 2.58                     | 0.42              |
| 2:C:175:ARG:HH11  | 2:C:175:ARG:CG    | 2.28                     | 0.42              |
| 2:C:405:ARG:HD2   | 2:C:631:GLY:CA    | 2.50                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:693:ILE:HD13  | 2:C:701:ILE:HD13 | 2.02                     | 0.42              |
| 7:H:148:GLU:HB2   | 7:H:160:ILE:O    | 2.20                     | 0.42              |
| 7:H:45:ILE:HD13   | 7:H:45:ILE:HA    | 1.89                     | 0.42              |
| 10:K:3:VAL:HG12   | 10:K:15:GLY:HA2  | 2.00                     | 0.42              |
| 2:C:1039:GLY:HA2  | 10:K:51:LEU:CD2  | 2.49                     | 0.42              |
| 11:L:31:VAL:HG12  | 11:L:32:VAL:H    | 1.81                     | 0.42              |
| 1:B:106:VAL:HG13  | 1:B:112:LYS:C    | 2.40                     | 0.42              |
| 1:B:1163:ILE:HG22 | 1:B:1164:PRO:HD2 | 2.02                     | 0.42              |
| 1:B:1173:HIS:O    | 1:B:1174:PHE:HD1 | 2.03                     | 0.42              |
| 1:B:1446:ASP:HB2  | 6:G:133:VAL:HG23 | 2.01                     | 0.42              |
| 1:B:266:LEU:O     | 1:B:267:ALA:C    | 2.57                     | 0.42              |
| 1:B:92:HIS:CD2    | 1:B:304:MET:HE3  | 2.54                     | 0.42              |
| 1:B:337:ARG:O     | 1:B:337:ARG:HG2  | 2.19                     | 0.42              |
| 1:B:509:LEU:C     | 1:B:511:ILE:H    | 2.22                     | 0.42              |
| 1:B:600:PRO:CG    | 1:B:601:LYS:H    | 2.30                     | 0.42              |
| 1:B:644:LYS:O     | 1:B:647:GLY:N    | 2.53                     | 0.42              |
| 1:B:786:HIS:CD2   | 1:B:786:HIS:N    | 2.86                     | 0.42              |
| 1:B:337:ARG:NH2   | 1:B:839:ARG:HH12 | 2.18                     | 0.42              |
| 2:C:1203:LEU:O    | 2:C:1207:LEU:HG  | 2.20                     | 0.42              |
| 2:C:364:ILE:CG1   | 2:C:585:VAL:HG13 | 2.49                     | 0.42              |
| 2:C:843:GLN:CB    | 2:C:994:TYR:O    | 2.68                     | 0.42              |
| 2:C:910:VAL:HG12  | 2:C:912:ILE:N    | 2.29                     | 0.42              |
| 2:C:970:THR:HG22  | 2:C:971:THR:N    | 2.34                     | 0.42              |
| 4:E:187:THR:HG22  | 4:E:188:ALA:N    | 2.35                     | 0.42              |
| 4:E:119:ARG:HD3   | 4:E:221:TYR:CD2  | 2.55                     | 0.42              |
| 1:B:1341:ILE:HG22 | 5:F:182:ASP:OD2  | 2.20                     | 0.42              |
| 6:G:109:VAL:CG1   | 6:G:110:ASP:H    | 2.26                     | 0.42              |
| 8:I:83:GLN:O      | 8:I:85:GLY:N     | 2.53                     | 0.42              |
| 8:I:93:TYR:HA     | 8:I:145:ARG:HB3  | 2.02                     | 0.42              |
| 9:J:100:PHE:HD1   | 9:J:100:PHE:N    | 2.18                     | 0.42              |
| 10:K:1:MET:HE2    | 10:K:56:LEU:HD12 | 2.02                     | 0.42              |
| 1:B:1313:LEU:HD11 | 1:B:1317:MET:HE1 | 2.02                     | 0.41              |
| 1:B:382:PRO:CB    | 1:B:428:TYR:CE2  | 2.96                     | 0.41              |
| 1:B:552:TRP:HE1   | 11:L:62:LYS:CB   | 2.33                     | 0.41              |
| 1:B:65:LEU:O      | 1:B:66:LYS:C     | 2.59                     | 0.41              |
| 1:B:709:THR:CG2   | 9:J:93:LYS:O     | 2.68                     | 0.41              |
| 1:B:853:ASP:OD1   | 1:B:855:THR:HB   | 2.20                     | 0.41              |
| 2:C:1135:ARG:NH2  | 2:C:1136:ASP:OD1 | 2.52                     | 0.41              |
| 2:C:345:LYS:O     | 2:C:346:GLU:HB2  | 2.20                     | 0.41              |
| 2:C:449:ASN:C     | 2:C:451:LYS:N    | 2.73                     | 0.41              |
| 2:C:519:TRP:NE1   | 2:C:635:ARG:NH2  | 2.67                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:882:THR:C     | 2:C:884:ARG:H     | 2.23                     | 0.41              |
| 3:D:116:LYS:HG3   | 3:D:117:ASP:H     | 1.84                     | 0.41              |
| 3:D:148:ARG:HD3   | 3:D:149:LYS:H     | 1.85                     | 0.41              |
| 3:D:66:ARG:NH1    | 10:K:2:ILE:CG2    | 2.78                     | 0.41              |
| 4:E:118:THR:HB    | 4:E:121:LYS:HB2   | 2.01                     | 0.41              |
| 4:E:139:LYS:C     | 4:E:139:LYS:HD3   | 2.40                     | 0.41              |
| 4:E:13:ARG:HH11   | 4:E:13:ARG:HG2    | 1.85                     | 0.41              |
| 4:E:185:CYS:O     | 4:E:211:LEU:HD22  | 2.19                     | 0.41              |
| 8:I:16:ASP:HA     | 8:I:17:PRO:HD3    | 1.91                     | 0.41              |
| 3:D:174:ALA:O     | 10:K:10:CYS:O     | 2.38                     | 0.41              |
| 10:K:44:TYR:O     | 10:K:47:ARG:HB2   | 2.19                     | 0.41              |
| 1:B:1313:LEU:HD23 | 1:B:1338:VAL:CG2  | 2.50                     | 0.41              |
| 1:B:1370:LEU:O    | 1:B:1374:VAL:HG23 | 2.20                     | 0.41              |
| 1:B:1405:THR:HB   | 1:B:1406:VAL:H    | 1.54                     | 0.41              |
| 1:B:860:LEU:HA    | 1:B:1422:ARG:NH1  | 2.34                     | 0.41              |
| 1:B:1437:GLY:CA   | 6:G:88:TYR:CD2    | 3.03                     | 0.41              |
| 1:B:174:ILE:HG13  | 1:B:174:ILE:H     | 1.66                     | 0.41              |
| 1:B:224:PHE:CE2   | 1:B:234:MET:HE2   | 2.55                     | 0.41              |
| 1:B:414:ASP:OD1   | 1:B:416:ARG:HG2   | 2.21                     | 0.41              |
| 1:B:471:ASN:OD1   | 1:B:473:SER:N     | 2.54                     | 0.41              |
| 2:C:1002:THR:O    | 2:C:1003:ALA:C    | 2.57                     | 0.41              |
| 2:C:34:ILE:HD13   | 2:C:747:MET:CE    | 2.51                     | 0.41              |
| 3:D:104:PHE:HD2   | 3:D:105:GLY:N     | 2.17                     | 0.41              |
| 4:E:137:ASN:N     | 4:E:137:ASN:ND2   | 2.67                     | 0.41              |
| 4:E:220:LEU:HB3   | 4:E:221:TYR:H     | 1.57                     | 0.41              |
| 5:F:167:ARG:HA    | 5:F:167:ARG:HD3   | 1.72                     | 0.41              |
| 6:G:130:ILE:HB    | 6:G:148:VAL:HG21  | 2.01                     | 0.41              |
| 8:I:142:LEU:C     | 8:I:143:LEU:HD12  | 2.41                     | 0.41              |
| 8:I:91:ASP:O      | 8:I:93:TYR:N      | 2.49                     | 0.41              |
| 1:B:1332:PHE:HD2  | 1:B:1332:PHE:N    | 2.17                     | 0.41              |
| 1:B:345:VAL:HG23  | 1:B:346:ASP:O     | 2.20                     | 0.41              |
| 1:B:405:VAL:HG23  | 1:B:415:LEU:HD11  | 2.03                     | 0.41              |
| 1:B:836:TYR:HE1   | 15:T:17:DC:OP1    | 2.03                     | 0.41              |
| 1:B:855:THR:HG23  | 1:B:857:ARG:HG3   | 2.01                     | 0.41              |
| 2:C:24:PRO:O      | 2:C:655:LYS:HB2   | 2.21                     | 0.41              |
| 2:C:210:LYS:HG3   | 2:C:461:LEU:O     | 2.20                     | 0.41              |
| 2:C:593:PRO:HG2   | 2:C:617:ARG:CZ    | 2.51                     | 0.41              |
| 4:E:180:LEU:CD2   | 4:E:195:ILE:HD12  | 2.48                     | 0.41              |
| 5:F:129:PRO:O     | 5:F:130:ALA:C     | 2.58                     | 0.41              |
| 7:H:15:PRO:HD3    | 7:H:67:SER:N      | 2.36                     | 0.41              |
| 7:H:27:LYS:O      | 7:H:28:THR:C      | 2.58                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:H:7:LEU:HD12    | 7:H:74:TYR:CZ     | 2.55                     | 0.41              |
| 9:J:13:MET:HG3    | 9:J:14:LEU:N      | 2.35                     | 0.41              |
| 9:J:84:VAL:O      | 9:J:84:VAL:HG13   | 2.20                     | 0.41              |
| 2:C:992:ILE:CD1   | 11:L:66:PRO:HB2   | 2.49                     | 0.41              |
| 11:L:49:GLU:OE2   | 11:L:97:LYS:HE3   | 2.20                     | 0.41              |
| 12:M:55:ILE:H     | 12:M:55:ILE:HG12  | 1.60                     | 0.41              |
| 1:B:1134:ILE:O    | 1:B:1137:ALA:HB3  | 2.21                     | 0.41              |
| 1:B:1148:ILE:HD11 | 1:B:1198:ASP:CA   | 2.43                     | 0.41              |
| 1:B:1215:ARG:NH1  | 1:B:1215:ARG:HG2  | 2.35                     | 0.41              |
| 1:B:1425:SER:O    | 1:B:1429:ILE:HG13 | 2.20                     | 0.41              |
| 1:B:344:ARG:NH1   | 1:B:344:ARG:HG2   | 2.35                     | 0.41              |
| 1:B:384:ASN:HB2   | 1:B:388:LEU:HD12  | 2.02                     | 0.41              |
| 1:B:613:ILE:HG22  | 1:B:614:PHE:HD2   | 1.85                     | 0.41              |
| 1:B:710:LEU:CD1   | 1:B:710:LEU:H     | 2.33                     | 0.41              |
| 1:B:758:ILE:H     | 1:B:758:ILE:HG13  | 1.73                     | 0.41              |
| 2:C:1034:VAL:C    | 2:C:1036:ALA:H    | 2.23                     | 0.41              |
| 2:C:446:LEU:HD23  | 2:C:446:LEU:N     | 2.36                     | 0.41              |
| 2:C:54:PHE:O      | 2:C:58:THR:HB     | 2.21                     | 0.41              |
| 2:C:613:VAL:CG1   | 2:C:627:PHE:O     | 2.68                     | 0.41              |
| 2:C:711:GLU:H     | 2:C:712:PRO:HD2   | 1.86                     | 0.41              |
| 2:C:809:MET:HE1   | 2:C:814:PHE:CD2   | 2.55                     | 0.41              |
| 4:E:173:HIS:HA    | 4:E:174:PRO:HD2   | 1.64                     | 0.41              |
| 4:E:7:THR:O       | 4:E:9:GLN:N       | 2.53                     | 0.41              |
| 5:F:142:VAL:HG12  | 5:F:143:ASN:N     | 2.36                     | 0.41              |
| 5:F:76:GLY:HA3    | 5:F:106:GLN:HB3   | 2.02                     | 0.41              |
| 6:G:89:GLU:HB3    | 6:G:134:ILE:HD11  | 2.00                     | 0.41              |
| 11:L:15:GLY:O     | 11:L:16:GLU:HG3   | 2.20                     | 0.41              |
| 11:L:35:PHE:HE1   | 11:L:73:LEU:HB3   | 1.85                     | 0.41              |
| 11:L:89:ASN:O     | 11:L:90:ALA:C     | 2.59                     | 0.41              |
| 1:B:1303:GLU:HG3  | 1:B:1303:GLU:O    | 2.19                     | 0.41              |
| 1:B:1349:TYR:O    | 1:B:1350:LYS:C    | 2.58                     | 0.41              |
| 1:B:289:ILE:CG2   | 1:B:290:GLU:N     | 2.84                     | 0.41              |
| 1:B:382:PRO:HB3   | 1:B:428:TYR:OH    | 2.20                     | 0.41              |
| 1:B:577:ILE:O     | 1:B:579:SER:N     | 2.53                     | 0.41              |
| 1:B:61:ILE:CG2    | 1:B:62:ASP:H      | 2.23                     | 0.41              |
| 1:B:849:MET:CE    | 1:B:1061:GLY:CA   | 2.92                     | 0.41              |
| 1:B:874:ASP:O     | 1:B:875:ALA:C     | 2.57                     | 0.41              |
| 2:C:280:ILE:CG2   | 2:C:285:ILE:HG13  | 2.50                     | 0.41              |
| 2:C:594:ALA:HA    | 2:C:617:ARG:NH1   | 2.36                     | 0.41              |
| 2:C:661:LEU:HD11  | 2:C:684:LEU:HD11  | 2.03                     | 0.41              |
| 2:C:780:VAL:HG21  | 10:K:56:LEU:CD1   | 2.46                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:781:PHE:HE1  | 2:C:788:ARG:HD3   | 1.84                     | 0.41              |
| 2:C:873:THR:O    | 2:C:914:LYS:HA    | 2.20                     | 0.41              |
| 1:B:568:PRO:HB2  | 3:D:221:TYR:CE1   | 2.55                     | 0.41              |
| 3:D:236:GLY:C    | 3:D:238:ILE:N     | 2.73                     | 0.41              |
| 5:F:16:PHE:O     | 5:F:19:VAL:HG23   | 2.21                     | 0.41              |
| 5:F:144:ILE:HD13 | 5:F:183:PRO:HB3   | 2.02                     | 0.41              |
| 5:F:190:LEU:C    | 5:F:191:LYS:HG2   | 2.40                     | 0.41              |
| 5:F:42:PHE:HZ    | 5:F:58:MET:HE1    | 1.85                     | 0.41              |
| 1:B:1446:ASP:HB2 | 6:G:133:VAL:CG2   | 2.50                     | 0.41              |
| 6:G:128:LYS:HD3  | 6:G:149:GLU:O     | 2.20                     | 0.41              |
| 7:H:139:ILE:CG2  | 7:H:140:LYS:N     | 2.70                     | 0.41              |
| 7:H:23:LYS:HE2   | 7:H:27:LYS:HE3    | 2.03                     | 0.41              |
| 7:H:77:VAL:CG1   | 7:H:77:VAL:O      | 2.68                     | 0.41              |
| 8:I:100:THR:CG2  | 8:I:101:ALA:N     | 2.84                     | 0.41              |
| 9:J:82:GLU:C     | 9:J:104:LEU:HG    | 2.40                     | 0.41              |
| 12:M:38:LEU:CD1  | 12:M:49:LYS:HE2   | 2.51                     | 0.41              |
| 1:B:1029:ARG:HD2 | 1:B:1033:GLN:HE22 | 1.81                     | 0.41              |
| 1:B:1104:ILE:O   | 1:B:1106:ASN:N    | 2.53                     | 0.41              |
| 1:B:1268:LEU:O   | 1:B:1269:GLU:HG2  | 2.21                     | 0.41              |
| 1:B:944:ARG:NE   | 1:B:1298:TYR:HE1  | 2.18                     | 0.41              |
| 1:B:567:LYS:HZ3  | 8:I:47:PHE:HB3    | 1.85                     | 0.41              |
| 1:B:49:LYS:HZ3   | 1:B:61:ILE:HG13   | 1.84                     | 0.41              |
| 1:B:650:GLN:C    | 1:B:654:ASN:ND2   | 2.74                     | 0.41              |
| 1:B:779:PHE:HD2  | 1:B:779:PHE:HA    | 1.79                     | 0.41              |
| 1:B:932:GLU:O    | 1:B:935:GLN:N     | 2.52                     | 0.41              |
| 2:C:181:LEU:HD21 | 2:C:194:GLU:HG3   | 2.03                     | 0.41              |
| 2:C:376:PHE:HB3  | 2:C:586:TRP:CZ3   | 2.55                     | 0.41              |
| 2:C:486:TYR:CE1  | 2:C:1096:ARG:NH2  | 2.85                     | 0.41              |
| 2:C:527:THR:OG1  | 2:C:528:PRO:HD2   | 2.19                     | 0.41              |
| 2:C:597:MET:HE3  | 2:C:601:ARG:HG3   | 2.03                     | 0.41              |
| 3:D:146:LYS:C    | 3:D:147:LEU:HD23  | 2.41                     | 0.41              |
| 3:D:22:LEU:HD13  | 3:D:230:MET:CE    | 2.50                     | 0.41              |
| 3:D:252:GLN:O    | 3:D:253:LYS:C     | 2.59                     | 0.41              |
| 3:D:75:MET:HE2   | 3:D:239:PRO:HD3   | 2.02                     | 0.41              |
| 5:F:190:LEU:N    | 5:F:190:LEU:HD23  | 2.36                     | 0.41              |
| 4:E:32:GLU:HG3   | 7:H:5:LYS:HE2     | 2.03                     | 0.41              |
| 9:J:59:VAL:O     | 9:J:62:ILE:HG22   | 2.20                     | 0.41              |
| 1:B:320:ARG:NH2  | 14:P:3:C:O2'      | 2.54                     | 0.41              |
| 1:B:63:ARG:HA    | 1:B:74:MET:CE     | 2.51                     | 0.41              |
| 2:C:186:GLU:HB3  | 2:C:187:SER:H     | 1.67                     | 0.41              |
| 2:C:34:ILE:O     | 2:C:35:SER:C      | 2.57                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:282:ILE:HG21 | 2:C:382:ILE:CD1  | 2.51                     | 0.41              |
| 2:C:512:ARG:HG2  | 2:C:512:ARG:HH11 | 1.86                     | 0.41              |
| 2:C:566:LEU:O    | 2:C:567:GLU:C    | 2.59                     | 0.41              |
| 2:C:681:TRP:O    | 2:C:682:SER:C    | 2.59                     | 0.41              |
| 2:C:526:GLU:CB   | 2:C:771:SER:HB3  | 2.51                     | 0.41              |
| 2:C:797:TYR:CE1  | 2:C:854:LEU:HD23 | 2.56                     | 0.41              |
| 2:C:911:ILE:O    | 2:C:912:ILE:HG13 | 2.20                     | 0.41              |
| 3:D:11:ARG:HB3   | 3:D:12:GLU:H     | 1.67                     | 0.41              |
| 3:D:113:VAL:O    | 3:D:143:LEU:HD12 | 2.20                     | 0.41              |
| 3:D:241:ASP:O    | 3:D:244:VAL:HB   | 2.21                     | 0.41              |
| 3:D:260:LEU:O    | 3:D:263:THR:HB   | 2.21                     | 0.41              |
| 5:F:13:TRP:HB2   | 5:F:42:PHE:CE2   | 2.56                     | 0.41              |
| 6:G:114:GLU:HA   | 6:G:114:GLU:OE2  | 2.21                     | 0.41              |
| 10:K:28:ASP:O    | 10:K:29:GLU:C    | 2.58                     | 0.41              |
| 12:M:28:LYS:C    | 12:M:29:TYR:HD2  | 2.23                     | 0.41              |
| 14:P:7:A:H2'     | 14:P:7:A:N3      | 2.35                     | 0.41              |
| 15:T:20:DT:H2''  | 15:T:21:DA:C5'   | 2.47                     | 0.41              |
| 1:B:1068:ALA:HB1 | 1:B:1367:HIS:HA  | 2.02                     | 0.41              |
| 1:B:12:ARG:NE    | 2:C:1192:TYR:HE2 | 2.18                     | 0.41              |
| 1:B:498:ARG:O    | 1:B:501:LEU:N    | 2.54                     | 0.41              |
| 1:B:600:PRO:HG2  | 1:B:601:LYS:N    | 2.31                     | 0.41              |
| 1:B:672:ASP:O    | 1:B:673:GLY:C    | 2.59                     | 0.41              |
| 1:B:919:ILE:O    | 1:B:920:LEU:C    | 2.59                     | 0.41              |
| 2:C:1074:ASN:N   | 2:C:1081:LEU:CD2 | 2.84                     | 0.41              |
| 2:C:308:TRP:HA   | 2:C:311:LEU:HD12 | 2.02                     | 0.41              |
| 2:C:324:ILE:HD13 | 2:C:330:ALA:HA   | 2.02                     | 0.41              |
| 2:C:370:PHE:HD2  | 2:C:373:ARG:HD3  | 1.86                     | 0.41              |
| 2:C:51:PHE:HZ    | 2:C:172:ILE:HA   | 1.86                     | 0.41              |
| 2:C:706:GLN:H    | 2:C:710:LEU:HD12 | 1.85                     | 0.41              |
| 2:C:519:TRP:CZ3  | 2:C:748:ILE:HD13 | 2.56                     | 0.41              |
| 2:C:752:ALA:O    | 2:C:753:ALA:C    | 2.59                     | 0.41              |
| 2:C:802:PRO:HG2  | 2:C:805:THR:CG2  | 2.51                     | 0.41              |
| 2:C:890:TYR:CE2  | 2:C:910:VAL:HG21 | 2.56                     | 0.41              |
| 2:C:95:ILE:CG1   | 2:C:130:VAL:HG22 | 2.50                     | 0.41              |
| 3:D:258:ILE:CD1  | 3:D:258:ILE:N    | 2.84                     | 0.41              |
| 3:D:264:GLN:H    | 3:D:264:GLN:HG3  | 1.51                     | 0.41              |
| 4:E:156:ASP:HB3  | 4:E:158:GLU:H    | 1.86                     | 0.41              |
| 4:E:214:LEU:O    | 4:E:218:GLU:HB2  | 2.21                     | 0.41              |
| 4:E:67:ARG:HG2   | 4:E:67:ARG:O     | 2.21                     | 0.41              |
| 8:I:101:ALA:HA   | 8:I:116:TYR:HA   | 2.03                     | 0.41              |
| 8:I:61:SER:O     | 8:I:62:SER:HB2   | 2.21                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:J:36:GLU:O      | 9:J:37:GLU:O      | 2.38                     | 0.41              |
| 10:K:32:GLU:H     | 10:K:32:GLU:CD    | 2.23                     | 0.41              |
| 10:K:48:ARG:O     | 10:K:49:MET:C     | 2.59                     | 0.41              |
| 11:L:58:PHE:HB3   | 11:L:76:GLN:HE21  | 1.86                     | 0.41              |
| 12:M:54:ARG:HG3   | 12:M:54:ARG:H     | 1.55                     | 0.41              |
| 13:N:2:DA:OP1     | 13:N:2:DA:H4'     | 2.21                     | 0.41              |
| 1:B:447:GLN:NE2   | 15:T:20:DT:H4'    | 2.29                     | 0.41              |
| 1:B:1101:LEU:HD11 | 1:B:1105:LEU:CD1  | 2.49                     | 0.41              |
| 1:B:1114:PRO:CG   | 1:B:1115:SER:H    | 2.34                     | 0.41              |
| 1:B:1068:ALA:HA   | 1:B:1367:HIS:ND1  | 2.36                     | 0.41              |
| 1:B:22:PHE:HE2    | 1:B:30:ILE:HD12   | 1.84                     | 0.41              |
| 1:B:384:ASN:O     | 1:B:386:ASP:N     | 2.53                     | 0.41              |
| 1:B:464:PRO:O     | 1:B:465:TYR:HB2   | 2.21                     | 0.41              |
| 1:B:503:GLN:HE21  | 6:G:90:ARG:NH2    | 2.17                     | 0.41              |
| 1:B:72:GLU:OE2    | 2:C:1175:LEU:HD12 | 2.20                     | 0.41              |
| 1:B:850:VAL:HG21  | 1:B:1058:VAL:HG11 | 2.03                     | 0.41              |
| 2:C:1064:TYR:O    | 2:C:1065:GLN:C    | 2.58                     | 0.41              |
| 2:C:287:ARG:C     | 2:C:289:LEU:N     | 2.74                     | 0.41              |
| 2:C:303:TYR:N     | 2:C:303:TYR:CD2   | 2.88                     | 0.41              |
| 2:C:38:PHE:CD2    | 2:C:43:LEU:HD23   | 2.56                     | 0.41              |
| 2:C:523:CYS:SG    | 2:C:524:PRO:HD2   | 2.61                     | 0.41              |
| 2:C:589:VAL:CG1   | 2:C:590:HIS:H     | 2.28                     | 0.41              |
| 2:C:784:ASN:O     | 2:C:788:ARG:HG3   | 2.21                     | 0.41              |
| 2:C:910:VAL:C     | 2:C:911:ILE:HG13  | 2.42                     | 0.41              |
| 3:D:98:VAL:O      | 3:D:99:LEU:HD23   | 2.20                     | 0.41              |
| 5:F:84:ASP:O      | 5:F:86:PRO:HD3    | 2.21                     | 0.41              |
| 6:G:81:THR:HG23   | 6:G:144:GLU:CD    | 2.42                     | 0.41              |
| 6:G:81:THR:HG23   | 6:G:144:GLU:OE2   | 2.21                     | 0.41              |
| 12:M:30:ILE:CG2   | 12:M:31:CYS:N     | 2.84                     | 0.41              |
| 15:T:14:DC:H2"    | 15:T:15:DT:C7     | 2.46                     | 0.41              |
| 1:B:1151:GLU:HB3  | 1:B:1153:TYR:HE1  | 1.86                     | 0.41              |
| 1:B:265:LYS:HG3   | 1:B:303:TYR:HB2   | 2.02                     | 0.41              |
| 1:B:316:GLN:O     | 1:B:318:SER:N     | 2.54                     | 0.41              |
| 2:C:1069:PHE:N    | 2:C:1069:PHE:HD1  | 2.04                     | 0.41              |
| 2:C:1104:HIS:CG   | 2:C:1122:ARG:HB2  | 2.56                     | 0.41              |
| 2:C:281:PRO:HB3   | 2:C:320:ASP:OD2   | 2.21                     | 0.41              |
| 2:C:466:TRP:HA    | 2:C:466:TRP:CE3   | 2.55                     | 0.41              |
| 2:C:469:GLN:HB2   | 2:C:470:LYS:H     | 1.60                     | 0.41              |
| 2:C:882:THR:HG21  | 2:C:935:ARG:HA    | 2.02                     | 0.41              |
| 4:E:137:ASN:HD22  | 4:E:137:ASN:N     | 2.19                     | 0.41              |
| 7:H:79:PHE:CE2    | 7:H:105:PRO:HD2   | 2.55                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:H:13:LEU:HD22  | 7:H:14:HIS:O      | 2.20                     | 0.41              |
| 7:H:59:GLY:CA    | 7:H:70:PHE:CD2    | 3.00                     | 0.41              |
| 10:K:10:CYS:SG   | 10:K:11:GLY:N     | 2.94                     | 0.41              |
| 10:K:44:TYR:CA   | 10:K:47:ARG:HB2   | 2.39                     | 0.41              |
| 11:L:102:LYS:O   | 11:L:106:GLU:HG3  | 2.21                     | 0.41              |
| 12:M:33:GLU:C    | 12:M:35:SER:H     | 2.24                     | 0.41              |
| 1:B:332:LYS:NZ   | 15:T:19:DT:OP2    | 2.51                     | 0.41              |
| 1:B:1147:THR:HB  | 9:J:48:LEU:HD12   | 2.03                     | 0.41              |
| 1:B:1306:LEU:HA  | 1:B:1306:LEU:HD23 | 1.83                     | 0.41              |
| 1:B:1392:SER:O   | 1:B:1394:THR:N    | 2.53                     | 0.41              |
| 1:B:1409:LEU:CD1 | 2:C:1207:LEU:HD11 | 2.50                     | 0.41              |
| 1:B:196:GLU:CG   | 1:B:197:PRO:HD2   | 2.40                     | 0.41              |
| 1:B:289:ILE:HG22 | 1:B:290:GLU:N     | 2.36                     | 0.41              |
| 2:C:273:LEU:HB2  | 2:C:276:ILE:CG1   | 2.51                     | 0.41              |
| 2:C:899:ILE:CG1  | 2:C:911:ILE:HA    | 2.51                     | 0.41              |
| 3:D:52:GLU:HA    | 12:M:64:LEU:CD2   | 2.50                     | 0.41              |
| 4:E:137:ASN:H    | 4:E:137:ASN:HD22  | 1.69                     | 0.41              |
| 4:E:75:LYS:O     | 4:E:76:LYS:HB2    | 2.21                     | 0.41              |
| 1:B:560:ILE:HG13 | 8:I:79:TRP:H      | 1.85                     | 0.41              |
| 10:K:47:ARG:NH1  | 10:K:47:ARG:HG2   | 2.36                     | 0.41              |
| 10:K:41:LEU:HD11 | 10:K:50:ILE:HG13  | 2.03                     | 0.41              |
| 2:C:815:ARG:O    | 10:K:54:VAL:HG21  | 2.20                     | 0.41              |
| 11:L:76:GLN:HG2  | 11:L:77:THR:N     | 2.35                     | 0.41              |
| 12:M:70:ARG:NH1  | 12:M:70:ARG:HG2   | 2.36                     | 0.41              |
| 1:B:1127:ASP:O   | 1:B:1130:GLN:N    | 2.54                     | 0.40              |
| 1:B:506:ALA:O    | 1:B:509:LEU:HB2   | 2.21                     | 0.40              |
| 1:B:719:VAL:O    | 1:B:721:PHE:N     | 2.54                     | 0.40              |
| 1:B:767:GLN:NE2  | 1:B:798:GLY:O     | 2.54                     | 0.40              |
| 1:B:808:LEU:HD23 | 1:B:813:PHE:CA    | 2.51                     | 0.40              |
| 1:B:870:GLU:HG2  | 5:F:208:TYR:CD1   | 2.56                     | 0.40              |
| 1:B:973:ILE:HD11 | 1:B:1038:THR:H    | 1.86                     | 0.40              |
| 2:C:287:ARG:C    | 2:C:289:LEU:H     | 2.24                     | 0.40              |
| 2:C:69:LEU:HD13  | 2:C:429:PHE:CD1   | 2.57                     | 0.40              |
| 2:C:498:THR:HG22 | 2:C:537:LYS:N     | 2.36                     | 0.40              |
| 2:C:592:ASN:OD1  | 2:C:595:ARG:HG3   | 2.20                     | 0.40              |
| 3:D:100:THR:HB   | 3:D:119:VAL:HB    | 2.03                     | 0.40              |
| 4:E:63:LEU:O     | 4:E:129:LEU:HD11  | 2.21                     | 0.40              |
| 9:J:10:CYS:SG    | 9:J:31:THR:HB     | 2.62                     | 0.40              |
| 9:J:35:VAL:CG1   | 9:J:36:GLU:N      | 2.83                     | 0.40              |
| 11:L:44:ASN:N    | 11:L:61:TYR:CE1   | 2.89                     | 0.40              |
| 11:L:58:PHE:CE2  | 11:L:74:ARG:NE    | 2.77                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:998:LEU:HD22  | 1:B:1001:ARG:HG3  | 2.04                     | 0.40              |
| 1:B:1226:VAL:HG12 | 1:B:1227:ILE:N    | 2.36                     | 0.40              |
| 1:B:1376:THR:CG2  | 1:B:1377:THR:N    | 2.84                     | 0.40              |
| 1:B:218:ASP:O     | 1:B:219:PHE:O     | 2.39                     | 0.40              |
| 1:B:282:ASN:O     | 1:B:284:ALA:N     | 2.55                     | 0.40              |
| 1:B:426:LEU:HD13  | 1:B:432:VAL:HG21  | 2.03                     | 0.40              |
| 1:B:608:ILE:O     | 1:B:610:GLY:N     | 2.55                     | 0.40              |
| 1:B:6:TYR:CD1     | 1:B:6:TYR:C       | 2.93                     | 0.40              |
| 1:B:853:ASP:OD1   | 1:B:855:THR:CG2   | 2.70                     | 0.40              |
| 1:B:956:LEU:HD23  | 1:B:956:LEU:HA    | 1.79                     | 0.40              |
| 1:B:964:ILE:HG22  | 1:B:965:GLN:N     | 2.36                     | 0.40              |
| 2:C:1223:ASP:O    | 2:C:1224:PHE:HB2  | 2.21                     | 0.40              |
| 2:C:165:VAL:HG11  | 2:C:448:ILE:CD1   | 2.50                     | 0.40              |
| 2:C:118:ARG:CG    | 2:C:204:ILE:HD13  | 2.49                     | 0.40              |
| 2:C:472:ALA:C     | 2:C:474:SER:H     | 2.24                     | 0.40              |
| 2:C:515:HIS:CD2   | 2:C:516:ASN:N     | 2.90                     | 0.40              |
| 2:C:877:PRO:C     | 2:C:878:GLN:HG3   | 2.42                     | 0.40              |
| 2:C:899:ILE:CG2   | 2:C:903:VAL:HG21  | 2.52                     | 0.40              |
| 4:E:51:ASN:ND2    | 4:E:54:GLU:OE2    | 2.53                     | 0.40              |
| 1:B:1442:ASP:HB2  | 6:G:135:ARG:HB3   | 2.04                     | 0.40              |
| 8:I:98:TYR:C      | 8:I:118:PHE:HD2   | 2.24                     | 0.40              |
| 8:I:92:ASP:C      | 8:I:93:TYR:CD1    | 2.94                     | 0.40              |
| 9:J:98:VAL:HG12   | 9:J:111:THR:HG22  | 2.03                     | 0.40              |
| 1:B:466:SER:CB    | 11:L:2:ASN:ND2    | 2.82                     | 0.40              |
| 1:B:112:LYS:HG2   | 1:B:113:LEU:N     | 2.36                     | 0.40              |
| 1:B:1341:ILE:O    | 1:B:1344:GLY:N    | 2.54                     | 0.40              |
| 1:B:1389:PHE:C    | 1:B:1389:PHE:CD1  | 2.94                     | 0.40              |
| 1:B:269:ILE:HG23  | 1:B:300:VAL:HG22  | 2.03                     | 0.40              |
| 1:B:534:LEU:HD13  | 1:B:656:TRP:CG    | 2.56                     | 0.40              |
| 1:B:685:GLU:HG3   | 1:B:686:ALA:N     | 2.35                     | 0.40              |
| 1:B:784:LEU:HB3   | 1:B:785:PRO:HD2   | 2.02                     | 0.40              |
| 1:B:848:ILE:HB    | 1:B:1065:GLY:HA3  | 2.03                     | 0.40              |
| 1:B:661:GLY:HA3   | 2:C:1081:LEU:HD12 | 2.03                     | 0.40              |
| 2:C:31:TRP:HA     | 2:C:31:TRP:CE3    | 2.55                     | 0.40              |
| 2:C:487:THR:O     | 2:C:488:TYR:C     | 2.59                     | 0.40              |
| 2:C:899:ILE:HD11  | 2:C:910:VAL:O     | 2.21                     | 0.40              |
| 2:C:975:GLN:HG2   | 2:C:976:ILE:H     | 1.86                     | 0.40              |
| 3:D:66:ARG:NH2    | 10:K:5:VAL:HG23   | 2.36                     | 0.40              |
| 4:E:151:PHE:CD1   | 4:E:151:PHE:N     | 2.89                     | 0.40              |
| 4:E:191:ALA:O     | 4:E:193:THR:N     | 2.55                     | 0.40              |
| 6:G:103:MET:O     | 6:G:104:ASN:HB2   | 2.22                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:G:143:PHE:CD1   | 6:G:143:PHE:N     | 2.88                     | 0.40              |
| 8:I:104:PHE:CZ    | 8:I:136:LYS:HG2   | 2.56                     | 0.40              |
| 10:K:13:VAL:C     | 10:K:14:VAL:HG23  | 2.41                     | 0.40              |
| 14:P:5:C:H2'      | 14:P:6:A:H8       | 1.85                     | 0.40              |
| 1:B:1260:LEU:HD12 | 1:B:1260:LEU:C    | 2.42                     | 0.40              |
| 1:B:231:PRO:C     | 1:B:233:TRP:H     | 2.25                     | 0.40              |
| 1:B:523:ILE:CD1   | 1:B:649:ILE:HG21  | 2.51                     | 0.40              |
| 2:C:1115:THR:HG22 | 2:C:1117:GLN:CG   | 2.51                     | 0.40              |
| 2:C:1221:SER:O    | 2:C:1223:ASP:N    | 2.55                     | 0.40              |
| 2:C:308:TRP:O     | 2:C:312:GLU:N     | 2.46                     | 0.40              |
| 2:C:458:LYS:O     | 2:C:459:TYR:C     | 2.60                     | 0.40              |
| 2:C:460:ALA:O     | 2:C:462:ALA:N     | 2.47                     | 0.40              |
| 2:C:611:PRO:HB3   | 2:C:685:LEU:HD11  | 2.03                     | 0.40              |
| 2:C:540:SER:HB3   | 2:C:747:MET:O     | 2.21                     | 0.40              |
| 2:C:999:MET:HG2   | 2:C:1007:VAL:CG2  | 2.52                     | 0.40              |
| 3:D:131:HIS:HA    | 3:D:132:PRO:HD3   | 1.78                     | 0.40              |
| 4:E:141:LEU:HD12  | 4:E:145:MET:HG2   | 2.03                     | 0.40              |
| 4:E:40:HIS:CE1    | 4:E:41:GLN:CG     | 3.04                     | 0.40              |
| 5:F:117:THR:C     | 5:F:119:SER:H     | 2.23                     | 0.40              |
| 5:F:11:ARG:O      | 5:F:13:TRP:N      | 2.54                     | 0.40              |
| 5:F:147:HIS:CD2   | 5:F:149:LEU:HB2   | 2.52                     | 0.40              |
| 6:G:82:THR:HA     | 6:G:83:PRO:HD3    | 1.79                     | 0.40              |
| 8:I:128:ASN:CG    | 8:I:128:ASN:O     | 2.59                     | 0.40              |
| 8:I:63:LEU:C      | 8:I:90:ALA:CB     | 2.86                     | 0.40              |
| 1:B:1010:ALA:O    | 1:B:1013:ASP:HB2  | 2.20                     | 0.40              |
| 1:B:1019:CYS:O    | 1:B:1020:CYS:C    | 2.59                     | 0.40              |
| 1:B:1140:HIS:CE1  | 1:B:1272:THR:HG23 | 2.56                     | 0.40              |
| 1:B:1317:MET:C    | 1:B:1319:VAL:H    | 2.24                     | 0.40              |
| 1:B:376:TYR:CD2   | 1:B:376:TYR:C     | 2.95                     | 0.40              |
| 1:B:666:ILE:HG12  | 2:C:1030:LEU:HD22 | 2.04                     | 0.40              |
| 1:B:735:VAL:HG12  | 1:B:735:VAL:O     | 2.21                     | 0.40              |
| 1:B:754:SER:N     | 1:B:757:ASN:HD22  | 2.00                     | 0.40              |
| 1:B:767:GLN:HE21  | 1:B:774:ARG:HB3   | 1.79                     | 0.40              |
| 1:B:844:ALA:C     | 1:B:845:LEU:HD23  | 2.41                     | 0.40              |
| 1:B:874:ASP:C     | 1:B:874:ASP:OD1   | 2.60                     | 0.40              |
| 2:C:193:LYS:HD3   | 2:C:787:VAL:HG11  | 2.03                     | 0.40              |
| 2:C:237:VAL:HG12  | 2:C:238:ALA:N     | 2.36                     | 0.40              |
| 2:C:293:PRO:HG2   | 2:C:296:GLU:CB    | 2.51                     | 0.40              |
| 2:C:416:LEU:HD11  | 2:C:466:TRP:CZ2   | 2.57                     | 0.40              |
| 2:C:882:THR:HG22  | 2:C:884:ARG:CB    | 2.50                     | 0.40              |
| 4:E:12:ARG:NH1    | 4:E:14:ARG:HG3    | 2.36                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:F:16:PHE:O     | 5:F:17:ARG:C     | 2.59                     | 0.40              |
| 6:G:89:GLU:HB3   | 6:G:134:ILE:HD13 | 2.03                     | 0.40              |
| 7:H:114:LEU:HD23 | 7:H:161:GLY:C    | 2.41                     | 0.40              |
| 7:H:88:ASP:CB    | 7:H:144:ARG:HA   | 2.44                     | 0.40              |
| 8:I:24:CYS:CB    | 8:I:44:VAL:HG21  | 2.48                     | 0.40              |
| 9:J:34:TYR:C     | 9:J:35:VAL:HG23  | 2.42                     | 0.40              |
| 9:J:61:ASP:C     | 9:J:63:GLY:H     | 2.24                     | 0.40              |
| 9:J:7:CYS:C      | 9:J:8:ARG:O      | 2.57                     | 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   | B     | 1406/1733 (81%) | 965 (69%)  | 284 (20%) | 157 (11%) | 0           | 9  |
| 2   | C     | 1090/1224 (89%) | 719 (66%)  | 243 (22%) | 128 (12%) | 0           | 8  |
| 3   | D     | 264/318 (83%)   | 163 (62%)  | 70 (26%)  | 31 (12%)  | 0           | 8  |
| 4   | E     | 173/221 (78%)   | 107 (62%)  | 43 (25%)  | 23 (13%)  | 0           | 5  |
| 5   | F     | 212/215 (99%)   | 154 (73%)  | 36 (17%)  | 22 (10%)  | 0           | 10 |
| 6   | G     | 82/155 (53%)    | 62 (76%)   | 13 (16%)  | 7 (8%)    | 1           | 15 |
| 7   | H     | 169/171 (99%)   | 129 (76%)  | 26 (15%)  | 14 (8%)   | 1           | 16 |
| 8   | I     | 129/146 (88%)   | 79 (61%)   | 30 (23%)  | 20 (16%)  | 0           | 4  |
| 9   | J     | 117/122 (96%)   | 80 (68%)   | 24 (20%)  | 13 (11%)  | 0           | 9  |
| 10  | K     | 63/70 (90%)     | 38 (60%)   | 12 (19%)  | 13 (21%)  | 0           | 2  |
| 11  | L     | 112/120 (93%)   | 81 (72%)   | 24 (21%)  | 7 (6%)    | 1           | 24 |
| 12  | M     | 44/70 (63%)     | 22 (50%)   | 8 (18%)   | 14 (32%)  | 0           | 0  |
| All | All   | 3861/4565 (85%) | 2599 (67%) | 813 (21%) | 449 (12%) | 0           | 8  |

All (449) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 4    | GLN  |
| 1   | B     | 41   | MET  |
| 1   | B     | 48   | ALA  |
| 1   | B     | 54   | ASN  |
| 1   | B     | 57   | ARG  |
| 1   | B     | 62   | ASP  |
| 1   | B     | 67   | CYS  |
| 1   | B     | 93   | VAL  |
| 1   | B     | 130  | ASP  |
| 1   | B     | 149  | GLU  |
| 1   | B     | 154  | SER  |
| 1   | B     | 223  | GLY  |
| 1   | B     | 245  | PRO  |
| 1   | B     | 250  | ILE  |
| 1   | B     | 286  | HIS  |
| 1   | B     | 311  | GLN  |
| 1   | B     | 312  | PRO  |
| 1   | B     | 318  | SER  |
| 1   | B     | 322  | VAL  |
| 1   | B     | 331  | GLY  |
| 1   | B     | 332  | LYS  |
| 1   | B     | 335  | ARG  |
| 1   | B     | 336  | ILE  |
| 1   | B     | 409  | SER  |
| 1   | B     | 419  | LYS  |
| 1   | B     | 536  | LEU  |
| 1   | B     | 543  | LEU  |
| 1   | B     | 567  | LYS  |
| 1   | B     | 752  | LYS  |
| 1   | B     | 755  | PHE  |
| 1   | B     | 765  | VAL  |
| 1   | B     | 780  | VAL  |
| 1   | B     | 789  | LYS  |
| 1   | B     | 980  | ASP  |
| 1   | B     | 986  | ILE  |
| 1   | B     | 995  | GLU  |
| 1   | B     | 1002 | GLY  |
| 1   | B     | 1016 | THR  |
| 1   | B     | 1114 | PRO  |
| 1   | B     | 1115 | SER  |
| 1   | B     | 1120 | LEU  |
| 1   | B     | 1124 | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 1212 | VAL  |
| 1   | B     | 1223 | ASP  |
| 1   | B     | 1231 | ASP  |
| 1   | B     | 1242 | VAL  |
| 1   | B     | 1255 | GLU  |
| 1   | B     | 1261 | LYS  |
| 1   | B     | 1341 | ILE  |
| 1   | B     | 1365 | TYR  |
| 1   | B     | 1377 | THR  |
| 1   | B     | 1378 | GLN  |
| 1   | B     | 1393 | ASN  |
| 2   | C     | 21   | GLU  |
| 2   | C     | 45   | SER  |
| 2   | C     | 46   | GLN  |
| 2   | C     | 108  | VAL  |
| 2   | C     | 186  | GLU  |
| 2   | C     | 367  | LEU  |
| 2   | C     | 401  | PHE  |
| 2   | C     | 448  | ILE  |
| 2   | C     | 470  | LYS  |
| 2   | C     | 472  | ALA  |
| 2   | C     | 509  | ALA  |
| 2   | C     | 510  | LYS  |
| 2   | C     | 591  | ARG  |
| 2   | C     | 708  | GLU  |
| 2   | C     | 709  | ASP  |
| 2   | C     | 731  | VAL  |
| 2   | C     | 751  | VAL  |
| 2   | C     | 826  | ALA  |
| 2   | C     | 907  | GLY  |
| 2   | C     | 909  | ASP  |
| 2   | C     | 943  | SER  |
| 2   | C     | 1003 | ALA  |
| 2   | C     | 1006 | ILE  |
| 2   | C     | 1011 | ILE  |
| 2   | C     | 1045 | SER  |
| 2   | C     | 1046 | PRO  |
| 2   | C     | 1156 | ASP  |
| 2   | C     | 1171 | VAL  |
| 2   | C     | 1175 | LEU  |
| 2   | C     | 1181 | GLU  |
| 2   | C     | 1182 | CYS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | C     | 1183 | LYS  |
| 3   | D     | 81   | GLU  |
| 3   | D     | 117  | ASP  |
| 3   | D     | 149  | LYS  |
| 3   | D     | 156  | THR  |
| 3   | D     | 175  | ALA  |
| 3   | D     | 184  | ASN  |
| 3   | D     | 209  | TYR  |
| 4   | E     | 9    | GLN  |
| 4   | E     | 19   | GLU  |
| 4   | E     | 21   | GLU  |
| 4   | E     | 31   | GLN  |
| 4   | E     | 169  | SER  |
| 4   | E     | 173  | HIS  |
| 4   | E     | 174  | PRO  |
| 4   | E     | 199  | ASN  |
| 4   | E     | 218  | GLU  |
| 4   | E     | 220  | LEU  |
| 5   | F     | 43   | LYS  |
| 5   | F     | 44   | ALA  |
| 5   | F     | 48   | ASP  |
| 5   | F     | 59   | SER  |
| 5   | F     | 73   | PRO  |
| 5   | F     | 129  | PRO  |
| 5   | F     | 192  | ARG  |
| 5   | F     | 206  | GLY  |
| 6   | G     | 73   | ALA  |
| 7   | H     | 66   | GLY  |
| 7   | H     | 154  | VAL  |
| 8   | I     | 17   | PRO  |
| 8   | I     | 77   | ARG  |
| 8   | I     | 78   | SER  |
| 8   | I     | 81   | PRO  |
| 8   | I     | 84   | ALA  |
| 8   | I     | 108  | SER  |
| 8   | I     | 128  | ASN  |
| 8   | I     | 140  | ALA  |
| 9   | J     | 11   | ASN  |
| 9   | J     | 37   | GLU  |
| 9   | J     | 106  | CYS  |
| 10  | K     | 6    | ARG  |
| 10  | K     | 32   | GLU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 10  | K     | 64   | ASN  |
| 11  | L     | 29   | ASN  |
| 12  | M     | 35   | SER  |
| 12  | M     | 37   | LYS  |
| 12  | M     | 50   | ASP  |
| 12  | M     | 53   | HIS  |
| 12  | M     | 55   | ILE  |
| 12  | M     | 59   | ALA  |
| 12  | M     | 60   | ARG  |
| 1   | B     | 42   | ASP  |
| 1   | B     | 44   | THR  |
| 1   | B     | 51   | GLY  |
| 1   | B     | 58   | LEU  |
| 1   | B     | 66   | LYS  |
| 1   | B     | 70   | CYS  |
| 1   | B     | 73   | GLY  |
| 1   | B     | 76   | GLU  |
| 1   | B     | 167  | CYS  |
| 1   | B     | 257  | ARG  |
| 1   | B     | 283  | GLY  |
| 1   | B     | 303  | TYR  |
| 1   | B     | 317  | LYS  |
| 1   | B     | 410  | GLY  |
| 1   | B     | 415  | LEU  |
| 1   | B     | 666  | ILE  |
| 1   | B     | 718  | VAL  |
| 1   | B     | 719  | VAL  |
| 1   | B     | 829  | VAL  |
| 1   | B     | 846  | GLU  |
| 1   | B     | 847  | ASP  |
| 1   | B     | 871  | ASP  |
| 1   | B     | 968  | GLN  |
| 1   | B     | 979  | SER  |
| 1   | B     | 1050 | GLU  |
| 1   | B     | 1064 | VAL  |
| 1   | B     | 1116 | LEU  |
| 1   | B     | 1221 | LYS  |
| 1   | B     | 1314 | SER  |
| 1   | B     | 1335 | ILE  |
| 1   | B     | 1366 | ARG  |
| 1   | B     | 1405 | THR  |
| 1   | B     | 1438 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | C     | 184  | ALA  |
| 2   | C     | 206  | ASN  |
| 2   | C     | 229  | ALA  |
| 2   | C     | 260  | GLY  |
| 2   | C     | 304  | ASP  |
| 2   | C     | 305  | VAL  |
| 2   | C     | 365  | THR  |
| 2   | C     | 368  | GLU  |
| 2   | C     | 369  | GLY  |
| 2   | C     | 389  | ALA  |
| 2   | C     | 450  | ALA  |
| 2   | C     | 460  | ALA  |
| 2   | C     | 466  | TRP  |
| 2   | C     | 467  | GLY  |
| 2   | C     | 471  | LYS  |
| 2   | C     | 480  | SER  |
| 2   | C     | 511  | PRO  |
| 2   | C     | 543  | SER  |
| 2   | C     | 643  | ASP  |
| 2   | C     | 655  | LYS  |
| 2   | C     | 688  | GLY  |
| 2   | C     | 728  | ARG  |
| 2   | C     | 734  | HIS  |
| 2   | C     | 746  | SER  |
| 2   | C     | 825  | VAL  |
| 2   | C     | 827  | ILE  |
| 2   | C     | 883  | LEU  |
| 2   | C     | 1041 | GLU  |
| 2   | C     | 1082 | MET  |
| 2   | C     | 1096 | ARG  |
| 2   | C     | 1108 | ARG  |
| 2   | C     | 1112 | GLN  |
| 2   | C     | 1126 | GLY  |
| 2   | C     | 1155 | SER  |
| 2   | C     | 1167 | GLY  |
| 2   | C     | 1186 | ASP  |
| 2   | C     | 1188 | LYS  |
| 3   | D     | 94   | LYS  |
| 3   | D     | 110  | THR  |
| 3   | D     | 133  | ILE  |
| 3   | D     | 161  | LYS  |
| 3   | D     | 214  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | E     | 20  | GLU  |
| 4   | E     | 52  | LEU  |
| 5   | F     | 74  | ASP  |
| 5   | F     | 76  | GLY  |
| 5   | F     | 106 | GLN  |
| 5   | F     | 121 | MET  |
| 5   | F     | 174 | GLN  |
| 7   | H     | 17  | PHE  |
| 7   | H     | 64  | THR  |
| 7   | H     | 118 | ASP  |
| 7   | H     | 140 | LYS  |
| 8   | I     | 12  | VAL  |
| 8   | I     | 60  | ALA  |
| 8   | I     | 82  | PRO  |
| 8   | I     | 90  | ALA  |
| 8   | I     | 134 | ASN  |
| 8   | I     | 139 | ASN  |
| 9   | J     | 3   | THR  |
| 9   | J     | 8   | ARG  |
| 9   | J     | 33  | SER  |
| 9   | J     | 47  | GLU  |
| 9   | J     | 58  | VAL  |
| 9   | J     | 79  | HIS  |
| 10  | K     | 2   | ILE  |
| 10  | K     | 17  | LYS  |
| 10  | K     | 24  | LEU  |
| 10  | K     | 27  | GLU  |
| 10  | K     | 28  | ASP  |
| 10  | K     | 29  | GLU  |
| 10  | K     | 39  | LEU  |
| 11  | L     | 7   | PHE  |
| 11  | L     | 14  | GLU  |
| 11  | L     | 15  | GLY  |
| 1   | B     | 3   | GLY  |
| 1   | B     | 43  | GLU  |
| 1   | B     | 59  | GLY  |
| 1   | B     | 69  | THR  |
| 1   | B     | 131 | SER  |
| 1   | B     | 219 | PHE  |
| 1   | B     | 232 | GLU  |
| 1   | B     | 244 | PRO  |
| 1   | B     | 253 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 361  | LEU  |
| 1   | B     | 399  | HIS  |
| 1   | B     | 526  | ASP  |
| 1   | B     | 591  | PHE  |
| 1   | B     | 639  | PRO  |
| 1   | B     | 706  | HIS  |
| 1   | B     | 720  | ARG  |
| 1   | B     | 922  | ASP  |
| 1   | B     | 997  | LEU  |
| 1   | B     | 1139 | GLU  |
| 1   | B     | 1402 | PHE  |
| 1   | B     | 1448 | GLU  |
| 2   | C     | 219  | ALA  |
| 2   | C     | 266  | ALA  |
| 2   | C     | 295  | GLY  |
| 2   | C     | 427  | ASP  |
| 2   | C     | 430  | ARG  |
| 2   | C     | 613  | VAL  |
| 2   | C     | 711  | GLU  |
| 2   | C     | 712  | PRO  |
| 2   | C     | 792  | MET  |
| 2   | C     | 836  | GLU  |
| 2   | C     | 848  | ARG  |
| 2   | C     | 881  | ASN  |
| 2   | C     | 888  | GLY  |
| 2   | C     | 894  | ASP  |
| 2   | C     | 1018 | PRO  |
| 2   | C     | 1035 | ALA  |
| 2   | C     | 1074 | ASN  |
| 2   | C     | 1075 | GLY  |
| 2   | C     | 1100 | ASP  |
| 2   | C     | 1157 | ALA  |
| 2   | C     | 1176 | ASN  |
| 3   | D     | 60   | ASP  |
| 3   | D     | 95   | CYS  |
| 3   | D     | 138  | GLU  |
| 3   | D     | 148  | ARG  |
| 3   | D     | 240  | VAL  |
| 4   | E     | 8    | PHE  |
| 4   | E     | 131  | GLU  |
| 4   | E     | 139  | LYS  |
| 4   | E     | 198  | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 5   | F     | 3    | GLN  |
| 5   | F     | 50   | MET  |
| 5   | F     | 130  | ALA  |
| 5   | F     | 205  | SER  |
| 7   | H     | 20   | PRO  |
| 7   | H     | 67   | SER  |
| 7   | H     | 96   | GLN  |
| 8   | I     | 120  | GLY  |
| 9   | J     | 34   | TYR  |
| 9   | J     | 78   | CYS  |
| 12  | M     | 54   | ARG  |
| 1   | B     | 128  | ILE  |
| 1   | B     | 220  | THR  |
| 1   | B     | 424  | ILE  |
| 1   | B     | 428  | TYR  |
| 1   | B     | 465  | TYR  |
| 1   | B     | 510  | GLN  |
| 1   | B     | 587  | HIS  |
| 1   | B     | 636  | GLU  |
| 1   | B     | 825  | ILE  |
| 1   | B     | 958  | VAL  |
| 1   | B     | 1013 | ASP  |
| 1   | B     | 1051 | ALA  |
| 1   | B     | 1054 | LEU  |
| 1   | B     | 1105 | LEU  |
| 1   | B     | 1109 | LYS  |
| 1   | B     | 1229 | SER  |
| 1   | B     | 1330 | ASN  |
| 1   | B     | 1390 | ASN  |
| 2   | C     | 56   | ASP  |
| 2   | C     | 94   | LYS  |
| 2   | C     | 115  | GLN  |
| 2   | C     | 198  | ASP  |
| 2   | C     | 282  | ILE  |
| 2   | C     | 394  | ASP  |
| 2   | C     | 402  | GLY  |
| 2   | C     | 436  | VAL  |
| 2   | C     | 461  | LEU  |
| 2   | C     | 465  | ASN  |
| 2   | C     | 605  | ARG  |
| 2   | C     | 879  | ARG  |
| 2   | C     | 978  | ASP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | C     | 1143 | ALA  |
| 3   | D     | 87   | PHE  |
| 3   | D     | 90   | ASP  |
| 3   | D     | 206  | ASN  |
| 3   | D     | 213  | PRO  |
| 4   | E     | 25   | ALA  |
| 4   | E     | 192  | LYS  |
| 4   | E     | 217  | LEU  |
| 5   | F     | 115  | ASN  |
| 5   | F     | 120  | ALA  |
| 5   | F     | 122  | LYS  |
| 6   | G     | 112  | GLU  |
| 6   | G     | 150  | GLU  |
| 7   | H     | 16   | SER  |
| 7   | H     | 50   | ASP  |
| 7   | H     | 139  | ILE  |
| 8   | I     | 52   | GLN  |
| 9   | J     | 9    | ASP  |
| 12  | M     | 26   | THR  |
| 12  | M     | 39   | SER  |
| 12  | M     | 45   | ALA  |
| 12  | M     | 56   | LEU  |
| 1   | B     | 61   | ILE  |
| 1   | B     | 71   | GLN  |
| 1   | B     | 196  | GLU  |
| 1   | B     | 382  | PRO  |
| 1   | B     | 497  | THR  |
| 1   | B     | 661  | GLY  |
| 1   | B     | 775  | ILE  |
| 1   | B     | 821  | ARG  |
| 1   | B     | 972  | HIS  |
| 1   | B     | 1067 | LEU  |
| 1   | B     | 1324 | PRO  |
| 1   | B     | 1379 | GLY  |
| 1   | B     | 1394 | THR  |
| 2   | C     | 261  | ARG  |
| 2   | C     | 283  | VAL  |
| 2   | C     | 577  | ALA  |
| 2   | C     | 684  | LEU  |
| 2   | C     | 764  | SER  |
| 2   | C     | 800  | GLN  |
| 2   | C     | 832  | GLY  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | C     | 946  | ASN  |
| 2   | C     | 982  | SER  |
| 2   | C     | 1097 | HIS  |
| 3   | D     | 9    | LYS  |
| 3   | D     | 132  | PRO  |
| 3   | D     | 173  | ALA  |
| 3   | D     | 208  | GLU  |
| 4   | E     | 32   | GLU  |
| 4   | E     | 155  | ARG  |
| 4   | E     | 168  | LYS  |
| 5   | F     | 40   | GLU  |
| 6   | G     | 111  | LEU  |
| 6   | G     | 139  | PRO  |
| 7   | H     | 128  | PRO  |
| 8   | I     | 32   | THR  |
| 8   | I     | 62   | SER  |
| 8   | I     | 92   | ASP  |
| 8   | I     | 119  | GLY  |
| 9   | J     | 57   | GLY  |
| 10  | K     | 33   | GLY  |
| 11  | L     | 41   | THR  |
| 12  | M     | 40   | LEU  |
| 1   | B     | 321  | PRO  |
| 1   | B     | 400  | PRO  |
| 1   | B     | 759  | ALA  |
| 1   | B     | 975  | HIS  |
| 1   | B     | 1128 | GLN  |
| 2   | C     | 259  | TYR  |
| 2   | C     | 325  | GLN  |
| 2   | C     | 763  | GLN  |
| 2   | C     | 1131 | GLY  |
| 2   | C     | 1165 | ILE  |
| 2   | C     | 1170 | THR  |
| 3   | D     | 142  | VAL  |
| 3   | D     | 217  | ASP  |
| 5   | F     | 104  | ASN  |
| 10  | K     | 14   | VAL  |
| 10  | K     | 57   | ILE  |
| 11  | L     | 53   | ASP  |
| 1   | B     | 492  | PRO  |
| 1   | B     | 546  | VAL  |
| 1   | B     | 673  | GLY  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 916  | GLY  |
| 2   | C     | 524  | PRO  |
| 2   | C     | 1017 | ILE  |
| 3   | D     | 139  | GLY  |
| 3   | D     | 243  | VAL  |
| 6   | G     | 74   | ILE  |
| 6   | G     | 117  | PRO  |
| 7   | H     | 34   | VAL  |
| 11  | L     | 66   | PRO  |
| 1   | B     | 35   | ILE  |
| 1   | B     | 78   | PRO  |
| 1   | B     | 138  | ILE  |
| 1   | B     | 380  | VAL  |
| 1   | B     | 1006 | ILE  |
| 2   | C     | 562  | GLY  |
| 3   | D     | 255  | VAL  |
| 4   | E     | 202  | ILE  |
| 12  | M     | 46   | VAL  |
| 1   | B     | 38   | PRO  |
| 1   | B     | 396  | PRO  |
| 1   | B     | 948  | VAL  |
| 2   | C     | 911  | ILE  |
| 2   | C     | 1214 | PRO  |
| 3   | D     | 70   | ILE  |
| 1   | B     | 1435 | PRO  |
| 2   | C     | 571  | PRO  |
| 2   | C     | 636  | PRO  |
| 2   | C     | 867  | GLY  |
| 1   | B     | 1107 | VAL  |

### 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   | B     | 1239/1520 (82%) | 1113 (90%) | 126 (10%) | 8           | 37 |
| 2   | C     | 962/1061 (91%)  | 867 (90%)  | 95 (10%)  | 9           | 39 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 3   | D     | 234/274 (85%)   | 209 (89%)  | 25 (11%)  | 8           | 36 |
| 4   | E     | 159/200 (80%)   | 136 (86%)  | 23 (14%)  | 4           | 24 |
| 5   | F     | 196/197 (100%)  | 182 (93%)  | 14 (7%)   | 17          | 53 |
| 6   | G     | 74/137 (54%)    | 69 (93%)   | 5 (7%)    | 18          | 55 |
| 7   | H     | 152/152 (100%)  | 136 (90%)  | 16 (10%)  | 8           | 36 |
| 8   | I     | 117/128 (91%)   | 107 (92%)  | 10 (8%)   | 12          | 47 |
| 9   | J     | 113/116 (97%)   | 103 (91%)  | 10 (9%)   | 12          | 44 |
| 10  | K     | 60/65 (92%)     | 54 (90%)   | 6 (10%)   | 9           | 38 |
| 11  | L     | 99/102 (97%)    | 84 (85%)   | 15 (15%)  | 3           | 22 |
| 12  | M     | 40/57 (70%)     | 36 (90%)   | 4 (10%)   | 9           | 38 |
| All | All   | 3445/4009 (86%) | 3096 (90%) | 349 (10%) | 9           | 38 |

All (349) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 18  | GLN  |
| 1   | B     | 22  | PHE  |
| 1   | B     | 34  | LYS  |
| 1   | B     | 37  | PHE  |
| 1   | B     | 41  | MET  |
| 1   | B     | 43  | GLU  |
| 1   | B     | 57  | ARG  |
| 1   | B     | 62  | ASP  |
| 1   | B     | 67  | CYS  |
| 1   | B     | 68  | GLN  |
| 1   | B     | 70  | CYS  |
| 1   | B     | 83  | HIS  |
| 1   | B     | 93  | VAL  |
| 1   | B     | 108 | MET  |
| 1   | B     | 157 | ASP  |
| 1   | B     | 174 | ILE  |
| 1   | B     | 200 | ARG  |
| 1   | B     | 221 | SER  |
| 1   | B     | 245 | PRO  |
| 1   | B     | 261 | ASP  |
| 1   | B     | 265 | LYS  |
| 1   | B     | 270 | LEU  |
| 1   | B     | 282 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 312 | PRO  |
| 1   | B     | 320 | ARG  |
| 1   | B     | 322 | VAL  |
| 1   | B     | 326 | ARG  |
| 1   | B     | 335 | ARG  |
| 1   | B     | 360 | GLU  |
| 1   | B     | 375 | THR  |
| 1   | B     | 379 | VAL  |
| 1   | B     | 381 | THR  |
| 1   | B     | 385 | ILE  |
| 1   | B     | 394 | ASN  |
| 1   | B     | 396 | PRO  |
| 1   | B     | 406 | ILE  |
| 1   | B     | 408 | ASP  |
| 1   | B     | 417 | TYR  |
| 1   | B     | 434 | ARG  |
| 1   | B     | 442 | VAL  |
| 1   | B     | 443 | LEU  |
| 1   | B     | 445 | ASN  |
| 1   | B     | 450 | LEU  |
| 1   | B     | 451 | HIS  |
| 1   | B     | 462 | VAL  |
| 1   | B     | 466 | SER  |
| 1   | B     | 469 | ARG  |
| 1   | B     | 503 | GLN  |
| 1   | B     | 504 | LEU  |
| 1   | B     | 512 | VAL  |
| 1   | B     | 518 | LYS  |
| 1   | B     | 526 | ASP  |
| 1   | B     | 560 | ILE  |
| 1   | B     | 562 | THR  |
| 1   | B     | 590 | ARG  |
| 1   | B     | 616 | VAL  |
| 1   | B     | 618 | GLU  |
| 1   | B     | 629 | LEU  |
| 1   | B     | 635 | ARG  |
| 1   | B     | 642 | CYS  |
| 1   | B     | 657 | LEU  |
| 1   | B     | 664 | THR  |
| 1   | B     | 666 | ILE  |
| 1   | B     | 690 | VAL  |
| 1   | B     | 711 | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 727  | ASP  |
| 1   | B     | 741  | ASN  |
| 1   | B     | 764  | CYS  |
| 1   | B     | 768  | GLN  |
| 1   | B     | 774  | ARG  |
| 1   | B     | 779  | PHE  |
| 1   | B     | 821  | ARG  |
| 1   | B     | 827  | THR  |
| 1   | B     | 852  | TYR  |
| 1   | B     | 858  | ASN  |
| 1   | B     | 890  | ASP  |
| 1   | B     | 903  | ASN  |
| 1   | B     | 904  | THR  |
| 1   | B     | 906  | HIS  |
| 1   | B     | 907  | THR  |
| 1   | B     | 941  | LYS  |
| 1   | B     | 942  | PHE  |
| 1   | B     | 947  | PHE  |
| 1   | B     | 998  | LEU  |
| 1   | B     | 1035 | TYR  |
| 1   | B     | 1037 | LEU  |
| 1   | B     | 1067 | LEU  |
| 1   | B     | 1095 | THR  |
| 1   | B     | 1116 | LEU  |
| 1   | B     | 1120 | LEU  |
| 1   | B     | 1122 | PRO  |
| 1   | B     | 1138 | ILE  |
| 1   | B     | 1146 | VAL  |
| 1   | B     | 1147 | THR  |
| 1   | B     | 1152 | ILE  |
| 1   | B     | 1163 | ILE  |
| 1   | B     | 1170 | ILE  |
| 1   | B     | 1173 | HIS  |
| 1   | B     | 1194 | ARG  |
| 1   | B     | 1206 | ASP  |
| 1   | B     | 1240 | CYS  |
| 1   | B     | 1264 | GLU  |
| 1   | B     | 1271 | ILE  |
| 1   | B     | 1291 | VAL  |
| 1   | B     | 1295 | THR  |
| 1   | B     | 1298 | TYR  |
| 1   | B     | 1309 | ASP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 1332 | PHE  |
| 1   | B     | 1333 | ILE  |
| 1   | B     | 1351 | GLU  |
| 1   | B     | 1359 | ASP  |
| 1   | B     | 1366 | ARG  |
| 1   | B     | 1372 | VAL  |
| 1   | B     | 1385 | THR  |
| 1   | B     | 1386 | ARG  |
| 1   | B     | 1389 | PHE  |
| 1   | B     | 1391 | ARG  |
| 1   | B     | 1393 | ASN  |
| 1   | B     | 1400 | CYS  |
| 1   | B     | 1405 | THR  |
| 1   | B     | 1425 | SER  |
| 1   | B     | 1428 | VAL  |
| 1   | B     | 1432 | GLN  |
| 1   | B     | 1442 | ASP  |
| 1   | B     | 1444 | MET  |
| 1   | B     | 1445 | ILE  |
| 2   | C     | 20   | ASP  |
| 2   | C     | 25   | ILE  |
| 2   | C     | 44   | VAL  |
| 2   | C     | 57   | TYR  |
| 2   | C     | 61   | ASP  |
| 2   | C     | 63   | ILE  |
| 2   | C     | 98   | THR  |
| 2   | C     | 104  | GLU  |
| 2   | C     | 175  | ARG  |
| 2   | C     | 180  | TYR  |
| 2   | C     | 199  | MET  |
| 2   | C     | 203  | PHE  |
| 2   | C     | 217  | ARG  |
| 2   | C     | 250  | PHE  |
| 2   | C     | 258  | LEU  |
| 2   | C     | 283  | VAL  |
| 2   | C     | 286  | PHE  |
| 2   | C     | 289  | LEU  |
| 2   | C     | 323  | VAL  |
| 2   | C     | 365  | THR  |
| 2   | C     | 371  | GLU  |
| 2   | C     | 378  | LEU  |
| 2   | C     | 385  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | C     | 393 | LYS  |
| 2   | C     | 396 | ASP  |
| 2   | C     | 427 | ASP  |
| 2   | C     | 429 | PHE  |
| 2   | C     | 466 | TRP  |
| 2   | C     | 482 | VAL  |
| 2   | C     | 485 | ARG  |
| 2   | C     | 498 | THR  |
| 2   | C     | 502 | ILE  |
| 2   | C     | 511 | PRO  |
| 2   | C     | 513 | GLN  |
| 2   | C     | 516 | ASN  |
| 2   | C     | 539 | LEU  |
| 2   | C     | 544 | CYS  |
| 2   | C     | 582 | VAL  |
| 2   | C     | 602 | THR  |
| 2   | C     | 603 | LEU  |
| 2   | C     | 615 | MET  |
| 2   | C     | 616 | ILE  |
| 2   | C     | 619 | ILE  |
| 2   | C     | 629 | ASP  |
| 2   | C     | 635 | ARG  |
| 2   | C     | 644 | GLU  |
| 2   | C     | 683 | SER  |
| 2   | C     | 737 | THR  |
| 2   | C     | 742 | GLU  |
| 2   | C     | 748 | ILE  |
| 2   | C     | 755 | ILE  |
| 2   | C     | 790 | ASP  |
| 2   | C     | 797 | TYR  |
| 2   | C     | 807 | ARG  |
| 2   | C     | 811 | TYR  |
| 2   | C     | 830 | TYR  |
| 2   | C     | 833 | TYR  |
| 2   | C     | 835 | GLN  |
| 2   | C     | 837 | ASP  |
| 2   | C     | 839 | MET  |
| 2   | C     | 844 | SER  |
| 2   | C     | 862 | GLN  |
| 2   | C     | 866 | TYR  |
| 2   | C     | 878 | GLN  |
| 2   | C     | 894 | ASP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | C     | 909  | ASP  |
| 2   | C     | 944  | THR  |
| 2   | C     | 953  | LEU  |
| 2   | C     | 978  | ASP  |
| 2   | C     | 999  | MET  |
| 2   | C     | 1002 | THR  |
| 2   | C     | 1010 | LEU  |
| 2   | C     | 1045 | SER  |
| 2   | C     | 1046 | PRO  |
| 2   | C     | 1047 | PHE  |
| 2   | C     | 1060 | ARG  |
| 2   | C     | 1069 | PHE  |
| 2   | C     | 1076 | HIS  |
| 2   | C     | 1077 | THR  |
| 2   | C     | 1084 | GLN  |
| 2   | C     | 1092 | TYR  |
| 2   | C     | 1095 | LEU  |
| 2   | C     | 1098 | MET  |
| 2   | C     | 1108 | ARG  |
| 2   | C     | 1122 | ARG  |
| 2   | C     | 1151 | LEU  |
| 2   | C     | 1159 | ARG  |
| 2   | C     | 1170 | THR  |
| 2   | C     | 1182 | CYS  |
| 2   | C     | 1183 | LYS  |
| 2   | C     | 1185 | CYS  |
| 2   | C     | 1192 | TYR  |
| 2   | C     | 1202 | LEU  |
| 2   | C     | 1212 | ILE  |
| 2   | C     | 1222 | ARG  |
| 3   | D     | 3    | GLU  |
| 3   | D     | 8    | VAL  |
| 3   | D     | 26   | ASP  |
| 3   | D     | 29   | MET  |
| 3   | D     | 58   | LEU  |
| 3   | D     | 62   | PHE  |
| 3   | D     | 74   | SER  |
| 3   | D     | 77   | ILE  |
| 3   | D     | 83   | SER  |
| 3   | D     | 91   | HIS  |
| 3   | D     | 104  | PHE  |
| 3   | D     | 138  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | D     | 140 | ASN  |
| 3   | D     | 147 | LEU  |
| 3   | D     | 148 | ARG  |
| 3   | D     | 163 | ILE  |
| 3   | D     | 170 | TRP  |
| 3   | D     | 190 | ASP  |
| 3   | D     | 193 | TYR  |
| 3   | D     | 209 | TYR  |
| 3   | D     | 226 | ASP  |
| 3   | D     | 228 | PHE  |
| 3   | D     | 235 | VAL  |
| 3   | D     | 240 | VAL  |
| 3   | D     | 266 | ASP  |
| 4   | E     | 5   | THR  |
| 4   | E     | 8   | PHE  |
| 4   | E     | 9   | GLN  |
| 4   | E     | 11  | ARG  |
| 4   | E     | 13  | ARG  |
| 4   | E     | 14  | ARG  |
| 4   | E     | 20  | GLU  |
| 4   | E     | 22  | GLU  |
| 4   | E     | 31  | GLN  |
| 4   | E     | 40  | HIS  |
| 4   | E     | 47  | LEU  |
| 4   | E     | 50  | LEU  |
| 4   | E     | 63  | LEU  |
| 4   | E     | 70  | PHE  |
| 4   | E     | 137 | ASN  |
| 4   | E     | 139 | LYS  |
| 4   | E     | 146 | GLN  |
| 4   | E     | 148 | LEU  |
| 4   | E     | 170 | THR  |
| 4   | E     | 174 | PRO  |
| 4   | E     | 211 | LEU  |
| 4   | E     | 214 | LEU  |
| 4   | E     | 221 | TYR  |
| 5   | F     | 7   | ARG  |
| 5   | F     | 46  | TYR  |
| 5   | F     | 60  | PHE  |
| 5   | F     | 74  | ASP  |
| 5   | F     | 77  | SER  |
| 5   | F     | 82  | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | F     | 92  | THR  |
| 5   | F     | 93  | MET  |
| 5   | F     | 94  | LYS  |
| 5   | F     | 104 | ASN  |
| 5   | F     | 114 | ASN  |
| 5   | F     | 132 | ILE  |
| 5   | F     | 198 | ILE  |
| 5   | F     | 207 | ARG  |
| 6   | G     | 74  | ILE  |
| 6   | G     | 90  | ARG  |
| 6   | G     | 107 | VAL  |
| 6   | G     | 111 | LEU  |
| 6   | G     | 143 | PHE  |
| 7   | H     | 1   | MET  |
| 7   | H     | 7   | LEU  |
| 7   | H     | 11  | ILE  |
| 7   | H     | 13  | LEU  |
| 7   | H     | 45  | ILE  |
| 7   | H     | 49  | LEU  |
| 7   | H     | 56  | ILE  |
| 7   | H     | 74  | TYR  |
| 7   | H     | 77  | VAL  |
| 7   | H     | 79  | PHE  |
| 7   | H     | 80  | LYS  |
| 7   | H     | 88  | ASP  |
| 7   | H     | 140 | LYS  |
| 7   | H     | 152 | SER  |
| 7   | H     | 165 | GLU  |
| 7   | H     | 171 | ILE  |
| 8   | I     | 7   | ASP  |
| 8   | I     | 10  | PHE  |
| 8   | I     | 17  | PRO  |
| 8   | I     | 26  | ILE  |
| 8   | I     | 95  | TYR  |
| 8   | I     | 96  | VAL  |
| 8   | I     | 102 | TYR  |
| 8   | I     | 106 | GLU  |
| 8   | I     | 110 | ASP  |
| 8   | I     | 130 | ARG  |
| 9   | J     | 8   | ARG  |
| 9   | J     | 9   | ASP  |
| 9   | J     | 15  | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | J     | 31  | THR  |
| 9   | J     | 52  | ILE  |
| 9   | J     | 59  | VAL  |
| 9   | J     | 85  | PHE  |
| 9   | J     | 86  | PHE  |
| 9   | J     | 99  | LEU  |
| 9   | J     | 100 | PHE  |
| 10  | K     | 16  | ASP  |
| 10  | K     | 19  | GLU  |
| 10  | K     | 28  | ASP  |
| 10  | K     | 43  | ARG  |
| 10  | K     | 44  | TYR  |
| 10  | K     | 48  | ARG  |
| 11  | L     | 7   | PHE  |
| 11  | L     | 10  | PHE  |
| 11  | L     | 12  | LEU  |
| 11  | L     | 47  | ARG  |
| 11  | L     | 50  | LEU  |
| 11  | L     | 61  | TYR  |
| 11  | L     | 65  | HIS  |
| 11  | L     | 68  | PHE  |
| 11  | L     | 78  | THR  |
| 11  | L     | 81  | TYR  |
| 11  | L     | 89  | ASN  |
| 11  | L     | 102 | LYS  |
| 11  | L     | 111 | LEU  |
| 11  | L     | 113 | THR  |
| 11  | L     | 114 | LEU  |
| 12  | M     | 44  | ASP  |
| 12  | M     | 54  | ARG  |
| 12  | M     | 55  | ILE  |
| 12  | M     | 70  | ARG  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (106) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 54  | ASN  |
| 1   | B     | 64  | ASN  |
| 1   | B     | 68  | GLN  |
| 1   | B     | 71  | GLN  |
| 1   | B     | 169 | ASN  |
| 1   | B     | 171 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 225  | ASN  |
| 1   | B     | 256  | GLN  |
| 1   | B     | 297  | GLN  |
| 1   | B     | 339  | ASN  |
| 1   | B     | 358  | ASN  |
| 1   | B     | 394  | ASN  |
| 1   | B     | 435  | HIS  |
| 1   | B     | 493  | GLN  |
| 1   | B     | 603  | ASN  |
| 1   | B     | 654  | ASN  |
| 1   | B     | 698  | GLN  |
| 1   | B     | 723  | ASN  |
| 1   | B     | 736  | ASN  |
| 1   | B     | 741  | ASN  |
| 1   | B     | 757  | ASN  |
| 1   | B     | 760  | GLN  |
| 1   | B     | 786  | HIS  |
| 1   | B     | 858  | ASN  |
| 1   | B     | 881  | GLN  |
| 1   | B     | 903  | ASN  |
| 1   | B     | 926  | GLN  |
| 1   | B     | 965  | GLN  |
| 1   | B     | 1033 | GLN  |
| 1   | B     | 1106 | ASN  |
| 1   | B     | 1124 | HIS  |
| 1   | B     | 1130 | GLN  |
| 1   | B     | 1140 | HIS  |
| 1   | B     | 1173 | HIS  |
| 1   | B     | 1188 | GLN  |
| 1   | B     | 1203 | ASN  |
| 1   | B     | 1218 | GLN  |
| 1   | B     | 1258 | HIS  |
| 1   | B     | 1270 | ASN  |
| 1   | B     | 1354 | ASN  |
| 1   | B     | 1393 | ASN  |
| 2   | C     | 60   | GLN  |
| 2   | C     | 110  | HIS  |
| 2   | C     | 121  | ASN  |
| 2   | C     | 178  | ASN  |
| 2   | C     | 236  | HIS  |
| 2   | C     | 363  | HIS  |
| 2   | C     | 366  | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | C     | 383  | ASN  |
| 2   | C     | 465  | ASN  |
| 2   | C     | 515  | HIS  |
| 2   | C     | 516  | ASN  |
| 2   | C     | 518  | HIS  |
| 2   | C     | 538  | ASN  |
| 2   | C     | 734  | HIS  |
| 2   | C     | 744  | HIS  |
| 2   | C     | 763  | GLN  |
| 2   | C     | 770  | GLN  |
| 2   | C     | 776  | GLN  |
| 2   | C     | 821  | GLN  |
| 2   | C     | 842  | ASN  |
| 2   | C     | 862  | GLN  |
| 2   | C     | 957  | ASN  |
| 2   | C     | 958  | GLN  |
| 2   | C     | 1065 | GLN  |
| 2   | C     | 1074 | ASN  |
| 2   | C     | 1084 | GLN  |
| 2   | C     | 1093 | GLN  |
| 2   | C     | 1117 | GLN  |
| 2   | C     | 1161 | HIS  |
| 2   | C     | 1176 | ASN  |
| 2   | C     | 1179 | GLN  |
| 3   | D     | 24   | ASN  |
| 3   | D     | 65   | HIS  |
| 3   | D     | 73   | GLN  |
| 3   | D     | 91   | HIS  |
| 3   | D     | 102  | GLN  |
| 3   | D     | 112  | ASN  |
| 3   | D     | 167  | HIS  |
| 4   | E     | 39   | ASN  |
| 4   | E     | 74   | GLN  |
| 4   | E     | 137  | ASN  |
| 4   | E     | 143  | ASN  |
| 4   | E     | 173  | HIS  |
| 4   | E     | 199  | ASN  |
| 5   | F     | 101  | GLN  |
| 5   | F     | 104  | ASN  |
| 5   | F     | 114  | ASN  |
| 5   | F     | 147  | HIS  |
| 7   | H     | 14   | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | H     | 53  | ASN  |
| 7   | H     | 97  | HIS  |
| 7   | H     | 122 | ASN  |
| 7   | H     | 126 | ASN  |
| 7   | H     | 153 | GLN  |
| 7   | H     | 158 | HIS  |
| 8   | I     | 137 | GLN  |
| 9   | J     | 12  | ASN  |
| 9   | J     | 90  | GLN  |
| 9   | J     | 108 | HIS  |
| 11  | L     | 44  | ASN  |
| 11  | L     | 65  | HIS  |
| 11  | L     | 76  | GLN  |
| 11  | L     | 89  | ASN  |
| 11  | L     | 110 | ASN  |
| 12  | M     | 53  | HIS  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed   | Backbone Outliers | Pucker Outliers |
|-----|-------|------------|-------------------|-----------------|
| 14  | P     | 7/16 (43%) | 1 (14%)           | 0               |

All (1) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | P     | 7   | A    |

There are no RNA pucker outliers to report.

## 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 carbohydrates in this entry.

## 5.6 Ligand geometry

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

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   | B     | 1416/1733 (81%) | -0.37  | 4 (0%) 93 91  | 76, 129, 175, 200     | 0       |
| 2   | C     | 1108/1224 (90%) | -0.32  | 2 (0%) 94 93  | 79, 140, 185, 200     | 0       |
| 3   | D     | 266/318 (83%)   | -0.41  | 0 100 100     | 93, 126, 168, 188     | 0       |
| 4   | E     | 177/221 (80%)   | -0.34  | 0 100 100     | 106, 142, 182, 190    | 0       |
| 5   | F     | 214/215 (99%)   | -0.33  | 0 100 100     | 99, 161, 187, 200     | 0       |
| 6   | G     | 84/155 (54%)    | -0.52  | 0 100 100     | 73, 107, 138, 147     | 0       |
| 7   | H     | 171/171 (100%)  | -0.34  | 0 100 100     | 98, 127, 164, 174     | 0       |
| 8   | I     | 133/146 (91%)   | 0.02   | 1 (0%) 86 79  | 134, 165, 186, 196    | 0       |
| 9   | J     | 119/122 (97%)   | -0.31  | 0 100 100     | 122, 165, 189, 200    | 0       |
| 10  | K     | 65/70 (92%)     | -0.59  | 0 100 100     | 92, 121, 158, 169     | 0       |
| 11  | L     | 114/120 (95%)   | -0.40  | 0 100 100     | 94, 128, 156, 170     | 0       |
| 12  | M     | 46/70 (65%)     | -0.03  | 0 100 100     | 120, 172, 195, 198    | 0       |
| 13  | N     | 7/14 (50%)      | 1.19   | 2 (28%) 1 1   | 199, 200, 200, 200    | 1 (14%) |
| 14  | P     | 8/16 (50%)      | 0.05   | 0 100 100     | 198, 199, 200, 200    | 0       |
| 15  | T     | 18/26 (69%)     | 0.65   | 2 (11%) 6 6   | 178, 199, 200, 200    | 1 (5%)  |
| All | All   | 3946/4621 (85%) | -0.34  | 11 (0%) 93 91 | 73, 136, 184, 200     | 2 (0%)  |

All (11) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | B     | 1176 | LEU  | 3.7  |
| 15  | T     | 11   | DT   | 2.8  |
| 13  | N     | 7    | DC   | 2.8  |
| 2   | C     | 471  | LYS  | 2.8  |
| 8   | I     | 105  | GLU  | 2.3  |
| 1   | B     | 1455 | PRO  | 2.2  |
| 1   | B     | 145  | LYS  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | C     | 865 | LYS  | 2.2  |
| 13  | N     | 6   | DA   | 2.2  |
| 15  | T     | 10  | DG   | 2.0  |
| 1   | B     | 164 | ARG  | 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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 16  | ZN   | J     | 123  | 1/1   | 0.99 | 0.16 | 0.27  | 136,136,136,136             | 0     |
| 16  | ZN   | K     | 71   | 1/1   | 0.99 | 0.25 | 0.14  | 113,113,113,113             | 0     |
| 16  | ZN   | D     | 319  | 1/1   | 0.99 | 0.13 | -0.66 | 98,98,98,98                 | 0     |
| 16  | ZN   | B     | 1735 | 1/1   | 0.99 | 0.12 | -1.49 | 110,110,110,110             | 0     |
| 16  | ZN   | M     | 71   | 1/1   | 0.98 | 0.05 | -1.61 | 174,174,174,174             | 0     |
| 16  | ZN   | B     | 1734 | 1/1   | 0.99 | 0.04 | -2.66 | 149,149,149,149             | 0     |
| 16  | ZN   | J     | 124  | 1/1   | 0.92 | 0.03 | -2.80 | 200,200,200,200             | 0     |
| 17  | MG   | B     | 1736 | 1/1   | 0.86 | 0.10 | -     | 153,153,153,153             | 0     |
| 16  | ZN   | C     | 1225 | 1/1   | 0.99 | 0.23 | -     | 104,104,104,104             | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.