



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:33 PM UTC

PDB ID : 1NIK / pdb\_00001nik  
Title : Wild Type RNA Polymerase II  
Authors : Bushnell, D.A.; Kornberg, R.D.  
Deposited on : 2002-12-24  
Resolution : 4.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

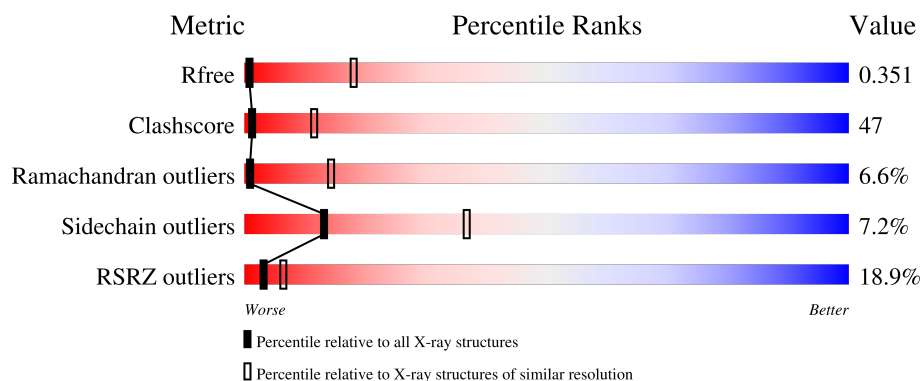
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.10 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1243 (4.40-3.80)                                      |
| Clashscore            | 190562                      | 1293 (4.40-3.80)                                      |
| Ramachandran outliers | 187476                      | 1206 (4.40-3.80)                                      |
| Sidechain outliers    | 187428                      | 1193 (4.40-3.80)                                      |
| RSRZ outliers         | 180081                      | 1240 (4.40-3.80)                                      |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 1733   |                  |
| 2   | B     | 1224   |                  |
| 3   | C     | 318    |                  |
| 4   | D     | 161    |                  |
| 5   | E     | 215    |                  |

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| Mol | Chain | Length | Quality of chain                                                                                         |
|-----|-------|--------|----------------------------------------------------------------------------------------------------------|
| 6   | F     | 155    | <div><div></div><div>9%</div><div>15%</div><div>34%</div><div>5%</div><div>46%</div></div>               |
| 7   | G     | 170    | <div><div></div><div>95%</div><div>5%</div></div>                                                        |
| 8   | H     | 146    | <div><div></div><div>30%</div><div>26%</div><div>53%</div><div>12%</div><div>•</div><div>9%</div></div>  |
| 9   | I     | 122    | <div><div></div><div>41%</div><div>32%</div><div>52%</div><div>12%</div><div>• •</div></div>             |
| 10  | J     | 70     | <div><div></div><div>9%</div><div>27%</div><div>51%</div><div>13%</div><div>•</div><div>7%</div></div>   |
| 11  | K     | 120    | <div><div></div><div>8%</div><div>35%</div><div>53%</div><div>6%</div><div>•</div><div>5%</div></div>    |
| 12  | L     | 70     | <div><div></div><div>30%</div><div>11%</div><div>33%</div><div>19%</div><div>•</div><div>34%</div></div> |

## 2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 28295 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 RPB1.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 1   | A     | 1388     | Total | C    | N    | O    | S  | 0       | 0       | 7     |
|     |       |          | 10864 | 6858 | 1899 | 2046 | 61 |         |         |       |

- Molecule 2 is a protein called ORF YOR151c.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 2   | B     | 1097     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 8721  | 5526 | 1523 | 1618 | 54 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 3   | C     | 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, chain RPB4.

| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------------|---------|---------|-------|
| 4   | D     | 153      | Total C<br>153 153 | 0       | 0       | 153   |

- Molecule 5 is a protein called DNA-directed RNA polymerase II, chain RPB5.

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

- Molecule 6 is a protein called DNA-directed RNA polymerase I, II and III 23 kDa polypeptide.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | F     | 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, chain RPB7.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|---------|---------|-------|
| 7   | G     | 170      | Total | C   | 0       | 0       | 170   |
|     |       |          | 170   | 170 |         |         |       |

- Molecule 8 is a protein called DNA-directed RNA polymerase subunit RPB8.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | H     | 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, chain RPB9.

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

- Molecule 10 is a protein called DNA-directed RNA polymerase II, chain RPB10.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 10  | J     | 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, chain RPB11.

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

- Molecule 12 is a protein called DNA-directed RNA polymerase II, chain RPB12.

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

- Molecule 13 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 13  | A     | 2        | Total | Zn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 13  | B     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

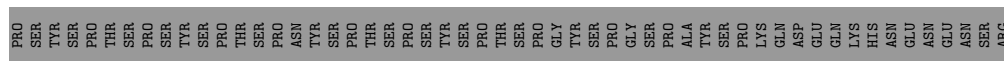
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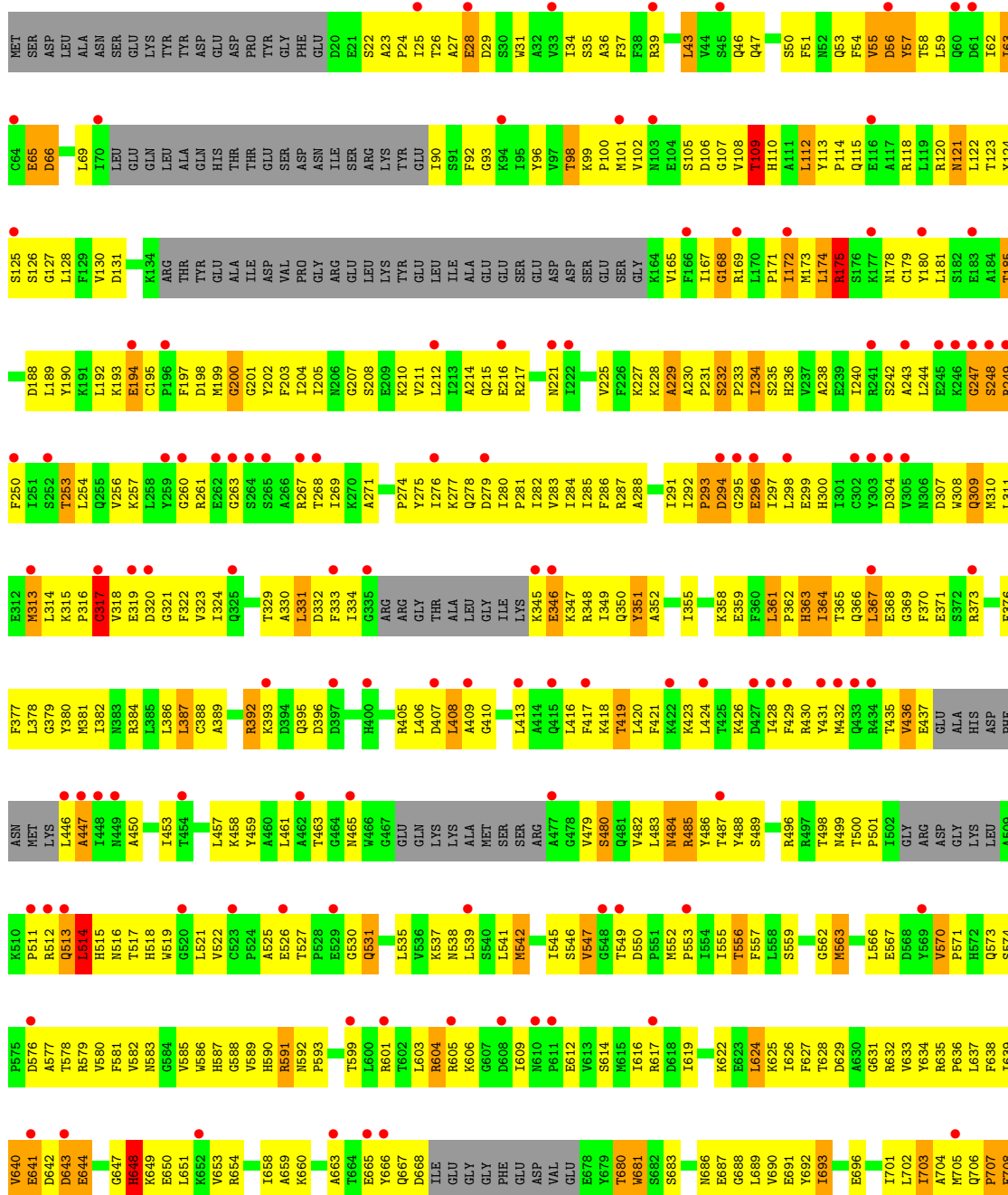
| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 13  | C     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 13  | I     | 2        | Total<br>2 | Zn<br>2 | 0       | 0       |
| 13  | J     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |

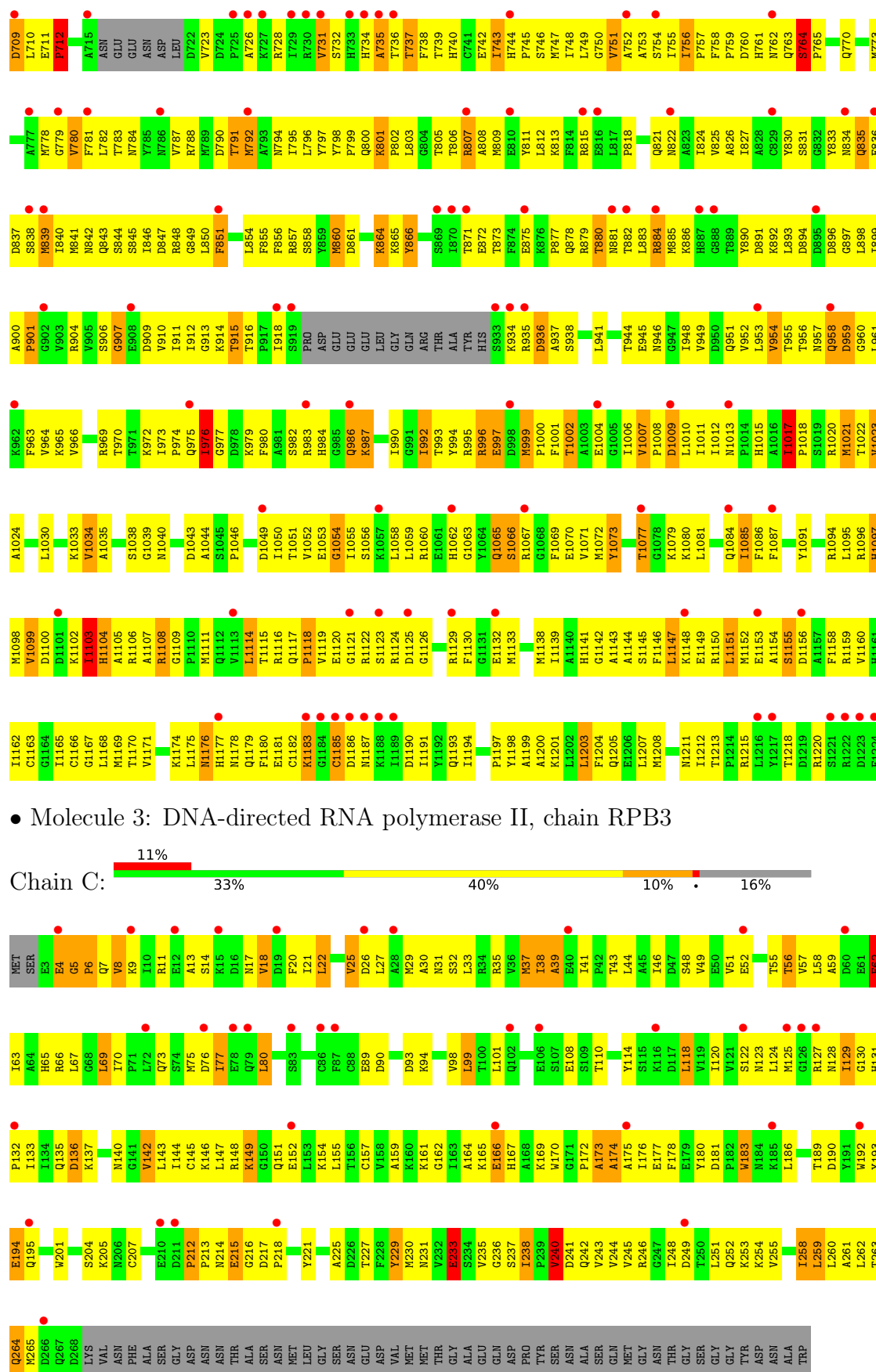


|     |       |       |       |       |       |       |       |       |      |      |      |      |
|-----|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|------|
| SER | A1440 | G1379 | M1317 | GLU   | S1189 | Q1128 | G1065 | R1001 | L928 | Q885 | Y804 | L658 |
| ASN | G1380 | T1318 | T1319 | THR   | P1190 | E1129 | V1066 | G1002 | L929 | P866 | L905 | H659 |
| ASP | L1381 | GLU   | GLU   | THR   | W1191 | Q1130 | L1067 | K1003 | D930 | I867 | R906 | N660 |
| MET | V1443 | P1320 | A1254 | E1255 | L1192 | A1131 | A1068 | N1004 | E931 | Y868 | G907 | G661 |
| ALA | M1444 | E1383 | G1321 | E1256 | L1193 | K1132 | L1193 | E1005 | E932 | G869 | L908 | F662 |
| ALA | L1445 | V1384 | I1322 | E1257 | R1194 | L1133 | A1069 |       | Y933 | E870 | T909 | S663 |
| GLY | L1446 | T1385 | I1323 | D1257 | L1195 | I1134 | G1073 | Q1008 | L936 | D871 | P810 | T664 |
| GLY | E1447 | R1386 | F1324 | H1258 | E1196 | R1135 | E1074 | M1009 | L937 | G872 | Q911 | G665 |
| PHE | E1448 | G1387 | M1259 | H1259 | L1197 | A1010 | P1075 | A1010 | Y937 | M873 | E812 | L666 |
| THR | S1449 | L1326 | L1325 | L1198 | D1198 | A1137 | A1076 |       | X938 | D874 | F813 | L667 |
| THR | F1389 | I1327 | K1261 | E1138 | R1199 | I1139 | T1077 | A1014 | D939 | F814 | N742 |      |
| TYR | L1450 | V1328 | K1262 | E1139 |       | E1139 | Q1078 | V1015 | R940 | F815 | F815 | L670 |
| TYR | V1451 | K1262 | L1328 | H1263 | M1202 | H1140 | M1079 | T1016 |      | I878 | H816 | A671 |
| GLY | K1452 | R1391 | T1329 | E1264 | M1203 | T1141 | T1080 | L1017 | L943 | E879 | A817 | A671 |
| GLY | TYR   | S1392 | M1330 | E1264 | M1203 | T1141 | T1080 | L1017 | L943 | E879 | A817 | A671 |
| ALA | MET   | F1394 | A1331 |       | D1204 | T1142 | ASN   | F1018 | Y948 | K880 | M818 | D672 |
| ASP | PRO   | T1394 | F1332 |       | K1205 | L1143 | THR   | C1019 | G949 | Q881 | G819 | P674 |
| TYR | GLU   | G1395 | E1333 |       | K1206 | L1143 | PHE   | G1020 | D949 | G882 | G820 | G750 |
| GLN | L1396 | D1334 | D1269 | E1269 | L1207 | S1145 | HIS   | L1021 | G950 | T885 | R821 | S751 |
| GLY | LYS   | L1397 | I1335 | E1270 | T1208 | V1146 | THR   | L1022 | E951 | E886 | E822 | K752 |
| GLY | LYS   | L1397 | I1335 | E1270 | T1208 | V1146 | PHE   | R1023 | A952 | I886 | G923 | G753 |
| ALA | ILE   | M1398 | M1336 | E1337 | L1271 | I1147 | ALA   | S1024 | Y954 | G887 | L824 | S754 |
| THR | THR   | E1337 | E1337 | L1272 | Q1211 | A1148 | GLY   | R1025 | X954 | G888 | I825 | F755 |
| SER | GLU   | C1400 | L1273 | L1273 | Q1211 | A1149 | VAL   | L1026 | P855 | S889 | D826 | T682 |
| PRO | ILE   | S1401 | L1339 | E1274 | V1212 | S1150 | ALA   | A1027 | L956 | D890 | T827 | T683 |
| PHE | GLU   | F1402 | G1340 | G1275 | E1151 | E1151 | SER   | T1028 | P857 | A891 | N757 | I683 |
| GLY | ASP   | E1403 | I1341 | V1276 | E1214 | I1152 | THR   | R1029 | Y958 | A892 | A828 | A686 |
| GLY | GLN   | E1404 | E1342 | E1277 | Y1153 | Y1153 | K1093 | R1030 | X959 | F893 | G830 | A686 |
| GLY | GLY   | T1405 | A1343 | T1278 | I1216 | Y1154 | V1094 | E1031 | R960 | E894 | K830 | Q760 |
| GLY | ASP   | V1406 | G1344 | E1279 | K1217 | D1155 | T1095 | L1032 | R961 | K895 | T831 | K689 |
| GLY | GLY   | E1407 | R1345 | E1280 | Q1218 | E1217 | S1096 | L1032 | P862 | R896 | T834 | K689 |
| ALA | GLY   | A1408 | A1346 | R1281 | T1219 | P1158 | G1097 | Y1035 | P863 | Y897 | G835 | L691 |
| PRO | VAL   | L1409 | A1347 | V1282 | F1220 | R1159 | G1097 | R1036 | P864 | R898 | Y836 | D692 |
| THR | THR   | F1410 | L1348 | V1283 | K1221 | S1160 | P1098 | D1043 | Q942 | P899 | I837 | V693 |
| SER | PRO   | E1411 | Y1349 | M1284 | M1222 | T1161 | P1099 | T1038 | Q965 | T899 | Q838 | T694 |
| SER | TYR   | A1412 | K1350 | L1223 | V1162 | R1100 | R1100 | T1038 | Q968 | D900 | L901 | K695 |
| GLY | SER   | G1413 | E1351 | K1290 | L1224 | L1163 | L1101 | K1039 |      | L901 | R839 | E696 |
| PHE | ASN   | A1414 | Y1352 | T1225 | F1225 | P1164 | K1102 | Q1040 |      | L902 | R840 | E697 |
| GLY | GLU   | S1415 | Y1353 | V1226 | E1165 | E1165 | E1103 | Q1041 | P971 | N903 | L941 | Q698 |
| VAL | SER   | A1416 | P1294 | P1294 | I1227 | D1166 | T1104 | F1042 | H972 | T904 | K842 | L701 |
| SER | GLY   | E1417 | V1355 | T1295 | W1228 | E1167 | L1104 | D1043 | Q943 | D905 | K943 | L702 |
| SER | LEU   | L1418 | G1296 | S1229 | E1168 | E1168 | W1044 | D974  | H975 | H906 | A844 | T763 |
| PRO | VAL   | D1419 | E1297 | E1297 | I1169 | I1170 | A1108 | V1045 | H975 | T907 | L845 | T763 |
| GLY | ASN   | D1369 | D1291 | Y1298 | D1291 | I1170 | K1109 | L1046 | P976 | L908 | E846 | A704 |
| PHE | ALA   | C1421 | G1360 | V1299 | M1232 | Q1171 | M1110 | S1047 | D947 | D909 | D847 |      |
| SER | ASP   | R1422 | S1361 | K1300 | M1232 | L1172 | M1111 | S1047 | S979 | P910 | I848 | T709 |
| LEU | LEU   | G1423 | Y1362 | E1301 | K1235 | H1173 | L1112 | E1059 | D980 | S911 | M849 | L710 |
| THR | ASP   | V1424 | V1363 | P1302 | L1236 | T1113 | T1113 | E1050 | L981 | L912 | V850 | R711 |
| SER | VAL   | S1425 | M1364 | E1303 | I1237 | S1175 | P1114 | Q1051 | T982 | L913 | H851 | E712 |
| PRO | LYS   |       | Y1365 | W1304 | I1238 | L1176 | S1115 | Q1052 | L983 | E914 | X852 | S713 |
| THR | ASP   | Y1428 | R1366 | V1305 | R1239 | LEU   | L1116 | F1053 | X984 | S915 | D953 | F714 |
| GLU | GLU   | I1429 | H1367 | L1306 | C1240 | ASP   | T1117 | L1054 | D985 |      | N854 | E715 |
| TYR | LEU   | L1430 | E1307 | L1306 | GLU   | GLU   | V1118 | R1055 | P986 | E918 | T855 |      |
| PRO | MET   | G1431 | T1308 | W1242 | GLU   | GLU   | Y1119 | S1056 | X987 | I919 | T856 | V719 |
| THR | PHE   | Q1432 | D1309 | V1243 | ALA   | ALA   | L1120 | V1057 | L988 | L920 | R857 | R720 |
| SER | SER   | M1433 | GLU   | ARG   | GLU   | GLU   | E1121 | V1058 |      | C921 | X858 | F721 |
| PRO | PRO   | D1372 | D1373 | PRO   | GLN   | GLN   | E1121 | V1058 |      | D922 | Y795 | L722 |
| ALA | LEU   | P1435 | V1374 | LYS   | THR   | SER   | P1122 | H1059 | Q994 | L923 | S959 |      |
| TYR | VAL   | T1436 | M1375 | GLI   | SER   | PHE   | L1223 | E1060 | E995 | G924 | L860 |      |
| ASP | ASP   | G1437 | T1376 | LEU   | ASP   | THR   | H1124 | E1061 | X996 | K924 | X861 | A725 |
| PRO | SER   | T1438 | T1377 | ASP   | LEU   | ASP   | A1125 | G1062 | L997 | L925 | N862 | R726 |
| PRO | GLY   | C1439 | D1377 | ALA   | ASP   | GLI   | A1126 | V1063 | L998 | Q926 | V863 | D727 |
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|     |       |       |       |       |       |       |       |       |      |      |      |      |



Chain B:  17% 28% 50% 10% 10%





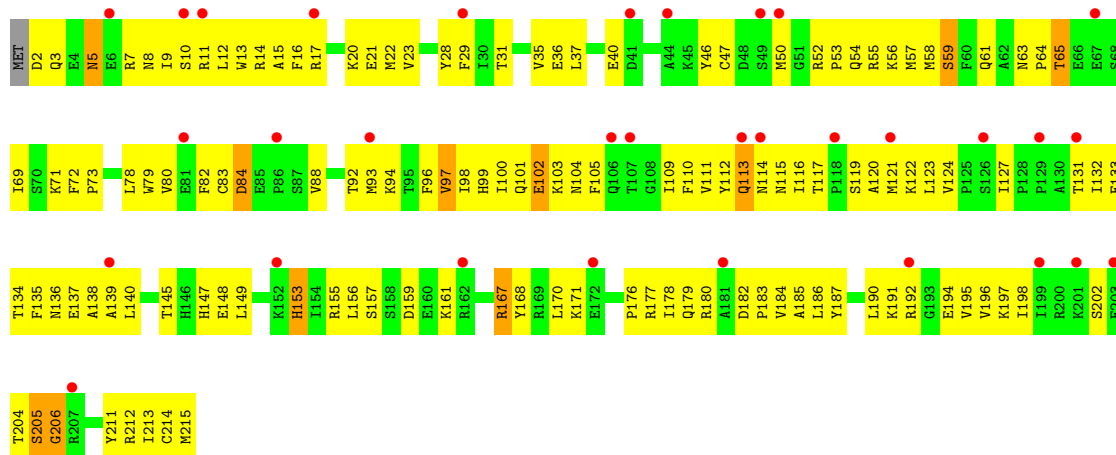
- Molecule 4: DNA-directed RNA polymerase II, chain RPB4

Chain D:  91% 5%

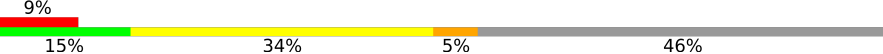


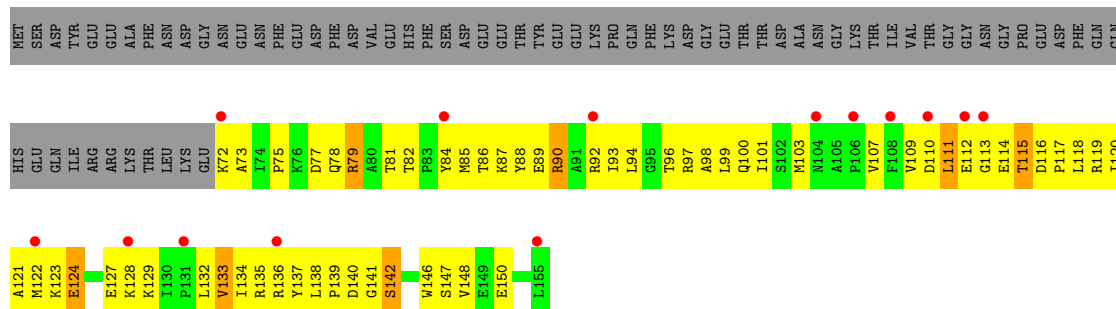
- Molecule 5: DNA-directed RNA polymerase II, chain RPB5

Chain E:  15% 38% 56% 5%

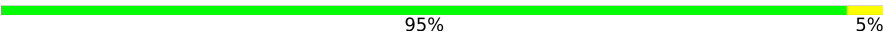


- Molecule 6: DNA-directed RNA polymerase I, II and III 23 kDa polypeptide

Chain F:  9% 15% 34% 5% 46%

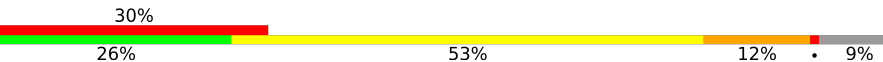


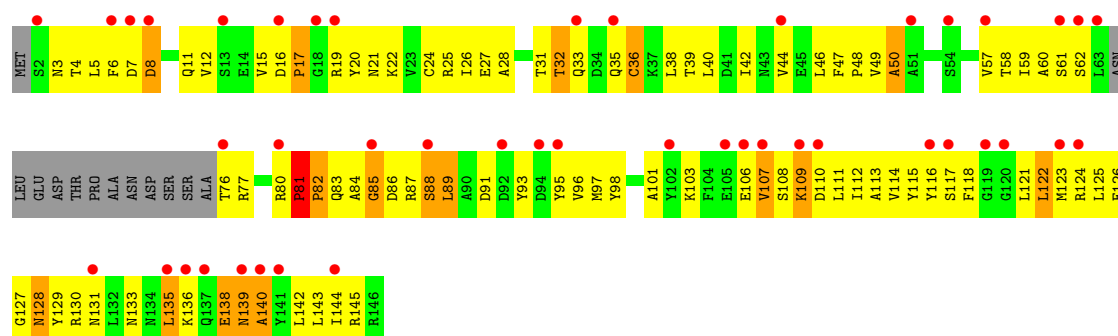
- Molecule 7: DNA-directed RNA polymerase II, chain RPB7

Chain G:  95% 5%

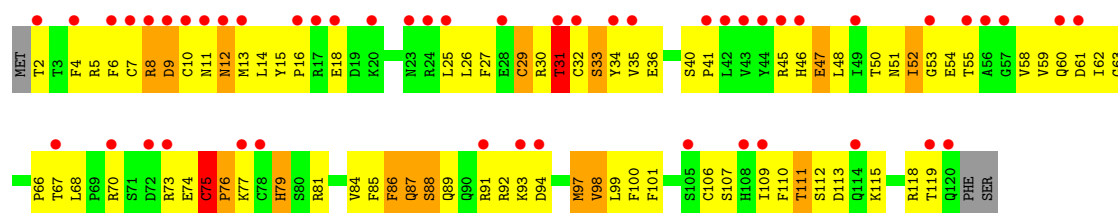


- Molecule 8: DNA-directed RNA polymerase subunit RPB8

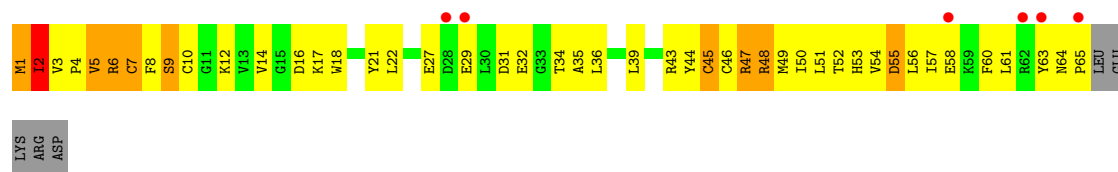
Chain H:  30% 26% 53% 12% 9%



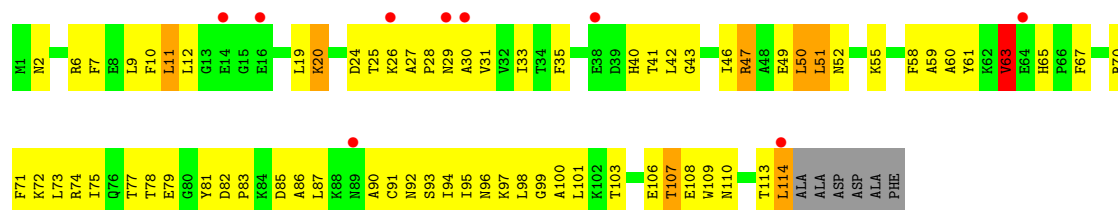
- Molecule 9: DNA-directed RNA polymerase II, chain RPB9



- Molecule 10: DNA-directed RNA polymerase II, chain RPB10

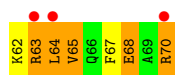


- Molecule 11: DNA-directed RNA polymerase II, chain RPB11



- Molecule 12: DNA-directed RNA polymerase II, chain RPB12





## 4 Data and refinement statistics

| Property                                                                | Value                                                                         | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------------------------|------------------|
| Space group                                                             | C 2 2 21                                                                      | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 224.10Å 394.46Å 284.34Å<br>90.00° 90.00° 90.00°                               | Depositor        |
| Resolution (Å)                                                          | 40.00 – 4.10<br>40.00 – 4.11                                                  | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | (Not available) (40.00-4.10)<br>86.2 (40.00-4.11)                             | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                                               | Depositor        |
| $R_{sym}$                                                               | 0.11                                                                          | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.58 (at 4.13Å)                                                               | Xtriage          |
| Refinement program                                                      | CNS                                                                           | Depositor        |
| R, $R_{free}$                                                           | 0.334 , 0.360<br>0.330 , 0.351                                                | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 3272 reflections (3.38%)                                                      | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 114.0                                                                         | Xtriage          |
| Anisotropy                                                              | 0.378                                                                         | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.30 , 262.1                                                                  | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$                   | Xtriage          |
| Estimated twinning fraction                                             | 0.044 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l<br>0.047 for 1/2*h+1/2*k,3/2*h-1/2*k,-l | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.78                                                                          | EDS              |
| Total number of atoms                                                   | 28295                                                                         | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 194.0                                                                         | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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

| Mol | Chain | Bond lengths |         | Bond angles |                  |
|-----|-------|--------------|---------|-------------|------------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5          |
| 1   | A     | 0.53         | 0/11048 | 1.07        | 74/14936 (0.5%)  |
| 2   | B     | 0.56         | 0/8891  | 1.07        | 58/11990 (0.5%)  |
| 3   | C     | 0.60         | 0/2133  | 1.19        | 27/2891 (0.9%)   |
| 5   | E     | 0.42         | 0/1788  | 1.04        | 13/2406 (0.5%)   |
| 6   | F     | 0.48         | 0/691   | 0.99        | 2/933 (0.2%)     |
| 8   | H     | 0.46         | 0/1086  | 1.11        | 11/1470 (0.7%)   |
| 9   | I     | 0.53         | 0/989   | 1.10        | 7/1331 (0.5%)    |
| 10  | J     | 0.67         | 0/541   | 1.09        | 4/727 (0.6%)     |
| 11  | K     | 0.54         | 0/937   | 0.95        | 3/1265 (0.2%)    |
| 12  | L     | 0.54         | 0/366   | 1.10        | 5/485 (1.0%)     |
| All | All   | 0.54         | 0/28470 | 1.08        | 204/38434 (0.5%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2   | B     | 0                   | 1                   |

There are no bond length outliers.

All (204) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 2   | B     | 296 | GLU  | N-CA-C | -12.34 | 97.59       | 112.89   |
| 3   | C     | 173 | ALA  | N-CA-C | 11.19  | 123.47      | 111.28   |
| 1   | A     | 452 | LYS  | N-CA-C | -10.89 | 97.32       | 112.45   |
| 1   | A     | 474 | VAL  | N-CA-C | -10.80 | 102.54      | 112.90   |
| 9   | I     | 75  | CYS  | N-CA-C | -9.93  | 97.14       | 109.65   |
| 3   | C     | 39  | ALA  | N-CA-C | 9.52   | 127.35      | 114.12   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | C     | 183  | TRP  | N-CA-C  | -9.09 | 95.86       | 110.32   |
| 1   | A     | 1311 | VAL  | N-CA-C  | 8.80  | 121.16      | 108.48   |
| 2   | B     | 976  | ILE  | N-CA-C  | 8.79  | 118.86      | 110.42   |
| 8   | H     | 85   | GLY  | N-CA-C  | -8.48 | 104.99      | 114.40   |
| 2   | B     | 736  | THR  | N-CA-C  | -8.41 | 100.05      | 110.65   |
| 8   | H     | 80   | ARG  | CA-C-N  | -8.30 | 111.83      | 120.38   |
| 8   | H     | 80   | ARG  | C-N-CA  | -8.30 | 111.83      | 120.38   |
| 1   | A     | 1392 | SER  | N-CA-C  | 8.13  | 128.13      | 110.80   |
| 1   | A     | 693  | VAL  | N-CA-C  | -7.90 | 103.55      | 110.74   |
| 2   | B     | 606  | LYS  | N-CA-C  | -7.61 | 103.26      | 112.54   |
| 1   | A     | 241  | VAL  | N-CA-C  | 7.60  | 115.08      | 107.55   |
| 5   | E     | 171  | LYS  | N-CA-C  | -7.60 | 100.73      | 110.53   |
| 1   | A     | 950  | GLY  | N-CA-C  | -7.59 | 104.56      | 115.27   |
| 2   | B     | 392  | ARG  | N-CA-C  | -7.50 | 104.27      | 113.50   |
| 1   | A     | 398  | GLU  | N-CA-C  | -7.49 | 95.43       | 108.69   |
| 2   | B     | 514  | LEU  | N-CA-C  | -7.48 | 98.74       | 109.96   |
| 8   | H     | 81   | PRO  | N-CA-C  | 7.46  | 119.80      | 110.70   |
| 2   | B     | 591  | ARG  | N-CA-C  | -7.41 | 101.30      | 110.41   |
| 1   | A     | 1215 | ARG  | N-CA-C  | -7.39 | 102.60      | 111.69   |
| 1   | A     | 564  | ALA  | N-CA-C  | -7.33 | 103.32      | 111.82   |
| 1   | A     | 481  | ASP  | N-CA-C  | -7.29 | 97.64       | 108.79   |
| 2   | B     | 851  | PHE  | N-CA-C  | 7.24  | 121.38      | 111.39   |
| 1   | A     | 417  | TYR  | N-CA-C  | -7.20 | 98.12       | 109.50   |
| 5   | E     | 5    | ASN  | N-CA-C  | -7.16 | 102.89      | 111.69   |
| 12  | L     | 58   | LYS  | N-CA-C  | 7.05  | 121.63      | 110.70   |
| 2   | B     | 1077 | THR  | N-CA-C  | 6.96  | 121.00      | 112.23   |
| 1   | A     | 1440 | ALA  | N-CA-C  | -6.95 | 104.67      | 113.43   |
| 3   | C     | 137  | LYS  | N-CA-C  | -6.94 | 103.45      | 112.68   |
| 9   | I     | 119  | THR  | N-CA-C  | -6.93 | 104.86      | 113.38   |
| 1   | A     | 1338 | VAL  | N-CA-C  | 6.92  | 117.88      | 111.45   |
| 6   | F     | 112  | GLU  | N-CA-C  | -6.86 | 104.99      | 113.15   |
| 2   | B     | 363  | HIS  | N-CA-C  | -6.85 | 101.50      | 110.33   |
| 2   | B     | 351  | TYR  | N-CA-C  | -6.84 | 102.90      | 111.11   |
| 3   | C     | 233  | GLU  | N-CA-C  | -6.83 | 100.40      | 110.52   |
| 1   | A     | 296  | LEU  | N-CA-C  | -6.83 | 103.76      | 111.07   |
| 5   | E     | 202  | SER  | N-CA-C  | 6.83  | 119.81      | 109.23   |
| 5   | E     | 65   | THR  | N-CA-C  | -6.79 | 102.06      | 110.41   |
| 1   | A     | 71   | GLN  | CB-CA-C | -6.77 | 108.75      | 116.54   |
| 1   | A     | 1403 | GLU  | N-CA-C  | 6.71  | 125.08      | 110.80   |
| 8   | H     | 122  | LEU  | N-CA-C  | 6.68  | 120.77      | 110.42   |
| 2   | B     | 1130 | PHE  | N-CA-C  | -6.61 | 102.50      | 111.55   |
| 1   | A     | 797  | LYS  | N-CA-C  | 6.59  | 120.02      | 112.57   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 1   | A     | 1269 | GLU  | N-CA-C | 6.59  | 122.41      | 113.97   |
| 3   | C     | 89   | GLU  | N-CA-C | -6.59 | 98.48       | 108.96   |
| 12  | L     | 65   | VAL  | N-CA-C | 6.52  | 117.97      | 108.58   |
| 2   | B     | 703  | ILE  | N-CA-C | 6.52  | 117.27      | 107.75   |
| 2   | B     | 712  | PRO  | N-CA-C | -6.48 | 99.12       | 112.47   |
| 1   | A     | 466  | SER  | N-CA-C | 6.47  | 124.59      | 110.80   |
| 3   | C     | 194  | GLU  | N-CA-C | -6.44 | 106.01      | 114.31   |
| 1   | A     | 643  | ALA  | N-CA-C | -6.40 | 104.22      | 111.07   |
| 10  | J     | 2    | ILE  | N-CA-C | 6.39  | 122.63      | 109.34   |
| 2   | B     | 99   | LYS  | N-CA-C | -6.38 | 101.81      | 110.36   |
| 2   | B     | 761  | HIS  | N-CA-C | -6.38 | 102.90      | 112.54   |
| 1   | A     | 729  | ALA  | N-CA-C | -6.37 | 104.34      | 111.28   |
| 1   | A     | 1010 | ALA  | N-CA-C | -6.37 | 103.97      | 111.03   |
| 1   | A     | 491  | VAL  | N-CA-C | 6.35  | 114.81      | 107.89   |
| 1   | A     | 1262 | LYS  | N-CA-C | -6.34 | 104.81      | 112.54   |
| 5   | E     | 97   | VAL  | N-CA-C | -6.31 | 104.18      | 110.62   |
| 9   | I     | 111  | THR  | N-CA-C | 6.31  | 119.92      | 110.14   |
| 12  | L     | 67   | PHE  | N-CA-C | 6.30  | 119.77      | 109.24   |
| 2   | B     | 56   | ASP  | N-CA-C | 6.29  | 118.69      | 111.02   |
| 1   | A     | 776  | ALA  | N-CA-C | 6.28  | 119.02      | 110.35   |
| 3   | C     | 41   | ILE  | CA-C-N | 6.28  | 126.25      | 120.03   |
| 3   | C     | 41   | ILE  | C-N-CA | 6.28  | 126.25      | 120.03   |
| 5   | E     | 153  | HIS  | N-CA-C | -6.25 | 100.38      | 110.32   |
| 2   | B     | 1085 | ILE  | N-CA-C | 6.25  | 118.47      | 108.85   |
| 2   | B     | 801  | LYS  | N-CA-C | -6.19 | 101.97      | 109.83   |
| 2   | B     | 1009 | ASP  | N-CA-C | -6.17 | 105.58      | 113.23   |
| 2   | B     | 681  | TRP  | N-CA-C | -6.16 | 104.83      | 112.90   |
| 1   | A     | 399  | HIS  | N-CA-C | 6.16  | 123.42      | 109.81   |
| 1   | A     | 1021 | LEU  | N-CA-C | -6.14 | 103.53      | 111.02   |
| 8   | H     | 50   | ALA  | N-CA-C | 6.12  | 115.93      | 107.73   |
| 2   | B     | 1103 | ILE  | N-CA-C | 6.11  | 122.04      | 109.34   |
| 3   | C     | 166  | GLU  | N-CA-C | -6.10 | 104.74      | 111.82   |
| 1   | A     | 602  | ASP  | N-CA-C | -6.08 | 103.00      | 111.39   |
| 1   | A     | 938  | LYS  | N-CA-C | -6.07 | 104.74      | 111.36   |
| 1   | A     | 1148 | ILE  | N-CA-C | -6.07 | 105.22      | 110.74   |
| 1   | A     | 496  | GLU  | N-CA-C | -5.91 | 104.47      | 111.03   |
| 9   | I     | 31   | THR  | N-CA-C | -5.87 | 106.25      | 113.41   |
| 2   | B     | 706  | GLN  | N-CA-C | -5.86 | 102.22      | 110.31   |
| 1   | A     | 1170 | ILE  | N-CA-C | 5.85  | 116.03      | 110.53   |
| 1   | A     | 749  | ALA  | N-CA-C | -5.82 | 105.02      | 111.36   |
| 2   | B     | 599  | THR  | N-CA-C | -5.82 | 104.58      | 111.03   |
| 3   | C     | 108  | GLU  | N-CA-C | -5.80 | 106.01      | 112.57   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 8   | H     | 36   | CYS  | N-CA-C  | 5.80  | 118.99      | 109.76   |
| 2   | B     | 541  | LEU  | N-CA-C  | 5.78  | 117.38      | 111.14   |
| 9   | I     | 11   | ASN  | N-CA-C  | 5.77  | 119.52      | 111.90   |
| 1   | A     | 710  | LEU  | N-CA-C  | -5.76 | 104.38      | 111.75   |
| 1   | A     | 266  | LEU  | N-CA-C  | -5.75 | 106.10      | 113.23   |
| 3   | C     | 237  | SER  | N-CA-C  | -5.74 | 105.38      | 112.38   |
| 1   | A     | 325  | ILE  | N-CA-C  | -5.74 | 107.25      | 111.90   |
| 5   | E     | 111  | VAL  | N-CA-C  | 5.72  | 115.49      | 107.37   |
| 2   | B     | 165  | VAL  | N-CA-C  | 5.71  | 116.53      | 108.36   |
| 2   | B     | 172  | ILE  | N-CA-C  | 5.69  | 116.77      | 108.58   |
| 2   | B     | 900  | ALA  | CA-C-N  | 5.68  | 126.95      | 119.84   |
| 2   | B     | 900  | ALA  | C-N-CA  | 5.68  | 126.95      | 119.84   |
| 1   | A     | 468  | PHE  | N-CA-C  | -5.68 | 101.88      | 110.28   |
| 1   | A     | 553  | VAL  | CA-C-N  | 5.67  | 125.34      | 119.05   |
| 1   | A     | 553  | VAL  | C-N-CA  | 5.67  | 125.34      | 119.05   |
| 1   | A     | 399  | HIS  | CA-C-N  | -5.66 | 112.76      | 119.84   |
| 1   | A     | 399  | HIS  | C-N-CA  | -5.66 | 112.76      | 119.84   |
| 1   | A     | 524  | VAL  | N-CA-C  | 5.65  | 121.10      | 109.34   |
| 3   | C     | 259  | LEU  | N-CA-C  | -5.63 | 105.06      | 111.14   |
| 2   | B     | 294  | ASP  | N-CA-C  | -5.61 | 98.84       | 110.80   |
| 1   | A     | 395  | GLY  | CA-C-N  | 5.60  | 126.84      | 119.84   |
| 1   | A     | 395  | GLY  | C-N-CA  | 5.60  | 126.84      | 119.84   |
| 11  | K     | 63   | VAL  | N-CA-C  | -5.59 | 98.39       | 106.88   |
| 2   | B     | 640  | VAL  | N-CA-C  | 5.58  | 119.00      | 113.53   |
| 2   | B     | 109  | THR  | N-CA-C  | -5.57 | 100.16      | 109.24   |
| 10  | J     | 45   | CYS  | N-CA-C  | -5.57 | 105.21      | 111.28   |
| 8   | H     | 3    | ASN  | N-CA-C  | 5.54  | 115.60      | 108.34   |
| 2   | B     | 413  | LEU  | N-CA-C  | -5.53 | 105.25      | 111.28   |
| 1   | A     | 44   | THR  | N-CA-C  | -5.52 | 105.17      | 112.24   |
| 1   | A     | 330  | LYS  | N-CA-C  | 5.52  | 118.02      | 110.24   |
| 3   | C     | 8    | VAL  | N-CA-C  | 5.52  | 117.07      | 109.46   |
| 1   | A     | 1162 | VAL  | N-CA-C  | -5.51 | 105.57      | 113.07   |
| 6   | F     | 124  | GLU  | N-CA-C  | -5.51 | 106.06      | 112.89   |
| 2   | B     | 894  | ASP  | N-CA-C  | -5.51 | 101.85      | 110.17   |
| 3   | C     | 41   | ILE  | N-CA-C  | -5.50 | 103.90      | 108.63   |
| 1   | A     | 750  | GLY  | N-CA-C  | -5.48 | 100.18      | 113.18   |
| 1   | A     | 1391 | ARG  | N-CA-C  | -5.48 | 104.94      | 111.69   |
| 2   | B     | 936  | ASP  | N-CA-C  | 5.48  | 118.39      | 110.28   |
| 3   | C     | 62   | PHE  | N-CA-C  | -5.47 | 105.23      | 111.14   |
| 2   | B     | 647  | GLY  | N-CA-C  | 5.47  | 126.15      | 113.18   |
| 1   | A     | 666  | ILE  | CB-CA-C | -5.47 | 104.97      | 111.97   |
| 5   | E     | 180  | ARG  | N-CA-C  | -5.47 | 105.32      | 111.28   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | C     | 37   | MET  | N-CA-C  | -5.47 | 105.22      | 111.07   |
| 3   | C     | 94   | LYS  | N-CA-C  | -5.46 | 106.98      | 113.97   |
| 1   | A     | 827  | THR  | N-CA-C  | -5.45 | 105.25      | 111.14   |
| 3   | C     | 225  | ALA  | N-CA-C  | 5.45  | 117.12      | 108.67   |
| 1   | A     | 143  | LYS  | N-CA-C  | -5.43 | 107.02      | 113.97   |
| 3   | C     | 118  | LEU  | N-CA-C  | -5.43 | 102.96      | 110.35   |
| 5   | E     | 113  | GLN  | N-CA-C  | 5.43  | 119.91      | 113.12   |
| 11  | K     | 52   | ASN  | N-CA-C  | -5.43 | 106.82      | 113.50   |
| 5   | E     | 161  | LYS  | N-CA-C  | -5.42 | 105.37      | 111.28   |
| 1   | A     | 1307 | GLU  | N-CA-C  | -5.42 | 101.45      | 110.17   |
| 5   | E     | 63   | ASN  | CA-C-N  | 5.41  | 125.34      | 119.76   |
| 5   | E     | 63   | ASN  | C-N-CA  | 5.41  | 125.34      | 119.76   |
| 12  | L     | 68   | GLU  | N-CA-C  | -5.39 | 101.88      | 109.96   |
| 2   | B     | 693  | ILE  | N-CA-C  | 5.38  | 115.69      | 108.17   |
| 2   | B     | 1114 | LEU  | N-CA-C  | 5.37  | 117.22      | 111.36   |
| 1   | A     | 288  | ALA  | N-CA-C  | -5.37 | 105.41      | 113.89   |
| 8   | H     | 103  | LYS  | N-CA-C  | 5.36  | 117.64      | 108.90   |
| 2   | B     | 112  | LEU  | N-CA-C  | 5.35  | 118.34      | 109.46   |
| 3   | C     | 56   | THR  | N-CA-C  | 5.35  | 116.82      | 110.19   |
| 2   | B     | 1023 | VAL  | N-CA-C  | 5.33  | 116.05      | 110.62   |
| 1   | A     | 847  | ASP  | N-CA-C  | 5.32  | 119.48      | 113.15   |
| 1   | A     | 1389 | PHE  | N-CA-C  | 5.32  | 119.62      | 113.18   |
| 2   | B     | 648  | HIS  | N-CA-C  | 5.29  | 122.06      | 110.80   |
| 8   | H     | 16   | ASP  | N-CA-C  | 5.28  | 117.97      | 109.15   |
| 2   | B     | 253  | THR  | N-CA-C  | 5.28  | 118.16      | 109.76   |
| 9   | I     | 18   | GLU  | N-CA-C  | 5.28  | 117.85      | 109.24   |
| 1   | A     | 562  | THR  | CA-C-N  | 5.28  | 125.27      | 119.89   |
| 1   | A     | 562  | THR  | C-N-CA  | 5.28  | 125.27      | 119.89   |
| 8   | H     | 107  | VAL  | N-CA-C  | -5.27 | 106.07      | 112.76   |
| 2   | B     | 1123 | SER  | N-CA-C  | -5.25 | 105.98      | 112.38   |
| 2   | B     | 739  | THR  | N-CA-C  | -5.25 | 107.54      | 114.31   |
| 3   | C     | 80   | LEU  | N-CA-C  | -5.24 | 100.48      | 109.24   |
| 3   | C     | 258  | ILE  | N-CA-C  | -5.23 | 105.30      | 111.00   |
| 1   | A     | 1113 | THR  | CA-C-N  | 5.23  | 126.37      | 119.84   |
| 1   | A     | 1113 | THR  | C-N-CA  | 5.23  | 126.37      | 119.84   |
| 2   | B     | 1203 | LEU  | N-CA-C  | -5.23 | 105.27      | 110.97   |
| 1   | A     | 1216 | ILE  | CB-CA-C | -5.22 | 105.02      | 112.22   |
| 2   | B     | 69   | LEU  | N-CA-C  | 5.21  | 118.09      | 109.85   |
| 1   | A     | 693  | VAL  | CB-CA-C | -5.21 | 105.06      | 111.94   |
| 10  | J     | 5    | VAL  | N-CA-C  | -5.20 | 101.97      | 108.84   |
| 1   | A     | 580  | VAL  | N-CA-C  | -5.20 | 105.47      | 110.72   |
| 1   | A     | 861  | GLY  | N-CA-C  | -5.20 | 107.37      | 114.64   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | A     | 628  | GLY  | N-CA-C  | 5.18  | 125.47      | 113.18   |
| 1   | A     | 1188 | GLN  | N-CA-C  | 5.18  | 117.86      | 110.24   |
| 3   | C     | 193  | TYR  | N-CA-C  | 5.18  | 117.28      | 109.41   |
| 2   | B     | 278  | GLN  | N-CA-C  | 5.18  | 116.07      | 107.73   |
| 2   | B     | 110  | HIS  | N-CA-C  | 5.17  | 118.17      | 109.95   |
| 2   | B     | 317  | CYS  | N-CA-C  | -5.17 | 105.33      | 111.69   |
| 2   | B     | 756  | ILE  | CB-CA-C | -5.17 | 106.13      | 110.94   |
| 5   | E     | 205  | SER  | N-CA-C  | -5.16 | 99.69       | 108.26   |
| 2   | B     | 107  | GLY  | N-CA-C  | 5.16  | 118.52      | 110.88   |
| 3   | C     | 240  | VAL  | N-CA-C  | 5.16  | 115.78      | 110.36   |
| 2   | B     | 604  | ARG  | N-CA-C  | -5.15 | 106.84      | 113.23   |
| 2   | B     | 743  | ILE  | N-CA-C  | -5.14 | 105.49      | 110.42   |
| 2   | B     | 886  | LYS  | N-CA-C  | 5.12  | 117.45      | 109.52   |
| 1   | A     | 696  | GLU  | N-CA-C  | -5.11 | 105.40      | 110.97   |
| 12  | L     | 40   | LEU  | N-CA-C  | 5.11  | 116.57      | 108.96   |
| 2   | B     | 66   | ASP  | N-CA-C  | -5.11 | 106.80      | 112.57   |
| 9   | I     | 10   | CYS  | N-CA-C  | 5.10  | 119.13      | 113.01   |
| 1   | A     | 12   | ARG  | N-CA-C  | 5.09  | 116.55      | 108.96   |
| 1   | A     | 415  | LEU  | N-CA-C  | 5.07  | 121.60      | 110.80   |
| 2   | B     | 659  | ALA  | N-CA-C  | -5.07 | 105.89      | 111.71   |
| 10  | J     | 10   | CYS  | N-CA-C  | 5.06  | 119.73      | 113.50   |
| 1   | A     | 337  | ARG  | N-CA-C  | 5.06  | 116.60      | 111.14   |
| 1   | A     | 1078 | GLN  | N-CA-C  | -5.05 | 106.03      | 113.61   |
| 2   | B     | 854  | LEU  | N-CA-C  | -5.05 | 102.60      | 110.42   |
| 3   | C     | 38   | ILE  | N-CA-C  | 5.04  | 115.76      | 110.62   |
| 11  | K     | 20   | LYS  | N-CA-C  | -5.03 | 99.79       | 108.69   |
| 1   | A     | 886  | ILE  | N-CA-C  | 5.02  | 116.12      | 111.45   |
| 1   | A     | 445  | ASN  | N-CA-C  | 5.01  | 117.00      | 109.23   |
| 3   | C     | 129  | ILE  | N-CA-C  | 5.01  | 114.47      | 108.06   |
| 2   | B     | 293  | PRO  | N-CA-C  | 5.01  | 118.74      | 111.03   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 2   | B     | 811 | TYR  | Sidechain |

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 10864 | 0        | 10959    | 1096    | 1            |
| 2   | B     | 8721  | 0        | 8746     | 944     | 0            |
| 3   | C     | 2095  | 0        | 2052     | 172     | 1            |
| 4   | D     | 153   | 0        | 0        | 4       | 0            |
| 5   | E     | 1752  | 0        | 1776     | 142     | 0            |
| 6   | F     | 679   | 0        | 701      | 72      | 0            |
| 7   | G     | 170   | 0        | 0        | 5       | 0            |
| 8   | H     | 1068  | 0        | 1040     | 136     | 0            |
| 9   | I     | 971   | 0        | 933      | 105     | 0            |
| 10  | J     | 532   | 0        | 544      | 76      | 0            |
| 11  | K     | 919   | 0        | 929      | 91      | 0            |
| 12  | L     | 364   | 0        | 390      | 56      | 0            |
| 13  | A     | 2     | 0        | 0        | 0       | 0            |
| 13  | B     | 1     | 0        | 0        | 0       | 0            |
| 13  | C     | 1     | 0        | 0        | 0       | 0            |
| 13  | I     | 2     | 0        | 0        | 1       | 0            |
| 13  | J     | 1     | 0        | 0        | 1       | 0            |
| All | All   | 28295 | 0        | 28070    | 2652    | 1            |

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 47.

All (2652) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:132:UNK:CA    | 4:D:133:UNK:CA    | 2.01                     | 1.36              |
| 12:L:60:ARG:HG3   | 12:L:61:THR:H     | 1.05                     | 1.17              |
| 1:A:567:LYS:HB2   | 1:A:568:PRO:HD2   | 1.18                     | 1.15              |
| 9:I:111:THR:HG22  | 9:I:113:ASP:H     | 1.05                     | 1.14              |
| 1:A:353:ILE:HD13  | 1:A:487:MET:HE3   | 1.23                     | 1.13              |
| 1:A:1364:ASN:ND2  | 1:A:1366:ARG:HG2  | 1.65                     | 1.11              |
| 1:A:855:THR:HG21  | 1:A:857:ARG:HE    | 1.12                     | 1.10              |
| 1:A:93:VAL:HG13   | 1:A:301:ALA:HB1   | 1.33                     | 1.08              |
| 1:A:666:ILE:HD11  | 2:B:1030:LEU:HD13 | 1.27                     | 1.08              |
| 2:B:1051:THR:HG22 | 2:B:1053:GLU:H    | 1.00                     | 1.08              |
| 5:E:124:VAL:HG13  | 5:E:132:ILE:HB    | 1.33                     | 1.07              |
| 1:A:704:ALA:HB2   | 1:A:710:LEU:HG    | 1.34                     | 1.07              |
| 2:B:512:ARG:HH21  | 2:B:535:LEU:HD11  | 1.17                     | 1.06              |
| 2:B:708:GLU:HG3   | 2:B:709:ASP:H     | 1.17                     | 1.06              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1161:THR:HG22 | 1:A:1163:ILE:H    | 1.18                     | 1.05              |
| 2:B:345:LYS:HA    | 2:B:348:ARG:HE    | 1.11                     | 1.05              |
| 2:B:570:VAL:HB    | 2:B:573:GLN:HB3   | 1.36                     | 1.05              |
| 6:F:81:THR:HG21   | 6:F:136:ARG:HD3   | 1.38                     | 1.04              |
| 2:B:120:ARG:HG2   | 2:B:955:THR:HG21  | 1.40                     | 1.03              |
| 1:A:1329:THR:HG22 | 1:A:1331:SER:H    | 1.16                     | 1.03              |
| 1:A:902:LEU:HG    | 1:A:926:GLN:HG3   | 1.40                     | 1.02              |
| 2:B:287:ARG:HG2   | 2:B:292:ILE:HA    | 1.38                     | 1.02              |
| 2:B:1159:ARG:HE   | 2:B:1193:GLN:NE2  | 1.56                     | 1.02              |
| 1:A:1111:MET:HE2  | 1:A:1114:PRO:HA   | 1.39                     | 1.02              |
| 12:L:32:ALA:HB3   | 12:L:55:ILE:HD12  | 1.39                     | 1.02              |
| 2:B:1159:ARG:NE   | 2:B:1193:GLN:HE21 | 1.57                     | 1.02              |
| 1:A:913:LEU:HD12  | 1:A:914:GLU:H     | 1.25                     | 1.01              |
| 3:C:80:LEU:HD22   | 3:C:129:ILE:HD11  | 1.41                     | 1.00              |
| 1:A:567:LYS:CB    | 1:A:568:PRO:HD2   | 1.91                     | 1.00              |
| 2:B:977:GLY:HA3   | 2:B:1099:VAL:HG21 | 1.41                     | 0.99              |
| 3:C:57:VAL:HG11   | 10:J:60:PHE:HB3   | 1.44                     | 0.99              |
| 1:A:567:LYS:HB3   | 8:H:96:VAL:H      | 1.26                     | 0.99              |
| 2:B:1002:THR:HG22 | 2:B:1006:ILE:H    | 1.22                     | 0.98              |
| 1:A:115:LEU:HB2   | 1:A:122:MET:HE2   | 1.45                     | 0.98              |
| 5:E:135:PHE:HB3   | 5:E:140:LEU:HD11  | 1.45                     | 0.98              |
| 1:A:244:PRO:HG2   | 1:A:245:PRO:HD3   | 1.46                     | 0.98              |
| 11:K:113:THR:O    | 11:K:114:LEU:HB2  | 1.60                     | 0.97              |
| 2:B:842:ASN:ND2   | 2:B:845:SER:H     | 1.62                     | 0.97              |
| 9:I:7:CYS:HB2     | 9:I:14:LEU:HD21   | 1.47                     | 0.97              |
| 2:B:1100:ASP:HA   | 2:B:1103:ILE:HD11 | 1.46                     | 0.96              |
| 3:C:167:HIS:CD2   | 3:C:169:LYS:H     | 1.83                     | 0.96              |
| 2:B:955:THR:HG22  | 2:B:956:THR:H     | 1.31                     | 0.96              |
| 2:B:392:ARG:HH21  | 9:I:52:ILE:HD11   | 1.30                     | 0.96              |
| 2:B:1159:ARG:HD3  | 2:B:1193:GLN:HG3  | 1.47                     | 0.95              |
| 2:B:174:LEU:O     | 2:B:175:ARG:HB2   | 1.64                     | 0.95              |
| 2:B:200:GLY:HA2   | 2:B:202:TYR:CE2   | 2.01                     | 0.95              |
| 2:B:1051:THR:HG22 | 2:B:1053:GLU:N    | 1.81                     | 0.95              |
| 10:J:1:MET:H1     | 10:J:56:LEU:HB2   | 1.31                     | 0.94              |
| 3:C:56:THR:HG22   | 3:C:57:VAL:H      | 1.28                     | 0.94              |
| 2:B:737:THR:HG21  | 9:I:66:PRO:O      | 1.68                     | 0.94              |
| 1:A:1399:ARG:HB3  | 1:A:1408:ILE:HD13 | 1.50                     | 0.94              |
| 2:B:639:ILE:HD11  | 2:B:691:GLU:HG3   | 1.47                     | 0.94              |
| 10:J:46:CYS:HG    | 13:J:101:ZN:ZN    | 0.78                     | 0.94              |
| 1:A:783:THR:HG22  | 1:A:784:LEU:HG    | 1.49                     | 0.93              |
| 3:C:73:GLN:HE21   | 3:C:75:MET:H      | 1.14                     | 0.93              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1281:ARG:HD2  | 1:A:1309:ASP:OD2  | 1.68                     | 0.93              |
| 2:B:1002:THR:HG22 | 2:B:1006:ILE:N    | 1.84                     | 0.92              |
| 2:B:1159:ARG:HE   | 2:B:1193:GLN:HE21 | 0.93                     | 0.92              |
| 1:A:1116:LEU:HD12 | 1:A:1329:THR:OG1  | 1.67                     | 0.92              |
| 1:A:1445:ILE:O    | 1:A:1446:ASP:CA   | 2.16                     | 0.92              |
| 2:B:824:ILE:HG12  | 10:J:48:ARG:HH12  | 1.32                     | 0.92              |
| 5:E:5:ASN:HD21    | 5:E:52:ARG:HG2    | 1.35                     | 0.92              |
| 1:A:338:GLY:HA2   | 2:B:1129:ARG:HH22 | 1.33                     | 0.92              |
| 9:I:75:CYS:HG     | 13:I:204:ZN:ZN    | 0.68                     | 0.91              |
| 1:A:1435:PRO:HA   | 1:A:1439:GLY:O    | 1.69                     | 0.91              |
| 2:B:1077:THR:HG22 | 2:B:1079:LYS:H    | 1.35                     | 0.90              |
| 1:A:590:ARG:HG3   | 1:A:590:ARG:NH1   | 1.86                     | 0.90              |
| 1:A:567:LYS:HB2   | 1:A:568:PRO:CD    | 2.01                     | 0.90              |
| 1:A:1194:ARG:NH2  | 1:A:1237:ILE:HD13 | 1.87                     | 0.90              |
| 1:A:15:LYS:HB3    | 2:B:1220:ARG:HG2  | 1.51                     | 0.90              |
| 2:B:842:ASN:HD22  | 2:B:845:SER:H     | 1.17                     | 0.90              |
| 7:G:11:UNK:CA     | 7:G:66:UNK:CA     | 2.49                     | 0.90              |
| 1:A:549:MET:SD    | 1:A:577:ILE:HD12  | 2.12                     | 0.90              |
| 3:C:167:HIS:HD2   | 3:C:169:LYS:H     | 0.90                     | 0.90              |
| 1:A:381:THR:HG22  | 1:A:383:TYR:H     | 1.35                     | 0.89              |
| 3:C:22:LEU:HD22   | 3:C:25:VAL:HG21   | 1.53                     | 0.89              |
| 9:I:111:THR:HG22  | 9:I:113:ASP:N     | 1.86                     | 0.89              |
| 1:A:567:LYS:NZ    | 8:H:46:LEU:HB2    | 1.87                     | 0.89              |
| 1:A:962:ARG:HA    | 1:A:965:GLN:HE21  | 1.37                     | 0.89              |
| 1:A:61:ILE:HG22   | 1:A:62:ASP:H      | 1.37                     | 0.89              |
| 1:A:868:TYR:HD2   | 1:A:1058:VAL:HG21 | 1.38                     | 0.88              |
| 3:C:44:LEU:HB2    | 3:C:77:ILE:HD11   | 1.55                     | 0.88              |
| 1:A:886:ILE:HD11  | 1:A:943:LEU:HB3   | 1.56                     | 0.88              |
| 3:C:57:VAL:HG11   | 10:J:60:PHE:CB    | 2.03                     | 0.88              |
| 1:A:1410:PHE:CD2  | 2:B:1212:ILE:HD11 | 2.08                     | 0.88              |
| 2:B:956:THR:HA    | 2:B:961:LEU:O     | 1.71                     | 0.88              |
| 1:A:337:ARG:NH1   | 1:A:839:ARG:HH12  | 1.72                     | 0.88              |
| 2:B:800:GLN:HB3   | 10:J:52:THR:HG21  | 1.54                     | 0.88              |
| 1:A:1105:LEU:HD22 | 1:A:1384:VAL:HG21 | 1.53                     | 0.88              |
| 6:F:93:ILE:HD11   | 6:F:134:ILE:HD11  | 1.54                     | 0.88              |
| 2:B:1065:GLN:HE21 | 2:B:1067:ARG:N    | 1.72                     | 0.88              |
| 2:B:977:GLY:HA3   | 2:B:1099:VAL:CG2  | 2.04                     | 0.87              |
| 2:B:955:THR:CG2   | 2:B:956:THR:H     | 1.87                     | 0.87              |
| 1:A:590:ARG:HG3   | 1:A:590:ARG:HH11  | 1.37                     | 0.87              |
| 1:A:666:ILE:CD1   | 2:B:1030:LEU:HD13 | 2.04                     | 0.87              |
| 2:B:228:LYS:HD3   | 2:B:234:ILE:HD13  | 1.57                     | 0.86              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:269:ILE:HD11  | 1:A:300:VAL:HA    | 1.57                     | 0.86              |
| 1:A:351:THR:HG23  | 2:B:1103:ILE:HA   | 1.53                     | 0.86              |
| 1:A:1039:LYS:O    | 1:A:1043:ASP:HB2  | 1.75                     | 0.86              |
| 2:B:130:VAL:HG21  | 2:B:167:ILE:HD12  | 1.56                     | 0.86              |
| 2:B:512:ARG:HH21  | 2:B:535:LEU:CD1   | 1.88                     | 0.86              |
| 1:A:667:GLY:HA2   | 1:A:670:ILE:HD12  | 1.56                     | 0.86              |
| 1:A:1192:LEU:HD11 | 1:A:1239:ARG:HB3  | 1.57                     | 0.86              |
| 1:A:1242:VAL:HG12 | 1:A:1243:VAL:H    | 1.40                     | 0.86              |
| 2:B:345:LYS:CA    | 2:B:348:ARG:HE    | 1.87                     | 0.86              |
| 2:B:955:THR:HG22  | 2:B:956:THR:N     | 1.86                     | 0.85              |
| 2:B:519:TRP:HZ2   | 2:B:705:MET:HE1   | 1.37                     | 0.85              |
| 1:A:417:TYR:O     | 1:A:418:SER:HB2   | 1.75                     | 0.85              |
| 12:L:60:ARG:HG3   | 12:L:61:THR:N     | 1.85                     | 0.85              |
| 2:B:744:HIS:HD2   | 2:B:746:SER:H     | 1.23                     | 0.85              |
| 8:H:125:LEU:HG    | 8:H:130:ARG:NH1   | 1.92                     | 0.85              |
| 11:K:10:PHE:CD1   | 11:K:11:LEU:HD13  | 2.11                     | 0.85              |
| 2:B:801:LYS:O     | 10:J:52:THR:HG23  | 1.76                     | 0.85              |
| 2:B:519:TRP:CZ2   | 2:B:705:MET:HE1   | 2.11                     | 0.84              |
| 5:E:177:ARG:HD3   | 5:E:215:MET:SD    | 2.18                     | 0.84              |
| 11:K:12:LEU:H     | 11:K:12:LEU:HD12  | 1.42                     | 0.84              |
| 2:B:108:VAL:HG12  | 2:B:109:THR:H     | 1.42                     | 0.84              |
| 1:A:804:TYR:HE1   | 2:B:1021:MET:HE3  | 1.40                     | 0.84              |
| 2:B:345:LYS:HA    | 2:B:348:ARG:NE    | 1.91                     | 0.84              |
| 2:B:1106:ARG:HH21 | 2:B:1109:GLY:H    | 1.24                     | 0.84              |
| 10:J:48:ARG:HH21  | 10:J:49:MET:HE1   | 1.42                     | 0.84              |
| 2:B:912:ILE:O     | 2:B:938:SER:HB2   | 1.76                     | 0.83              |
| 2:B:1106:ARG:NH1  | 2:B:1118:PRO:HB3  | 1.91                     | 0.83              |
| 5:E:2:ASP:O       | 5:E:3:GLN:HG2     | 1.78                     | 0.83              |
| 1:A:709:THR:HG21  | 9:I:93:LYS:O      | 1.77                     | 0.83              |
| 1:A:1118:VAL:CG2  | 1:A:1306:LEU:HB2  | 2.08                     | 0.83              |
| 3:C:11:ARG:NH2    | 3:C:229:TYR:HD2   | 1.77                     | 0.83              |
| 6:F:147:SER:OG    | 6:F:150:GLU:HG3   | 1.78                     | 0.83              |
| 1:A:605:MET:HE3   | 1:A:614:PHE:O     | 1.79                     | 0.83              |
| 1:A:683:ILE:HD11  | 1:A:764:CYS:HB2   | 1.61                     | 0.83              |
| 1:A:443:LEU:HD22  | 1:A:455:MET:HE2   | 1.58                     | 0.83              |
| 1:A:535:THR:HG21  | 1:A:617:VAL:H     | 1.43                     | 0.83              |
| 2:B:1002:THR:CG2  | 2:B:1006:ILE:H    | 1.91                     | 0.83              |
| 1:A:1390:ASN:ND2  | 1:A:1399:ARG:HA   | 1.93                     | 0.82              |
| 2:B:200:GLY:HA2   | 2:B:202:TYR:HE2   | 1.42                     | 0.82              |
| 2:B:763:GLN:HG2   | 2:B:765:PRO:HD2   | 1.61                     | 0.82              |
| 1:A:1348:LEU:HD23 | 1:A:1372:VAL:HG13 | 1.59                     | 0.82              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:565:ILE:HG23  | 1:A:567:LYS:HG2   | 1.62                     | 0.82              |
| 2:B:637:LEU:HD12  | 2:B:693:ILE:HD12  | 1.60                     | 0.82              |
| 2:B:1106:ARG:HH21 | 2:B:1109:GLY:N    | 1.78                     | 0.81              |
| 8:H:93:TYR:HB3    | 8:H:144:ILE:O     | 1.80                     | 0.81              |
| 1:A:208:LEU:HD22  | 1:A:212:LYS:HE3   | 1.62                     | 0.81              |
| 2:B:1065:GLN:HE21 | 2:B:1067:ARG:H    | 1.29                     | 0.81              |
| 2:B:1106:ARG:HE   | 2:B:1109:GLY:N    | 1.79                     | 0.81              |
| 1:A:406:ILE:HB    | 1:A:431:LYS:HB2   | 1.61                     | 0.81              |
| 1:A:885:THR:HG23  | 1:A:893:PHE:HE1   | 1.44                     | 0.81              |
| 1:A:1017:LEU:HB2  | 5:E:206:GLY:H     | 1.44                     | 0.81              |
| 1:A:1111:MET:HE1  | 1:A:1330:ASN:OD1  | 1.79                     | 0.81              |
| 1:A:353:ILE:CD1   | 1:A:487:MET:HE3   | 2.07                     | 0.81              |
| 1:A:511:ILE:HG12  | 1:A:521:MET:HE3   | 1.62                     | 0.81              |
| 2:B:121:ASN:N     | 2:B:121:ASN:HD22  | 1.79                     | 0.81              |
| 1:A:742:ASN:HA    | 1:A:745:GLN:HB2   | 1.63                     | 0.81              |
| 3:C:148:ARG:NH1   | 10:J:64:ASN:HA    | 1.96                     | 0.81              |
| 10:J:3:VAL:HG21   | 10:J:18:TRP:HB2   | 1.61                     | 0.81              |
| 2:B:244:LEU:O     | 2:B:249:ARG:HG2   | 1.81                     | 0.81              |
| 1:A:563:PRO:HG3   | 1:A:572:TRP:CZ2   | 2.15                     | 0.80              |
| 2:B:1106:ARG:NH2  | 2:B:1109:GLY:H    | 1.79                     | 0.80              |
| 8:H:5:LEU:HD11    | 8:H:135:LEU:HG    | 1.63                     | 0.80              |
| 2:B:899:ILE:HD11  | 2:B:911:ILE:HA    | 1.63                     | 0.80              |
| 2:B:999:MET:HG3   | 2:B:1000:PRO:HD2  | 1.61                     | 0.80              |
| 1:A:855:THR:HG21  | 1:A:857:ARG:NE    | 1.95                     | 0.80              |
| 2:B:796:LEU:HB3   | 2:B:799:PRO:HG3   | 1.63                     | 0.80              |
| 8:H:81:PRO:HB2    | 8:H:82:PRO:CD     | 2.11                     | 0.80              |
| 2:B:800:GLN:HB3   | 10:J:52:THR:CG2   | 2.11                     | 0.80              |
| 2:B:834:ASN:HB3   | 2:B:840:ILE:HG13  | 1.63                     | 0.80              |
| 1:A:868:TYR:CE1   | 1:A:1064:VAL:HG11 | 2.17                     | 0.80              |
| 2:B:293:PRO:HG2   | 2:B:296:GLU:CB    | 2.12                     | 0.80              |
| 3:C:167:HIS:HD2   | 3:C:169:LYS:N     | 1.76                     | 0.80              |
| 8:H:89:LEU:C      | 8:H:91:ASP:H      | 1.90                     | 0.80              |
| 9:I:50:THR:CG2    | 9:I:52:ILE:HG23   | 2.11                     | 0.80              |
| 2:B:118:ARG:HH22  | 2:B:194:GLU:CD    | 1.90                     | 0.80              |
| 1:A:40:THR:HG22   | 1:A:41:MET:HG3    | 1.64                     | 0.80              |
| 10:J:3:VAL:HG21   | 10:J:18:TRP:CB    | 2.12                     | 0.79              |
| 1:A:1299:VAL:HG12 | 1:A:1300:LYS:H    | 1.47                     | 0.79              |
| 2:B:542:MET:HE3   | 2:B:747:MET:HG3   | 1.63                     | 0.79              |
| 3:C:37:MET:HG2    | 3:C:243:VAL:HG12  | 1.62                     | 0.79              |
| 8:H:81:PRO:HB2    | 8:H:82:PRO:HD3    | 1.62                     | 0.79              |
| 1:A:523:ILE:HD12  | 1:A:622:VAL:CG2   | 2.12                     | 0.79              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:32:VAL:HG21   | 1:A:68:GLN:NE2    | 1.97                     | 0.79              |
| 2:B:269:ILE:HD11  | 2:B:386:LEU:HD21  | 1.62                     | 0.79              |
| 2:B:1100:ASP:HA   | 2:B:1103:ILE:CD1  | 2.12                     | 0.79              |
| 1:A:93:VAL:CG1    | 1:A:301:ALA:HB1   | 2.11                     | 0.79              |
| 1:A:666:ILE:HD13  | 2:B:1030:LEU:HD22 | 1.65                     | 0.79              |
| 1:A:298:PHE:O     | 1:A:302:THR:HB    | 1.83                     | 0.79              |
| 1:A:337:ARG:NH1   | 1:A:839:ARG:NH1   | 2.29                     | 0.79              |
| 1:A:679:ILE:HG23  | 1:A:729:ALA:HB1   | 1.63                     | 0.79              |
| 1:A:768:GLN:CG    | 1:A:816:HIS:HA    | 2.13                     | 0.78              |
| 2:B:487:THR:HG22  | 2:B:489:SER:H     | 1.48                     | 0.78              |
| 2:B:855:PHE:HZ    | 2:B:857:ARG:NH1   | 1.81                     | 0.78              |
| 1:A:472:LEU:O     | 1:A:475:THR:HB    | 1.81                     | 0.78              |
| 1:A:783:THR:HG21  | 1:A:815:PHE:CZ    | 2.19                     | 0.78              |
| 10:J:64:ASN:HB3   | 10:J:65:PRO:HD3   | 1.63                     | 0.78              |
| 1:A:313:GLN:HB2   | 1:A:322:VAL:CG2   | 2.14                     | 0.78              |
| 1:A:1076:ALA:HA   | 1:A:1079:MET:HE2  | 1.65                     | 0.78              |
| 1:A:1438:THR:HB   | 2:B:1144:ALA:HB3  | 1.66                     | 0.78              |
| 2:B:842:ASN:ND2   | 2:B:845:SER:N     | 2.31                     | 0.78              |
| 1:A:313:GLN:HB2   | 1:A:322:VAL:HG23  | 1.64                     | 0.78              |
| 1:A:399:HIS:O     | 1:A:401:GLY:N     | 2.17                     | 0.78              |
| 2:B:583:ASN:HD21  | 2:B:628:THR:HB    | 1.49                     | 0.78              |
| 1:A:23:SER:HB3    | 1:A:233:TRP:CZ2   | 2.19                     | 0.78              |
| 1:A:58:LEU:HD22   | 1:A:80:HIS:O      | 1.83                     | 0.78              |
| 2:B:1106:ARG:HE   | 2:B:1109:GLY:H    | 1.29                     | 0.78              |
| 3:C:56:THR:HG22   | 3:C:57:VAL:N      | 1.97                     | 0.78              |
| 2:B:102:VAL:CG2   | 2:B:112:LEU:HB2   | 2.13                     | 0.77              |
| 2:B:392:ARG:NH2   | 9:I:52:ILE:HD11   | 1.98                     | 0.77              |
| 1:A:326:ARG:HG2   | 1:A:1406:VAL:HG21 | 1.66                     | 0.77              |
| 2:B:707:PRO:HG2   | 2:B:708:GLU:H     | 1.49                     | 0.77              |
| 2:B:1100:ASP:OD1  | 2:B:1103:ILE:HD11 | 1.84                     | 0.77              |
| 1:A:913:LEU:HD12  | 1:A:914:GLU:N     | 1.98                     | 0.77              |
| 1:A:1281:ARG:O    | 1:A:1282:VAL:HG23 | 1.83                     | 0.77              |
| 3:C:165:LYS:O     | 11:K:6:ARG:NH1    | 2.17                     | 0.77              |
| 1:A:849:MET:HE3   | 1:A:1061:GLY:HA2  | 1.67                     | 0.77              |
| 1:A:901:LEU:H     | 1:A:926:GLN:NE2   | 1.82                     | 0.77              |
| 1:A:31:SER:CB     | 1:A:83:HIS:HB2    | 2.15                     | 0.77              |
| 2:B:708:GLU:HG3   | 2:B:709:ASP:N     | 1.98                     | 0.77              |
| 3:C:124:LEU:O     | 3:C:127:ARG:HG2   | 1.85                     | 0.77              |
| 2:B:102:VAL:HG23  | 2:B:112:LEU:HB2   | 1.65                     | 0.77              |
| 1:A:1118:VAL:HG22 | 1:A:1306:LEU:HB2  | 1.64                     | 0.77              |
| 4:D:81:UNK:CA     | 4:D:82:UNK:CA     | 2.63                     | 0.77              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:70:CYS:O      | 1:A:72:GLU:HG2    | 1.84                     | 0.77              |
| 2:B:1096:ARG:O    | 2:B:1097:HIS:HB2  | 1.84                     | 0.77              |
| 1:A:1345:ARG:HD2  | 1:A:1373:ASP:OD1  | 1.84                     | 0.76              |
| 3:C:57:VAL:CG1    | 10:J:60:PHE:HB3   | 2.15                     | 0.76              |
| 11:K:47:ARG:HB3   | 11:K:47:ARG:HH11  | 1.49                     | 0.76              |
| 1:A:896:ARG:HD3   | 1:A:897:TYR:CE1   | 2.21                     | 0.76              |
| 3:C:166:GLU:HG3   | 11:K:10:PHE:HZ    | 1.51                     | 0.76              |
| 8:H:40:LEU:HD23   | 8:H:42:ILE:HD11   | 1.65                     | 0.76              |
| 2:B:232:SER:OG    | 2:B:234:ILE:HD12  | 1.84                     | 0.76              |
| 5:E:61:GLN:HE21   | 5:E:105:PHE:HE2   | 1.34                     | 0.76              |
| 8:H:93:TYR:HA     | 8:H:145:ARG:HB3   | 1.68                     | 0.76              |
| 11:K:55:LYS:HB3   | 11:K:81:TYR:HD1   | 1.50                     | 0.76              |
| 1:A:341:MET:HE1   | 1:A:1401:SER:HB2  | 1.68                     | 0.76              |
| 2:B:496:ARG:NH1   | 2:B:539:LEU:HB2   | 1.99                     | 0.76              |
| 2:B:899:ILE:CD1   | 2:B:911:ILE:HA    | 2.16                     | 0.76              |
| 2:B:770:GLN:HG2   | 2:B:983:ARG:O     | 1.86                     | 0.76              |
| 1:A:24:PRO:HB3    | 1:A:237:THR:HB    | 1.67                     | 0.76              |
| 2:B:708:GLU:CG    | 2:B:709:ASP:H     | 1.97                     | 0.76              |
| 2:B:996:ARG:NH2   | 3:C:174:ALA:O     | 2.19                     | 0.76              |
| 1:A:804:TYR:CE1   | 2:B:1021:MET:HE3  | 2.21                     | 0.76              |
| 1:A:1323:ASP:OD1  | 1:A:1325:THR:HB   | 1.86                     | 0.76              |
| 2:B:118:ARG:HG3   | 2:B:204:ILE:HD13  | 1.67                     | 0.75              |
| 2:B:842:ASN:HD22  | 2:B:845:SER:N     | 1.83                     | 0.75              |
| 1:A:95:PHE:O      | 1:A:99:ILE:HG13   | 1.85                     | 0.75              |
| 1:A:1094:VAL:HG13 | 1:A:1113:THR:HG21 | 1.66                     | 0.75              |
| 2:B:211:VAL:HG21  | 2:B:483:LEU:HD13  | 1.67                     | 0.75              |
| 2:B:542:MET:HG3   | 2:B:747:MET:HE3   | 1.66                     | 0.75              |
| 1:A:541:ILE:HG12  | 1:A:549:MET:HE1   | 1.66                     | 0.75              |
| 12:L:38:LEU:O     | 12:L:39:SER:HB3   | 1.85                     | 0.75              |
| 1:A:41:MET:HA     | 1:A:49:LYS:HA     | 1.68                     | 0.75              |
| 2:B:1166:CYS:O    | 2:B:1168:LEU:N    | 2.18                     | 0.75              |
| 10:J:12:LYS:O     | 10:J:14:VAL:HG23  | 1.85                     | 0.75              |
| 2:B:423:LYS:HA    | 2:B:426:LYS:HE2   | 1.68                     | 0.75              |
| 2:B:651:LEU:HD11  | 2:B:707:PRO:HB3   | 1.69                     | 0.75              |
| 1:A:223:GLY:O     | 1:A:1415:SER:HA   | 1.86                     | 0.75              |
| 1:A:265:LYS:NZ    | 1:A:323:LYS:H     | 1.84                     | 0.75              |
| 2:B:542:MET:HE1   | 2:B:743:ILE:HG21  | 1.69                     | 0.75              |
| 1:A:469:ARG:HH21  | 2:B:976:ILE:HD13  | 1.51                     | 0.75              |
| 5:E:69:ILE:HG23   | 5:E:73:PRO:HA     | 1.67                     | 0.75              |
| 1:A:336:ILE:HD12  | 1:A:1405:THR:HG21 | 1.68                     | 0.74              |
| 1:A:458:HIS:CE1   | 1:A:507:VAL:HG21  | 2.23                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:521:LEU:HD22  | 2:B:633:VAL:HG12  | 1.69                     | 0.74              |
| 2:B:711:GLU:N     | 2:B:712:PRO:HD3   | 2.01                     | 0.74              |
| 1:A:535:THR:CG2   | 1:A:616:VAL:HA    | 2.18                     | 0.74              |
| 1:A:1146:VAL:HG11 | 1:A:1202:MET:SD   | 2.27                     | 0.74              |
| 1:A:1436:ILE:HG22 | 1:A:1437:GLY:N    | 2.02                     | 0.74              |
| 1:A:1436:ILE:CG2  | 2:B:1142:GLY:HA2  | 2.17                     | 0.74              |
| 2:B:62:ILE:HG23   | 2:B:418:LYS:HG2   | 1.69                     | 0.74              |
| 6:F:111:LEU:HD12  | 6:F:111:LEU:N     | 2.02                     | 0.74              |
| 1:A:1399:ARG:HB2  | 1:A:1408:ILE:HG21 | 1.70                     | 0.74              |
| 1:A:693:VAL:HG21  | 1:A:721:PHE:HE1   | 1.51                     | 0.74              |
| 1:A:443:LEU:HD21  | 1:A:455:MET:HB3   | 1.70                     | 0.74              |
| 2:B:570:VAL:HB    | 2:B:573:GLN:CB    | 2.18                     | 0.74              |
| 1:A:858:ASN:C     | 1:A:858:ASN:HD22  | 1.96                     | 0.74              |
| 2:B:46:GLN:HG3    | 2:B:47:GLN:N      | 2.03                     | 0.74              |
| 2:B:879:ARG:HB3   | 2:B:883:LEU:HD23  | 1.70                     | 0.74              |
| 2:B:882:THR:HG22  | 2:B:884:ARG:H     | 1.50                     | 0.74              |
| 1:A:268:ASP:HB3   | 1:A:299:HIS:CE1   | 2.23                     | 0.74              |
| 1:A:575:LYS:HB3   | 1:A:612:ILE:CG2   | 2.17                     | 0.74              |
| 1:A:534:LEU:O     | 1:A:574:GLY:HA3   | 1.88                     | 0.74              |
| 1:A:853:ASP:OD1   | 1:A:855:THR:HB    | 1.88                     | 0.74              |
| 1:A:567:LYS:HB3   | 8:H:96:VAL:N      | 2.02                     | 0.73              |
| 5:E:61:GLN:NE2    | 5:E:105:PHE:HE2   | 1.86                     | 0.73              |
| 8:H:89:LEU:HB3    | 8:H:91:ASP:OD1    | 1.88                     | 0.73              |
| 1:A:925:LEU:O     | 1:A:929:LEU:HD23  | 1.88                     | 0.73              |
| 1:A:154:SER:HB3   | 1:A:162:VAL:CG2   | 2.17                     | 0.73              |
| 1:A:710:LEU:H     | 1:A:710:LEU:HD12  | 1.52                     | 0.73              |
| 2:B:172:ILE:HD13  | 2:B:178:ASN:HB3   | 1.70                     | 0.73              |
| 2:B:980:PHE:CE2   | 2:B:1094:ARG:HG3  | 2.23                     | 0.73              |
| 8:H:123:MET:HE1   | 8:H:142:LEU:CD1   | 2.17                     | 0.73              |
| 1:A:445:ASN:HB2   | 1:A:455:MET:HG2   | 1.70                     | 0.73              |
| 1:A:899:VAL:HB    | 1:A:929:LEU:HD12  | 1.71                     | 0.73              |
| 5:E:124:VAL:HA    | 5:E:132:ILE:HD12  | 1.70                     | 0.73              |
| 8:H:123:MET:HE1   | 8:H:142:LEU:HD13  | 1.69                     | 0.73              |
| 2:B:193:LYS:HD3   | 2:B:787:VAL:HG11  | 1.70                     | 0.73              |
| 8:H:35:GLN:HB3    | 8:H:111:LEU:HD21  | 1.70                     | 0.73              |
| 1:A:1258:HIS:ND1  | 1:A:1262:LYS:HE3  | 2.04                     | 0.73              |
| 2:B:313:MET:HE3   | 2:B:386:LEU:HD22  | 1.68                     | 0.73              |
| 2:B:363:HIS:O     | 2:B:364:ILE:HB    | 1.88                     | 0.73              |
| 2:B:1106:ARG:NE   | 2:B:1109:GLY:H    | 1.85                     | 0.73              |
| 1:A:500:GLU:OE2   | 2:B:1145:SER:HB2  | 1.88                     | 0.73              |
| 2:B:1072:MET:HE3  | 2:B:1085:ILE:HD12 | 1.70                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:321:PRO:O     | 1:A:322:VAL:HB    | 1.87                     | 0.73              |
| 1:A:445:ASN:CB    | 1:A:455:MET:HG2   | 2.19                     | 0.73              |
| 1:A:1441:PHE:CZ   | 6:F:89:GLU:HA     | 2.23                     | 0.73              |
| 1:A:868:TYR:CD2   | 1:A:1058:VAL:HG21 | 2.23                     | 0.72              |
| 1:A:901:LEU:HG    | 1:A:926:GLN:HE21  | 1.54                     | 0.72              |
| 1:A:1436:ILE:HG22 | 1:A:1437:GLY:H    | 1.52                     | 0.72              |
| 1:A:337:ARG:NE    | 1:A:839:ARG:HH22  | 1.88                     | 0.72              |
| 2:B:58:THR:O      | 2:B:62:ILE:HG13   | 1.89                     | 0.72              |
| 2:B:313:MET:CE    | 2:B:386:LEU:HD22  | 2.19                     | 0.72              |
| 1:A:32:VAL:HB     | 1:A:57:ARG:HD2    | 1.71                     | 0.72              |
| 2:B:570:VAL:HG21  | 2:B:573:GLN:NE2   | 2.04                     | 0.72              |
| 2:B:708:GLU:O     | 2:B:710:LEU:N     | 2.22                     | 0.72              |
| 2:B:745:PRO:O     | 2:B:748:ILE:HG12  | 1.89                     | 0.72              |
| 1:A:399:HIS:HB3   | 1:A:400:PRO:HD3   | 1.69                     | 0.72              |
| 1:A:855:THR:HG23  | 1:A:857:ARG:HG3   | 1.72                     | 0.72              |
| 1:A:1209:MET:SD   | 1:A:1236:LEU:HB3  | 2.30                     | 0.72              |
| 1:A:567:LYS:HZ1   | 8:H:46:LEU:HB2    | 1.55                     | 0.72              |
| 1:A:857:ARG:HD3   | 1:A:861:GLY:O     | 1.88                     | 0.72              |
| 11:K:65:HIS:CD2   | 11:K:67:PHE:H     | 2.06                     | 0.72              |
| 1:A:351:THR:HG21  | 2:B:1103:ILE:HG23 | 1.71                     | 0.72              |
| 1:A:575:LYS:HB3   | 1:A:612:ILE:HG23  | 1.71                     | 0.72              |
| 2:B:999:MET:HE2   | 2:B:1011:ILE:HD11 | 1.71                     | 0.72              |
| 9:I:74:GLU:HB3    | 9:I:79:HIS:HA     | 1.70                     | 0.72              |
| 1:A:567:LYS:HD3   | 8:H:95:TYR:CD1    | 2.25                     | 0.72              |
| 1:A:1299:VAL:HG12 | 1:A:1300:LYS:N    | 2.02                     | 0.72              |
| 1:A:994:GLN:HE22  | 1:A:1023:ARG:HE   | 1.38                     | 0.72              |
| 8:H:5:LEU:HB3     | 8:H:133:ASN:O     | 1.88                     | 0.72              |
| 1:A:828:ALA:HB2   | 2:B:530:GLY:HA2   | 1.70                     | 0.72              |
| 1:A:900:ASP:OD2   | 1:A:903:ASN:HB2   | 1.90                     | 0.72              |
| 2:B:955:THR:CG2   | 2:B:956:THR:N     | 2.49                     | 0.71              |
| 1:A:567:LYS:HE3   | 8:H:46:LEU:HD12   | 1.71                     | 0.71              |
| 1:A:1397:LEU:O    | 1:A:1400:CYS:HB2  | 1.89                     | 0.71              |
| 1:A:503:GLN:HE21  | 6:F:90:ARG:NH2    | 1.88                     | 0.71              |
| 2:B:108:VAL:HG12  | 2:B:109:THR:N     | 2.06                     | 0.71              |
| 2:B:309:GLN:HG3   | 9:I:52:ILE:HD13   | 1.72                     | 0.71              |
| 2:B:555:ILE:HD13  | 2:B:587:HIS:CE1   | 2.26                     | 0.71              |
| 11:K:7:PHE:HB2    | 11:K:11:LEU:HD22  | 1.72                     | 0.71              |
| 1:A:598:LEU:HD22  | 8:H:25:ARG:NH1    | 2.05                     | 0.71              |
| 2:B:234:ILE:HD12  | 2:B:234:ILE:H     | 1.53                     | 0.71              |
| 5:E:168:TYR:HB3   | 5:E:170:LEU:HD21  | 1.72                     | 0.71              |
| 1:A:417:TYR:O     | 1:A:418:SER:CB    | 2.36                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1007:VAL:HG22 | 2:B:1008:PRO:HD2  | 1.71                     | 0.71              |
| 3:C:98:VAL:C      | 3:C:99:LEU:HD23   | 2.16                     | 0.71              |
| 1:A:1152:ILE:HG23 | 1:A:1260:LEU:HD23 | 1.71                     | 0.71              |
| 1:A:44:THR:O      | 1:A:45:GLN:HB2    | 1.91                     | 0.71              |
| 1:A:75:ASN:O      | 1:A:76:GLU:HB3    | 1.88                     | 0.71              |
| 1:A:225:ASN:O     | 1:A:227:VAL:N     | 2.21                     | 0.71              |
| 1:A:340:LEU:HD21  | 2:B:1200:ALA:HB2  | 1.72                     | 0.71              |
| 1:A:383:TYR:HB3   | 6:F:115:THR:HG22  | 1.73                     | 0.71              |
| 1:A:672:ASP:HB2   | 1:A:736:ASN:OD1   | 1.90                     | 0.71              |
| 1:A:1332:PHE:H    | 1:A:1332:PHE:HD2  | 1.38                     | 0.71              |
| 1:A:367:PRO:HB3   | 1:A:466:SER:HA    | 1.73                     | 0.70              |
| 1:A:451:HIS:NE2   | 1:A:1074:GLU:HG3  | 2.07                     | 0.70              |
| 1:A:675:THR:HG21  | 1:A:736:ASN:ND2   | 2.06                     | 0.70              |
| 1:A:1015:VAL:HG12 | 1:A:1019:CYS:SG   | 2.32                     | 0.70              |
| 2:B:637:LEU:CD1   | 2:B:693:ILE:HD12  | 2.20                     | 0.70              |
| 11:K:65:HIS:HD2   | 11:K:67:PHE:H     | 1.35                     | 0.70              |
| 1:A:741:ASN:HD22  | 1:A:741:ASN:C     | 1.99                     | 0.70              |
| 1:A:48:ALA:O      | 1:A:49:LYS:HG3    | 1.89                     | 0.70              |
| 1:A:691:LEU:HD11  | 1:A:695:LYS:HE3   | 1.71                     | 0.70              |
| 2:B:636:PRO:O     | 2:B:637:LEU:HG    | 1.90                     | 0.70              |
| 2:B:737:THR:HG23  | 9:I:66:PRO:CB     | 2.20                     | 0.70              |
| 2:B:792:MET:HA    | 2:B:856:PHE:O     | 1.91                     | 0.70              |
| 1:A:463:ILE:HB    | 1:A:464:PRO:HD2   | 1.74                     | 0.70              |
| 3:C:18:VAL:HG23   | 3:C:240:VAL:HG11  | 1.72                     | 0.70              |
| 2:B:130:VAL:HG12  | 2:B:131:ASP:N     | 2.07                     | 0.70              |
| 2:B:463:THR:CG2   | 2:B:465:ASN:HD22  | 2.05                     | 0.70              |
| 2:B:542:MET:CE    | 2:B:747:MET:HG3   | 2.22                     | 0.70              |
| 11:K:55:LYS:HD3   | 11:K:78:THR:CB    | 2.20                     | 0.70              |
| 1:A:1208:THR:HB   | 1:A:1211:GLN:HG3  | 1.74                     | 0.70              |
| 1:A:1394:THR:HG23 | 1:A:1398:MET:HE3  | 1.74                     | 0.70              |
| 2:B:281:PRO:HG2   | 2:B:284:ILE:HD12  | 1.73                     | 0.70              |
| 2:B:957:ASN:HD22  | 2:B:961:LEU:HD12  | 1.57                     | 0.70              |
| 12:L:47:ARG:HG2   | 12:L:52:GLY:HA2   | 1.72                     | 0.70              |
| 1:A:335:ARG:HA    | 1:A:339:ASN:HD22  | 1.57                     | 0.70              |
| 2:B:65:GLU:HG3    | 2:B:66:ASP:H      | 1.56                     | 0.70              |
| 5:E:56:LYS:HG3    | 5:E:84:ASP:HB2    | 1.73                     | 0.70              |
| 1:A:567:LYS:HE3   | 8:H:46:LEU:CD1    | 2.22                     | 0.70              |
| 11:K:55:LYS:HD3   | 11:K:78:THR:HB    | 1.72                     | 0.70              |
| 2:B:1066:SER:O    | 2:B:1067:ARG:HD3  | 1.90                     | 0.69              |
| 8:H:36:CYS:SG     | 8:H:130:ARG:NH2   | 2.65                     | 0.69              |
| 1:A:72:GLU:OE2    | 2:B:1175:LEU:HD12 | 1.92                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:675:THR:CB    | 1:A:736:ASN:HD21  | 2.04                     | 0.69              |
| 2:B:293:PRO:HG2   | 2:B:296:GLU:HB3   | 1.74                     | 0.69              |
| 1:A:763:ALA:O     | 1:A:803:SER:HB3   | 1.92                     | 0.69              |
| 8:H:49:VAL:HG12   | 8:H:50:ALA:N      | 2.07                     | 0.69              |
| 1:A:472:LEU:HD11  | 2:B:835:GLN:NE2   | 2.08                     | 0.69              |
| 1:A:584:ASN:O     | 1:A:637:LYS:HE3   | 1.92                     | 0.69              |
| 2:B:839:MET:HE3   | 2:B:1010:LEU:HD11 | 1.74                     | 0.69              |
| 2:B:955:THR:HG23  | 12:L:54:ARG:O     | 1.91                     | 0.69              |
| 1:A:768:GLN:HG2   | 1:A:816:HIS:HA    | 1.75                     | 0.69              |
| 5:E:83:CYS:SG     | 5:E:88:VAL:HG22   | 2.32                     | 0.69              |
| 1:A:343:LYS:HE3   | 2:B:1151:LEU:O    | 1.92                     | 0.69              |
| 3:C:80:LEU:HD22   | 3:C:129:ILE:CD1   | 2.21                     | 0.69              |
| 1:A:414:ASP:OD1   | 1:A:416:ARG:HG2   | 1.93                     | 0.69              |
| 1:A:1445:ILE:C    | 1:A:1446:ASP:CA   | 2.65                     | 0.69              |
| 2:B:280:ILE:CD1   | 2:B:334:ILE:HG12  | 2.23                     | 0.69              |
| 2:B:638:PHE:CE1   | 2:B:743:ILE:HA    | 2.26                     | 0.69              |
| 1:A:340:LEU:HD13  | 1:A:1429:ILE:HG23 | 1.74                     | 0.69              |
| 2:B:378:LEU:O     | 2:B:382:ILE:HG13  | 1.92                     | 0.69              |
| 2:B:1056:SER:HB3  | 2:B:1066:SER:HB2  | 1.73                     | 0.68              |
| 1:A:392:VAL:HG13  | 1:A:415:LEU:HD11  | 1.74                     | 0.68              |
| 1:A:694:THR:O     | 1:A:698:GLN:HG3   | 1.94                     | 0.68              |
| 8:H:7:ASP:O       | 8:H:8:ASP:HB2     | 1.92                     | 0.68              |
| 1:A:599:SER:HB2   | 1:A:603:ASN:H     | 1.58                     | 0.68              |
| 1:A:391:LEU:HD22  | 1:A:400:PRO:O     | 1.93                     | 0.68              |
| 2:B:54:PHE:HA     | 2:B:58:THR:HB     | 1.74                     | 0.68              |
| 3:C:39:ALA:HA     | 3:C:164:ALA:HB3   | 1.74                     | 0.68              |
| 3:C:93:ASP:O      | 3:C:127:ARG:NH2   | 2.27                     | 0.68              |
| 2:B:22:SER:O      | 2:B:654:ARG:HD2   | 1.94                     | 0.68              |
| 2:B:884:ARG:O     | 2:B:936:ASP:HB3   | 1.93                     | 0.68              |
| 2:B:976:ILE:O     | 2:B:990:ILE:HB    | 1.94                     | 0.68              |
| 6:F:81:THR:HG21   | 6:F:136:ARG:CD    | 2.20                     | 0.68              |
| 1:A:381:THR:HG22  | 1:A:383:TYR:N     | 2.09                     | 0.68              |
| 2:B:314:LEU:O     | 2:B:317:CYS:HB2   | 1.92                     | 0.68              |
| 3:C:51:VAL:HG22   | 3:C:155:LEU:HD22  | 1.76                     | 0.68              |
| 9:I:53:GLY:O      | 9:I:89:GLN:HB2    | 1.94                     | 0.68              |
| 12:L:46:VAL:HG13  | 12:L:56:LEU:HD12  | 1.76                     | 0.68              |
| 1:A:446:ARG:HG2   | 1:A:446:ARG:HH11  | 1.59                     | 0.68              |
| 1:A:1095:THR:HG22 | 1:A:1100:ARG:HB2  | 1.74                     | 0.68              |
| 2:B:709:ASP:O     | 2:B:710:LEU:HD23  | 1.94                     | 0.68              |
| 2:B:986:GLN:OE1   | 2:B:986:GLN:HA    | 1.92                     | 0.68              |
| 3:C:166:GLU:HG3   | 11:K:10:PHE:CZ    | 2.29                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:254:LYS:HB3   | 11:K:42:LEU:HD11  | 1.75                     | 0.68              |
| 2:B:280:ILE:HG22  | 2:B:285:ILE:HG13  | 1.76                     | 0.68              |
| 2:B:842:ASN:ND2   | 2:B:844:SER:HB2   | 2.09                     | 0.68              |
| 2:B:954:VAL:O     | 12:L:55:ILE:O     | 2.11                     | 0.68              |
| 1:A:535:THR:HG21  | 1:A:616:VAL:HA    | 1.76                     | 0.67              |
| 2:B:562:GLY:HA3   | 2:B:590:HIS:CE1   | 2.29                     | 0.67              |
| 2:B:711:GLU:N     | 2:B:712:PRO:CD    | 2.57                     | 0.67              |
| 1:A:693:VAL:CG2   | 1:A:721:PHE:HE1   | 2.07                     | 0.67              |
| 2:B:288:ALA:HB1   | 2:B:331:LEU:HD12  | 1.75                     | 0.67              |
| 12:L:40:LEU:HD13  | 12:L:44:ASP:CG    | 2.19                     | 0.67              |
| 1:A:786:HIS:HE1   | 2:B:742:GLU:OE1   | 1.76                     | 0.67              |
| 1:A:351:THR:CG2   | 2:B:1103:ILE:HG23 | 2.24                     | 0.67              |
| 2:B:882:THR:HG21  | 2:B:935:ARG:HA    | 1.75                     | 0.67              |
| 2:B:1002:THR:HG23 | 2:B:1004:GLU:N    | 2.10                     | 0.67              |
| 1:A:994:GLN:HE21  | 1:A:1019:CYS:HB3  | 1.59                     | 0.67              |
| 2:B:603:LEU:HB3   | 2:B:609:ILE:HG13  | 1.76                     | 0.67              |
| 2:B:1106:ARG:CZ   | 2:B:1109:GLY:H    | 2.07                     | 0.67              |
| 1:A:16:GLU:HB3    | 1:A:1418:LEU:HD11 | 1.77                     | 0.67              |
| 1:A:1390:ASN:HD22 | 1:A:1399:ARG:HA   | 1.57                     | 0.67              |
| 2:B:287:ARG:NH2   | 2:B:294:ASP:OD2   | 2.28                     | 0.67              |
| 5:E:127:ILE:O     | 5:E:127:ILE:HG13  | 1.93                     | 0.67              |
| 8:H:115:TYR:CE2   | 8:H:124:ARG:HG3   | 2.30                     | 0.67              |
| 1:A:353:ILE:HD13  | 1:A:487:MET:CE    | 2.14                     | 0.67              |
| 1:A:453:MET:HB3   | 1:A:477:PRO:HB3   | 1.76                     | 0.67              |
| 3:C:260:LEU:O     | 3:C:264:GLN:HG3   | 1.95                     | 0.67              |
| 8:H:106:GLU:C     | 8:H:108:SER:H     | 2.02                     | 0.67              |
| 11:K:47:ARG:HB3   | 11:K:47:ARG:NH1   | 2.09                     | 0.67              |
| 1:A:306:ASN:HD21  | 1:A:324:SER:H     | 1.43                     | 0.67              |
| 3:C:8:VAL:HG12    | 3:C:9:LYS:N       | 2.09                     | 0.67              |
| 10:J:58:GLU:HA    | 10:J:61:LEU:HD12  | 1.76                     | 0.67              |
| 1:A:897:TYR:CD2   | 1:A:936:LEU:HD13  | 2.30                     | 0.67              |
| 2:B:1162:ILE:HD11 | 2:B:1194:ILE:HD13 | 1.77                     | 0.67              |
| 3:C:5:GLY:O       | 3:C:7:GLN:HG3     | 1.94                     | 0.67              |
| 8:H:26:ILE:HD12   | 8:H:42:ILE:HD12   | 1.76                     | 0.67              |
| 1:A:816:HIS:CE1   | 2:B:764:SER:HB2   | 2.30                     | 0.67              |
| 8:H:97:MET:HE2    | 8:H:142:LEU:HD23  | 1.76                     | 0.67              |
| 12:L:45:ALA:O     | 12:L:46:VAL:HG23  | 1.95                     | 0.67              |
| 1:A:76:GLU:OE2    | 2:B:1159:ARG:NH1  | 2.28                     | 0.66              |
| 1:A:1348:LEU:HD21 | 1:A:1375:MET:SD   | 2.35                     | 0.66              |
| 2:B:311:LEU:HB3   | 9:I:4:PHE:CZ      | 2.31                     | 0.66              |
| 2:B:864:LYS:HB3   | 2:B:872:GLU:H     | 1.59                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:814:PHE:O     | 1:A:817:ALA:HB3   | 1.95                     | 0.66              |
| 1:A:914:GLU:HB2   | 1:A:979:SER:O     | 1.95                     | 0.66              |
| 2:B:514:LEU:HD12  | 2:B:515:HIS:N     | 2.09                     | 0.66              |
| 3:C:22:LEU:HD22   | 3:C:25:VAL:CG2    | 2.25                     | 0.66              |
| 3:C:56:THR:HG21   | 3:C:145:CYS:SG    | 2.35                     | 0.66              |
| 1:A:381:THR:CG2   | 1:A:383:TYR:H     | 2.09                     | 0.66              |
| 1:A:563:PRO:HB2   | 1:A:565:ILE:O     | 1.94                     | 0.66              |
| 1:A:736:ASN:O     | 1:A:737:LEU:C     | 2.38                     | 0.66              |
| 1:A:828:ALA:CB    | 2:B:530:GLY:HA2   | 2.25                     | 0.66              |
| 1:A:1193:LEU:HD21 | 1:A:1267:MET:HE2  | 1.77                     | 0.66              |
| 1:A:1333:ILE:O    | 1:A:1336:MET:HB3  | 1.96                     | 0.66              |
| 1:A:1364:ASN:ND2  | 1:A:1365:TYR:N    | 2.43                     | 0.66              |
| 2:B:1147:LEU:HD22 | 2:B:1151:LEU:HD22 | 1.77                     | 0.66              |
| 1:A:88:LYS:HD2    | 1:A:293:GLU:CD    | 2.20                     | 0.66              |
| 1:A:1267:MET:HA   | 1:A:1271:ILE:HD12 | 1.77                     | 0.66              |
| 1:A:1342:GLU:OE2  | 5:E:212:ARG:NH1   | 2.28                     | 0.66              |
| 9:I:32:CYS:SG     | 9:I:33:SER:N      | 2.69                     | 0.66              |
| 9:I:55:THR:HG23   | 9:I:58:VAL:HG21   | 1.76                     | 0.66              |
| 2:B:121:ASN:HA    | 2:B:207:GLY:HA3   | 1.77                     | 0.66              |
| 2:B:363:HIS:O     | 2:B:364:ILE:CB    | 2.44                     | 0.66              |
| 1:A:590:ARG:HB3   | 1:A:605:MET:N     | 2.10                     | 0.66              |
| 5:E:78:LEU:HD23   | 5:E:78:LEU:C      | 2.20                     | 0.66              |
| 2:B:128:LEU:HB3   | 2:B:167:ILE:O     | 1.95                     | 0.66              |
| 2:B:566:LEU:HD13  | 2:B:588:GLY:HA2   | 1.78                     | 0.66              |
| 8:H:95:TYR:CE2    | 8:H:97:MET:HG3    | 2.31                     | 0.66              |
| 1:A:525:GLN:CB    | 2:B:835:GLN:HG2   | 2.25                     | 0.66              |
| 2:B:649:LYS:HE2   | 2:B:738:PHE:O     | 1.96                     | 0.66              |
| 6:F:109:VAL:HG12  | 6:F:110:ASP:N     | 2.10                     | 0.66              |
| 1:A:535:THR:HG21  | 1:A:617:VAL:N     | 2.08                     | 0.66              |
| 1:A:1364:ASN:HD22 | 1:A:1364:ASN:C    | 2.04                     | 0.66              |
| 2:B:986:GLN:HE22  | 2:B:1020:ARG:CZ   | 2.08                     | 0.66              |
| 7:G:113:UNK:CA    | 7:G:115:UNK:CA    | 2.74                     | 0.66              |
| 2:B:46:GLN:HE22   | 2:B:496:ARG:HA    | 1.61                     | 0.66              |
| 2:B:957:ASN:O     | 2:B:959:ASP:N     | 2.28                     | 0.66              |
| 1:A:541:ILE:HG21  | 1:A:549:MET:HE3   | 1.78                     | 0.65              |
| 1:A:90:VAL:CG1    | 1:A:297:GLN:HA    | 2.26                     | 0.65              |
| 1:A:95:PHE:HE2    | 1:A:1414:ALA:HB2  | 1.62                     | 0.65              |
| 8:H:38:LEU:HD13   | 8:H:125:LEU:HD13  | 1.77                     | 0.65              |
| 1:A:305:ASP:HB3   | 1:A:308:ILE:HD11  | 1.77                     | 0.65              |
| 1:A:381:THR:HG21  | 1:A:383:TYR:CD1   | 2.31                     | 0.65              |
| 1:A:751:SER:O     | 1:A:752:LYS:HG2   | 1.96                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:293:PRO:HG2   | 2:B:296:GLU:HB2   | 1.79                     | 0.65              |
| 2:B:1001:PHE:CZ   | 2:B:1073:TYR:HB2  | 2.30                     | 0.65              |
| 8:H:40:LEU:HD13   | 8:H:123:MET:HE3   | 1.79                     | 0.65              |
| 1:A:523:ILE:HD12  | 1:A:622:VAL:HG22  | 1.79                     | 0.65              |
| 1:A:590:ARG:HH11  | 1:A:590:ARG:CG    | 2.06                     | 0.65              |
| 1:A:1115:SER:HA   | 1:A:1308:THR:HG22 | 1.77                     | 0.65              |
| 2:B:46:GLN:HG3    | 2:B:47:GLN:H      | 1.59                     | 0.65              |
| 2:B:120:ARG:CG    | 2:B:955:THR:HG21  | 2.23                     | 0.65              |
| 2:B:211:VAL:HG23  | 2:B:483:LEU:HB2   | 1.79                     | 0.65              |
| 2:B:1039:GLY:HA2  | 10:J:51:LEU:HD21  | 1.77                     | 0.65              |
| 3:C:11:ARG:HH21   | 3:C:229:TYR:HD2   | 1.44                     | 0.65              |
| 2:B:751:VAL:O     | 2:B:754:SER:HB2   | 1.95                     | 0.65              |
| 5:E:176:PRO:O     | 5:E:212:ARG:HA    | 1.95                     | 0.65              |
| 1:A:102:VAL:HG21  | 1:A:234:MET:HE1   | 1.77                     | 0.65              |
| 1:A:1319:VAL:HG13 | 1:A:1320:PRO:HD2  | 1.79                     | 0.65              |
| 2:B:114:PRO:HG3   | 2:B:181:LEU:HD11  | 1.79                     | 0.65              |
| 2:B:911:ILE:CG2   | 2:B:966:VAL:HG11  | 2.26                     | 0.65              |
| 5:E:124:VAL:HG22  | 5:E:132:ILE:HG21  | 1.78                     | 0.65              |
| 12:L:51:CYS:O     | 12:L:53:HIS:N     | 2.28                     | 0.65              |
| 1:A:512:VAL:HA    | 1:A:519:PRO:HA    | 1.79                     | 0.65              |
| 8:H:24:CYS:HB2    | 8:H:44:VAL:CG2    | 2.27                     | 0.65              |
| 1:A:450:LEU:HD13  | 1:A:1074:GLU:HG2  | 1.77                     | 0.65              |
| 2:B:349:ILE:O     | 2:B:352:ALA:HB3   | 1.96                     | 0.65              |
| 3:C:8:VAL:HG12    | 3:C:9:LYS:H       | 1.60                     | 0.65              |
| 8:H:107:VAL:HG21  | 8:H:126:GLU:HG3   | 1.79                     | 0.65              |
| 9:I:111:THR:HG21  | 9:I:113:ASP:HB2   | 1.78                     | 0.65              |
| 1:A:87:ALA:HB3    | 1:A:276:LEU:HD23  | 1.79                     | 0.65              |
| 1:A:418:SER:O     | 1:A:419:LYS:C     | 2.40                     | 0.65              |
| 1:A:1042:PHE:CE2  | 1:A:1046:LEU:HD11 | 2.31                     | 0.65              |
| 1:A:1224:LEU:HD12 | 1:A:1241:ARG:O    | 1.97                     | 0.65              |
| 2:B:577:ALA:HB1   | 2:B:589:VAL:CG1   | 2.27                     | 0.64              |
| 2:B:805:THR:HG21  | 2:B:815:ARG:HE    | 1.62                     | 0.64              |
| 1:A:579:SER:OG    | 1:A:612:ILE:HG22  | 1.98                     | 0.64              |
| 1:A:1035:TYR:O    | 1:A:1037:LEU:N    | 2.30                     | 0.64              |
| 1:A:329:LEU:HD23  | 1:A:335:ARG:HG3   | 1.78                     | 0.64              |
| 2:B:666:TYR:C     | 2:B:668:ASP:H     | 2.06                     | 0.64              |
| 2:B:1170:THR:O    | 2:B:1170:THR:HG22 | 1.97                     | 0.64              |
| 2:B:25:ILE:HG22   | 2:B:29:ASP:HB2    | 1.79                     | 0.64              |
| 2:B:686:ASN:C     | 2:B:688:GLY:H     | 2.04                     | 0.64              |
| 2:B:879:ARG:HB3   | 2:B:883:LEU:CD2   | 2.26                     | 0.64              |
| 2:B:1072:MET:CE   | 2:B:1085:ILE:HB   | 2.28                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:241:ASP:HB3   | 11:K:109:TRP:CE2  | 2.32                     | 0.64              |
| 1:A:715:GLU:O     | 1:A:719:VAL:HG23  | 1.96                     | 0.64              |
| 2:B:101:MET:HE3   | 2:B:169:ARG:HH22  | 1.62                     | 0.64              |
| 2:B:515:HIS:HD2   | 2:B:517:THR:OG1   | 1.81                     | 0.64              |
| 1:A:901:LEU:HA    | 1:A:907:THR:HG23  | 1.80                     | 0.64              |
| 2:B:604:ARG:HG2   | 2:B:604:ARG:O     | 1.98                     | 0.64              |
| 6:F:96:THR:O      | 6:F:100:GLN:HG3   | 1.97                     | 0.64              |
| 6:F:86:THR:OG1    | 6:F:89:GLU:HG3    | 1.98                     | 0.64              |
| 1:A:629:LEU:HD13  | 1:A:645:LEU:HD21  | 1.79                     | 0.64              |
| 1:A:1193:LEU:HB2  | 1:A:1260:LEU:HD11 | 1.78                     | 0.64              |
| 1:A:1394:THR:CG2  | 1:A:1395:GLY:N    | 2.60                     | 0.64              |
| 8:H:89:LEU:C      | 8:H:91:ASP:N      | 2.55                     | 0.64              |
| 2:B:711:GLU:H     | 2:B:712:PRO:HD3   | 1.61                     | 0.64              |
| 1:A:1444:MET:HE1  | 6:F:135:ARG:CZ    | 2.28                     | 0.63              |
| 2:B:519:TRP:C     | 2:B:519:TRP:CD1   | 2.76                     | 0.63              |
| 1:A:523:ILE:HD12  | 1:A:622:VAL:HG21  | 1.80                     | 0.63              |
| 2:B:824:ILE:CG1   | 10:J:48:ARG:HH12  | 2.08                     | 0.63              |
| 2:B:1197:PRO:HG2  | 2:B:1200:ALA:HB2  | 1.79                     | 0.63              |
| 5:E:93:MET:HE3    | 5:E:120:ALA:O     | 1.98                     | 0.63              |
| 1:A:225:ASN:O     | 1:A:226:GLU:HG2   | 1.99                     | 0.63              |
| 1:A:709:THR:HB    | 1:A:712:GLU:H     | 1.64                     | 0.63              |
| 2:B:1001:PHE:CE1  | 2:B:1073:TYR:HB2  | 2.33                     | 0.63              |
| 8:H:49:VAL:HG12   | 8:H:50:ALA:H      | 1.62                     | 0.63              |
| 1:A:84:ILE:HG23   | 1:A:239:LEU:HB3   | 1.80                     | 0.63              |
| 1:A:994:GLN:HE22  | 1:A:1023:ARG:NE   | 1.95                     | 0.63              |
| 2:B:780:VAL:HG21  | 10:J:56:LEU:CD1   | 2.29                     | 0.63              |
| 2:B:842:ASN:HD21  | 2:B:844:SER:HB2   | 1.63                     | 0.63              |
| 2:B:1104:HIS:HB2  | 2:B:1122:ARG:HD2  | 1.80                     | 0.63              |
| 8:H:101:ALA:HB2   | 8:H:116:TYR:CE2   | 2.33                     | 0.63              |
| 10:J:9:SER:OG     | 10:J:48:ARG:NH2   | 2.30                     | 0.63              |
| 2:B:221:ASN:OD1   | 2:B:242:SER:HA    | 1.98                     | 0.63              |
| 1:A:108:MET:O     | 1:A:109:HIS:HB2   | 1.99                     | 0.63              |
| 1:A:354:SER:HA    | 1:A:482:PHE:CD2   | 2.34                     | 0.63              |
| 1:A:443:LEU:CD2   | 1:A:455:MET:HE2   | 2.27                     | 0.63              |
| 1:A:475:THR:HG22  | 1:A:476:SER:N     | 2.12                     | 0.63              |
| 2:B:525:ALA:O     | 2:B:527:THR:HG22  | 1.99                     | 0.63              |
| 6:F:109:VAL:HG21  | 6:F:124:GLU:HA    | 1.80                     | 0.63              |
| 8:H:31:THR:O      | 8:H:32:THR:CB     | 2.47                     | 0.63              |
| 1:A:268:ASP:HB3   | 1:A:299:HIS:ND1   | 2.14                     | 0.63              |
| 1:A:1242:VAL:HG12 | 1:A:1243:VAL:N    | 2.12                     | 0.63              |
| 1:A:1364:ASN:ND2  | 1:A:1364:ASN:C    | 2.56                     | 0.63              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:373:ARG:NE   | 2:B:567:GLU:OE2   | 2.29                     | 0.63              |
| 3:C:114:TYR:CD2  | 3:C:140:ASN:HB3   | 2.32                     | 0.63              |
| 5:E:96:PHE:CZ    | 5:E:100:ILE:HD11  | 2.32                     | 0.63              |
| 1:A:1074:GLU:HB3 | 1:A:1075:PRO:CD   | 2.29                     | 0.63              |
| 5:E:50:MET:HE3   | 5:E:50:MET:O      | 1.98                     | 0.63              |
| 6:F:135:ARG:HG2  | 6:F:137:TYR:CE1   | 2.34                     | 0.63              |
| 1:A:418:SER:O    | 1:A:420:ARG:N     | 2.32                     | 0.63              |
| 1:A:982:THR:HG22 | 1:A:984:LYS:H     | 1.64                     | 0.63              |
| 1:A:1317:MET:HA  | 1:A:1322:ILE:HD11 | 1.81                     | 0.63              |
| 1:A:1402:PHE:CD2 | 1:A:1403:GLU:HG3  | 2.33                     | 0.63              |
| 2:B:788:ARG:NH1  | 2:B:790:ASP:OD1   | 2.31                     | 0.63              |
| 2:B:1201:LYS:O   | 2:B:1205:GLN:HG3  | 1.97                     | 0.63              |
| 4:D:7:UNK:CA     | 7:G:8:UNK:CA      | 2.76                     | 0.62              |
| 6:F:111:LEU:HD12 | 6:F:111:LEU:H     | 1.61                     | 0.62              |
| 1:A:33:ALA:O     | 1:A:83:HIS:HB3    | 1.99                     | 0.62              |
| 1:A:821:ARG:HG3  | 1:A:825:ILE:HD11  | 1.81                     | 0.62              |
| 2:B:1106:ARG:HD2 | 2:B:1126:GLY:O    | 1.99                     | 0.62              |
| 6:F:97:ARG:O     | 6:F:101:ILE:HG13  | 1.99                     | 0.62              |
| 8:H:12:VAL:HA    | 8:H:28:ALA:CB     | 2.28                     | 0.62              |
| 1:A:73:GLY:O     | 1:A:75:ASN:N      | 2.32                     | 0.62              |
| 2:B:208:SER:OG   | 2:B:210:LYS:HD3   | 1.99                     | 0.62              |
| 2:B:446:LEU:O    | 2:B:447:ALA:HB3   | 1.97                     | 0.62              |
| 2:B:616:ILE:HD12 | 2:B:616:ILE:N     | 2.14                     | 0.62              |
| 2:B:914:LYS:HB3  | 2:B:937:ALA:O     | 1.98                     | 0.62              |
| 5:E:157:SER:C    | 5:E:159:ASP:H     | 2.07                     | 0.62              |
| 1:A:871:ASP:HB3  | 5:E:204:THR:HG22  | 1.82                     | 0.62              |
| 1:A:1054:LEU:O   | 1:A:1057:VAL:HG23 | 1.99                     | 0.62              |
| 2:B:25:ILE:HG22  | 2:B:26:THR:H      | 1.65                     | 0.62              |
| 2:B:1072:MET:HE3 | 2:B:1085:ILE:CD1  | 2.29                     | 0.62              |
| 3:C:173:ALA:O    | 3:C:174:ALA:HB3   | 2.00                     | 0.62              |
| 12:L:55:ILE:HG13 | 12:L:56:LEU:H     | 1.63                     | 0.62              |
| 1:A:915:SER:O    | 1:A:919:ILE:HG13  | 2.00                     | 0.62              |
| 1:A:1436:ILE:HB  | 2:B:1144:ALA:HB2  | 1.80                     | 0.62              |
| 5:E:96:PHE:O     | 5:E:100:ILE:HG13  | 1.98                     | 0.62              |
| 9:I:7:CYS:HB2    | 9:I:29:CYS:HB2    | 1.81                     | 0.62              |
| 1:A:445:ASN:HB2  | 1:A:454:SER:O     | 2.00                     | 0.62              |
| 2:B:195:CYS:HB3  | 2:B:782:LEU:HD22  | 1.81                     | 0.62              |
| 1:A:328:ARG:O    | 1:A:335:ARG:HG2   | 1.99                     | 0.62              |
| 1:A:672:ASP:OD1  | 1:A:674:PRO:HD2   | 2.00                     | 0.62              |
| 1:A:689:LYS:O    | 1:A:693:VAL:HG23  | 2.00                     | 0.62              |
| 1:A:898:ARG:HB2  | 1:A:933:TYR:CE1   | 2.35                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1212:VAL:O    | 1:A:1216:ILE:HG13 | 1.99                     | 0.62              |
| 1:A:871:ASP:HB3   | 5:E:204:THR:CG2   | 2.30                     | 0.62              |
| 2:B:39:ARG:HE     | 2:B:665:GLU:HG2   | 1.65                     | 0.62              |
| 2:B:446:LEU:O     | 2:B:447:ALA:CB    | 2.48                     | 0.62              |
| 2:B:787:VAL:O     | 2:B:787:VAL:HG12  | 2.00                     | 0.62              |
| 2:B:839:MET:HE3   | 2:B:1010:LEU:CD1  | 2.30                     | 0.62              |
| 2:B:1034:VAL:HG23 | 2:B:1059:LEU:HB2  | 1.80                     | 0.62              |
| 2:B:1051:THR:CG2  | 2:B:1053:GLU:H    | 1.93                     | 0.62              |
| 5:E:100:ILE:HG23  | 5:E:105:PHE:HB2   | 1.80                     | 0.62              |
| 1:A:590:ARG:HB3   | 1:A:605:MET:H     | 1.63                     | 0.62              |
| 6:F:101:ILE:HD12  | 6:F:121:ALA:HB2   | 1.82                     | 0.62              |
| 10:J:3:VAL:HG21   | 10:J:18:TRP:CG    | 2.34                     | 0.62              |
| 1:A:148:CYS:O     | 1:A:168:GLY:HA2   | 1.99                     | 0.61              |
| 1:A:778:GLY:HA3   | 2:B:516:ASN:HB2   | 1.80                     | 0.61              |
| 1:A:871:ASP:OD2   | 5:E:204:THR:HG23  | 1.99                     | 0.61              |
| 2:B:496:ARG:HH11  | 2:B:539:LEU:HB2   | 1.62                     | 0.61              |
| 2:B:999:MET:HE2   | 2:B:1011:ILE:CD1  | 2.30                     | 0.61              |
| 2:B:1187:ASN:OD1  | 2:B:1190:ASP:HB3  | 1.99                     | 0.61              |
| 5:E:178:ILE:HG23  | 5:E:214:CYS:HA    | 1.81                     | 0.61              |
| 12:L:51:CYS:HB2   | 12:L:53:HIS:CD2   | 2.35                     | 0.61              |
| 1:A:503:GLN:HE21  | 6:F:90:ARG:HH21   | 1.47                     | 0.61              |
| 1:A:1021:LEU:O    | 1:A:1025:ARG:HG2  | 2.00                     | 0.61              |
| 2:B:211:VAL:O     | 2:B:480:SER:HA    | 2.00                     | 0.61              |
| 5:E:93:MET:O      | 5:E:97:VAL:HG23   | 2.00                     | 0.61              |
| 6:F:111:LEU:H     | 6:F:111:LEU:CD1   | 2.12                     | 0.61              |
| 6:F:111:LEU:C     | 6:F:113:GLY:H     | 2.07                     | 0.61              |
| 2:B:913:GLY:HA2   | 2:B:938:SER:HB3   | 1.81                     | 0.61              |
| 5:E:156:LEU:HD12  | 5:E:195:VAL:HG12  | 1.81                     | 0.61              |
| 8:H:89:LEU:HD22   | 8:H:91:ASP:CG     | 2.25                     | 0.61              |
| 1:A:567:LYS:HZ2   | 8:H:46:LEU:HB2    | 1.64                     | 0.61              |
| 3:C:166:GLU:HA    | 11:K:6:ARG:HB3    | 1.82                     | 0.61              |
| 6:F:109:VAL:HG23  | 6:F:124:GLU:HG2   | 1.82                     | 0.61              |
| 1:A:961:ARG:O     | 1:A:965:GLN:HG3   | 2.00                     | 0.61              |
| 1:A:1329:THR:HG22 | 1:A:1331:SER:N    | 2.01                     | 0.61              |
| 3:C:123:ASN:HD22  | 3:C:125:MET:HG2   | 1.66                     | 0.61              |
| 3:C:235:VAL:HG21  | 10:J:6:ARG:HH21   | 1.65                     | 0.61              |
| 1:A:549:MET:SD    | 1:A:577:ILE:CD1   | 2.87                     | 0.61              |
| 2:B:101:MET:HE3   | 2:B:169:ARG:NH2   | 2.15                     | 0.61              |
| 2:B:512:ARG:NH2   | 2:B:535:LEU:CD1   | 2.62                     | 0.61              |
| 2:B:1002:THR:HG23 | 2:B:1004:GLU:H    | 1.64                     | 0.61              |
| 2:B:429:PHE:HA    | 2:B:432:MET:HE3   | 1.82                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:582:VAL:HG22  | 2:B:626:ILE:HB    | 1.82                     | 0.61              |
| 10:J:64:ASN:HB3   | 10:J:65:PRO:CD    | 2.29                     | 0.61              |
| 1:A:567:LYS:CG    | 1:A:568:PRO:HD2   | 2.31                     | 0.61              |
| 1:A:1437:GLY:HA3  | 6:F:88:TYR:CD2    | 2.36                     | 0.61              |
| 2:B:185:THR:HG23  | 2:B:188:ASP:OD2   | 2.01                     | 0.61              |
| 2:B:198:ASP:OD1   | 2:B:485:ARG:NH2   | 2.33                     | 0.61              |
| 2:B:1169:MET:HE1  | 2:B:1201:LYS:O    | 2.00                     | 0.61              |
| 3:C:131:HIS:O     | 3:C:132:PRO:C     | 2.43                     | 0.61              |
| 9:I:7:CYS:C       | 9:I:8:ARG:O       | 2.43                     | 0.61              |
| 1:A:506:ALA:HB1   | 1:A:508:PRO:HD2   | 1.83                     | 0.61              |
| 1:A:528:LEU:O     | 1:A:531:ILE:HG22  | 2.01                     | 0.61              |
| 1:A:1132:LYS:O    | 1:A:1135:ARG:HB3  | 2.01                     | 0.61              |
| 1:A:1192:LEU:HD22 | 1:A:1239:ARG:NH2  | 2.16                     | 0.61              |
| 6:F:138:LEU:HB3   | 6:F:139:PRO:HD2   | 1.83                     | 0.61              |
| 12:L:70:ARG:HG2   | 12:L:70:ARG:HH11  | 1.66                     | 0.61              |
| 1:A:401:GLY:C     | 1:A:435:HIS:CD2   | 2.79                     | 0.61              |
| 1:A:789:LYS:HG3   | 9:I:67:THR:HB     | 1.83                     | 0.61              |
| 2:B:29:ASP:HB3    | 2:B:658:ILE:CD1   | 2.30                     | 0.61              |
| 2:B:57:TYR:CD1    | 2:B:57:TYR:N      | 2.68                     | 0.61              |
| 12:L:26:THR:O     | 12:L:27:LEU:HB3   | 2.01                     | 0.61              |
| 3:C:46:ILE:HA     | 3:C:159:ALA:HA    | 1.82                     | 0.60              |
| 3:C:49:VAL:HG21   | 3:C:67:LEU:HD12   | 1.83                     | 0.60              |
| 5:E:29:PHE:HB2    | 5:E:65:THR:HG22   | 1.83                     | 0.60              |
| 12:L:48:CYS:SG    | 12:L:49:LYS:N     | 2.70                     | 0.60              |
| 1:A:244:PRO:CG    | 1:A:245:PRO:HD3   | 2.27                     | 0.60              |
| 1:A:1293:SER:OG   | 1:A:1294:PRO:HD2  | 2.01                     | 0.60              |
| 2:B:778:MET:CE    | 2:B:1094:ARG:HD3  | 2.32                     | 0.60              |
| 2:B:1138:MET:HE2  | 2:B:1146:PHE:CD2  | 2.36                     | 0.60              |
| 5:E:78:LEU:HD23   | 5:E:79:TRP:N      | 2.16                     | 0.60              |
| 8:H:106:GLU:C     | 8:H:108:SER:N     | 2.57                     | 0.60              |
| 11:K:63:VAL:CG2   | 11:K:63:VAL:O     | 2.49                     | 0.60              |
| 2:B:114:PRO:HB3   | 2:B:174:LEU:HD11  | 1.82                     | 0.60              |
| 2:B:463:THR:HG22  | 2:B:465:ASN:HD22  | 1.66                     | 0.60              |
| 1:A:565:ILE:CG2   | 1:A:567:LYS:HG2   | 2.31                     | 0.60              |
| 1:A:855:THR:CG2   | 1:A:857:ARG:HG3   | 2.30                     | 0.60              |
| 1:A:1365:TYR:O    | 1:A:1366:ARG:C    | 2.43                     | 0.60              |
| 9:I:5:ARG:HD3     | 9:I:36:GLU:OE2    | 2.01                     | 0.60              |
| 11:K:90:ALA:O     | 11:K:94:ILE:HG13  | 2.01                     | 0.60              |
| 1:A:663:SER:OG    | 1:A:664:THR:N     | 2.34                     | 0.60              |
| 1:A:779:PHE:CZ    | 2:B:517:THR:HA    | 2.37                     | 0.60              |
| 1:A:1208:THR:O    | 1:A:1212:VAL:HG23 | 2.01                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:118:ARG:NH2   | 2:B:194:GLU:CD    | 2.60                     | 0.60              |
| 2:B:299:GLU:OE1   | 2:B:571:PRO:HG2   | 2.01                     | 0.60              |
| 2:B:549:THR:HB    | 2:B:628:THR:CG2   | 2.30                     | 0.60              |
| 2:B:744:HIS:CD2   | 2:B:746:SER:H     | 2.14                     | 0.60              |
| 2:B:1039:GLY:HA2  | 10:J:51:LEU:CD2   | 2.31                     | 0.60              |
| 2:B:1051:THR:HG22 | 2:B:1052:VAL:N    | 2.17                     | 0.60              |
| 1:A:306:ASN:OD1   | 1:A:324:SER:HB3   | 2.01                     | 0.60              |
| 1:A:322:VAL:O     | 1:A:323:LYS:HG3   | 2.01                     | 0.60              |
| 2:B:975:GLN:HG2   | 2:B:976:ILE:H     | 1.67                     | 0.60              |
| 8:H:15:VAL:HG22   | 8:H:26:ILE:HG12   | 1.83                     | 0.60              |
| 11:K:49:GLU:HG3   | 11:K:94:ILE:HG12  | 1.83                     | 0.60              |
| 1:A:709:THR:OG1   | 1:A:712:GLU:HG3   | 2.00                     | 0.60              |
| 2:B:479:VAL:HG12  | 2:B:480:SER:N     | 2.17                     | 0.60              |
| 2:B:809:MET:HE1   | 2:B:983:ARG:NH2   | 2.16                     | 0.60              |
| 5:E:47:CYS:HA     | 5:E:53:PRO:HA     | 1.83                     | 0.60              |
| 1:A:338:GLY:HA2   | 2:B:1129:ARG:NH2  | 2.10                     | 0.60              |
| 1:A:1042:PHE:HE2  | 1:A:1046:LEU:HD11 | 1.67                     | 0.60              |
| 1:A:1223:ASP:HA   | 1:A:1243:VAL:CG1  | 2.32                     | 0.60              |
| 1:A:68:GLN:HE22   | 1:A:80:HIS:CB     | 2.15                     | 0.60              |
| 2:B:794:ASN:C     | 2:B:795:ILE:HD12  | 2.26                     | 0.60              |
| 1:A:97:ALA:HA     | 1:A:100:LYS:HE3   | 1.84                     | 0.60              |
| 1:A:1115:SER:O    | 1:A:1329:THR:HG23 | 2.02                     | 0.60              |
| 2:B:778:MET:HE3   | 2:B:1094:ARG:HD3  | 1.84                     | 0.60              |
| 2:B:995:ARG:NH1   | 2:B:995:ARG:HB2   | 2.16                     | 0.60              |
| 2:B:1171:VAL:CG1  | 2:B:1191:ILE:HD13 | 2.32                     | 0.60              |
| 1:A:337:ARG:CZ    | 1:A:839:ARG:NH1   | 2.64                     | 0.59              |
| 1:A:567:LYS:O     | 1:A:569:LYS:N     | 2.35                     | 0.59              |
| 1:A:886:ILE:CD1   | 1:A:943:LEU:HB3   | 2.31                     | 0.59              |
| 1:A:1158:PRO:HB3  | 1:A:1241:ARG:NH1  | 2.17                     | 0.59              |
| 1:A:1402:PHE:CE2  | 1:A:1403:GLU:HG3  | 2.37                     | 0.59              |
| 2:B:211:VAL:CG2   | 2:B:483:LEU:HD13  | 2.32                     | 0.59              |
| 2:B:28:GLU:CD     | 2:B:807:ARG:HH22  | 2.10                     | 0.59              |
| 2:B:1117:GLN:HG3  | 2:B:1156:ASP:OD1  | 2.02                     | 0.59              |
| 1:A:444:PHE:HB3   | 1:A:458:HIS:HD2   | 1.67                     | 0.59              |
| 1:A:756:ILE:HG22  | 1:A:757:ASN:N     | 2.17                     | 0.59              |
| 1:A:1149:ALA:HB2  | 9:I:47:GLU:HA     | 1.84                     | 0.59              |
| 1:A:1394:THR:HG22 | 1:A:1395:GLY:N    | 2.17                     | 0.59              |
| 2:B:803:LEU:H     | 2:B:822:ASN:HD21  | 1.48                     | 0.59              |
| 2:B:1159:ARG:CD   | 2:B:1193:GLN:HE21 | 2.15                     | 0.59              |
| 2:B:1174:LYS:HB2  | 2:B:1179:GLN:O    | 2.02                     | 0.59              |
| 9:I:8:ARG:HG3     | 9:I:9:ASP:N       | 2.15                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:107:CYS:HB2   | 1:A:114:LEU:CD2   | 2.33                     | 0.59              |
| 1:A:151:ASP:HA    | 1:A:162:VAL:O     | 2.02                     | 0.59              |
| 1:A:239:LEU:HD12  | 1:A:240:PRO:HD2   | 1.84                     | 0.59              |
| 1:A:824:LEU:O     | 1:A:827:THR:HB    | 2.00                     | 0.59              |
| 2:B:405:ARG:NH1   | 2:B:632:ARG:HG2   | 2.17                     | 0.59              |
| 1:A:1399:ARG:CB   | 1:A:1408:ILE:HD13 | 2.28                     | 0.59              |
| 6:F:85:MET:HE1    | 6:F:148:VAL:HG13  | 1.84                     | 0.59              |
| 9:I:15:TYR:O      | 9:I:27:PHE:HA     | 2.02                     | 0.59              |
| 1:A:93:VAL:HG11   | 1:A:308:ILE:CD1   | 2.33                     | 0.59              |
| 2:B:589:VAL:HG12  | 2:B:590:HIS:N     | 2.18                     | 0.59              |
| 9:I:85:PHE:CD1    | 9:I:99:LEU:HD22   | 2.37                     | 0.59              |
| 1:A:76:GLU:HG3    | 1:A:76:GLU:O      | 2.02                     | 0.59              |
| 3:C:166:GLU:CG    | 11:K:10:PHE:HZ    | 2.14                     | 0.59              |
| 11:K:49:GLU:HG3   | 11:K:94:ILE:CG1   | 2.33                     | 0.59              |
| 1:A:821:ARG:O     | 1:A:822:GLU:C     | 2.46                     | 0.59              |
| 1:A:840:ARG:HB3   | 1:A:1384:VAL:HG12 | 1.85                     | 0.59              |
| 1:A:896:ARG:NH2   | 1:A:1030:ARG:HH21 | 2.00                     | 0.59              |
| 1:A:1004:ASN:ND2  | 5:E:167:ARG:HD2   | 2.18                     | 0.59              |
| 2:B:90:ILE:HD12   | 2:B:432:MET:SD    | 2.42                     | 0.59              |
| 2:B:217:ARG:NH1   | 2:B:407:ASP:OD1   | 2.35                     | 0.59              |
| 8:H:24:CYS:HB2    | 8:H:44:VAL:HG21   | 1.85                     | 0.59              |
| 8:H:84:ALA:HA     | 8:H:87:ARG:CG     | 2.32                     | 0.59              |
| 9:I:111:THR:CG2   | 9:I:113:ASP:HB2   | 2.33                     | 0.59              |
| 1:A:469:ARG:NH2   | 2:B:976:ILE:HD13  | 2.18                     | 0.59              |
| 1:A:809:THR:O     | 1:A:810:PRO:C     | 2.46                     | 0.59              |
| 1:A:1385:THR:HG22 | 1:A:1386:ARG:H    | 1.68                     | 0.59              |
| 2:B:130:VAL:HG12  | 2:B:131:ASP:H     | 1.67                     | 0.59              |
| 1:A:57:ARG:O      | 1:A:68:GLN:HG3    | 2.03                     | 0.59              |
| 1:A:68:GLN:HE22   | 1:A:80:HIS:HB3    | 1.67                     | 0.59              |
| 1:A:1336:MET:CE   | 1:A:1381:LEU:HG   | 2.33                     | 0.59              |
| 1:A:1341:ILE:HD12 | 1:A:1379:GLY:C    | 2.28                     | 0.59              |
| 6:F:81:THR:HG22   | 6:F:82:THR:N      | 2.18                     | 0.59              |
| 6:F:127:GLU:O     | 6:F:129:LYS:HG3   | 2.03                     | 0.59              |
| 1:A:225:ASN:ND2   | 1:A:227:VAL:HB    | 2.18                     | 0.58              |
| 1:A:1018:PHE:O    | 1:A:1021:LEU:HB3  | 2.03                     | 0.58              |
| 2:B:642:ASP:O     | 2:B:644:GLU:N     | 2.36                     | 0.58              |
| 5:E:156:LEU:HD12  | 5:E:195:VAL:CG1   | 2.33                     | 0.58              |
| 8:H:109:LYS:HB2   | 8:H:109:LYS:NZ    | 2.18                     | 0.58              |
| 1:A:738:LYS:HZ1   | 3:C:194:GLU:C     | 2.11                     | 0.58              |
| 2:B:640:VAL:O     | 2:B:641:GLU:C     | 2.46                     | 0.58              |
| 2:B:912:ILE:HD11  | 2:B:966:VAL:HG23  | 1.84                     | 0.58              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 10:J:48:ARG:HE    | 10:J:49:MET:CE   | 2.16                     | 0.58              |
| 11:K:47:ARG:HD3   | 11:K:59:ALA:O    | 2.04                     | 0.58              |
| 2:B:779:GLY:HA2   | 2:B:796:LEU:HB2  | 1.85                     | 0.58              |
| 2:B:860:MET:HG2   | 2:B:861:ASP:N    | 2.18                     | 0.58              |
| 2:B:1102:LYS:O    | 2:B:1104:HIS:N   | 2.32                     | 0.58              |
| 2:B:1201:LYS:HE2  | 2:B:1205:GLN:NE2 | 2.18                     | 0.58              |
| 1:A:596:THR:O     | 1:A:598:LEU:N    | 2.36                     | 0.58              |
| 1:A:1325:THR:O    | 5:E:148:GLU:HB2  | 2.04                     | 0.58              |
| 1:A:1342:GLU:HG3  | 5:E:198:ILE:HG21 | 1.86                     | 0.58              |
| 1:A:1444:MET:HE1  | 6:F:135:ARG:NE   | 2.18                     | 0.58              |
| 1:A:90:VAL:HG11   | 1:A:297:GLN:HA   | 1.84                     | 0.58              |
| 1:A:567:LYS:NZ    | 8:H:95:TYR:CE1   | 2.71                     | 0.58              |
| 2:B:23:ALA:O      | 2:B:654:ARG:HB3  | 2.04                     | 0.58              |
| 2:B:46:GLN:O      | 2:B:408:LEU:HD23 | 2.03                     | 0.58              |
| 1:A:44:THR:O      | 1:A:44:THR:HG22  | 2.02                     | 0.58              |
| 1:A:50:ILE:C      | 1:A:52:GLY:H     | 2.09                     | 0.58              |
| 1:A:1295:THR:HG23 | 1:A:1297:GLU:OE1 | 2.03                     | 0.58              |
| 2:B:758:PHE:C     | 2:B:760:ASP:H    | 2.10                     | 0.58              |
| 2:B:983:ARG:HD2   | 2:B:1091:TYR:HB3 | 1.85                     | 0.58              |
| 2:B:1168:LEU:HD13 | 2:B:1208:MET:HE3 | 1.86                     | 0.58              |
| 11:K:46:ILE:HG22  | 11:K:50:LEU:HD12 | 1.86                     | 0.58              |
| 12:L:31:CYS:HG    | 12:L:34:CYS:HG   | 1.49                     | 0.58              |
| 1:A:219:PHE:O     | 1:A:222:LEU:N    | 2.33                     | 0.58              |
| 2:B:913:GLY:HA2   | 2:B:938:SER:CB   | 2.32                     | 0.58              |
| 3:C:37:MET:HG2    | 3:C:243:VAL:CG1  | 2.34                     | 0.58              |
| 3:C:244:VAL:O     | 3:C:248:ILE:HG13 | 2.03                     | 0.58              |
| 5:E:61:GLN:HB2    | 5:E:79:TRP:CE3   | 2.38                     | 0.58              |
| 9:I:16:PRO:HB3    | 9:I:27:PHE:CE2   | 2.38                     | 0.58              |
| 11:K:55:LYS:HB3   | 11:K:81:TYR:CD1  | 2.36                     | 0.58              |
| 1:A:260:ASP:OD1   | 1:A:261:ASP:N    | 2.37                     | 0.58              |
| 1:A:353:ILE:HG22  | 1:A:468:PHE:HB2  | 1.85                     | 0.58              |
| 1:A:1308:THR:HG21 | 1:A:1310:GLY:O   | 2.04                     | 0.58              |
| 2:B:287:ARG:NH1   | 2:B:324:ILE:O    | 2.37                     | 0.58              |
| 2:B:1077:THR:CG2  | 2:B:1079:LYS:HB2 | 2.34                     | 0.58              |
| 8:H:81:PRO:CB     | 8:H:82:PRO:CD    | 2.81                     | 0.58              |
| 11:K:65:HIS:HD2   | 11:K:67:PHE:N    | 2.02                     | 0.58              |
| 1:A:31:SER:OG     | 1:A:83:HIS:HB2   | 2.02                     | 0.58              |
| 1:A:86:LEU:HA     | 1:A:273:ASN:OD1  | 2.02                     | 0.58              |
| 1:A:93:VAL:HG22   | 1:A:301:ALA:HA   | 1.85                     | 0.58              |
| 1:A:1332:PHE:N    | 1:A:1332:PHE:CD2 | 2.72                     | 0.58              |
| 2:B:205:ILE:N     | 2:B:205:ILE:HD12 | 2.19                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1106:ARG:HH12 | 2:B:1118:PRO:HB3  | 1.67                     | 0.58              |
| 1:A:76:GLU:O      | 1:A:76:GLU:CG     | 2.52                     | 0.58              |
| 1:A:101:LYS:O     | 1:A:105:CYS:HB2   | 2.04                     | 0.58              |
| 1:A:225:ASN:HD22  | 1:A:227:VAL:HB    | 1.68                     | 0.58              |
| 1:A:1400:CYS:SG   | 1:A:1409:LEU:HG   | 2.44                     | 0.58              |
| 6:F:87:LYS:HE2    | 6:F:88:TYR:CZ     | 2.39                     | 0.58              |
| 11:K:33:ILE:HD13  | 11:K:87:LEU:HD22  | 1.85                     | 0.58              |
| 1:A:233:TRP:C     | 1:A:235:ILE:N     | 2.60                     | 0.57              |
| 1:A:385:ILE:HG22  | 1:A:386:ASP:N     | 2.18                     | 0.57              |
| 2:B:23:ALA:HB1    | 2:B:24:PRO:HD2    | 1.85                     | 0.57              |
| 2:B:980:PHE:CE1   | 2:B:990:ILE:HD11  | 2.39                     | 0.57              |
| 1:A:41:MET:HB3    | 1:A:48:ALA:O      | 2.04                     | 0.57              |
| 1:A:452:LYS:HB3   | 2:B:1141:HIS:CE1  | 2.40                     | 0.57              |
| 1:A:537:ARG:HB2   | 8:H:20:TYR:CE2    | 2.39                     | 0.57              |
| 1:A:1155:ASP:OD2  | 1:A:1161:THR:HG23 | 2.04                     | 0.57              |
| 2:B:25:ILE:HG22   | 2:B:29:ASP:CB     | 2.34                     | 0.57              |
| 2:B:101:MET:HB2   | 2:B:169:ARG:HH12  | 1.69                     | 0.57              |
| 2:B:756:ILE:O     | 2:B:759:PRO:HD3   | 2.04                     | 0.57              |
| 2:B:806:THR:HB    | 2:B:809:MET:HG3   | 1.85                     | 0.57              |
| 5:E:61:GLN:HB2    | 5:E:79:TRP:HE3    | 1.69                     | 0.57              |
| 6:F:111:LEU:N     | 6:F:111:LEU:CD1   | 2.67                     | 0.57              |
| 11:K:65:HIS:CD2   | 11:K:67:PHE:HB2   | 2.39                     | 0.57              |
| 1:A:399:HIS:O     | 1:A:435:HIS:HD2   | 1.87                     | 0.57              |
| 1:A:882:SER:HA    | 1:A:952:ALA:O     | 2.05                     | 0.57              |
| 1:A:901:LEU:N     | 1:A:926:GLN:NE2   | 2.50                     | 0.57              |
| 1:A:1143:LEU:HD23 | 1:A:1267:MET:HB3  | 1.86                     | 0.57              |
| 1:A:1281:ARG:HB2  | 1:A:1309:ASP:HB2  | 1.86                     | 0.57              |
| 1:A:1315:GLU:O    | 1:A:1318:THR:HG23 | 2.04                     | 0.57              |
| 2:B:653:VAL:HG22  | 2:B:689:LEU:HB3   | 1.85                     | 0.57              |
| 2:B:803:LEU:N     | 2:B:822:ASN:HD21  | 2.02                     | 0.57              |
| 5:E:5:ASN:ND2     | 5:E:52:ARG:HG2    | 2.12                     | 0.57              |
| 5:E:46:TYR:HA     | 5:E:57:MET:SD     | 2.43                     | 0.57              |
| 5:E:213:ILE:HG23  | 5:E:213:ILE:O     | 2.04                     | 0.57              |
| 8:H:24:CYS:SG     | 8:H:44:VAL:HG21   | 2.44                     | 0.57              |
| 8:H:139:ASN:O     | 8:H:140:ALA:HB2   | 2.02                     | 0.57              |
| 9:I:47:GLU:OE1    | 9:I:50:THR:HG23   | 2.04                     | 0.57              |
| 1:A:166:GLY:O     | 1:A:167:CYS:HB3   | 2.03                     | 0.57              |
| 1:A:482:PHE:CD1   | 2:B:836:GLU:HB2   | 2.38                     | 0.57              |
| 1:A:524:VAL:HG12  | 1:A:525:GLN:H     | 1.69                     | 0.57              |
| 2:B:547:VAL:H     | 2:B:612:GLU:CD    | 2.13                     | 0.57              |
| 2:B:642:ASP:HB3   | 2:B:649:LYS:HD2   | 1.85                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:806:THR:C     | 2:B:808:ALA:H     | 2.13                     | 0.57              |
| 3:C:18:VAL:HG23   | 3:C:240:VAL:CG1   | 2.33                     | 0.57              |
| 8:H:5:LEU:CD1     | 8:H:135:LEU:HG    | 2.34                     | 0.57              |
| 8:H:12:VAL:HA     | 8:H:28:ALA:HB2    | 1.86                     | 0.57              |
| 1:A:337:ARG:CD    | 1:A:839:ARG:HH22  | 2.17                     | 0.57              |
| 1:A:1074:GLU:O    | 1:A:1076:ALA:N    | 2.37                     | 0.57              |
| 1:A:1436:ILE:HG22 | 2:B:1142:GLY:HA2  | 1.87                     | 0.57              |
| 9:I:29:CYS:C      | 9:I:31:THR:H      | 2.13                     | 0.57              |
| 11:K:10:PHE:HD1   | 11:K:11:LEU:HD13  | 1.67                     | 0.57              |
| 1:A:401:GLY:O     | 1:A:435:HIS:CD2   | 2.58                     | 0.57              |
| 1:A:879:GLU:OE2   | 1:A:962:ARG:NH2   | 2.37                     | 0.57              |
| 2:B:1077:THR:HG22 | 2:B:1079:LYS:N    | 2.13                     | 0.57              |
| 2:B:1147:LEU:HD22 | 2:B:1151:LEU:CD2  | 2.35                     | 0.57              |
| 12:L:49:LYS:O     | 12:L:50:ASP:HB2   | 2.03                     | 0.57              |
| 1:A:567:LYS:NZ    | 8:H:46:LEU:CB     | 2.67                     | 0.57              |
| 2:B:429:PHE:HA    | 2:B:432:MET:CE    | 2.35                     | 0.57              |
| 2:B:855:PHE:HZ    | 2:B:857:ARG:HH11  | 1.52                     | 0.57              |
| 3:C:55:THR:HB     | 3:C:152:GLU:H     | 1.70                     | 0.57              |
| 9:I:75:CYS:C      | 9:I:77:LYS:N      | 2.59                     | 0.57              |
| 1:A:28:ARG:HG2    | 1:A:83:HIS:CE1    | 2.39                     | 0.57              |
| 2:B:311:LEU:HB3   | 9:I:4:PHE:CE2     | 2.40                     | 0.57              |
| 2:B:848:ARG:NH1   | 10:J:8:PHE:O      | 2.35                     | 0.57              |
| 3:C:148:ARG:HG3   | 10:J:61:LEU:O     | 2.03                     | 0.57              |
| 3:C:251:LEU:O     | 3:C:255:VAL:HG23  | 2.04                     | 0.57              |
| 1:A:40:THR:HG21   | 1:A:259:GLU:OE2   | 2.04                     | 0.57              |
| 1:A:414:ASP:O     | 1:A:417:TYR:O     | 2.22                     | 0.57              |
| 1:A:754:SER:O     | 1:A:755:PHE:C     | 2.48                     | 0.57              |
| 1:A:901:LEU:H     | 1:A:926:GLN:HE21  | 1.50                     | 0.57              |
| 2:B:973:ILE:HG23  | 2:B:974:PRO:HD2   | 1.87                     | 0.57              |
| 1:A:63:ARG:HA     | 1:A:74:MET:HE2    | 1.86                     | 0.57              |
| 1:A:399:HIS:C     | 1:A:401:GLY:H     | 2.10                     | 0.57              |
| 1:A:710:LEU:HD12  | 1:A:710:LEU:N     | 2.20                     | 0.57              |
| 1:A:1300:LYS:NZ   | 1:A:1300:LYS:HB3  | 2.20                     | 0.57              |
| 2:B:955:THR:OG1   | 12:L:55:ILE:HA    | 2.04                     | 0.57              |
| 2:B:1116:ARG:HD2  | 2:B:1198:TYR:CG   | 2.40                     | 0.57              |
| 5:E:46:TYR:CE2    | 5:E:58:MET:HA     | 2.40                     | 0.57              |
| 1:A:233:TRP:C     | 1:A:235:ILE:H     | 2.13                     | 0.56              |
| 1:A:714:PHE:HB2   | 9:I:97:MET:HE1    | 1.85                     | 0.56              |
| 1:A:1017:LEU:HD23 | 5:E:204:THR:O     | 2.05                     | 0.56              |
| 2:B:701:ILE:HD11  | 2:B:703:ILE:HD11  | 1.86                     | 0.56              |
| 2:B:979:LYS:HG2   | 2:B:1095:LEU:HD12 | 1.87                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:242:GLN:NE2   | 3:C:246:ARG:HE    | 2.02                     | 0.56              |
| 1:A:742:ASN:CA    | 1:A:745:GLN:HB2   | 2.33                     | 0.56              |
| 2:B:980:PHE:HE1   | 2:B:990:ILE:HD11  | 1.70                     | 0.56              |
| 2:B:1022:THR:HG23 | 2:B:1022:THR:O    | 2.05                     | 0.56              |
| 2:B:1072:MET:HE3  | 2:B:1085:ILE:HB   | 1.86                     | 0.56              |
| 2:B:1180:PHE:O    | 2:B:1181:GLU:HB2  | 2.05                     | 0.56              |
| 5:E:22:MET:HE1    | 5:E:135:PHE:CE2   | 2.40                     | 0.56              |
| 5:E:35:VAL:C      | 5:E:37:LEU:H      | 2.12                     | 0.56              |
| 8:H:89:LEU:HD22   | 8:H:91:ASP:OD2    | 2.05                     | 0.56              |
| 11:K:51:LEU:HD13  | 11:K:59:ALA:HB3   | 1.86                     | 0.56              |
| 12:L:51:CYS:C     | 12:L:53:HIS:H     | 2.11                     | 0.56              |
| 1:A:556:TRP:CE3   | 1:A:558:GLY:HA2   | 2.41                     | 0.56              |
| 1:A:619:LYS:O     | 1:A:623:GLY:N     | 2.38                     | 0.56              |
| 1:A:1193:LEU:CD2  | 1:A:1267:MET:HE2  | 2.35                     | 0.56              |
| 2:B:844:SER:OG    | 2:B:996:ARG:N     | 2.33                     | 0.56              |
| 2:B:864:LYS:HD3   | 2:B:871:THR:OG1   | 2.05                     | 0.56              |
| 3:C:229:TYR:N     | 3:C:229:TYR:CD1   | 2.74                     | 0.56              |
| 3:C:248:ILE:CD1   | 11:K:101:LEU:HD22 | 2.35                     | 0.56              |
| 8:H:82:PRO:O      | 8:H:83:GLN:HB2    | 2.04                     | 0.56              |
| 1:A:69:THR:HB     | 2:B:1174:LYS:HE2  | 1.87                     | 0.56              |
| 1:A:849:MET:HE3   | 1:A:1061:GLY:CA   | 2.35                     | 0.56              |
| 2:B:243:ALA:HA    | 2:B:250:PHE:O     | 2.05                     | 0.56              |
| 2:B:522:VAL:HG11  | 2:B:537:LYS:HB3   | 1.86                     | 0.56              |
| 2:B:704:ALA:HB1   | 2:B:710:LEU:HD12  | 1.87                     | 0.56              |
| 3:C:175:ALA:HB3   | 10:J:43:ARG:NH2   | 2.20                     | 0.56              |
| 3:C:258:ILE:O     | 3:C:261:ALA:HB3   | 2.04                     | 0.56              |
| 6:F:97:ARG:NE     | 6:F:124:GLU:OE1   | 2.31                     | 0.56              |
| 6:F:99:LEU:HD12   | 6:F:99:LEU:O      | 2.05                     | 0.56              |
| 1:A:98:LYS:O      | 1:A:102:VAL:HG23  | 2.05                     | 0.56              |
| 1:A:185:TRP:CZ3   | 1:A:200:ARG:HG2   | 2.40                     | 0.56              |
| 1:A:384:ASN:O     | 1:A:385:ILE:C     | 2.48                     | 0.56              |
| 1:A:577:ILE:O     | 1:A:580:VAL:HG23  | 2.04                     | 0.56              |
| 1:A:741:ASN:C     | 1:A:741:ASN:ND2   | 2.62                     | 0.56              |
| 2:B:1079:LYS:HA   | 3:C:27:LEU:HD21   | 1.87                     | 0.56              |
| 9:I:111:THR:HG22  | 9:I:112:SER:N     | 2.19                     | 0.56              |
| 1:A:548:ASN:HA    | 11:K:60:ALA:HB1   | 1.87                     | 0.56              |
| 1:A:1326:ARG:O    | 1:A:1327:ILE:C    | 2.49                     | 0.56              |
| 5:E:195:VAL:HG22  | 5:E:213:ILE:HB    | 1.88                     | 0.56              |
| 11:K:50:LEU:CD1   | 11:K:73:LEU:HD21  | 2.35                     | 0.56              |
| 1:A:1359:ASP:C    | 1:A:1361:SER:H    | 2.13                     | 0.56              |
| 10:J:1:MET:HG3    | 10:J:60:PHE:HE2   | 1.69                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:547:LEU:HD22  | 11:K:58:PHE:CD1   | 2.41                     | 0.56              |
| 1:A:974:ASP:HB2   | 8:H:136:LYS:NZ    | 2.21                     | 0.56              |
| 1:A:1364:ASN:ND2  | 1:A:1366:ARG:N    | 2.53                     | 0.56              |
| 2:B:839:MET:CE    | 2:B:980:PHE:HB2   | 2.35                     | 0.56              |
| 8:H:97:MET:CE     | 8:H:142:LEU:HD23  | 2.35                     | 0.56              |
| 12:L:26:THR:HG22  | 12:L:27:LEU:N     | 2.21                     | 0.56              |
| 2:B:120:ARG:NH1   | 12:L:54:ARG:NH1   | 2.54                     | 0.56              |
| 3:C:162:GLY:HA3   | 3:C:170:TRP:CE2   | 2.41                     | 0.56              |
| 5:E:121:MET:C     | 5:E:123:LEU:H     | 2.13                     | 0.56              |
| 1:A:896:ARG:HD3   | 1:A:897:TYR:HE1   | 1.67                     | 0.56              |
| 1:A:1420:ASP:O    | 1:A:1421:CYS:HB2  | 2.04                     | 0.56              |
| 3:C:99:LEU:HD23   | 3:C:99:LEU:N      | 2.20                     | 0.56              |
| 12:L:62:LYS:C     | 12:L:64:LEU:H     | 2.13                     | 0.56              |
| 1:A:596:THR:O     | 1:A:597:LEU:C     | 2.48                     | 0.55              |
| 1:A:825:ILE:HD12  | 2:B:513:GLN:NE2   | 2.21                     | 0.55              |
| 1:A:1161:THR:HG22 | 1:A:1163:ILE:N    | 2.03                     | 0.55              |
| 1:A:1328:TYR:CG   | 1:A:1329:THR:N    | 2.74                     | 0.55              |
| 1:A:1342:GLU:HG2  | 5:E:212:ARG:NH1   | 2.20                     | 0.55              |
| 2:B:864:LYS:N     | 2:B:872:GLU:OE1   | 2.39                     | 0.55              |
| 8:H:6:PHE:HE1     | 8:H:130:ARG:HE    | 1.53                     | 0.55              |
| 1:A:35:ILE:HG12   | 1:A:52:GLY:O      | 2.06                     | 0.55              |
| 1:A:1096:SER:O    | 1:A:1099:PRO:HG2  | 2.05                     | 0.55              |
| 1:A:1351:GLU:O    | 1:A:1352:VAL:C    | 2.49                     | 0.55              |
| 2:B:1171:VAL:HG11 | 2:B:1191:ILE:HD13 | 1.88                     | 0.55              |
| 1:A:92:HIS:HD2    | 1:A:94:GLY:H      | 1.53                     | 0.55              |
| 1:A:1261:LYS:HA   | 1:A:1264:GLU:HB3  | 1.88                     | 0.55              |
| 2:B:479:VAL:HG12  | 2:B:480:SER:H     | 1.72                     | 0.55              |
| 2:B:898:LEU:HD22  | 2:B:964:VAL:HG11  | 1.89                     | 0.55              |
| 2:B:984:HIS:HB3   | 2:B:1022:THR:OG1  | 2.05                     | 0.55              |
| 3:C:145:CYS:SG    | 3:C:146:LYS:N     | 2.79                     | 0.55              |
| 11:K:61:TYR:HA    | 11:K:72:LYS:O     | 2.07                     | 0.55              |
| 1:A:672:ASP:HB3   | 1:A:675:THR:OG1   | 2.05                     | 0.55              |
| 1:A:838:GLN:O     | 1:A:842:VAL:HG23  | 2.06                     | 0.55              |
| 1:A:867:ILE:HG22  | 1:A:872:GLY:N     | 2.22                     | 0.55              |
| 1:A:1389:PHE:O    | 1:A:1392:SER:HB3  | 2.06                     | 0.55              |
| 2:B:34:ILE:O      | 2:B:37:PHE:HB3    | 2.06                     | 0.55              |
| 2:B:57:TYR:N      | 2:B:57:TYR:HD1    | 2.03                     | 0.55              |
| 2:B:780:VAL:HG21  | 10:J:56:LEU:HD13  | 1.88                     | 0.55              |
| 2:B:1159:ARG:CD   | 2:B:1193:GLN:HG3  | 2.31                     | 0.55              |
| 3:C:56:THR:CG2    | 3:C:57:VAL:H      | 2.09                     | 0.55              |
| 3:C:70:ILE:HD11   | 3:C:144:ILE:HG12  | 1.88                     | 0.55              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 10:J:21:TYR:HA   | 10:J:39:LEU:HD11  | 1.89                     | 0.55              |
| 1:A:665:GLY:HA3  | 2:B:1086:PHE:CD1  | 2.41                     | 0.55              |
| 2:B:25:ILE:HD11  | 2:B:653:VAL:HB    | 1.89                     | 0.55              |
| 2:B:93:GLY:N     | 2:B:131:ASP:O     | 2.37                     | 0.55              |
| 2:B:361:LEU:N    | 2:B:362:PRO:CD    | 2.69                     | 0.55              |
| 2:B:1084:GLN:H   | 2:B:1084:GLN:CD   | 2.14                     | 0.55              |
| 1:A:885:THR:HG22 | 1:A:885:THR:O     | 2.05                     | 0.55              |
| 1:A:885:THR:O    | 1:A:940:ARG:HG3   | 2.07                     | 0.55              |
| 1:A:1222:ASN:O   | 1:A:1223:ASP:HB3  | 2.06                     | 0.55              |
| 2:B:556:THR:HG22 | 2:B:557:PHE:N     | 2.20                     | 0.55              |
| 2:B:801:LYS:O    | 10:J:52:THR:CG2   | 2.52                     | 0.55              |
| 1:A:23:SER:HB3   | 1:A:233:TRP:CE2   | 2.41                     | 0.55              |
| 1:A:517:ASN:ND2  | 1:A:1362:TYR:HE2  | 2.05                     | 0.55              |
| 2:B:566:LEU:HD22 | 2:B:586:TRP:O     | 2.06                     | 0.55              |
| 2:B:1051:THR:CG2 | 2:B:1052:VAL:N    | 2.70                     | 0.55              |
| 6:F:109:VAL:HG13 | 6:F:127:GLU:OE1   | 2.07                     | 0.55              |
| 8:H:17:PRO:HB3   | 8:H:24:CYS:SG     | 2.47                     | 0.55              |
| 1:A:15:LYS:HD2   | 2:B:1220:ARG:HE   | 1.72                     | 0.55              |
| 1:A:216:VAL:O    | 1:A:219:PHE:HB2   | 2.06                     | 0.55              |
| 1:A:463:ILE:HD11 | 1:A:469:ARG:HG3   | 1.89                     | 0.55              |
| 2:B:63:ILE:HA    | 2:B:421:PHE:CE2   | 2.42                     | 0.55              |
| 2:B:130:VAL:CG2  | 2:B:167:ILE:HD12  | 2.34                     | 0.55              |
| 2:B:515:HIS:H    | 2:B:518:HIS:CD2   | 2.24                     | 0.55              |
| 8:H:84:ALA:C     | 8:H:86:ASP:H      | 2.13                     | 0.55              |
| 9:I:7:CYS:O      | 9:I:8:ARG:O       | 2.24                     | 0.55              |
| 12:L:32:ALA:HB3  | 12:L:55:ILE:CD1   | 2.26                     | 0.55              |
| 1:A:399:HIS:O    | 1:A:435:HIS:CD2   | 2.60                     | 0.55              |
| 1:A:418:SER:C    | 1:A:420:ARG:N     | 2.63                     | 0.55              |
| 1:A:704:ALA:HB2  | 1:A:710:LEU:CG    | 2.23                     | 0.55              |
| 2:B:35:SER:O     | 2:B:36:ALA:C      | 2.50                     | 0.55              |
| 2:B:308:TRP:CH2  | 9:I:45:ARG:HG2    | 2.42                     | 0.55              |
| 2:B:406:LEU:HD12 | 2:B:545:ILE:HD11  | 1.89                     | 0.55              |
| 2:B:958:GLN:O    | 2:B:960:GLY:N     | 2.33                     | 0.55              |
| 3:C:248:ILE:HD13 | 11:K:101:LEU:HD22 | 1.89                     | 0.55              |
| 9:I:111:THR:CG2  | 9:I:112:SER:N     | 2.69                     | 0.55              |
| 1:A:843:LYS:HG3  | 1:A:1402:PHE:HD1  | 1.72                     | 0.55              |
| 1:A:852:TYR:CE2  | 6:F:136:ARG:HG2   | 2.42                     | 0.55              |
| 1:A:1116:LEU:O   | 1:A:1308:THR:HB   | 2.07                     | 0.55              |
| 2:B:755:ILE:CG2  | 2:B:755:ILE:O     | 2.55                     | 0.55              |
| 2:B:1053:GLU:O   | 2:B:1054:GLY:C    | 2.50                     | 0.55              |
| 5:E:168:TYR:HB3  | 5:E:170:LEU:CD2   | 2.36                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:339:ASN:O     | 1:A:343:LYS:HG2   | 2.07                     | 0.54              |
| 1:A:760:GLN:HB2   | 2:B:1021:MET:HE1  | 1.89                     | 0.54              |
| 1:A:1308:THR:CG2  | 1:A:1310:GLY:O    | 2.55                     | 0.54              |
| 2:B:179:CYS:SG    | 2:B:181:LEU:HB2   | 2.47                     | 0.54              |
| 2:B:195:CYS:CB    | 2:B:782:LEU:HD22  | 2.37                     | 0.54              |
| 2:B:566:LEU:HD13  | 2:B:588:GLY:CA    | 2.37                     | 0.54              |
| 5:E:176:PRO:HD2   | 5:E:211:TYR:O     | 2.07                     | 0.54              |
| 5:E:197:LYS:HG3   | 5:E:211:TYR:CE2   | 2.42                     | 0.54              |
| 8:H:83:GLN:C      | 8:H:85:GLY:H      | 2.14                     | 0.54              |
| 8:H:89:LEU:O      | 8:H:91:ASP:N      | 2.37                     | 0.54              |
| 9:I:2:THR:HG22    | 9:I:2:THR:O       | 2.07                     | 0.54              |
| 1:A:122:MET:O     | 1:A:126:LEU:HG    | 2.07                     | 0.54              |
| 1:A:346:ASP:CG    | 2:B:1108:ARG:HA   | 2.31                     | 0.54              |
| 1:A:646:PHE:O     | 1:A:650:GLN:HG3   | 2.07                     | 0.54              |
| 1:A:741:ASN:ND2   | 1:A:743:VAL:H     | 2.05                     | 0.54              |
| 1:A:819:GLY:O     | 1:A:820:GLY:C     | 2.49                     | 0.54              |
| 8:H:59:ILE:HG22   | 8:H:60:ALA:N      | 2.21                     | 0.54              |
| 1:A:590:ARG:O     | 1:A:591:PHE:HB2   | 2.08                     | 0.54              |
| 1:A:829:VAL:C     | 1:A:831:THR:H     | 2.15                     | 0.54              |
| 1:A:875:ALA:HB2   | 1:A:1366:ARG:HD2  | 1.88                     | 0.54              |
| 2:B:680:THR:HG22  | 2:B:681:TRP:H     | 1.72                     | 0.54              |
| 1:A:89:PRO:O      | 1:A:204:THR:HG21  | 2.07                     | 0.54              |
| 1:A:350:ARG:HB2   | 1:A:488:ASN:OD1   | 2.08                     | 0.54              |
| 1:A:556:TRP:CD2   | 1:A:558:GLY:HA2   | 2.42                     | 0.54              |
| 1:A:1073:GLY:O    | 1:A:1076:ALA:HB3  | 2.07                     | 0.54              |
| 2:B:172:ILE:HD13  | 2:B:178:ASN:CB    | 2.37                     | 0.54              |
| 2:B:708:GLU:C     | 2:B:710:LEU:H     | 2.16                     | 0.54              |
| 5:E:153:HIS:CE1   | 5:E:184:VAL:HG11  | 2.43                     | 0.54              |
| 1:A:451:HIS:CE1   | 1:A:1074:GLU:HG3  | 2.42                     | 0.54              |
| 1:A:1339:LEU:HD13 | 5:E:147:HIS:CD2   | 2.42                     | 0.54              |
| 2:B:542:MET:HE1   | 2:B:743:ILE:CG2   | 2.37                     | 0.54              |
| 2:B:783:THR:HA    | 10:J:60:PHE:HE1   | 1.72                     | 0.54              |
| 2:B:784:ASN:ND2   | 2:B:788:ARG:HD2   | 2.23                     | 0.54              |
| 2:B:911:ILE:HD11  | 2:B:941:LEU:CD1   | 2.37                     | 0.54              |
| 2:B:1034:VAL:HG12 | 2:B:1035:ALA:N    | 2.23                     | 0.54              |
| 3:C:13:ALA:O      | 11:K:114:LEU:HD13 | 2.08                     | 0.54              |
| 5:E:195:VAL:HG22  | 5:E:213:ILE:CB    | 2.36                     | 0.54              |
| 12:L:63:ARG:O     | 12:L:64:LEU:O     | 2.24                     | 0.54              |
| 1:A:963:ILE:HD12  | 1:A:1049:ILE:HG12 | 1.88                     | 0.54              |
| 1:A:1116:LEU:H    | 1:A:1308:THR:HG22 | 1.72                     | 0.54              |
| 1:A:1205:LYS:O    | 1:A:1207:LEU:N    | 2.41                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1225:PHE:CE2  | 1:A:1227:ILE:HD11 | 2.43                     | 0.54              |
| 1:A:1349:TYR:C    | 1:A:1349:TYR:CD2  | 2.84                     | 0.54              |
| 2:B:839:MET:HE1   | 2:B:980:PHE:HB2   | 1.89                     | 0.54              |
| 3:C:101:LEU:HD13  | 3:C:118:LEU:HD23  | 1.88                     | 0.54              |
| 5:E:46:TYR:CD2    | 5:E:58:MET:HG2    | 2.42                     | 0.54              |
| 6:F:72:LYS:N      | 6:F:142:SER:HA    | 2.22                     | 0.54              |
| 6:F:107:VAL:HG12  | 6:F:109:VAL:H     | 1.72                     | 0.54              |
| 8:H:84:ALA:HA     | 8:H:87:ARG:HG3    | 1.88                     | 0.54              |
| 1:A:515:GLN:HG3   | 1:A:516:SER:N     | 2.22                     | 0.54              |
| 1:A:563:PRO:HG3   | 1:A:572:TRP:CE2   | 2.42                     | 0.54              |
| 2:B:43:LEU:HD13   | 2:B:812:LEU:CD2   | 2.38                     | 0.54              |
| 2:B:292:ILE:H     | 2:B:293:PRO:HD2   | 1.73                     | 0.54              |
| 3:C:183:TRP:CZ2   | 3:C:207:CYS:HB3   | 2.42                     | 0.54              |
| 3:C:242:GLN:HE21  | 3:C:246:ARG:HE    | 1.54                     | 0.54              |
| 5:E:61:GLN:NE2    | 5:E:105:PHE:CE2   | 2.71                     | 0.54              |
| 1:A:367:PRO:HB3   | 1:A:465:TYR:O     | 2.08                     | 0.54              |
| 1:A:533:LYS:O     | 1:A:535:THR:N     | 2.40                     | 0.54              |
| 1:A:738:LYS:HB2   | 1:A:740:LEU:HG    | 1.89                     | 0.54              |
| 1:A:1366:ARG:O    | 1:A:1369:ALA:HB3  | 2.08                     | 0.54              |
| 2:B:102:VAL:HG22  | 2:B:112:LEU:HD22  | 1.88                     | 0.54              |
| 2:B:898:LEU:CD2   | 2:B:964:VAL:HG11  | 2.38                     | 0.54              |
| 3:C:238:ILE:HG23  | 3:C:242:GLN:HB2   | 1.89                     | 0.54              |
| 5:E:157:SER:C     | 5:E:159:ASP:N     | 2.64                     | 0.54              |
| 5:E:191:LYS:O     | 5:E:192:ARG:C     | 2.51                     | 0.54              |
| 10:J:7:CYS:O      | 10:J:8:PHE:C      | 2.50                     | 0.54              |
| 1:A:225:ASN:C     | 1:A:227:VAL:H     | 2.10                     | 0.54              |
| 1:A:356:ASP:OD2   | 11:K:65:HIS:HE1   | 1.91                     | 0.54              |
| 1:A:710:LEU:H     | 1:A:710:LEU:CD1   | 2.19                     | 0.54              |
| 2:B:43:LEU:HD13   | 2:B:812:LEU:HD23  | 1.90                     | 0.54              |
| 2:B:120:ARG:HE    | 2:B:955:THR:CG2   | 2.20                     | 0.54              |
| 2:B:288:ALA:HB1   | 2:B:331:LEU:CD1   | 2.38                     | 0.54              |
| 1:A:337:ARG:NE    | 1:A:839:ARG:NH2   | 2.55                     | 0.54              |
| 1:A:845:LEU:N     | 1:A:845:LEU:HD23  | 2.22                     | 0.54              |
| 2:B:864:LYS:HG3   | 2:B:865:LYS:N     | 2.22                     | 0.54              |
| 5:E:16:PHE:CD1    | 5:E:58:MET:HE2    | 2.42                     | 0.54              |
| 1:A:89:PRO:C      | 1:A:204:THR:HG21  | 2.33                     | 0.53              |
| 1:A:90:VAL:HG13   | 1:A:297:GLN:HA    | 1.90                     | 0.53              |
| 1:A:154:SER:HB3   | 1:A:162:VAL:HG23  | 1.89                     | 0.53              |
| 1:A:1341:ILE:HD12 | 1:A:1379:GLY:O    | 2.07                     | 0.53              |
| 2:B:287:ARG:CG    | 2:B:292:ILE:HA    | 2.26                     | 0.53              |
| 2:B:484:ASN:ND2   | 2:B:486:TYR:CD1   | 2.76                     | 0.53              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:906:SER:O     | 2:B:907:GLY:C    | 2.50                     | 0.53              |
| 6:F:94:LEU:HD21   | 6:F:122:MET:HA   | 1.89                     | 0.53              |
| 6:F:114:GLU:OE1   | 6:F:119:ARG:HG3  | 2.08                     | 0.53              |
| 10:J:32:GLU:O     | 10:J:36:LEU:HG   | 2.07                     | 0.53              |
| 10:J:36:LEU:HD12  | 10:J:47:ARG:NH1  | 2.23                     | 0.53              |
| 12:L:60:ARG:CG    | 12:L:61:THR:H    | 1.94                     | 0.53              |
| 1:A:61:ILE:HG22   | 1:A:62:ASP:N     | 2.16                     | 0.53              |
| 1:A:444:PHE:HB3   | 1:A:458:HIS:CD2  | 2.43                     | 0.53              |
| 1:A:1392:SER:O    | 1:A:1393:ASN:CG  | 2.52                     | 0.53              |
| 2:B:549:THR:HB    | 2:B:628:THR:HG23 | 1.89                     | 0.53              |
| 2:B:837:ASP:OD1   | 2:B:1020:ARG:NH2 | 2.41                     | 0.53              |
| 1:A:92:HIS:CD2    | 1:A:94:GLY:H     | 2.26                     | 0.53              |
| 1:A:898:ARG:HD2   | 1:A:899:VAL:H    | 1.73                     | 0.53              |
| 1:A:1375:MET:HG2  | 1:A:1382:THR:O   | 2.08                     | 0.53              |
| 2:B:956:THR:CG2   | 2:B:960:GLY:HA2  | 2.38                     | 0.53              |
| 2:B:1106:ARG:NH2  | 2:B:1109:GLY:C   | 2.67                     | 0.53              |
| 12:L:27:LEU:HD13  | 12:L:37:LYS:HB3  | 1.90                     | 0.53              |
| 1:A:696:GLU:OE2   | 1:A:702:LEU:HD23 | 2.08                     | 0.53              |
| 1:A:768:GLN:HG2   | 1:A:816:HIS:CA   | 2.38                     | 0.53              |
| 1:A:1116:LEU:HD12 | 1:A:1329:THR:HG1 | 1.73                     | 0.53              |
| 2:B:644:GLU:HG3   | 2:B:654:ARG:HH22 | 1.74                     | 0.53              |
| 2:B:756:ILE:HG21  | 2:B:759:PRO:HB3  | 1.90                     | 0.53              |
| 2:B:899:ILE:HD11  | 2:B:910:VAL:O    | 2.09                     | 0.53              |
| 3:C:189:THR:HG22  | 3:C:190:ASP:N    | 2.24                     | 0.53              |
| 9:I:29:CYS:SG     | 9:I:29:CYS:O     | 2.66                     | 0.53              |
| 1:A:32:VAL:HG21   | 1:A:68:GLN:HE22  | 1.74                     | 0.53              |
| 1:A:38:PRO:N      | 1:A:270:LEU:HD23 | 2.22                     | 0.53              |
| 1:A:557:ASP:OD2   | 1:A:559:VAL:HB   | 2.08                     | 0.53              |
| 1:A:567:LYS:HZ2   | 8:H:46:LEU:CB    | 2.21                     | 0.53              |
| 1:A:693:VAL:HG21  | 1:A:721:PHE:CE1  | 2.39                     | 0.53              |
| 1:A:1029:ARG:HH11 | 1:A:1029:ARG:HG3 | 1.74                     | 0.53              |
| 2:B:235:SER:OG    | 2:B:236:HIS:HD2  | 1.91                     | 0.53              |
| 2:B:405:ARG:HA    | 2:B:631:GLY:O    | 2.09                     | 0.53              |
| 9:I:62:ILE:HG23   | 9:I:63:GLY:N     | 2.22                     | 0.53              |
| 12:L:70:ARG:HG2   | 12:L:70:ARG:NH1  | 2.22                     | 0.53              |
| 1:A:529:CYS:HB2   | 2:B:1015:HIS:CE1 | 2.44                     | 0.53              |
| 1:A:608:ILE:HD12  | 1:A:613:ILE:CD1  | 2.38                     | 0.53              |
| 1:A:683:ILE:HD11  | 1:A:764:CYS:CB   | 2.35                     | 0.53              |
| 2:B:287:ARG:HA    | 2:B:291:ILE:O    | 2.09                     | 0.53              |
| 5:E:23:VAL:HG12   | 5:E:28:TYR:HB2   | 1.89                     | 0.53              |
| 6:F:118:LEU:O     | 6:F:122:MET:HG3  | 2.08                     | 0.53              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:13:THR:HG23   | 1:A:1432:GLN:NE2 | 2.24                     | 0.53              |
| 1:A:407:ARG:HD2   | 1:A:413:ILE:HD11 | 1.91                     | 0.53              |
| 1:A:552:TRP:NE1   | 1:A:655:PHE:CD1  | 2.77                     | 0.53              |
| 2:B:205:ILE:HD11  | 2:B:461:LEU:HD23 | 1.90                     | 0.53              |
| 8:H:38:LEU:CD1    | 8:H:125:LEU:HD13 | 2.38                     | 0.53              |
| 1:A:114:LEU:HD22  | 1:A:171:GLN:NE2  | 2.23                     | 0.53              |
| 1:A:185:TRP:HZ3   | 1:A:200:ARG:HG2  | 1.74                     | 0.53              |
| 1:A:384:ASN:OD1   | 1:A:385:ILE:N    | 2.42                     | 0.53              |
| 1:A:852:TYR:CZ    | 6:F:136:ARG:HG2  | 2.44                     | 0.53              |
| 1:A:1220:PHE:O    | 1:A:1222:ASN:N   | 2.42                     | 0.53              |
| 2:B:90:ILE:CD1    | 2:B:432:MET:SD   | 2.97                     | 0.53              |
| 2:B:577:ALA:HB1   | 2:B:589:VAL:HG11 | 1.91                     | 0.53              |
| 2:B:857:ARG:HD2   | 2:B:945:GLU:OE1  | 2.08                     | 0.53              |
| 2:B:1069:PHE:HA   | 2:B:1085:ILE:O   | 2.08                     | 0.53              |
| 2:B:1106:ARG:HH21 | 2:B:1109:GLY:C   | 2.16                     | 0.53              |
| 6:F:132:LEU:O     | 6:F:148:VAL:HG23 | 2.09                     | 0.53              |
| 8:H:84:ALA:C      | 8:H:86:ASP:N     | 2.64                     | 0.53              |
| 9:I:46:HIS:CD2    | 9:I:48:LEU:HD21  | 2.44                     | 0.53              |
| 1:A:442:VAL:O     | 1:A:457:ALA:HA   | 2.09                     | 0.53              |
| 1:A:902:LEU:HD21  | 1:A:923:LEU:HD23 | 1.90                     | 0.53              |
| 1:A:1161:THR:HG22 | 1:A:1162:VAL:N   | 2.24                     | 0.53              |
| 1:A:1436:ILE:CG2  | 1:A:1437:GLY:H   | 2.22                     | 0.53              |
| 2:B:59:LEU:HD11   | 2:B:417:PHE:CZ   | 2.44                     | 0.53              |
| 1:A:91:PHE:HB2    | 1:A:297:GLN:OE1  | 2.09                     | 0.53              |
| 1:A:376:TYR:C     | 1:A:376:TYR:CD2  | 2.87                     | 0.53              |
| 2:B:120:ARG:NH2   | 12:L:54:ARG:HD2  | 2.24                     | 0.53              |
| 2:B:240:ILE:HG23  | 2:B:240:ILE:O    | 2.09                     | 0.53              |
| 3:C:46:ILE:HD13   | 3:C:157:CYS:CB   | 2.39                     | 0.53              |
| 3:C:57:VAL:HG11   | 10:J:60:PHE:HB2  | 1.88                     | 0.53              |
| 5:E:28:TYR:CE1    | 5:E:78:LEU:HD12  | 2.44                     | 0.53              |
| 8:H:6:PHE:O       | 8:H:58:THR:HA    | 2.08                     | 0.53              |
| 9:I:73:ARG:O      | 9:I:81:ARG:HA    | 2.09                     | 0.53              |
| 1:A:134:ARG:HH12  | 1:A:220:THR:HG22 | 1.74                     | 0.52              |
| 1:A:928:LEU:O     | 1:A:931:GLU:N    | 2.43                     | 0.52              |
| 2:B:121:ASN:N     | 2:B:121:ASN:ND2  | 2.50                     | 0.52              |
| 2:B:234:ILE:H     | 2:B:234:ILE:CD1  | 2.16                     | 0.52              |
| 2:B:234:ILE:HG21  | 2:B:257:LYS:HB3  | 1.91                     | 0.52              |
| 2:B:293:PRO:HA    | 9:I:12:ASN:HD21  | 1.74                     | 0.52              |
| 2:B:484:ASN:ND2   | 2:B:486:TYR:CE1  | 2.77                     | 0.52              |
| 3:C:241:ASP:O     | 3:C:245:VAL:HG23 | 2.08                     | 0.52              |
| 5:E:12:LEU:HD22   | 5:E:55:ARG:CZ    | 2.39                     | 0.52              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:E:17:ARG:O     | 5:E:21:GLU:HG3    | 2.09                     | 0.52              |
| 5:E:78:LEU:HD21  | 5:E:109:ILE:HD12  | 1.90                     | 0.52              |
| 8:H:32:THR:HG22  | 8:H:33:GLN:HG3    | 1.90                     | 0.52              |
| 12:L:38:LEU:HG   | 12:L:39:SER:N     | 2.24                     | 0.52              |
| 1:A:225:ASN:O    | 1:A:227:VAL:HG23  | 2.08                     | 0.52              |
| 1:A:226:GLU:HG2  | 1:A:227:VAL:HG23  | 1.90                     | 0.52              |
| 1:A:666:ILE:HD11 | 2:B:1030:LEU:CD1  | 2.20                     | 0.52              |
| 1:A:1074:GLU:C   | 1:A:1076:ALA:N    | 2.67                     | 0.52              |
| 1:A:1116:LEU:N   | 1:A:1308:THR:HG22 | 2.24                     | 0.52              |
| 1:A:1365:TYR:O   | 1:A:1367:HIS:N    | 2.42                     | 0.52              |
| 2:B:284:ILE:HD13 | 2:B:324:ILE:HD12  | 1.91                     | 0.52              |
| 2:B:542:MET:CG   | 2:B:747:MET:HE3   | 2.36                     | 0.52              |
| 2:B:875:GLU:O    | 2:B:877:PRO:HD3   | 2.09                     | 0.52              |
| 2:B:911:ILE:HD11 | 2:B:941:LEU:HD12  | 1.91                     | 0.52              |
| 5:E:155:ARG:HD2  | 5:E:194:GLU:OE2   | 2.09                     | 0.52              |
| 6:F:77:ASP:O     | 6:F:78:GLN:HB2    | 2.09                     | 0.52              |
| 1:A:670:ILE:HD13 | 2:B:1067:ARG:CZ   | 2.39                     | 0.52              |
| 1:A:1299:VAL:CG1 | 1:A:1300:LYS:N    | 2.72                     | 0.52              |
| 2:B:46:GLN:NE2   | 2:B:496:ARG:HA    | 2.24                     | 0.52              |
| 2:B:916:THR:HG22 | 2:B:918:ILE:HG13  | 1.90                     | 0.52              |
| 3:C:93:ASP:OD1   | 3:C:122:SER:HB2   | 2.09                     | 0.52              |
| 8:H:138:GLU:O    | 8:H:139:ASN:C     | 2.53                     | 0.52              |
| 11:K:46:ILE:O    | 11:K:50:LEU:HB2   | 2.09                     | 0.52              |
| 1:A:387:ARG:O    | 1:A:391:LEU:HG    | 2.09                     | 0.52              |
| 1:A:1147:THR:HA  | 1:A:1197:LEU:HD23 | 1.90                     | 0.52              |
| 1:A:1392:SER:O   | 1:A:1393:ASN:CB   | 2.58                     | 0.52              |
| 2:B:25:ILE:HG22  | 2:B:26:THR:N      | 2.24                     | 0.52              |
| 10:J:9:SER:CB    | 10:J:45:CYS:HB2   | 2.40                     | 0.52              |
| 12:L:38:LEU:O    | 12:L:39:SER:CB    | 2.56                     | 0.52              |
| 1:A:507:VAL:N    | 1:A:508:PRO:CD    | 2.72                     | 0.52              |
| 1:A:1319:VAL:CG1 | 1:A:1320:PRO:HD2  | 2.39                     | 0.52              |
| 2:B:98:THR:OG1   | 2:B:127:GLY:HA3   | 2.09                     | 0.52              |
| 2:B:271:ALA:HB3  | 2:B:285:ILE:CD1   | 2.40                     | 0.52              |
| 2:B:428:ILE:HG22 | 2:B:432:MET:HE2   | 1.91                     | 0.52              |
| 7:G:141:UNK:CA   | 7:G:168:UNK:CA    | 2.87                     | 0.52              |
| 9:I:50:THR:HG22  | 9:I:52:ILE:H      | 1.75                     | 0.52              |
| 10:J:52:THR:O    | 10:J:52:THR:HG22  | 2.08                     | 0.52              |
| 11:K:65:HIS:HD2  | 11:K:67:PHE:HB2   | 1.74                     | 0.52              |
| 1:A:261:ASP:OD2  | 1:A:323:LYS:HD2   | 2.10                     | 0.52              |
| 1:A:340:LEU:HD21 | 2:B:1200:ALA:CB   | 2.40                     | 0.52              |
| 2:B:552:MET:N    | 2:B:553:PRO:HD2   | 2.24                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:842:ASN:HD22 | 2:B:845:SER:CB   | 2.21                     | 0.52              |
| 1:A:167:CYS:HB2  | 1:A:169:ASN:ND2  | 2.24                     | 0.52              |
| 1:A:219:PHE:O    | 1:A:222:LEU:O    | 2.28                     | 0.52              |
| 1:A:858:ASN:C    | 1:A:858:ASN:ND2  | 2.68                     | 0.52              |
| 2:B:108:VAL:CG1  | 2:B:109:THR:H    | 2.18                     | 0.52              |
| 2:B:614:SER:OG   | 2:B:627:PHE:HB2  | 2.09                     | 0.52              |
| 2:B:1084:GLN:HG2 | 3:C:201:TRP:CZ2  | 2.45                     | 0.52              |
| 3:C:164:ALA:HA   | 3:C:167:HIS:O    | 2.10                     | 0.52              |
| 6:F:109:VAL:CG1  | 6:F:110:ASP:N    | 2.73                     | 0.52              |
| 9:I:75:CYS:O     | 9:I:76:PRO:C     | 2.52                     | 0.52              |
| 1:A:326:ARG:HG2  | 1:A:1406:VAL:CG2 | 2.39                     | 0.52              |
| 1:A:365:GLY:HA3  | 1:A:469:ARG:HB2  | 1.91                     | 0.52              |
| 1:A:714:PHE:CB   | 9:I:97:MET:HE1   | 2.40                     | 0.52              |
| 1:A:817:ALA:HA   | 2:B:764:SER:OG   | 2.10                     | 0.52              |
| 2:B:230:ALA:C    | 2:B:232:SER:H    | 2.17                     | 0.52              |
| 11:K:49:GLU:OE2  | 11:K:97:LYS:HE3  | 2.10                     | 0.52              |
| 1:A:167:CYS:C    | 1:A:169:ASN:H    | 2.18                     | 0.52              |
| 1:A:443:LEU:HD11 | 2:B:1138:MET:SD  | 2.50                     | 0.52              |
| 1:A:715:GLU:OE2  | 1:A:774:ARG:NH1  | 2.43                     | 0.52              |
| 1:A:974:ASP:HB2  | 8:H:136:LYS:HZ1  | 1.74                     | 0.52              |
| 2:B:750:GLY:O    | 2:B:751:VAL:C    | 2.53                     | 0.52              |
| 2:B:1065:GLN:NE2 | 2:B:1067:ARG:HG2 | 2.24                     | 0.52              |
| 2:B:1197:PRO:HG2 | 2:B:1200:ALA:CB  | 2.40                     | 0.52              |
| 1:A:22:PHE:HB2   | 2:B:1211:ASN:CG  | 2.35                     | 0.52              |
| 1:A:41:MET:HG2   | 1:A:49:LYS:HG2   | 1.92                     | 0.52              |
| 1:A:96:ILE:O     | 1:A:100:LYS:HG3  | 2.10                     | 0.52              |
| 1:A:384:ASN:OD1  | 1:A:388:LEU:HD12 | 2.10                     | 0.52              |
| 1:A:666:ILE:O    | 1:A:667:GLY:C    | 2.53                     | 0.52              |
| 1:A:737:LEU:HD11 | 1:A:758:ILE:HG21 | 1.92                     | 0.52              |
| 1:A:907:THR:HG22 | 1:A:908:LEU:N    | 2.25                     | 0.52              |
| 1:A:1074:GLU:C   | 1:A:1076:ALA:H   | 2.18                     | 0.52              |
| 2:B:25:ILE:CG2   | 2:B:29:ASP:HB3   | 2.40                     | 0.52              |
| 2:B:248:SER:O    | 2:B:249:ARG:HB2  | 2.09                     | 0.52              |
| 2:B:332:ASP:C    | 2:B:334:ILE:N    | 2.68                     | 0.52              |
| 2:B:515:HIS:H    | 2:B:518:HIS:HD2  | 1.55                     | 0.52              |
| 2:B:563:MET:HE2  | 2:B:588:GLY:HA3  | 1.92                     | 0.52              |
| 2:B:755:ILE:O    | 2:B:755:ILE:HG22 | 2.09                     | 0.52              |
| 5:E:58:MET:O     | 5:E:59:SER:C     | 2.53                     | 0.52              |
| 2:B:287:ARG:HG2  | 2:B:292:ILE:CA   | 2.27                     | 0.51              |
| 2:B:864:LYS:HD3  | 2:B:871:THR:HA   | 1.91                     | 0.51              |
| 2:B:1163:CYS:SG  | 2:B:1182:CYS:SG  | 3.09                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:E:7:ARG:C      | 5:E:9:ILE:H       | 2.17                     | 0.51              |
| 11:K:63:VAL:O    | 11:K:63:VAL:HG23  | 2.08                     | 0.51              |
| 1:A:50:ILE:HG22  | 1:A:51:GLY:N      | 2.24                     | 0.51              |
| 1:A:134:ARG:NH1  | 1:A:220:THR:O     | 2.42                     | 0.51              |
| 1:A:1375:MET:HE3 | 1:A:1384:VAL:HG23 | 1.91                     | 0.51              |
| 2:B:563:MET:HG3  | 2:B:563:MET:O     | 2.10                     | 0.51              |
| 2:B:737:THR:CG2  | 9:I:66:PRO:HB2    | 2.40                     | 0.51              |
| 2:B:751:VAL:HG12 | 2:B:752:ALA:N     | 2.26                     | 0.51              |
| 2:B:846:ILE:HD13 | 2:B:974:PRO:HG2   | 1.91                     | 0.51              |
| 3:C:73:GLN:HE21  | 3:C:75:MET:N      | 1.97                     | 0.51              |
| 12:L:27:LEU:HD13 | 12:L:37:LYS:CG    | 2.41                     | 0.51              |
| 1:A:530:GLY:O    | 1:A:531:ILE:C     | 2.54                     | 0.51              |
| 5:E:5:ASN:O      | 5:E:9:ILE:HG13    | 2.11                     | 0.51              |
| 12:L:47:ARG:HG2  | 12:L:52:GLY:CA    | 2.39                     | 0.51              |
| 1:A:540:PHE:C    | 1:A:541:ILE:HD12  | 2.35                     | 0.51              |
| 1:A:568:PRO:HB2  | 3:C:221:TYR:CE1   | 2.45                     | 0.51              |
| 1:A:675:THR:CG2  | 1:A:736:ASN:HD21  | 2.22                     | 0.51              |
| 1:A:821:ARG:HG3  | 1:A:825:ILE:CD1   | 2.40                     | 0.51              |
| 1:A:836:TYR:CE2  | 1:A:840:ARG:HD2   | 2.45                     | 0.51              |
| 1:A:1299:VAL:CG1 | 1:A:1300:LYS:H    | 2.20                     | 0.51              |
| 2:B:130:VAL:CG1  | 2:B:131:ASP:N     | 2.74                     | 0.51              |
| 2:B:314:LEU:O    | 2:B:315:LYS:C     | 2.53                     | 0.51              |
| 2:B:1035:ALA:HB1 | 2:B:1040:ASN:O    | 2.10                     | 0.51              |
| 3:C:80:LEU:CD2   | 3:C:129:ILE:HD11  | 2.28                     | 0.51              |
| 5:E:124:VAL:HG22 | 5:E:132:ILE:CG2   | 2.39                     | 0.51              |
| 9:I:75:CYS:HG    | 9:I:106:CYS:HG    | 1.59                     | 0.51              |
| 10:J:14:VAL:HG12 | 10:J:50:ILE:HD11  | 1.92                     | 0.51              |
| 1:A:357:PRO:HG2  | 2:B:833:TYR:CE1   | 2.45                     | 0.51              |
| 1:A:753:GLY:HA2  | 1:A:757:ASN:HD22  | 1.74                     | 0.51              |
| 1:A:898:ARG:HD2  | 1:A:899:VAL:N     | 2.26                     | 0.51              |
| 1:A:929:LEU:H    | 1:A:929:LEU:CD2   | 2.23                     | 0.51              |
| 2:B:31:TRP:CD1   | 2:B:807:ARG:NH1   | 2.78                     | 0.51              |
| 3:C:177:GLU:HG3  | 3:C:231:ASN:HB3   | 1.93                     | 0.51              |
| 5:E:23:VAL:HG13  | 5:E:28:TYR:CD1    | 2.45                     | 0.51              |
| 6:F:109:VAL:CG2  | 6:F:124:GLU:HG2   | 2.40                     | 0.51              |
| 1:A:27:VAL:HG13  | 1:A:240:PRO:HB3   | 1.91                     | 0.51              |
| 1:A:306:ASN:HD21 | 1:A:324:SER:N     | 2.09                     | 0.51              |
| 1:A:444:PHE:CB   | 1:A:458:HIS:HD2   | 2.24                     | 0.51              |
| 1:A:847:ASP:OD2  | 1:A:858:ASN:HB2   | 2.10                     | 0.51              |
| 1:A:1150:SER:HB2 | 1:A:1195:LEU:HD23 | 1.93                     | 0.51              |
| 1:A:1362:TYR:OH  | 1:A:1364:ASN:HA   | 2.11                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:120:ARG:HB2  | 2:B:122:LEU:HG    | 1.91                     | 0.51              |
| 2:B:463:THR:HG21 | 2:B:465:ASN:HD22  | 1.74                     | 0.51              |
| 2:B:514:LEU:HD12 | 2:B:515:HIS:H     | 1.74                     | 0.51              |
| 2:B:825:VAL:HG12 | 2:B:826:ALA:N     | 2.24                     | 0.51              |
| 2:B:834:ASN:O    | 2:B:1013:ASN:HB2  | 2.10                     | 0.51              |
| 11:K:24:ASP:HB3  | 11:K:30:ALA:HB3   | 1.93                     | 0.51              |
| 1:A:567:LYS:HD2  | 1:A:568:PRO:HD2   | 1.92                     | 0.51              |
| 1:A:1017:LEU:O   | 1:A:1018:PHE:C    | 2.53                     | 0.51              |
| 1:A:1152:ILE:CG2 | 1:A:1260:LEU:HD23 | 2.38                     | 0.51              |
| 1:A:1364:ASN:ND2 | 1:A:1366:ARG:HH11 | 2.09                     | 0.51              |
| 2:B:321:GLY:C    | 2:B:323:VAL:H     | 2.17                     | 0.51              |
| 2:B:864:LYS:HG2  | 2:B:871:THR:HG23  | 1.93                     | 0.51              |
| 5:E:102:GLU:C    | 5:E:104:ASN:N     | 2.67                     | 0.51              |
| 6:F:101:ILE:HD13 | 6:F:120:ILE:HG22  | 1.91                     | 0.51              |
| 10:J:7:CYS:SG    | 10:J:9:SER:HB2    | 2.50                     | 0.51              |
| 12:L:62:LYS:O    | 12:L:64:LEU:HG    | 2.11                     | 0.51              |
| 1:A:332:LYS:H    | 1:A:337:ARG:HD2   | 1.76                     | 0.51              |
| 1:A:649:ILE:O    | 1:A:653:VAL:HG23  | 2.11                     | 0.51              |
| 1:A:849:MET:CE   | 1:A:1061:GLY:HA2  | 2.36                     | 0.51              |
| 1:A:1214:GLU:O   | 1:A:1218:GLN:HG2  | 2.10                     | 0.51              |
| 1:A:1444:MET:HE2 | 6:F:135:ARG:HB2   | 1.92                     | 0.51              |
| 2:B:185:THR:O    | 2:B:189:LEU:HG    | 2.11                     | 0.51              |
| 2:B:271:ALA:O    | 2:B:279:ASP:HA    | 2.11                     | 0.51              |
| 2:B:283:VAL:HG13 | 2:B:297:ILE:CD1   | 2.41                     | 0.51              |
| 2:B:428:ILE:O    | 2:B:431:TYR:HB3   | 2.10                     | 0.51              |
| 2:B:707:PRO:CG   | 2:B:708:GLU:H     | 2.21                     | 0.51              |
| 3:C:263:THR:C    | 3:C:265:MET:H     | 2.18                     | 0.51              |
| 11:K:101:LEU:O   | 11:K:101:LEU:HD23 | 2.11                     | 0.51              |
| 1:A:15:LYS:CB    | 2:B:1220:ARG:HG2  | 2.33                     | 0.51              |
| 1:A:722:LEU:HD11 | 1:A:794:PRO:HB3   | 1.92                     | 0.51              |
| 1:A:859:SER:OG   | 1:A:1398:MET:HE1  | 2.10                     | 0.51              |
| 1:A:1269:GLU:OE2 | 2:B:263:GLY:HA3   | 2.10                     | 0.51              |
| 1:A:1410:PHE:C   | 1:A:1412:ALA:N    | 2.67                     | 0.51              |
| 2:B:332:ASP:C    | 2:B:334:ILE:H     | 2.17                     | 0.51              |
| 2:B:653:VAL:C    | 2:B:654:ARG:HG2   | 2.36                     | 0.51              |
| 3:C:18:VAL:HG12  | 3:C:20:PHE:HD2    | 1.76                     | 0.51              |
| 3:C:62:PHE:C     | 3:C:62:PHE:CD2    | 2.89                     | 0.51              |
| 5:E:54:GLN:O     | 5:E:57:MET:HB3    | 2.11                     | 0.51              |
| 5:E:168:TYR:HB3  | 5:E:170:LEU:CG    | 2.41                     | 0.51              |
| 1:A:107:CYS:HB2  | 1:A:114:LEU:HD23  | 1.93                     | 0.51              |
| 1:A:376:TYR:OH   | 1:A:498:ARG:HD2   | 2.10                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:500:GLU:OE1   | 2:B:1143:ALA:HB1  | 2.11                     | 0.51              |
| 1:A:901:LEU:HD23  | 1:A:907:THR:HG23  | 1.92                     | 0.51              |
| 2:B:100:PRO:HG3   | 2:B:172:ILE:HD12  | 1.92                     | 0.51              |
| 2:B:365:THR:HG23  | 2:B:367:LEU:HG    | 1.93                     | 0.51              |
| 1:A:49:LYS:HB3    | 1:A:55:ASP:HB2    | 1.92                     | 0.50              |
| 1:A:709:THR:CB    | 1:A:712:GLU:HG3   | 2.41                     | 0.50              |
| 1:A:1312:ASN:O    | 1:A:1316:VAL:HG23 | 2.11                     | 0.50              |
| 2:B:1169:MET:HE3  | 2:B:1205:GLN:HG2  | 1.93                     | 0.50              |
| 2:B:1177:HIS:HB3  | 2:B:1179:GLN:HE21 | 1.74                     | 0.50              |
| 1:A:451:HIS:CD2   | 1:A:1074:GLU:HG3  | 2.45                     | 0.50              |
| 2:B:827:ILE:HG12  | 2:B:1012:ILE:HD11 | 1.93                     | 0.50              |
| 2:B:1106:ARG:HH12 | 2:B:1118:PRO:CB   | 2.24                     | 0.50              |
| 11:K:47:ARG:HH11  | 11:K:47:ARG:CB    | 2.23                     | 0.50              |
| 1:A:857:ARG:HG2   | 1:A:863:VAL:HA    | 1.94                     | 0.50              |
| 1:A:1376:THR:HG23 | 1:A:1376:THR:O    | 2.12                     | 0.50              |
| 1:A:1376:THR:HG23 | 5:E:212:ARG:NH2   | 2.26                     | 0.50              |
| 2:B:1177:HIS:CB   | 2:B:1179:GLN:HE21 | 2.24                     | 0.50              |
| 8:H:95:TYR:HE2    | 8:H:97:MET:HG3    | 1.74                     | 0.50              |
| 8:H:128:ASN:O     | 8:H:131:ASN:ND2   | 2.45                     | 0.50              |
| 10:J:32:GLU:CD    | 10:J:32:GLU:H     | 2.19                     | 0.50              |
| 1:A:587:HIS:HA    | 1:A:607:ILE:O     | 2.11                     | 0.50              |
| 2:B:485:ARG:NH2   | 2:B:782:LEU:HD11  | 2.27                     | 0.50              |
| 2:B:581:PHE:HB2   | 2:B:625:LYS:HG2   | 1.93                     | 0.50              |
| 2:B:686:ASN:C     | 2:B:688:GLY:N     | 2.70                     | 0.50              |
| 2:B:737:THR:HG23  | 9:I:66:PRO:HB2    | 1.93                     | 0.50              |
| 2:B:890:TYR:C     | 2:B:892:LYS:H     | 2.19                     | 0.50              |
| 2:B:1119:VAL:O    | 2:B:1126:GLY:HA3  | 2.11                     | 0.50              |
| 9:I:68:LEU:HB3    | 9:I:84:VAL:HG22   | 1.94                     | 0.50              |
| 10:J:36:LEU:HD13  | 10:J:47:ARG:HG2   | 1.92                     | 0.50              |
| 11:K:91:CYS:O     | 11:K:95:ILE:HG13  | 2.11                     | 0.50              |
| 1:A:573:SER:O     | 1:A:576:GLN:HB2   | 2.11                     | 0.50              |
| 1:A:810:PRO:O     | 1:A:813:PHE:HB3   | 2.11                     | 0.50              |
| 1:A:1384:VAL:HG12 | 1:A:1384:VAL:O    | 2.11                     | 0.50              |
| 1:A:1410:PHE:C    | 1:A:1412:ALA:H    | 2.19                     | 0.50              |
| 2:B:271:ALA:HB3   | 2:B:285:ILE:HD11  | 1.93                     | 0.50              |
| 2:B:559:SER:HA    | 2:B:563:MET:HB3   | 1.91                     | 0.50              |
| 2:B:1098:MET:O    | 2:B:1099:VAL:C    | 2.53                     | 0.50              |
| 2:B:1200:ALA:O    | 2:B:1201:LYS:C    | 2.54                     | 0.50              |
| 10:J:54:VAL:O     | 10:J:56:LEU:N     | 2.43                     | 0.50              |
| 1:A:542:GLU:C     | 1:A:546:VAL:HG23  | 2.36                     | 0.50              |
| 1:A:1111:MET:CE   | 1:A:1330:ASN:OD1  | 2.57                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1155:ASP:CG   | 1:A:1162:VAL:HG23 | 2.37                     | 0.50              |
| 2:B:292:ILE:N     | 2:B:293:PRO:HD2   | 2.25                     | 0.50              |
| 2:B:758:PHE:C     | 2:B:760:ASP:N     | 2.68                     | 0.50              |
| 2:B:800:GLN:OE1   | 2:B:822:ASN:HB2   | 2.12                     | 0.50              |
| 3:C:66:ARG:NH2    | 10:J:2:ILE:CG2    | 2.74                     | 0.50              |
| 9:I:15:TYR:N      | 9:I:15:TYR:CD1    | 2.79                     | 0.50              |
| 9:I:25:LEU:HD12   | 9:I:26:LEU:H      | 1.76                     | 0.50              |
| 9:I:75:CYS:O      | 9:I:77:LYS:N      | 2.44                     | 0.50              |
| 9:I:101:PHE:O     | 9:I:109:ILE:HA    | 2.12                     | 0.50              |
| 1:A:100:LYS:NZ    | 1:A:176:LYS:HD2   | 2.27                     | 0.50              |
| 1:A:341:MET:CE    | 1:A:1401:SER:HB2  | 2.40                     | 0.50              |
| 1:A:751:SER:O     | 1:A:752:LYS:CG    | 2.59                     | 0.50              |
| 2:B:515:HIS:O     | 2:B:516:ASN:C     | 2.54                     | 0.50              |
| 2:B:879:ARG:HD3   | 2:B:885:MET:HE2   | 1.92                     | 0.50              |
| 3:C:22:LEU:CD1    | 3:C:230:MET:HE1   | 2.42                     | 0.50              |
| 5:E:177:ARG:O     | 5:E:212:ARG:HD3   | 2.11                     | 0.50              |
| 11:K:61:TYR:CD1   | 11:K:61:TYR:C     | 2.89                     | 0.50              |
| 1:A:535:THR:HG23  | 1:A:575:LYS:HE2   | 1.93                     | 0.50              |
| 1:A:888:GLY:O     | 1:A:940:ARG:NH2   | 2.44                     | 0.50              |
| 1:A:893:PHE:CE1   | 1:A:940:ARG:HD2   | 2.46                     | 0.50              |
| 1:A:1153:TYR:HA   | 9:I:41:PRO:O      | 2.12                     | 0.50              |
| 1:A:1300:LYS:HB3  | 1:A:1300:LYS:HZ3  | 1.77                     | 0.50              |
| 2:B:642:ASP:HB3   | 2:B:649:LYS:CD    | 2.41                     | 0.50              |
| 2:B:653:VAL:CG2   | 2:B:689:LEU:HB3   | 2.42                     | 0.50              |
| 2:B:858:SER:HA    | 2:B:966:VAL:O     | 2.12                     | 0.50              |
| 2:B:975:GLN:O     | 2:B:990:ILE:HD12  | 2.12                     | 0.50              |
| 2:B:977:GLY:CA    | 2:B:1099:VAL:CG2  | 2.86                     | 0.50              |
| 3:C:142:VAL:H     | 10:J:16:ASP:HB3   | 1.77                     | 0.50              |
| 5:E:80:VAL:HG22   | 5:E:109:ILE:HD12  | 1.94                     | 0.50              |
| 5:E:205:SER:O     | 5:E:206:GLY:C     | 2.54                     | 0.50              |
| 12:L:40:LEU:HD13  | 12:L:44:ASP:OD1   | 2.11                     | 0.50              |
| 1:A:329:LEU:HD22  | 2:B:1203:LEU:CD1  | 2.41                     | 0.50              |
| 1:A:612:ILE:HG23  | 1:A:612:ILE:O     | 2.12                     | 0.50              |
| 1:A:1094:VAL:HG13 | 1:A:1113:THR:CG2  | 2.37                     | 0.50              |
| 1:A:1194:ARG:HH22 | 1:A:1237:ILE:HD13 | 1.73                     | 0.50              |
| 2:B:542:MET:HE2   | 2:B:747:MET:HE2   | 1.93                     | 0.50              |
| 2:B:648:HIS:NE2   | 2:B:650:GLU:OE1   | 2.43                     | 0.50              |
| 2:B:977:GLY:C     | 2:B:1099:VAL:HG23 | 2.37                     | 0.50              |
| 3:C:5:GLY:O       | 3:C:6:PRO:C       | 2.54                     | 0.50              |
| 3:C:254:LYS:HE2   | 11:K:42:LEU:HD13  | 1.94                     | 0.50              |
| 5:E:46:TYR:HE2    | 5:E:58:MET:HA     | 1.76                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:E:98:ILE:O     | 5:E:102:GLU:HG3   | 2.12                     | 0.50              |
| 6:F:82:THR:HG22  | 6:F:84:TYR:N      | 2.27                     | 0.50              |
| 9:I:29:CYS:SG    | 9:I:31:THR:HG22   | 2.52                     | 0.50              |
| 9:I:99:LEU:HB2   | 9:I:112:SER:HB3   | 1.94                     | 0.50              |
| 1:A:105:CYS:SG   | 1:A:138:ILE:HG22  | 2.52                     | 0.49              |
| 1:A:332:LYS:HG3  | 1:A:333:GLU:HG2   | 1.94                     | 0.49              |
| 1:A:466:SER:HB3  | 11:K:2:ASN:ND2    | 2.27                     | 0.49              |
| 1:A:929:LEU:HD21 | 1:A:983:ILE:HG21  | 1.94                     | 0.49              |
| 1:A:1405:THR:O   | 1:A:1406:VAL:C    | 2.54                     | 0.49              |
| 2:B:195:CYS:SG   | 2:B:197:PHE:HB2   | 2.51                     | 0.49              |
| 2:B:240:ILE:O    | 2:B:253:THR:HG23  | 2.11                     | 0.49              |
| 3:C:33:LEU:HG    | 3:C:37:MET:CE     | 2.41                     | 0.49              |
| 3:C:62:PHE:C     | 3:C:62:PHE:HD2    | 2.20                     | 0.49              |
| 8:H:76:THR:O     | 8:H:76:THR:HG22   | 2.11                     | 0.49              |
| 8:H:84:ALA:HB1   | 8:H:87:ARG:HB2    | 1.94                     | 0.49              |
| 9:I:55:THR:HG21  | 9:I:109:ILE:HD13  | 1.93                     | 0.49              |
| 1:A:741:ASN:ND2  | 1:A:743:VAL:N     | 2.60                     | 0.49              |
| 1:A:808:LEU:O    | 2:B:728:ARG:NH1   | 2.43                     | 0.49              |
| 1:A:1142:THR:O   | 1:A:1273:LEU:HD22 | 2.12                     | 0.49              |
| 2:B:579:ARG:HB2  | 2:B:586:TRP:NE1   | 2.27                     | 0.49              |
| 2:B:873:THR:O    | 2:B:914:LYS:HA    | 2.12                     | 0.49              |
| 2:B:1043:ASP:O   | 2:B:1050:ILE:HD12 | 2.12                     | 0.49              |
| 3:C:75:MET:HG3   | 3:C:246:ARG:NH2   | 2.28                     | 0.49              |
| 5:E:56:LYS:HG3   | 5:E:84:ASP:CB     | 2.42                     | 0.49              |
| 1:A:135:PHE:HD1  | 1:A:222:LEU:HD22  | 1.76                     | 0.49              |
| 1:A:394:ASN:OD1  | 1:A:398:GLU:OE1   | 2.30                     | 0.49              |
| 1:A:675:THR:HG21 | 1:A:736:ASN:HD21  | 1.77                     | 0.49              |
| 1:A:821:ARG:CG   | 1:A:825:ILE:HD11  | 2.41                     | 0.49              |
| 1:A:829:VAL:C    | 1:A:831:THR:N     | 2.70                     | 0.49              |
| 2:B:260:GLY:O    | 2:B:267:ARG:HD3   | 2.12                     | 0.49              |
| 2:B:542:MET:HG3  | 2:B:747:MET:CE    | 2.38                     | 0.49              |
| 2:B:570:VAL:HG11 | 2:B:573:GLN:OE1   | 2.13                     | 0.49              |
| 2:B:734:HIS:O    | 2:B:735:ALA:HB2   | 2.12                     | 0.49              |
| 3:C:77:ILE:HG23  | 3:C:161:LYS:HE3   | 1.94                     | 0.49              |
| 6:F:133:VAL:HG22 | 6:F:147:SER:HA    | 1.94                     | 0.49              |
| 8:H:6:PHE:HE1    | 8:H:130:ARG:NE    | 2.10                     | 0.49              |
| 8:H:93:TYR:HA    | 8:H:145:ARG:CB    | 2.41                     | 0.49              |
| 9:I:8:ARG:HG3    | 9:I:9:ASP:CG      | 2.37                     | 0.49              |
| 9:I:75:CYS:C     | 9:I:77:LYS:H      | 2.20                     | 0.49              |
| 1:A:50:ILE:C     | 1:A:52:GLY:N      | 2.69                     | 0.49              |
| 1:A:78:PRO:O     | 1:A:79:GLY:C      | 2.56                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:65:GLU:HG3   | 2:B:66:ASP:N      | 2.27                     | 0.49              |
| 2:B:660:LYS:O    | 2:B:663:ALA:HB3   | 2.13                     | 0.49              |
| 2:B:1118:PRO:HD3 | 2:B:1155:SER:HA   | 1.95                     | 0.49              |
| 8:H:31:THR:O     | 8:H:32:THR:HB     | 2.11                     | 0.49              |
| 8:H:47:PHE:HB2   | 8:H:95:TYR:HD1    | 1.76                     | 0.49              |
| 1:A:738:LYS:NZ   | 3:C:194:GLU:HA    | 2.26                     | 0.49              |
| 1:A:1099:PRO:O   | 1:A:1102:LYS:HB3  | 2.13                     | 0.49              |
| 1:A:1134:ILE:O   | 1:A:1138:ILE:HG13 | 2.12                     | 0.49              |
| 1:A:1166:ASP:CG  | 1:A:1194:ARG:HH21 | 2.19                     | 0.49              |
| 2:B:896:ASP:OD2  | 12:L:58:LYS:HE3   | 2.13                     | 0.49              |
| 3:C:43:THR:CG2   | 3:C:44:LEU:N      | 2.75                     | 0.49              |
| 6:F:81:THR:HG22  | 6:F:82:THR:H      | 1.78                     | 0.49              |
| 8:H:44:VAL:O     | 8:H:44:VAL:HG12   | 2.12                     | 0.49              |
| 11:K:97:LYS:O    | 11:K:100:ALA:HB3  | 2.12                     | 0.49              |
| 12:L:52:GLY:O    | 12:L:54:ARG:HG3   | 2.12                     | 0.49              |
| 1:A:474:VAL:HG13 | 1:A:478:TYR:CE1   | 2.48                     | 0.49              |
| 1:A:538:ASP:OD1  | 8:H:22:LYS:HB2    | 2.12                     | 0.49              |
| 1:A:1436:ILE:O   | 1:A:1437:GLY:C    | 2.56                     | 0.49              |
| 2:B:171:PRO:HD2  | 2:B:457:LEU:CD1   | 2.43                     | 0.49              |
| 3:C:75:MET:HG3   | 3:C:246:ARG:HH22  | 1.77                     | 0.49              |
| 5:E:102:GLU:C    | 5:E:104:ASN:H     | 2.20                     | 0.49              |
| 11:K:78:THR:O    | 11:K:79:GLU:C     | 2.56                     | 0.49              |
| 1:A:74:MET:O     | 1:A:75:ASN:HB2    | 2.13                     | 0.49              |
| 1:A:226:GLU:CG   | 1:A:227:VAL:N     | 2.75                     | 0.49              |
| 1:A:391:LEU:O    | 1:A:394:ASN:N     | 2.46                     | 0.49              |
| 1:A:545:GLN:O    | 1:A:548:ASN:N     | 2.44                     | 0.49              |
| 1:A:709:THR:C    | 1:A:711:ARG:N     | 2.67                     | 0.49              |
| 2:B:726:ALA:HB1  | 2:B:1051:THR:CG2  | 2.43                     | 0.49              |
| 2:B:1208:MET:HA  | 2:B:1212:ILE:O    | 2.12                     | 0.49              |
| 6:F:111:LEU:C    | 6:F:113:GLY:N     | 2.71                     | 0.49              |
| 8:H:88:SER:O     | 8:H:89:LEU:HG     | 2.12                     | 0.49              |
| 9:I:85:PHE:O     | 9:I:86:PHE:HB3    | 2.12                     | 0.49              |
| 1:A:418:SER:HB3  | 1:A:421:ALA:HB2   | 1.94                     | 0.49              |
| 1:A:795:GLU:HG2  | 2:B:731:VAL:HG21  | 1.93                     | 0.49              |
| 2:B:25:ILE:CG2   | 2:B:29:ASP:CB     | 2.91                     | 0.49              |
| 2:B:635:ARG:NH1  | 2:B:742:GLU:OE2   | 2.45                     | 0.49              |
| 3:C:4:GLU:O      | 3:C:5:GLY:O       | 2.31                     | 0.49              |
| 5:E:7:ARG:C      | 5:E:9:ILE:N       | 2.71                     | 0.49              |
| 11:K:55:LYS:CD   | 11:K:78:THR:HB    | 2.42                     | 0.49              |
| 1:A:1100:ARG:NH2 | 1:A:1330:ASN:HB2  | 2.28                     | 0.49              |
| 2:B:225:VAL:HG11 | 2:B:388:CYS:HB3   | 1.95                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:291:ILE:HD13  | 2:B:300:HIS:CD2   | 2.48                     | 0.49              |
| 2:B:380:TYR:CE1   | 2:B:384:ARG:HD3   | 2.48                     | 0.49              |
| 2:B:488:TYR:CE2   | 2:B:813:LYS:HB2   | 2.48                     | 0.49              |
| 2:B:642:ASP:O     | 2:B:643:ASP:C     | 2.56                     | 0.49              |
| 2:B:737:THR:CG2   | 9:I:66:PRO:CB     | 2.89                     | 0.49              |
| 2:B:756:ILE:CG2   | 2:B:759:PRO:HB3   | 2.42                     | 0.49              |
| 2:B:890:TYR:O     | 2:B:892:LYS:N     | 2.46                     | 0.49              |
| 10:J:16:ASP:OD1   | 10:J:17:LYS:HE3   | 2.12                     | 0.49              |
| 1:A:5:GLN:O       | 2:B:1159:ARG:NH2  | 2.46                     | 0.49              |
| 1:A:337:ARG:CZ    | 1:A:839:ARG:HH12  | 2.22                     | 0.49              |
| 1:A:378:GLU:HG2   | 1:A:388:LEU:HD11  | 1.94                     | 0.49              |
| 1:A:1121:GLU:O    | 1:A:1122:PRO:C    | 2.56                     | 0.49              |
| 2:B:781:PHE:O     | 2:B:782:LEU:HG    | 2.12                     | 0.49              |
| 2:B:1177:HIS:C    | 2:B:1179:GLN:N    | 2.68                     | 0.49              |
| 4:D:118:UNK:CA    | 4:D:119:UNK:CA    | 2.91                     | 0.49              |
| 8:H:59:ILE:O      | 8:H:60:ALA:HB3    | 2.12                     | 0.49              |
| 11:K:83:PRO:HA    | 11:K:86:ALA:HB3   | 1.95                     | 0.49              |
| 1:A:1001:ARG:HG2  | 1:A:1001:ARG:HH11 | 1.77                     | 0.48              |
| 1:A:1046:LEU:O    | 1:A:1047:SER:C    | 2.55                     | 0.48              |
| 2:B:821:GLN:OE1   | 2:B:850:LEU:HD12  | 2.13                     | 0.48              |
| 2:B:1053:GLU:O    | 2:B:1055:ILE:N    | 2.46                     | 0.48              |
| 1:A:13:THR:HG23   | 1:A:1432:GLN:CD   | 2.38                     | 0.48              |
| 1:A:61:ILE:HA     | 1:A:74:MET:SD     | 2.53                     | 0.48              |
| 1:A:69:THR:O      | 1:A:69:THR:HG22   | 2.12                     | 0.48              |
| 1:A:332:LYS:N     | 1:A:337:ARG:HD2   | 2.28                     | 0.48              |
| 1:A:491:VAL:O     | 1:A:493:GLN:NE2   | 2.46                     | 0.48              |
| 1:A:589:GLN:OE1   | 1:A:591:PHE:HE1   | 1.96                     | 0.48              |
| 1:A:738:LYS:HB3   | 8:H:19:ARG:HH22   | 1.79                     | 0.48              |
| 1:A:918:GLU:HG3   | 1:A:918:GLU:O     | 2.12                     | 0.48              |
| 2:B:726:ALA:HB1   | 2:B:1051:THR:HG21 | 1.95                     | 0.48              |
| 2:B:1060:ARG:O    | 2:B:1063:GLY:N    | 2.45                     | 0.48              |
| 2:B:1065:GLN:HE22 | 2:B:1067:ARG:HG2  | 1.79                     | 0.48              |
| 2:B:1160:VAL:HG11 | 2:B:1169:MET:SD   | 2.53                     | 0.48              |
| 5:E:100:ILE:CG2   | 5:E:105:PHE:HB2   | 2.42                     | 0.48              |
| 8:H:39:THR:O      | 8:H:123:MET:HA    | 2.14                     | 0.48              |
| 8:H:49:VAL:CG1    | 8:H:50:ALA:N      | 2.75                     | 0.48              |
| 1:A:68:GLN:NE2    | 1:A:80:HIS:CB     | 2.76                     | 0.48              |
| 1:A:1189:SER:OG   | 1:A:1190:PRO:HD2  | 2.12                     | 0.48              |
| 1:A:1415:SER:O    | 1:A:1416:ALA:C    | 2.56                     | 0.48              |
| 2:B:227:LYS:HB2   | 2:B:395:GLN:OE1   | 2.13                     | 0.48              |
| 2:B:283:VAL:O     | 2:B:286:PHE:HB2   | 2.11                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:351:TYR:O     | 2:B:355:ILE:HG13  | 2.12                     | 0.48              |
| 5:E:138:ALA:C     | 5:E:140:LEU:H     | 2.21                     | 0.48              |
| 1:A:606:LEU:HB2   | 1:A:614:PHE:CE2   | 2.47                     | 0.48              |
| 1:A:742:ASN:C     | 1:A:745:GLN:HB2   | 2.38                     | 0.48              |
| 1:A:783:THR:HG21  | 1:A:815:PHE:CE2   | 2.48                     | 0.48              |
| 1:A:1097:GLY:C    | 1:A:1099:PRO:HD2  | 2.39                     | 0.48              |
| 1:A:1406:VAL:CG1  | 1:A:1410:PHE:HE1  | 2.26                     | 0.48              |
| 1:A:1436:ILE:CG2  | 1:A:1437:GLY:N    | 2.72                     | 0.48              |
| 2:B:526:GLU:CD    | 2:B:752:ALA:HB3   | 2.38                     | 0.48              |
| 2:B:911:ILE:HD11  | 2:B:941:LEU:HB2   | 1.94                     | 0.48              |
| 2:B:957:ASN:O     | 2:B:958:GLN:C     | 2.55                     | 0.48              |
| 2:B:1162:ILE:HD11 | 2:B:1194:ILE:CD1  | 2.41                     | 0.48              |
| 3:C:11:ARG:NH2    | 3:C:229:TYR:CD2   | 2.68                     | 0.48              |
| 3:C:135:GLN:C     | 3:C:136:ASP:O     | 2.56                     | 0.48              |
| 3:C:142:VAL:H     | 10:J:16:ASP:CB    | 2.26                     | 0.48              |
| 3:C:254:LYS:O     | 3:C:258:ILE:HD13  | 2.13                     | 0.48              |
| 5:E:102:GLU:O     | 5:E:104:ASN:N     | 2.46                     | 0.48              |
| 6:F:87:LYS:HE2    | 6:F:88:TYR:CE1    | 2.48                     | 0.48              |
| 1:A:154:SER:HB3   | 1:A:162:VAL:HG21  | 1.92                     | 0.48              |
| 1:A:381:THR:O     | 1:A:384:ASN:N     | 2.41                     | 0.48              |
| 1:A:475:THR:CG2   | 1:A:476:SER:N     | 2.76                     | 0.48              |
| 1:A:874:ASP:HA    | 1:A:1058:VAL:HG22 | 1.95                     | 0.48              |
| 1:A:913:LEU:HD11  | 1:A:981:LEU:O     | 2.14                     | 0.48              |
| 1:A:1356:ILE:HD12 | 1:A:1368:MET:SD   | 2.54                     | 0.48              |
| 1:A:1412:ALA:HA   | 1:A:1417:GLU:OE2  | 2.14                     | 0.48              |
| 2:B:745:PRO:C     | 2:B:747:MET:N     | 2.70                     | 0.48              |
| 2:B:1175:LEU:O    | 2:B:1176:ASN:CG   | 2.56                     | 0.48              |
| 6:F:82:THR:HG22   | 6:F:84:TYR:H      | 1.77                     | 0.48              |
| 7:G:136:UNK:CA    | 7:G:137:UNK:CA    | 2.91                     | 0.48              |
| 11:K:43:GLY:HA2   | 11:K:71:PHE:CZ    | 2.49                     | 0.48              |
| 1:A:31:SER:HB2    | 1:A:83:HIS:HB2    | 1.91                     | 0.48              |
| 1:A:89:PRO:HG3    | 1:A:208:LEU:CD1   | 2.44                     | 0.48              |
| 1:A:365:GLY:O     | 1:A:468:PHE:HA    | 2.14                     | 0.48              |
| 1:A:545:GLN:OE1   | 1:A:549:MET:HE2   | 2.14                     | 0.48              |
| 1:A:674:PRO:O     | 1:A:677:ARG:HB3   | 2.13                     | 0.48              |
| 2:B:298:LEU:N     | 2:B:298:LEU:HD23  | 2.29                     | 0.48              |
| 2:B:363:HIS:CD2   | 2:B:585:VAL:HG22  | 2.49                     | 0.48              |
| 3:C:212:PRO:HB3   | 3:C:213:PRO:HD2   | 1.95                     | 0.48              |
| 9:I:62:ILE:CG2    | 9:I:63:GLY:N      | 2.77                     | 0.48              |
| 11:K:27:ALA:HB1   | 11:K:28:PRO:HD2   | 1.96                     | 0.48              |
| 11:K:92:ASN:O     | 11:K:93:SER:C     | 2.56                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:742:ASN:O     | 1:A:745:GLN:HB2   | 2.13                     | 0.48              |
| 1:A:873:MET:HE3   | 1:A:957:PRO:HG3   | 1.94                     | 0.48              |
| 1:A:1394:THR:CG2  | 1:A:1398:MET:HE3  | 2.40                     | 0.48              |
| 2:B:1077:THR:HG22 | 2:B:1079:LYS:HB2  | 1.94                     | 0.48              |
| 8:H:33:GLN:OE1    | 8:H:129:TYR:CE2   | 2.67                     | 0.48              |
| 8:H:36:CYS:HA     | 8:H:126:GLU:O     | 2.13                     | 0.48              |
| 1:A:112:LYS:HG2   | 1:A:113:LEU:H     | 1.79                     | 0.48              |
| 1:A:178:GLY:O     | 1:A:179:LEU:HD23  | 2.13                     | 0.48              |
| 1:A:531:ILE:CD1   | 1:A:617:VAL:HG11  | 2.44                     | 0.48              |
| 2:B:284:ILE:CD1   | 2:B:324:ILE:HD12  | 2.43                     | 0.48              |
| 2:B:562:GLY:O     | 2:B:563:MET:C     | 2.56                     | 0.48              |
| 2:B:709:ASP:C     | 2:B:710:LEU:HD23  | 2.38                     | 0.48              |
| 2:B:806:THR:C     | 2:B:808:ALA:N     | 2.71                     | 0.48              |
| 2:B:821:GLN:HB2   | 2:B:851:PHE:CE2   | 2.49                     | 0.48              |
| 2:B:1060:ARG:C    | 2:B:1062:HIS:N    | 2.69                     | 0.48              |
| 1:A:167:CYS:O     | 1:A:169:ASN:N     | 2.45                     | 0.48              |
| 1:A:774:ARG:O     | 1:A:775:ILE:C     | 2.57                     | 0.48              |
| 1:A:1277:GLU:O    | 1:A:1278:ASN:HB2  | 2.14                     | 0.48              |
| 1:A:1410:PHE:CE2  | 2:B:1212:ILE:HD11 | 2.45                     | 0.48              |
| 2:B:566:LEU:CD1   | 2:B:588:GLY:HA2   | 2.44                     | 0.48              |
| 2:B:825:VAL:CG1   | 2:B:826:ALA:N     | 2.76                     | 0.48              |
| 1:A:18:GLN:O      | 2:B:1215:ARG:CG   | 2.62                     | 0.48              |
| 1:A:54:ASN:HA     | 1:A:58:LEU:HD12   | 1.95                     | 0.48              |
| 1:A:226:GLU:HG2   | 1:A:227:VAL:N     | 2.29                     | 0.48              |
| 1:A:834:THR:HG21  | 1:A:1077:THR:CA   | 2.43                     | 0.48              |
| 1:A:954:TRP:O     | 1:A:956:LEU:HG    | 2.14                     | 0.48              |
| 1:A:1066:VAL:O    | 1:A:1068:ALA:N    | 2.46                     | 0.48              |
| 2:B:315:LYS:O     | 2:B:318:VAL:N     | 2.46                     | 0.48              |
| 6:F:79:ARG:HG2    | 6:F:146:TRP:CZ2   | 2.49                     | 0.48              |
| 6:F:98:ALA:O      | 6:F:117:PRO:HB2   | 2.14                     | 0.48              |
| 11:K:10:PHE:CE1   | 11:K:11:LEU:HD13  | 2.49                     | 0.48              |
| 12:L:62:LYS:O     | 12:L:64:LEU:N     | 2.37                     | 0.48              |
| 1:A:644:LYS:O     | 1:A:645:LEU:C     | 2.55                     | 0.47              |
| 1:A:1192:LEU:HD11 | 1:A:1239:ARG:CB   | 2.37                     | 0.47              |
| 1:A:1284:MET:HG2  | 1:A:1306:LEU:CD2  | 2.43                     | 0.47              |
| 2:B:55:VAL:HG12   | 2:B:56:ASP:N      | 2.27                     | 0.47              |
| 3:C:258:ILE:HG23  | 11:K:19:LEU:HD11  | 1.96                     | 0.47              |
| 8:H:118:PHE:HB2   | 8:H:121:LEU:HB2   | 1.95                     | 0.47              |
| 9:I:50:THR:HG22   | 9:I:51:ASN:N      | 2.28                     | 0.47              |
| 1:A:443:LEU:CD2   | 1:A:455:MET:HB3   | 2.42                     | 0.47              |
| 1:A:533:LYS:C     | 1:A:535:THR:N     | 2.72                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:291:ILE:HD13  | 2:B:300:HIS:NE2   | 2.29                     | 0.47              |
| 2:B:324:ILE:HG23  | 2:B:329:THR:HB    | 1.96                     | 0.47              |
| 2:B:864:LYS:HB3   | 2:B:871:THR:HA    | 1.96                     | 0.47              |
| 2:B:1156:ASP:HB3  | 2:B:1197:PRO:HA   | 1.95                     | 0.47              |
| 3:C:35:ARG:O      | 3:C:38:ILE:N      | 2.47                     | 0.47              |
| 3:C:67:LEU:HD11   | 3:C:155:LEU:HD13  | 1.95                     | 0.47              |
| 1:A:1386:ARG:HE   | 1:A:1387:HIS:CE1  | 2.32                     | 0.47              |
| 2:B:269:ILE:CD1   | 2:B:386:LEU:HD21  | 2.39                     | 0.47              |
| 2:B:284:ILE:HD13  | 2:B:333:PHE:CD2   | 2.49                     | 0.47              |
| 2:B:484:ASN:CG    | 2:B:486:TYR:HE1   | 2.23                     | 0.47              |
| 2:B:871:THR:HG22  | 2:B:872:GLU:O     | 2.14                     | 0.47              |
| 2:B:1103:ILE:O    | 2:B:1104:HIS:C    | 2.56                     | 0.47              |
| 2:B:1158:PHE:HE2  | 2:B:1201:LYS:HE3  | 1.80                     | 0.47              |
| 3:C:62:PHE:O      | 3:C:66:ARG:HG3    | 2.13                     | 0.47              |
| 3:C:66:ARG:CZ     | 10:J:2:ILE:HG21   | 2.44                     | 0.47              |
| 8:H:83:GLN:C      | 8:H:85:GLY:N      | 2.73                     | 0.47              |
| 9:I:54:GLU:O      | 9:I:89:GLN:HG2    | 2.14                     | 0.47              |
| 10:J:57:ILE:HG12  | 10:J:61:LEU:HD11  | 1.94                     | 0.47              |
| 11:K:59:ALA:HA    | 11:K:74:ARG:O     | 2.15                     | 0.47              |
| 1:A:545:GLN:O     | 1:A:546:VAL:C     | 2.55                     | 0.47              |
| 1:A:1134:ILE:HD11 | 1:A:1321:GLY:HA3  | 1.96                     | 0.47              |
| 1:A:1225:PHE:O    | 1:A:1240:CYS:HA   | 2.14                     | 0.47              |
| 1:A:1237:ILE:HG22 | 1:A:1238:ILE:N    | 2.29                     | 0.47              |
| 2:B:46:GLN:HE21   | 2:B:496:ARG:HG2   | 1.78                     | 0.47              |
| 2:B:51:PHE:CD2    | 2:B:173:MET:HB3   | 2.49                     | 0.47              |
| 2:B:653:VAL:HG12  | 2:B:654:ARG:N     | 2.28                     | 0.47              |
| 2:B:726:ALA:CB    | 2:B:1051:THR:HG21 | 2.45                     | 0.47              |
| 2:B:1182:CYS:O    | 2:B:1183:LYS:O    | 2.31                     | 0.47              |
| 5:E:78:LEU:HD21   | 5:E:80:VAL:HG22   | 1.95                     | 0.47              |
| 8:H:40:LEU:CD2    | 8:H:42:ILE:HD11   | 2.39                     | 0.47              |
| 12:L:30:ILE:CD1   | 12:L:59:ALA:HA    | 2.45                     | 0.47              |
| 1:A:20:GLY:HA2    | 1:A:1413:GLY:O    | 2.14                     | 0.47              |
| 1:A:563:PRO:HG3   | 1:A:572:TRP:CH2   | 2.48                     | 0.47              |
| 1:A:614:PHE:CD1   | 1:A:614:PHE:C     | 2.92                     | 0.47              |
| 1:A:994:GLN:NE2   | 1:A:1019:CYS:HB3  | 2.27                     | 0.47              |
| 1:A:1364:ASN:HD21 | 1:A:1366:ARG:HH11 | 1.60                     | 0.47              |
| 2:B:780:VAL:HG21  | 10:J:56:LEU:HD11  | 1.97                     | 0.47              |
| 2:B:842:ASN:HD22  | 2:B:845:SER:HB3   | 1.80                     | 0.47              |
| 2:B:1054:GLY:O    | 2:B:1058:LEU:HG   | 2.13                     | 0.47              |
| 2:B:1072:MET:HE2  | 2:B:1085:ILE:HB   | 1.96                     | 0.47              |
| 2:B:1169:MET:SD   | 2:B:1201:LYS:HG2  | 2.54                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:43:THR:HG22   | 3:C:44:LEU:N      | 2.29                     | 0.47              |
| 5:E:117:THR:C     | 5:E:119:SER:N     | 2.73                     | 0.47              |
| 8:H:47:PHE:CD1    | 8:H:95:TYR:HB2    | 2.50                     | 0.47              |
| 10:J:44:TYR:HA    | 10:J:47:ARG:HB2   | 1.95                     | 0.47              |
| 1:A:14:VAL:H      | 1:A:1432:GLN:HE22 | 1.61                     | 0.47              |
| 1:A:845:LEU:O     | 1:A:846:GLU:C     | 2.57                     | 0.47              |
| 2:B:123:THR:O     | 2:B:125:SER:N     | 2.47                     | 0.47              |
| 2:B:845:SER:HB2   | 10:J:8:PHE:HB3    | 1.96                     | 0.47              |
| 2:B:1051:THR:HG21 | 2:B:1053:GLU:HB2  | 1.97                     | 0.47              |
| 2:B:1124:ARG:O    | 2:B:1125:ASP:HB3  | 2.14                     | 0.47              |
| 1:A:12:ARG:HD3    | 2:B:1218:THR:HB   | 1.97                     | 0.47              |
| 1:A:83:HIS:CE1    | 1:A:238:CYS:SG    | 3.08                     | 0.47              |
| 1:A:381:THR:CG2   | 1:A:383:TYR:CD1   | 2.98                     | 0.47              |
| 1:A:517:ASN:ND2   | 1:A:1362:TYR:CE2  | 2.83                     | 0.47              |
| 1:A:848:ILE:CD1   | 1:A:1374:VAL:HG21 | 2.45                     | 0.47              |
| 1:A:890:ASP:H     | 1:A:1296:GLY:HA3  | 1.78                     | 0.47              |
| 1:A:1066:VAL:O    | 1:A:1067:LEU:C    | 2.55                     | 0.47              |
| 1:A:1336:MET:HE1  | 1:A:1380:GLY:C    | 2.40                     | 0.47              |
| 1:A:1347:ALA:O    | 1:A:1348:LEU:C    | 2.55                     | 0.47              |
| 2:B:62:ILE:HG21   | 2:B:417:PHE:HD2   | 1.80                     | 0.47              |
| 2:B:236:HIS:CE1   | 2:B:389:ALA:HA    | 2.49                     | 0.47              |
| 2:B:860:MET:HB2   | 2:B:965:LYS:HG2   | 1.97                     | 0.47              |
| 2:B:892:LYS:NZ    | 2:B:909:ASP:OD2   | 2.47                     | 0.47              |
| 2:B:1013:ASN:OD1  | 2:B:1015:HIS:HB2  | 2.15                     | 0.47              |
| 2:B:1116:ARG:NH1  | 2:B:1198:TYR:CD1  | 2.83                     | 0.47              |
| 3:C:262:LEU:O     | 3:C:265:MET:HB3   | 2.15                     | 0.47              |
| 6:F:109:VAL:HG11  | 6:F:123:LYS:HG2   | 1.96                     | 0.47              |
| 1:A:90:VAL:HG21   | 1:A:296:LEU:HG    | 1.95                     | 0.47              |
| 1:A:294:SER:HA    | 1:A:297:GLN:HB3   | 1.96                     | 0.47              |
| 1:A:515:GLN:HA    | 1:A:1367:HIS:NE2  | 2.29                     | 0.47              |
| 1:A:1227:ILE:HG22 | 1:A:1228:TRP:N    | 2.30                     | 0.47              |
| 2:B:512:ARG:NH2   | 2:B:535:LEU:HD11  | 2.02                     | 0.47              |
| 3:C:31:ASN:O      | 3:C:32:SER:C      | 2.56                     | 0.47              |
| 8:H:125:LEU:HG    | 8:H:130:ARG:CZ    | 2.43                     | 0.47              |
| 9:I:100:PHE:HZ    | 9:I:118:ARG:HH12  | 1.62                     | 0.47              |
| 1:A:783:THR:CG2   | 1:A:815:PHE:CE2   | 2.97                     | 0.47              |
| 1:A:829:VAL:O     | 1:A:831:THR:N     | 2.48                     | 0.47              |
| 1:A:873:MET:C     | 1:A:1058:VAL:HG23 | 2.40                     | 0.47              |
| 2:B:666:TYR:C     | 2:B:668:ASP:N     | 2.72                     | 0.47              |
| 2:B:773:MET:SD    | 2:B:987:LYS:HD2   | 2.54                     | 0.47              |
| 2:B:798:TYR:CD2   | 10:J:4:PRO:HG3    | 2.49                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1177:HIS:C    | 2:B:1179:GLN:H    | 2.22                     | 0.47              |
| 6:F:101:ILE:HD11  | 6:F:124:GLU:OE1   | 2.15                     | 0.47              |
| 9:I:74:GLU:OE1    | 9:I:79:HIS:ND1    | 2.47                     | 0.47              |
| 11:K:83:PRO:O     | 11:K:87:LEU:N     | 2.46                     | 0.47              |
| 1:A:116:ASP:HB2   | 1:A:118:HIS:CD2   | 2.49                     | 0.47              |
| 1:A:152:VAL:CG1   | 1:A:153:PRO:HD2   | 2.45                     | 0.47              |
| 1:A:533:LYS:C     | 1:A:535:THR:H     | 2.23                     | 0.47              |
| 1:A:567:LYS:CD    | 1:A:568:PRO:HD2   | 2.45                     | 0.47              |
| 1:A:866:PHE:C     | 1:A:867:ILE:HG13  | 2.40                     | 0.47              |
| 1:A:908:LEU:O     | 1:A:909:ASP:C     | 2.58                     | 0.47              |
| 1:A:1237:ILE:CG2  | 1:A:1238:ILE:N    | 2.78                     | 0.47              |
| 1:A:1392:SER:O    | 1:A:1393:ASN:ND2  | 2.48                     | 0.47              |
| 2:B:210:LYS:HE2   | 2:B:461:LEU:O     | 2.14                     | 0.47              |
| 2:B:487:THR:O     | 2:B:488:TYR:C     | 2.56                     | 0.47              |
| 5:E:96:PHE:CE1    | 5:E:100:ILE:HD11  | 2.50                     | 0.47              |
| 5:E:137:GLU:O     | 5:E:138:ALA:C     | 2.57                     | 0.47              |
| 8:H:49:VAL:CG1    | 8:H:50:ALA:H      | 2.27                     | 0.47              |
| 1:A:67:CYS:SG     | 1:A:77:CYS:SG     | 3.11                     | 0.46              |
| 1:A:352:VAL:HG12  | 1:A:353:ILE:N     | 2.29                     | 0.46              |
| 1:A:645:LEU:O     | 1:A:649:ILE:HG13  | 2.16                     | 0.46              |
| 1:A:964:ILE:HD13  | 1:A:1035:TYR:CZ   | 2.50                     | 0.46              |
| 1:A:975:HIS:ND1   | 1:A:1036:ARG:HG3  | 2.30                     | 0.46              |
| 1:A:1349:TYR:O    | 1:A:1350:LYS:C    | 2.56                     | 0.46              |
| 1:A:1364:ASN:HD21 | 1:A:1366:ARG:HG2  | 1.67                     | 0.46              |
| 2:B:96:TYR:N      | 2:B:96:TYR:CD1    | 2.83                     | 0.46              |
| 2:B:640:VAL:O     | 2:B:640:VAL:HG12  | 2.15                     | 0.46              |
| 3:C:236:GLY:C     | 3:C:238:ILE:N     | 2.69                     | 0.46              |
| 5:E:100:ILE:O     | 5:E:101:GLN:C     | 2.58                     | 0.46              |
| 5:E:135:PHE:HD2   | 5:E:140:LEU:HD21  | 1.79                     | 0.46              |
| 6:F:101:ILE:HD13  | 6:F:120:ILE:CG2   | 2.45                     | 0.46              |
| 8:H:113:ALA:HA    | 8:H:125:LEU:O     | 2.15                     | 0.46              |
| 1:A:481:ASP:C     | 1:A:481:ASP:OD1   | 2.58                     | 0.46              |
| 1:A:573:SER:OG    | 1:A:576:GLN:HG3   | 2.15                     | 0.46              |
| 1:A:825:ILE:C     | 1:A:827:THR:N     | 2.70                     | 0.46              |
| 1:A:1173:HIS:CD2  | 1:A:1227:ILE:HG23 | 2.51                     | 0.46              |
| 2:B:377:PHE:C     | 2:B:379:GLY:N     | 2.68                     | 0.46              |
| 2:B:487:THR:HG22  | 2:B:489:SER:N     | 2.24                     | 0.46              |
| 2:B:519:TRP:HE1   | 2:B:635:ARG:HH22  | 1.64                     | 0.46              |
| 2:B:802:PRO:HA    | 2:B:822:ASN:HD21  | 1.79                     | 0.46              |
| 2:B:806:THR:HG22  | 2:B:808:ALA:H     | 1.79                     | 0.46              |
| 2:B:906:SER:CB    | 2:B:946:ASN:HB2   | 2.45                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:258:ILE:HD12  | 3:C:258:ILE:N     | 2.30                     | 0.46              |
| 8:H:26:ILE:HD13   | 8:H:49:VAL:HG11   | 1.97                     | 0.46              |
| 1:A:568:PRO:HB2   | 3:C:221:TYR:CZ    | 2.50                     | 0.46              |
| 1:A:849:MET:HB2   | 1:A:1063:MET:SD   | 2.55                     | 0.46              |
| 1:A:1049:ILE:O    | 1:A:1050:GLU:C    | 2.56                     | 0.46              |
| 1:A:1068:ALA:O    | 1:A:1069:ALA:C    | 2.55                     | 0.46              |
| 2:B:100:PRO:O     | 2:B:180:TYR:OH    | 2.31                     | 0.46              |
| 2:B:864:LYS:H     | 2:B:872:GLU:CG    | 2.28                     | 0.46              |
| 10:J:1:MET:O      | 10:J:2:ILE:O      | 2.33                     | 0.46              |
| 10:J:27:GLU:C     | 10:J:29:GLU:H     | 2.23                     | 0.46              |
| 1:A:222:LEU:O     | 1:A:224:PHE:N     | 2.46                     | 0.46              |
| 1:A:869:GLY:O     | 5:E:204:THR:HG21  | 2.14                     | 0.46              |
| 1:A:923:LEU:O     | 1:A:927:VAL:HG23  | 2.14                     | 0.46              |
| 1:A:982:THR:HB    | 1:A:985:ASP:CG    | 2.40                     | 0.46              |
| 1:A:1209:MET:CG   | 1:A:1236:LEU:HD22 | 2.45                     | 0.46              |
| 2:B:31:TRP:CE3    | 2:B:34:ILE:HD12   | 2.50                     | 0.46              |
| 2:B:100:PRO:HD2   | 2:B:180:TYR:CE1   | 2.50                     | 0.46              |
| 2:B:851:PHE:O     | 2:B:974:PRO:HD3   | 2.15                     | 0.46              |
| 1:A:329:LEU:HA    | 1:A:335:ARG:HB2   | 1.98                     | 0.46              |
| 1:A:399:HIS:C     | 1:A:401:GLY:N     | 2.71                     | 0.46              |
| 1:A:477:PRO:HG2   | 1:A:521:MET:HG2   | 1.98                     | 0.46              |
| 2:B:167:ILE:O     | 2:B:167:ILE:HG22  | 2.14                     | 0.46              |
| 2:B:350:GLN:O     | 2:B:351:TYR:C     | 2.59                     | 0.46              |
| 11:K:91:CYS:O     | 11:K:94:ILE:HB    | 2.16                     | 0.46              |
| 1:A:113:LEU:C     | 1:A:115:LEU:H     | 2.23                     | 0.46              |
| 1:A:889:SER:HB3   | 1:A:1297:GLU:HG3  | 1.98                     | 0.46              |
| 1:A:894:GLU:C     | 1:A:896:ARG:N     | 2.74                     | 0.46              |
| 1:A:897:TYR:HD2   | 1:A:936:LEU:HD13  | 1.78                     | 0.46              |
| 1:A:1140:HIS:HB2  | 1:A:1276:VAL:O    | 2.16                     | 0.46              |
| 2:B:230:ALA:N     | 2:B:231:PRO:HD2   | 2.31                     | 0.46              |
| 2:B:800:GLN:HB3   | 10:J:52:THR:HG22  | 1.97                     | 0.46              |
| 3:C:38:ILE:HG13   | 3:C:176:ILE:HD12  | 1.97                     | 0.46              |
| 6:F:117:PRO:O     | 6:F:120:ILE:HB    | 2.16                     | 0.46              |
| 9:I:7:CYS:CB      | 9:I:14:LEU:HD21   | 2.33                     | 0.46              |
| 1:A:658:LEU:HD13  | 2:B:831:SER:HA    | 1.98                     | 0.46              |
| 1:A:666:ILE:CD1   | 2:B:1030:LEU:HD22 | 2.41                     | 0.46              |
| 1:A:852:TYR:OH    | 6:F:89:GLU:OE2    | 2.28                     | 0.46              |
| 1:A:1390:ASN:HD21 | 1:A:1399:ARG:HA   | 1.78                     | 0.46              |
| 2:B:201:GLY:H     | 2:B:202:TYR:HD2   | 1.63                     | 0.46              |
| 2:B:282:ILE:HG13  | 2:B:283:VAL:N     | 2.31                     | 0.46              |
| 2:B:294:ASP:H     | 9:I:12:ASN:ND2    | 2.13                     | 0.46              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:307:ASP:O     | 2:B:308:TRP:C    | 2.59                     | 0.46              |
| 2:B:316:PRO:HA    | 2:B:319:GLU:HG2  | 1.98                     | 0.46              |
| 2:B:680:THR:O     | 2:B:683:SER:OG   | 2.34                     | 0.46              |
| 2:B:1020:ARG:O    | 2:B:1021:MET:C   | 2.58                     | 0.46              |
| 2:B:1100:ASP:HA   | 2:B:1103:ILE:CG1 | 2.46                     | 0.46              |
| 3:C:180:TYR:O     | 3:C:181:ASP:HB3  | 2.15                     | 0.46              |
| 5:E:71:LYS:C      | 5:E:73:PRO:HD3   | 2.40                     | 0.46              |
| 5:E:179:GLN:HA    | 5:E:179:GLN:OE1  | 2.16                     | 0.46              |
| 8:H:114:VAL:O     | 8:H:124:ARG:HA   | 2.16                     | 0.46              |
| 9:I:2:THR:OG1     | 9:I:45:ARG:HB3   | 2.15                     | 0.46              |
| 11:K:71:PHE:CD1   | 11:K:71:PHE:C    | 2.93                     | 0.46              |
| 1:A:55:ASP:HB3    | 1:A:56:PRO:HD3   | 1.98                     | 0.46              |
| 1:A:420:ARG:O     | 1:A:424:ILE:HG13 | 2.16                     | 0.46              |
| 1:A:679:ILE:HG23  | 1:A:729:ALA:CB   | 2.39                     | 0.46              |
| 1:A:960:ILE:O     | 1:A:961:ARG:C    | 2.57                     | 0.46              |
| 2:B:300:HIS:ND1   | 2:B:376:PHE:CE2  | 2.83                     | 0.46              |
| 2:B:1017:ILE:HB   | 2:B:1018:PRO:HD3 | 1.98                     | 0.46              |
| 2:B:1072:MET:O    | 2:B:1081:LEU:HB2 | 2.15                     | 0.46              |
| 3:C:252:GLN:CG    | 11:K:95:ILE:HG23 | 2.46                     | 0.46              |
| 5:E:190:LEU:HD11  | 5:E:196:VAL:HG11 | 1.98                     | 0.46              |
| 1:A:112:LYS:HG2   | 1:A:113:LEU:N    | 2.30                     | 0.46              |
| 1:A:383:TYR:HB3   | 6:F:115:THR:CG2  | 2.44                     | 0.46              |
| 1:A:701:LEU:HA    | 9:I:115:LYS:HE3  | 1.98                     | 0.46              |
| 1:A:881:GLN:OE1   | 1:A:959:ASN:HA   | 2.15                     | 0.46              |
| 1:A:890:ASP:N     | 1:A:1296:GLY:HA3 | 2.30                     | 0.46              |
| 1:A:1327:ILE:O    | 5:E:147:HIS:HE1  | 1.98                     | 0.46              |
| 2:B:240:ILE:C     | 2:B:253:THR:HG23 | 2.41                     | 0.46              |
| 2:B:322:PHE:CG    | 2:B:322:PHE:O    | 2.69                     | 0.46              |
| 2:B:346:GLU:O     | 2:B:347:LYS:C    | 2.58                     | 0.46              |
| 2:B:1085:ILE:HG22 | 2:B:1086:PHE:N   | 2.31                     | 0.46              |
| 8:H:26:ILE:CD1    | 8:H:49:VAL:HG11  | 2.46                     | 0.46              |
| 9:I:34:TYR:O      | 9:I:35:VAL:HG23  | 2.16                     | 0.46              |
| 1:A:50:ILE:HG22   | 1:A:51:GLY:H     | 1.81                     | 0.46              |
| 1:A:53:LEU:HD13   | 1:A:263:THR:HG23 | 1.97                     | 0.46              |
| 1:A:87:ALA:HB3    | 1:A:276:LEU:CD2  | 2.45                     | 0.46              |
| 1:A:446:ARG:HG2   | 1:A:446:ARG:NH1  | 2.28                     | 0.46              |
| 1:A:517:ASN:OD1   | 1:A:517:ASN:O    | 2.34                     | 0.46              |
| 1:A:535:THR:HG22  | 1:A:616:VAL:HA   | 1.98                     | 0.46              |
| 1:A:598:LEU:O     | 1:A:599:SER:C    | 2.59                     | 0.46              |
| 1:A:738:LYS:NZ    | 3:C:194:GLU:CA   | 2.79                     | 0.46              |
| 1:A:786:HIS:CE1   | 2:B:742:GLU:OE1  | 2.64                     | 0.46              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:958:VAL:HG22  | 1:A:1052:GLN:HB3 | 1.98                     | 0.46              |
| 1:A:1394:THR:HG21 | 1:A:1398:MET:SD  | 2.56                     | 0.46              |
| 2:B:280:ILE:HD13  | 2:B:334:ILE:HG12 | 1.95                     | 0.46              |
| 2:B:589:VAL:HG12  | 2:B:590:HIS:H    | 1.81                     | 0.46              |
| 2:B:893:LEU:HD22  | 2:B:897:GLY:O    | 2.16                     | 0.46              |
| 2:B:1085:ILE:CG2  | 2:B:1086:PHE:N   | 2.78                     | 0.46              |
| 2:B:1104:HIS:HB2  | 2:B:1122:ARG:CD  | 2.44                     | 0.46              |
| 2:B:1106:ARG:CD   | 2:B:1126:GLY:O   | 2.62                     | 0.46              |
| 5:E:112:TYR:CE2   | 5:E:134:THR:HB   | 2.51                     | 0.46              |
| 9:I:7:CYS:HB2     | 9:I:14:LEU:CD2   | 2.34                     | 0.46              |
| 1:A:556:TRP:CZ3   | 1:A:558:GLY:HA2  | 2.51                     | 0.45              |
| 1:A:893:PHE:CD1   | 1:A:940:ARG:HD2  | 2.51                     | 0.45              |
| 1:A:1041:ALA:O    | 1:A:1044:TRP:HB3 | 2.15                     | 0.45              |
| 2:B:50:SER:O      | 2:B:53:GLN:HB3   | 2.16                     | 0.45              |
| 2:B:229:ALA:HB1   | 2:B:231:PRO:HD2  | 1.99                     | 0.45              |
| 2:B:844:SER:HG    | 2:B:996:ARG:H    | 1.60                     | 0.45              |
| 2:B:1106:ARG:HG2  | 2:B:1107:ALA:N   | 2.31                     | 0.45              |
| 5:E:96:PHE:CE2    | 5:E:110:PHE:HB2  | 2.50                     | 0.45              |
| 9:I:91:ARG:HD3    | 9:I:91:ARG:HA    | 1.75                     | 0.45              |
| 12:L:45:ALA:O     | 12:L:46:VAL:CG2  | 2.64                     | 0.45              |
| 1:A:592:ASP:N     | 1:A:595:THR:OG1  | 2.48                     | 0.45              |
| 1:A:1208:THR:HG22 | 1:A:1210:GLY:H   | 1.81                     | 0.45              |
| 1:A:1433:MET:HE1  | 6:F:92:ARG:CZ    | 2.47                     | 0.45              |
| 2:B:25:ILE:HD11   | 2:B:653:VAL:CB   | 2.46                     | 0.45              |
| 2:B:345:LYS:O     | 2:B:347:LYS:N    | 2.49                     | 0.45              |
| 2:B:515:HIS:CD2   | 2:B:517:THR:OG1  | 2.66                     | 0.45              |
| 2:B:704:ALA:HB2   | 2:B:738:PHE:CE1  | 2.51                     | 0.45              |
| 2:B:806:THR:OG1   | 2:B:809:MET:HE3  | 2.15                     | 0.45              |
| 2:B:830:TYR:CE2   | 2:B:1000:PRO:HD3 | 2.50                     | 0.45              |
| 2:B:914:LYS:H     | 2:B:938:SER:HB3  | 1.81                     | 0.45              |
| 2:B:956:THR:HG21  | 2:B:960:GLY:HA2  | 1.96                     | 0.45              |
| 3:C:18:VAL:HG12   | 3:C:18:VAL:O     | 2.15                     | 0.45              |
| 9:I:34:TYR:C      | 9:I:35:VAL:HG23  | 2.41                     | 0.45              |
| 11:K:98:LEU:O     | 11:K:99:GLY:C    | 2.58                     | 0.45              |
| 1:A:223:GLY:HA3   | 1:A:1415:SER:HB3 | 1.98                     | 0.45              |
| 1:A:567:LYS:CB    | 1:A:568:PRO:CD   | 2.67                     | 0.45              |
| 1:A:848:ILE:HD13  | 1:A:864:ILE:HD13 | 1.98                     | 0.45              |
| 1:A:1037:LEU:HD13 | 1:A:1042:PHE:HA  | 1.98                     | 0.45              |
| 2:B:168:GLY:H     | 2:B:450:ALA:HB1  | 1.82                     | 0.45              |
| 2:B:238:ALA:HB3   | 2:B:256:VAL:HB   | 1.98                     | 0.45              |
| 2:B:574:SER:HB3   | 2:B:577:ALA:HB2  | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:963:PHE:HE2   | 2:B:965:LYS:HE3   | 1.81                     | 0.45              |
| 5:E:10:SER:O      | 5:E:14:ARG:HG3    | 2.16                     | 0.45              |
| 10:J:34:THR:O     | 10:J:35:ALA:C     | 2.58                     | 0.45              |
| 1:A:962:ARG:O     | 1:A:963:ILE:C     | 2.57                     | 0.45              |
| 1:A:1336:MET:SD   | 1:A:1381:LEU:HG   | 2.56                     | 0.45              |
| 2:B:295:GLY:O     | 2:B:299:GLU:HG3   | 2.16                     | 0.45              |
| 2:B:371:GLU:OE1   | 2:B:371:GLU:N     | 2.49                     | 0.45              |
| 2:B:549:THR:H     | 2:B:628:THR:HG22  | 1.81                     | 0.45              |
| 2:B:1171:VAL:HG13 | 2:B:1191:ILE:HD13 | 1.99                     | 0.45              |
| 3:C:29:MET:O      | 3:C:30:ALA:C      | 2.59                     | 0.45              |
| 5:E:94:LYS:O      | 5:E:98:ILE:HG13   | 2.16                     | 0.45              |
| 8:H:40:LEU:HD13   | 8:H:123:MET:HB2   | 1.99                     | 0.45              |
| 1:A:456:MET:HB2   | 1:A:478:TYR:OH    | 2.17                     | 0.45              |
| 1:A:1209:MET:CE   | 1:A:1236:LEU:HB3  | 2.47                     | 0.45              |
| 2:B:205:ILE:HG12  | 2:B:461:LEU:HB3   | 1.99                     | 0.45              |
| 2:B:707:PRO:O     | 2:B:708:GLU:C     | 2.59                     | 0.45              |
| 2:B:1182:CYS:O    | 2:B:1183:LYS:HD2  | 2.15                     | 0.45              |
| 3:C:249:ASP:O     | 3:C:252:GLN:HB3   | 2.16                     | 0.45              |
| 5:E:185:ALA:CB    | 5:E:190:LEU:HD12  | 2.47                     | 0.45              |
| 8:H:111:LEU:HA    | 8:H:127:GLY:O     | 2.17                     | 0.45              |
| 9:I:92:ARG:CG     | 9:I:93:LYS:H      | 2.30                     | 0.45              |
| 1:A:35:ILE:HD12   | 1:A:241:VAL:HG21  | 1.98                     | 0.45              |
| 1:A:1155:ASP:OD1  | 1:A:1162:VAL:HG23 | 2.17                     | 0.45              |
| 1:A:1410:PHE:HD2  | 2:B:1212:ILE:HD11 | 1.70                     | 0.45              |
| 2:B:100:PRO:HA    | 2:B:125:SER:O     | 2.16                     | 0.45              |
| 2:B:121:ASN:HA    | 2:B:207:GLY:CA    | 2.46                     | 0.45              |
| 2:B:215:GLN:HB2   | 2:B:407:ASP:HB2   | 1.98                     | 0.45              |
| 2:B:260:GLY:HA3   | 2:B:267:ARG:HG2   | 1.98                     | 0.45              |
| 2:B:276:ILE:HD13  | 2:B:334:ILE:CG2   | 2.46                     | 0.45              |
| 2:B:824:ILE:CG2   | 2:B:1087:PHE:CE2  | 3.00                     | 0.45              |
| 2:B:995:ARG:HB2   | 2:B:995:ARG:HH11  | 1.81                     | 0.45              |
| 3:C:242:GLN:OE1   | 3:C:242:GLN:HA    | 2.16                     | 0.45              |
| 8:H:84:ALA:HA     | 8:H:87:ARG:HB2    | 1.98                     | 0.45              |
| 9:I:29:CYS:O      | 9:I:31:THR:N      | 2.49                     | 0.45              |
| 10:J:48:ARG:NH2   | 10:J:49:MET:HE1   | 2.20                     | 0.45              |
| 1:A:335:ARG:HA    | 1:A:335:ARG:HD3   | 1.87                     | 0.45              |
| 1:A:418:SER:O     | 1:A:421:ALA:N     | 2.49                     | 0.45              |
| 1:A:535:THR:HG21  | 1:A:616:VAL:CA    | 2.43                     | 0.45              |
| 1:A:535:THR:O     | 1:A:536:LEU:C     | 2.59                     | 0.45              |
| 1:A:573:SER:H     | 1:A:576:GLN:HG3   | 1.81                     | 0.45              |
| 1:A:845:LEU:O     | 1:A:848:ILE:HG13  | 2.17                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:994:GLN:HE21  | 1:A:1019:CYS:CB   | 2.26                     | 0.45              |
| 1:A:1220:PHE:O    | 1:A:1221:LYS:C    | 2.60                     | 0.45              |
| 2:B:348:ARG:O     | 2:B:349:ILE:C     | 2.60                     | 0.45              |
| 2:B:408:LEU:HD12  | 2:B:408:LEU:HA    | 1.71                     | 0.45              |
| 2:B:763:GLN:CG    | 2:B:765:PRO:HD2   | 2.40                     | 0.45              |
| 2:B:1117:GLN:NE2  | 2:B:1156:ASP:OD2  | 2.48                     | 0.45              |
| 2:B:1185:CYS:O    | 2:B:1186:ASP:HB2  | 2.17                     | 0.45              |
| 3:C:52:GLU:HB3    | 3:C:154:LYS:HB3   | 1.99                     | 0.45              |
| 8:H:38:LEU:HD13   | 8:H:125:LEU:CD1   | 2.46                     | 0.45              |
| 8:H:101:ALA:HB2   | 8:H:116:TYR:CD2   | 2.51                     | 0.45              |
| 10:J:5:VAL:O      | 10:J:6:ARG:HB2    | 2.15                     | 0.45              |
| 1:A:152:VAL:HG13  | 1:A:153:PRO:HD2   | 1.99                     | 0.45              |
| 1:A:340:LEU:HD21  | 2:B:1200:ALA:CA   | 2.47                     | 0.45              |
| 1:A:738:LYS:NZ    | 3:C:194:GLU:C     | 2.74                     | 0.45              |
| 1:A:960:ILE:HD12  | 1:A:1021:LEU:HD21 | 1.99                     | 0.45              |
| 1:A:1208:THR:HG22 | 1:A:1210:GLY:N    | 2.31                     | 0.45              |
| 1:A:1317:MET:CA   | 1:A:1322:ILE:HD11 | 2.46                     | 0.45              |
| 2:B:57:TYR:O      | 2:B:58:THR:C      | 2.60                     | 0.45              |
| 2:B:361:LEU:O     | 2:B:363:HIS:O     | 2.35                     | 0.45              |
| 3:C:69:LEU:HD12   | 3:C:69:LEU:HA     | 1.76                     | 0.45              |
| 9:I:34:TYR:O      | 9:I:35:VAL:CG2    | 2.65                     | 0.45              |
| 1:A:53:LEU:O      | 1:A:54:ASN:C      | 2.60                     | 0.45              |
| 1:A:68:GLN:C      | 1:A:70:CYS:N      | 2.73                     | 0.45              |
| 1:A:79:GLY:C      | 1:A:243:PRO:HG3   | 2.41                     | 0.45              |
| 1:A:351:THR:CG2   | 2:B:1103:ILE:HA   | 2.36                     | 0.45              |
| 1:A:778:GLY:HA3   | 2:B:516:ASN:CB    | 2.46                     | 0.45              |
| 1:A:1114:PRO:O    | 1:A:1330:ASN:OD1  | 2.35                     | 0.45              |
| 2:B:321:GLY:C     | 2:B:323:VAL:N     | 2.74                     | 0.45              |
| 2:B:973:ILE:CG2   | 2:B:974:PRO:HD2   | 2.47                     | 0.45              |
| 2:B:995:ARG:NH1   | 2:B:997:GLU:OE1   | 2.49                     | 0.45              |
| 2:B:1013:ASN:OD1  | 2:B:1015:HIS:N    | 2.44                     | 0.45              |
| 2:B:1096:ARG:O    | 2:B:1097:HIS:CB   | 2.59                     | 0.45              |
| 2:B:1158:PHE:CD2  | 2:B:1198:TYR:HD1  | 2.35                     | 0.45              |
| 3:C:8:VAL:CG1     | 3:C:9:LYS:N       | 2.80                     | 0.45              |
| 3:C:17:ASN:OD1    | 3:C:233:GLU:HG2   | 2.16                     | 0.45              |
| 8:H:116:TYR:HE2   | 8:H:140:ALA:CB    | 2.30                     | 0.45              |
| 12:L:38:LEU:HG    | 12:L:39:SER:H     | 1.82                     | 0.45              |
| 1:A:47:ARG:O      | 1:A:48:ALA:HB2    | 2.16                     | 0.45              |
| 1:A:80:HIS:O      | 1:A:243:PRO:HB3   | 2.17                     | 0.45              |
| 1:A:210:ILE:O     | 1:A:214:ILE:HG13  | 2.17                     | 0.45              |
| 1:A:771:GLU:H     | 1:A:822:GLU:CD    | 2.25                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:815:PHE:O     | 1:A:818:MET:N     | 2.50                     | 0.45              |
| 1:A:1336:MET:HE1  | 1:A:1381:LEU:N    | 2.31                     | 0.45              |
| 1:A:1377:THR:C    | 1:A:1379:GLY:H    | 2.25                     | 0.45              |
| 2:B:361:LEU:N     | 2:B:362:PRO:HD2   | 2.31                     | 0.45              |
| 2:B:365:THR:CG2   | 2:B:367:LEU:H     | 2.30                     | 0.45              |
| 2:B:370:PHE:N     | 2:B:371:GLU:OE1   | 2.50                     | 0.45              |
| 2:B:426:LYS:O     | 2:B:430:ARG:HG3   | 2.17                     | 0.45              |
| 2:B:605:ARG:CZ    | 2:B:639:ILE:HD13  | 2.46                     | 0.45              |
| 2:B:640:VAL:HG23  | 2:B:740:HIS:HA    | 1.97                     | 0.45              |
| 2:B:1159:ARG:NE   | 2:B:1193:GLN:NE2  | 2.33                     | 0.45              |
| 3:C:76:ASP:OD2    | 3:C:128:ASN:N     | 2.47                     | 0.45              |
| 5:E:121:MET:C     | 5:E:123:LEU:N     | 2.75                     | 0.45              |
| 8:H:98:TYR:O      | 8:H:118:PHE:HD2   | 1.99                     | 0.45              |
| 11:K:73:LEU:CD2   | 11:K:75:ILE:HD11  | 2.46                     | 0.45              |
| 1:A:388:LEU:O     | 1:A:392:VAL:HG23  | 2.17                     | 0.44              |
| 1:A:1208:THR:N    | 1:A:1211:GLN:OE1  | 2.49                     | 0.44              |
| 1:A:1428:VAL:HG13 | 2:B:1151:LEU:HD23 | 2.00                     | 0.44              |
| 2:B:707:PRO:O     | 2:B:708:GLU:O     | 2.35                     | 0.44              |
| 2:B:737:THR:O     | 2:B:738:PHE:C     | 2.60                     | 0.44              |
| 2:B:1154:ALA:O    | 2:B:1155:SER:CB   | 2.64                     | 0.44              |
| 3:C:31:ASN:O      | 3:C:35:ARG:HG3    | 2.17                     | 0.44              |
| 3:C:73:GLN:NE2    | 3:C:75:MET:H      | 1.97                     | 0.44              |
| 5:E:147:HIS:CD2   | 5:E:149:LEU:H     | 2.35                     | 0.44              |
| 8:H:57:VAL:HG12   | 8:H:58:THR:N      | 2.32                     | 0.44              |
| 1:A:243:PRO:HB2   | 1:A:245:PRO:HD2   | 1.99                     | 0.44              |
| 1:A:1074:GLU:HB3  | 1:A:1075:PRO:HD3  | 1.97                     | 0.44              |
| 1:A:1152:ILE:HG23 | 1:A:1260:LEU:CD2  | 2.43                     | 0.44              |
| 2:B:332:ASP:O     | 2:B:334:ILE:N     | 2.50                     | 0.44              |
| 2:B:758:PHE:CZ    | 2:B:1044:ALA:HA   | 2.52                     | 0.44              |
| 2:B:847:ASP:O     | 3:C:65:HIS:HE1    | 2.01                     | 0.44              |
| 11:K:24:ASP:HB3   | 11:K:30:ALA:CB    | 2.47                     | 0.44              |
| 1:A:219:PHE:CE2   | 1:A:231:PRO:HD2   | 2.52                     | 0.44              |
| 1:A:815:PHE:C     | 1:A:817:ALA:N     | 2.72                     | 0.44              |
| 1:A:885:THR:HG23  | 1:A:893:PHE:CE1   | 2.36                     | 0.44              |
| 1:A:921:GLY:O     | 1:A:922:ASP:C     | 2.59                     | 0.44              |
| 1:A:1207:LEU:HA   | 1:A:1211:GLN:OE1  | 2.17                     | 0.44              |
| 2:B:293:PRO:C     | 2:B:294:ASP:O     | 2.57                     | 0.44              |
| 2:B:986:GLN:OE1   | 2:B:986:GLN:CA    | 2.64                     | 0.44              |
| 2:B:1163:CYS:C    | 2:B:1165:ILE:H    | 2.26                     | 0.44              |
| 3:C:120:ILE:HD11  | 3:C:130:GLY:O     | 2.17                     | 0.44              |
| 3:C:148:ARG:HD3   | 3:C:149:LYS:H     | 1.83                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:I:106:CYS:O     | 9:I:107:SER:HB2   | 2.18                     | 0.44              |
| 1:A:55:ASP:O      | 1:A:56:PRO:C      | 2.61                     | 0.44              |
| 1:A:244:PRO:O     | 1:A:245:PRO:C     | 2.59                     | 0.44              |
| 1:A:571:LEU:HD22  | 8:H:46:LEU:HD11   | 1.99                     | 0.44              |
| 1:A:1098:VAL:O    | 1:A:1099:PRO:C    | 2.59                     | 0.44              |
| 1:A:1441:PHE:HB2  | 6:F:134:ILE:HG23  | 2.00                     | 0.44              |
| 2:B:189:LEU:O     | 2:B:190:TYR:C     | 2.57                     | 0.44              |
| 2:B:247:GLY:O     | 2:B:248:SER:HB3   | 2.17                     | 0.44              |
| 2:B:972:LYS:CD    | 2:B:1098:MET:HE1  | 2.48                     | 0.44              |
| 3:C:77:ILE:CG2    | 3:C:161:LYS:HE3   | 2.48                     | 0.44              |
| 5:E:136:ASN:C     | 5:E:136:ASN:OD1   | 2.60                     | 0.44              |
| 8:H:5:LEU:O       | 8:H:133:ASN:HB3   | 2.17                     | 0.44              |
| 8:H:40:LEU:HG     | 8:H:42:ILE:HG13   | 1.98                     | 0.44              |
| 1:A:233:TRP:O     | 1:A:235:ILE:N     | 2.50                     | 0.44              |
| 1:A:574:GLY:O     | 1:A:575:LYS:C     | 2.61                     | 0.44              |
| 1:A:1149:ALA:CB   | 9:I:47:GLU:HA     | 2.45                     | 0.44              |
| 1:A:1348:LEU:CD2  | 1:A:1372:VAL:HG13 | 2.39                     | 0.44              |
| 2:B:281:PRO:HG2   | 2:B:284:ILE:CD1   | 2.45                     | 0.44              |
| 2:B:578:THR:HG23  | 2:B:622:LYS:C     | 2.41                     | 0.44              |
| 2:B:744:HIS:CD2   | 2:B:746:SER:OG    | 2.70                     | 0.44              |
| 2:B:904:ARG:CZ    | 2:B:948:ILE:HD11  | 2.48                     | 0.44              |
| 2:B:915:THR:HG21  | 2:B:934:LYS:HG2   | 2.00                     | 0.44              |
| 9:I:84:VAL:O      | 9:I:84:VAL:CG1    | 2.65                     | 0.44              |
| 9:I:99:LEU:HB2    | 9:I:112:SER:CB    | 2.46                     | 0.44              |
| 1:A:42:ASP:OD1    | 1:A:45:GLN:O      | 2.36                     | 0.44              |
| 1:A:974:ASP:CB    | 8:H:136:LYS:NZ    | 2.80                     | 0.44              |
| 1:A:1384:VAL:O    | 1:A:1389:PHE:HE2  | 2.01                     | 0.44              |
| 1:A:1424:VAL:HG11 | 2:B:1139:ILE:HD13 | 2.00                     | 0.44              |
| 2:B:200:GLY:HA2   | 2:B:202:TYR:CD2   | 2.50                     | 0.44              |
| 2:B:204:ILE:C     | 2:B:205:ILE:HD12  | 2.43                     | 0.44              |
| 2:B:288:ALA:HA    | 2:B:331:LEU:HD13  | 1.99                     | 0.44              |
| 2:B:563:MET:HE1   | 2:B:580:VAL:HB    | 2.00                     | 0.44              |
| 2:B:1002:THR:HG21 | 2:B:1006:ILE:HB   | 2.00                     | 0.44              |
| 2:B:1070:GLU:O    | 2:B:1071:VAL:C    | 2.59                     | 0.44              |
| 3:C:22:LEU:HD12   | 3:C:230:MET:HE1   | 1.99                     | 0.44              |
| 1:A:326:ARG:HE    | 1:A:1406:VAL:HG11 | 1.82                     | 0.44              |
| 1:A:367:PRO:CB    | 1:A:466:SER:HA    | 2.47                     | 0.44              |
| 1:A:381:THR:O     | 1:A:382:PRO:C     | 2.60                     | 0.44              |
| 1:A:968:GLN:NE2   | 1:A:1035:TYR:HB2  | 2.32                     | 0.44              |
| 2:B:113:TYR:CD2   | 2:B:192:LEU:HD22  | 2.53                     | 0.44              |
| 2:B:800:GLN:CB    | 10:J:52:THR:HG22  | 2.47                     | 0.44              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:872:GLU:CD    | 2:B:914:LYS:HE2  | 2.43                     | 0.44              |
| 2:B:1002:THR:CG2  | 2:B:1004:GLU:HB2 | 2.47                     | 0.44              |
| 5:E:16:PHE:O      | 5:E:17:ARG:C     | 2.60                     | 0.44              |
| 5:E:28:TYR:CE2    | 5:E:64:PRO:HG3   | 2.53                     | 0.44              |
| 6:F:147:SER:HG    | 6:F:150:GLU:HG3  | 1.78                     | 0.44              |
| 8:H:47:PHE:CB     | 8:H:95:TYR:HD1   | 2.31                     | 0.44              |
| 10:J:16:ASP:OD1   | 10:J:17:LYS:HG3  | 2.17                     | 0.44              |
| 11:K:24:ASP:OD1   | 11:K:26:LYS:N    | 2.51                     | 0.44              |
| 12:L:51:CYS:C     | 12:L:53:HIS:N    | 2.75                     | 0.44              |
| 1:A:21:LEU:HD21   | 1:A:95:PHE:CZ    | 2.53                     | 0.44              |
| 1:A:367:PRO:O     | 1:A:368:LYS:C    | 2.61                     | 0.44              |
| 1:A:591:PHE:HD2   | 1:A:595:THR:HB   | 1.83                     | 0.44              |
| 1:A:1046:LEU:C    | 1:A:1048:ASN:N   | 2.75                     | 0.44              |
| 1:A:1441:PHE:HB2  | 6:F:134:ILE:CG2  | 2.47                     | 0.44              |
| 2:B:56:ASP:HB3    | 2:B:57:TYR:CD1   | 2.52                     | 0.44              |
| 2:B:185:THR:H     | 2:B:188:ASP:HB2  | 1.81                     | 0.44              |
| 2:B:315:LYS:N     | 2:B:316:PRO:HD2  | 2.32                     | 0.44              |
| 2:B:650:GLU:HG2   | 2:B:654:ARG:NH1  | 2.33                     | 0.44              |
| 2:B:702:LEU:HD21  | 2:B:735:ALA:HB1  | 1.98                     | 0.44              |
| 2:B:864:LYS:HD3   | 2:B:871:THR:CB   | 2.47                     | 0.44              |
| 3:C:22:LEU:CD2    | 3:C:25:VAL:HG21  | 2.37                     | 0.44              |
| 3:C:186:LEU:HD12  | 3:C:186:LEU:HA   | 1.86                     | 0.44              |
| 5:E:133:GLU:HB3   | 5:E:135:PHE:HE1  | 1.83                     | 0.44              |
| 1:A:1094:VAL:HG12 | 1:A:1095:THR:N   | 2.32                     | 0.44              |
| 1:A:1097:GLY:O    | 1:A:1098:VAL:C   | 2.60                     | 0.44              |
| 2:B:216:GLU:OE1   | 2:B:537:LYS:CE   | 2.66                     | 0.44              |
| 2:B:274:PRO:O     | 2:B:276:ILE:N    | 2.51                     | 0.44              |
| 2:B:640:VAL:HG23  | 2:B:740:HIS:CA   | 2.48                     | 0.44              |
| 2:B:809:MET:HE1   | 2:B:983:ARG:HH22 | 1.82                     | 0.44              |
| 2:B:1120:GLU:HG2  | 2:B:1121:GLY:N   | 2.31                     | 0.44              |
| 3:C:39:ALA:HA     | 3:C:164:ALA:CB   | 2.46                     | 0.44              |
| 1:A:54:ASN:O      | 1:A:55:ASP:HB2   | 2.18                     | 0.43              |
| 1:A:69:THR:O      | 2:B:1174:LYS:HG2 | 2.17                     | 0.43              |
| 1:A:92:HIS:CD2    | 1:A:92:HIS:C     | 2.96                     | 0.43              |
| 1:A:148:CYS:HB3   | 1:A:167:CYS:O    | 2.18                     | 0.43              |
| 1:A:401:GLY:H     | 1:A:435:HIS:HD2  | 1.66                     | 0.43              |
| 1:A:466:SER:HB3   | 11:K:2:ASN:HD22  | 1.82                     | 0.43              |
| 1:A:496:GLU:O     | 1:A:497:THR:C    | 2.60                     | 0.43              |
| 1:A:595:THR:HG22  | 1:A:596:THR:N    | 2.33                     | 0.43              |
| 1:A:741:ASN:HD22  | 1:A:743:VAL:N    | 2.16                     | 0.43              |
| 2:B:102:VAL:HG21  | 2:B:112:LEU:HD13 | 1.99                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:130:VAL:CG1   | 2:B:131:ASP:H    | 2.29                     | 0.43              |
| 2:B:203:PHE:HE1   | 2:B:212:LEU:CD1  | 2.31                     | 0.43              |
| 2:B:212:LEU:HD13  | 2:B:409:ALA:HA   | 2.00                     | 0.43              |
| 2:B:849:GLY:O     | 2:B:850:LEU:C    | 2.59                     | 0.43              |
| 2:B:855:PHE:HZ    | 2:B:857:ARG:HH12 | 1.64                     | 0.43              |
| 3:C:143:LEU:HD21  | 3:C:146:LYS:HE3  | 1.99                     | 0.43              |
| 8:H:11:GLN:C      | 8:H:28:ALA:HB1   | 2.42                     | 0.43              |
| 11:K:40:HIS:O     | 11:K:41:THR:C    | 2.60                     | 0.43              |
| 11:K:47:ARG:C     | 11:K:47:ARG:HD2  | 2.43                     | 0.43              |
| 11:K:55:LYS:HD3   | 11:K:78:THR:OG1  | 2.18                     | 0.43              |
| 11:K:92:ASN:C     | 11:K:94:ILE:N    | 2.75                     | 0.43              |
| 12:L:26:THR:C     | 12:L:27:LEU:HD23 | 2.43                     | 0.43              |
| 1:A:7:SER:OG      | 2:B:1193:GLN:NE2 | 2.51                     | 0.43              |
| 1:A:84:ILE:HG23   | 1:A:84:ILE:O     | 2.17                     | 0.43              |
| 1:A:131:SER:OG    | 1:A:132:LYS:N    | 2.51                     | 0.43              |
| 1:A:306:ASN:OD1   | 1:A:313:GLN:NE2  | 2.51                     | 0.43              |
| 1:A:650:GLN:O     | 1:A:651:LYS:C    | 2.58                     | 0.43              |
| 1:A:673:GLY:N     | 1:A:674:PRO:HD2  | 2.33                     | 0.43              |
| 1:A:1148:ILE:HD12 | 1:A:1196:GLU:HG2 | 2.01                     | 0.43              |
| 1:A:1342:GLU:HG2  | 5:E:212:ARG:HH11 | 1.83                     | 0.43              |
| 1:A:1364:ASN:HD22 | 1:A:1366:ARG:N   | 2.16                     | 0.43              |
| 2:B:577:ALA:HB1   | 2:B:589:VAL:HG12 | 2.00                     | 0.43              |
| 2:B:806:THR:N     | 2:B:809:MET:HE3  | 2.33                     | 0.43              |
| 2:B:864:LYS:HD3   | 2:B:871:THR:CA   | 2.47                     | 0.43              |
| 2:B:1116:ARG:CZ   | 2:B:1198:TYR:CE1 | 3.01                     | 0.43              |
| 2:B:1117:GLN:HG3  | 2:B:1156:ASP:CG  | 2.43                     | 0.43              |
| 3:C:59:ALA:O      | 3:C:63:ILE:HG13  | 2.18                     | 0.43              |
| 3:C:263:THR:C     | 3:C:265:MET:N    | 2.77                     | 0.43              |
| 5:E:138:ALA:O     | 5:E:140:LEU:N    | 2.50                     | 0.43              |
| 5:E:145:THR:HG21  | 5:E:187:TYR:CE2  | 2.53                     | 0.43              |
| 8:H:81:PRO:HD2    | 8:H:82:PRO:HD2   | 1.98                     | 0.43              |
| 9:I:55:THR:HG21   | 9:I:109:ILE:CD1  | 2.48                     | 0.43              |
| 9:I:98:VAL:CG1    | 9:I:99:LEU:N     | 2.81                     | 0.43              |
| 12:L:27:LEU:HD13  | 12:L:37:LYS:CB   | 2.48                     | 0.43              |
| 1:A:103:CYS:O     | 1:A:106:VAL:O    | 2.35                     | 0.43              |
| 1:A:362:ASP:OD1   | 1:A:459:ARG:HD3  | 2.18                     | 0.43              |
| 1:A:518:LYS:HB2   | 1:A:519:PRO:HD2  | 2.00                     | 0.43              |
| 1:A:852:TYR:CE2   | 6:F:136:ARG:NE   | 2.86                     | 0.43              |
| 1:A:901:LEU:HD13  | 1:A:919:ILE:CG2  | 2.48                     | 0.43              |
| 1:A:928:LEU:O     | 1:A:929:LEU:C    | 2.59                     | 0.43              |
| 2:B:56:ASP:HB3    | 2:B:57:TYR:CE1   | 2.53                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:295:GLY:H    | 2:B:298:LEU:HG    | 1.84                     | 0.43              |
| 2:B:358:LYS:O    | 2:B:359:GLU:OE1   | 2.36                     | 0.43              |
| 2:B:705:MET:H    | 2:B:710:LEU:CD1   | 2.32                     | 0.43              |
| 2:B:1038:SER:HB3 | 2:B:1062:HIS:NE2  | 2.32                     | 0.43              |
| 3:C:8:VAL:HA     | 3:C:21:ILE:O      | 2.19                     | 0.43              |
| 9:I:46:HIS:O     | 9:I:47:GLU:HB2    | 2.18                     | 0.43              |
| 12:L:43:THR:HG22 | 12:L:43:THR:O     | 2.18                     | 0.43              |
| 1:A:84:ILE:CG2   | 1:A:239:LEU:HB3   | 2.48                     | 0.43              |
| 1:A:343:LYS:NZ   | 2:B:1156:ASP:OD2  | 2.49                     | 0.43              |
| 1:A:494:SER:HB2  | 1:A:497:THR:OG1   | 2.18                     | 0.43              |
| 1:A:751:SER:OG   | 2:B:1015:HIS:CE1  | 2.71                     | 0.43              |
| 1:A:850:VAL:O    | 1:A:1060:PRO:HA   | 2.18                     | 0.43              |
| 2:B:958:GLN:C    | 2:B:960:GLY:H     | 2.20                     | 0.43              |
| 2:B:1106:ARG:NH1 | 2:B:1118:PRO:CB   | 2.72                     | 0.43              |
| 5:E:69:ILE:O     | 5:E:73:PRO:HG3    | 2.19                     | 0.43              |
| 5:E:138:ALA:C    | 5:E:140:LEU:N     | 2.76                     | 0.43              |
| 1:A:86:LEU:HB3   | 1:A:296:LEU:HD21  | 1.99                     | 0.43              |
| 1:A:99:ILE:O     | 1:A:100:LYS:C     | 2.61                     | 0.43              |
| 1:A:344:ARG:O    | 2:B:1118:PRO:HG2  | 2.19                     | 0.43              |
| 1:A:834:THR:HG21 | 1:A:1077:THR:HA   | 2.00                     | 0.43              |
| 2:B:194:GLU:OE1  | 2:B:194:GLU:HA    | 2.18                     | 0.43              |
| 2:B:276:ILE:HD13 | 2:B:334:ILE:HG23  | 1.99                     | 0.43              |
| 2:B:781:PHE:CE2  | 2:B:795:ILE:HD11  | 2.53                     | 0.43              |
| 3:C:9:LYS:HB2    | 3:C:21:ILE:HB     | 1.98                     | 0.43              |
| 3:C:135:GLN:O    | 3:C:136:ASP:O     | 2.37                     | 0.43              |
| 3:C:249:ASP:OD1  | 3:C:253:LYS:HE3   | 2.19                     | 0.43              |
| 8:H:12:VAL:HG13  | 8:H:26:ILE:HG23   | 2.01                     | 0.43              |
| 1:A:68:GLN:O     | 1:A:70:CYS:N      | 2.52                     | 0.43              |
| 1:A:1118:VAL:O   | 1:A:1305:VAL:HG13 | 2.18                     | 0.43              |
| 2:B:690:VAL:HG12 | 2:B:691:GLU:N     | 2.33                     | 0.43              |
| 2:B:969:ARG:HG2  | 2:B:970:THR:N     | 2.33                     | 0.43              |
| 3:C:123:ASN:ND2  | 3:C:125:MET:HG2   | 2.31                     | 0.43              |
| 8:H:109:LYS:HB2  | 8:H:109:LYS:HZ2   | 1.83                     | 0.43              |
| 1:A:404:TYR:HA   | 1:A:413:ILE:O     | 2.18                     | 0.43              |
| 1:A:565:ILE:HD13 | 1:A:567:LYS:HE2   | 2.01                     | 0.43              |
| 1:A:1158:PRO:HB3 | 1:A:1241:ARG:HH12 | 1.83                     | 0.43              |
| 2:B:781:PHE:HE2  | 2:B:795:ILE:HD11  | 1.83                     | 0.43              |
| 2:B:1152:MET:SD  | 2:B:1197:PRO:HD3  | 2.59                     | 0.43              |
| 3:C:5:GLY:O      | 3:C:6:PRO:O       | 2.37                     | 0.43              |
| 5:E:59:SER:HA    | 5:E:80:VAL:O      | 2.19                     | 0.43              |
| 6:F:89:GLU:HB3   | 6:F:134:ILE:HD13  | 2.00                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 9:I:50:THR:HG22   | 9:I:52:ILE:N     | 2.33                     | 0.43              |
| 1:A:31:SER:HB2    | 1:A:82:GLY:C     | 2.43                     | 0.43              |
| 1:A:709:THR:HG23  | 9:I:94:ASP:HA    | 2.00                     | 0.43              |
| 1:A:853:ASP:OD1   | 1:A:855:THR:CB   | 2.64                     | 0.43              |
| 1:A:879:GLU:CD    | 1:A:962:ARG:HH22 | 2.26                     | 0.43              |
| 1:A:907:THR:HG22  | 1:A:908:LEU:H    | 1.82                     | 0.43              |
| 2:B:126:SER:OG    | 2:B:172:ILE:HD11 | 2.18                     | 0.43              |
| 2:B:214:ALA:HB2   | 2:B:408:LEU:CD1  | 2.48                     | 0.43              |
| 2:B:329:THR:O     | 2:B:332:ASP:HB3  | 2.19                     | 0.43              |
| 2:B:416:LEU:O     | 2:B:417:PHE:C    | 2.61                     | 0.43              |
| 2:B:446:LEU:N     | 2:B:446:LEU:HD23 | 2.33                     | 0.43              |
| 2:B:579:ARG:HB2   | 2:B:586:TRP:HE1  | 1.84                     | 0.43              |
| 2:B:834:ASN:HB2   | 2:B:838:SER:O    | 2.19                     | 0.43              |
| 2:B:835:GLN:O     | 2:B:836:GLU:C    | 2.62                     | 0.43              |
| 2:B:1108:ARG:O    | 2:B:1108:ARG:CG  | 2.67                     | 0.43              |
| 3:C:46:ILE:HG23   | 3:C:157:CYS:HB3  | 2.00                     | 0.43              |
| 5:E:82:PHE:CD1    | 5:E:82:PHE:N     | 2.85                     | 0.43              |
| 6:F:140:ASP:OD1   | 6:F:141:GLY:N    | 2.52                     | 0.43              |
| 10:J:9:SER:HB2    | 10:J:45:CYS:HB2  | 2.01                     | 0.43              |
| 10:J:21:TYR:CA    | 10:J:39:LEU:HD11 | 2.49                     | 0.43              |
| 11:K:95:ILE:O     | 11:K:98:LEU:HB2  | 2.19                     | 0.43              |
| 1:A:113:LEU:HG    | 1:A:218:ASP:OD1  | 2.19                     | 0.43              |
| 1:A:114:LEU:HD12  | 1:A:142:CYS:O    | 2.18                     | 0.43              |
| 1:A:266:LEU:HD23  | 1:A:266:LEU:HA   | 1.81                     | 0.43              |
| 1:A:396:PRO:HG3   | 1:A:416:ARG:HB3  | 2.00                     | 0.43              |
| 1:A:457:ALA:O     | 1:A:507:VAL:HG23 | 2.19                     | 0.43              |
| 1:A:458:HIS:ND1   | 1:A:507:VAL:HG21 | 2.33                     | 0.43              |
| 1:A:709:THR:O     | 1:A:712:GLU:N    | 2.52                     | 0.43              |
| 2:B:436:VAL:O     | 2:B:437:GLU:C    | 2.61                     | 0.43              |
| 2:B:702:LEU:HD22  | 2:B:737:THR:CG2  | 2.49                     | 0.43              |
| 2:B:839:MET:HE1   | 2:B:980:PHE:CB   | 2.49                     | 0.43              |
| 2:B:878:GLN:O     | 2:B:879:ARG:C    | 2.61                     | 0.43              |
| 9:I:84:VAL:O      | 9:I:84:VAL:HG13  | 2.19                     | 0.43              |
| 9:I:87:GLN:O      | 9:I:88:SER:C     | 2.62                     | 0.43              |
| 1:A:89:PRO:HG3    | 1:A:208:LEU:HD12 | 2.00                     | 0.43              |
| 1:A:633:VAL:HG11  | 1:A:645:LEU:HD22 | 2.00                     | 0.43              |
| 1:A:672:ASP:O     | 1:A:675:THR:HB   | 2.19                     | 0.43              |
| 1:A:679:ILE:O     | 1:A:682:THR:HB   | 2.18                     | 0.43              |
| 1:A:1150:SER:HB2  | 1:A:1195:LEU:CD2 | 2.49                     | 0.43              |
| 1:A:1343:ALA:O    | 1:A:1344:GLY:C   | 2.61                     | 0.43              |
| 1:A:1409:LEU:HD23 | 1:A:1409:LEU:HA  | 1.83                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:55:VAL:O      | 2:B:59:LEU:HB3   | 2.19                     | 0.43              |
| 2:B:202:TYR:CD2   | 2:B:202:TYR:N    | 2.87                     | 0.43              |
| 2:B:850:LEU:CD2   | 2:B:1009:ASP:HB3 | 2.48                     | 0.43              |
| 5:E:117:THR:C     | 5:E:119:SER:H    | 2.25                     | 0.43              |
| 6:F:94:LEU:HD23   | 6:F:94:LEU:HA    | 1.83                     | 0.43              |
| 8:H:84:ALA:CA     | 8:H:87:ARG:HB2   | 2.48                     | 0.43              |
| 9:I:50:THR:HG22   | 9:I:52:ILE:HG23  | 1.98                     | 0.43              |
| 1:A:30:ILE:O      | 1:A:31:SER:O     | 2.37                     | 0.42              |
| 1:A:337:ARG:CZ    | 1:A:839:ARG:CZ   | 2.97                     | 0.42              |
| 1:A:1028:THR:O    | 1:A:1029:ARG:C   | 2.61                     | 0.42              |
| 2:B:115:GLN:HG2   | 2:B:193:LYS:HB2  | 2.01                     | 0.42              |
| 2:B:313:MET:HE1   | 2:B:386:LEU:HD22 | 1.99                     | 0.42              |
| 2:B:366:GLN:O     | 2:B:367:LEU:O    | 2.36                     | 0.42              |
| 2:B:877:PRO:O     | 2:B:878:GLN:HG2  | 2.19                     | 0.42              |
| 3:C:214:ASN:O     | 3:C:215:GLU:C    | 2.62                     | 0.42              |
| 5:E:114:ASN:O     | 5:E:115:ASN:HB3  | 2.18                     | 0.42              |
| 5:E:168:TYR:O     | 5:E:170:LEU:HD23 | 2.19                     | 0.42              |
| 8:H:111:LEU:HD23  | 8:H:127:GLY:O    | 2.18                     | 0.42              |
| 12:L:61:THR:HG22  | 12:L:62:LYS:N    | 2.33                     | 0.42              |
| 1:A:265:LYS:HZ1   | 1:A:323:LYS:H    | 1.63                     | 0.42              |
| 1:A:373:THR:HG21  | 2:B:1105:ALA:O   | 2.18                     | 0.42              |
| 1:A:412:ARG:CZ    | 2:B:1108:ARG:NH2 | 2.81                     | 0.42              |
| 1:A:534:LEU:HD13  | 1:A:656:TRP:CD1  | 2.54                     | 0.42              |
| 1:A:645:LEU:HD11  | 1:A:649:ILE:HD11 | 2.01                     | 0.42              |
| 1:A:648:ASN:O     | 1:A:649:ILE:C    | 2.59                     | 0.42              |
| 1:A:782:ARG:NH2   | 9:I:67:THR:HG22  | 2.34                     | 0.42              |
| 1:A:922:ASP:CG    | 1:A:925:LEU:HG   | 2.43                     | 0.42              |
| 1:A:1048:ASN:O    | 1:A:1049:ILE:C   | 2.61                     | 0.42              |
| 1:A:1390:ASN:HD22 | 1:A:1399:ARG:CA  | 2.30                     | 0.42              |
| 2:B:310:MET:O     | 2:B:313:MET:HB2  | 2.18                     | 0.42              |
| 2:B:362:PRO:C     | 2:B:363:HIS:O    | 2.58                     | 0.42              |
| 2:B:705:MET:N     | 2:B:710:LEU:HD12 | 2.34                     | 0.42              |
| 3:C:148:ARG:H     | 3:C:151:GLN:HG3  | 1.84                     | 0.42              |
| 5:E:9:ILE:C       | 5:E:11:ARG:N     | 2.71                     | 0.42              |
| 5:E:134:THR:C     | 5:E:135:PHE:HD1  | 2.28                     | 0.42              |
| 8:H:93:TYR:CA     | 8:H:145:ARG:HB3  | 2.45                     | 0.42              |
| 8:H:143:LEU:HD12  | 8:H:143:LEU:N    | 2.34                     | 0.42              |
| 10:J:31:ASP:O     | 10:J:32:GLU:C    | 2.61                     | 0.42              |
| 12:L:58:LYS:O     | 12:L:59:ALA:C    | 2.63                     | 0.42              |
| 1:A:49:LYS:NZ     | 1:A:60:SER:HA    | 2.34                     | 0.42              |
| 1:A:134:ARG:O     | 1:A:137:ALA:N    | 2.52                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1155:ASP:O    | 1:A:1190:PRO:O    | 2.37                     | 0.42              |
| 2:B:784:ASN:HB3   | 10:J:63:TYR:OH    | 2.18                     | 0.42              |
| 2:B:880:THR:O     | 2:B:881:ASN:HB2   | 2.20                     | 0.42              |
| 2:B:995:ARG:O     | 2:B:996:ARG:C     | 2.63                     | 0.42              |
| 2:B:1073:TYR:N    | 2:B:1073:TYR:CD1  | 2.87                     | 0.42              |
| 3:C:20:PHE:CD1    | 3:C:20:PHE:C      | 2.97                     | 0.42              |
| 5:E:78:LEU:C      | 5:E:78:LEU:CD2    | 2.89                     | 0.42              |
| 5:E:79:TRP:HD1    | 5:E:96:PHE:HE1    | 1.67                     | 0.42              |
| 10:J:27:GLU:C     | 10:J:29:GLU:N     | 2.77                     | 0.42              |
| 1:A:80:HIS:N      | 1:A:243:PRO:HB3   | 2.34                     | 0.42              |
| 1:A:151:ASP:OD1   | 1:A:163:SER:HA    | 2.19                     | 0.42              |
| 1:A:541:ILE:HD12  | 1:A:541:ILE:N     | 2.34                     | 0.42              |
| 1:A:753:GLY:HA2   | 1:A:757:ASN:ND2   | 2.34                     | 0.42              |
| 1:A:1004:ASN:O    | 1:A:1008:GLN:HB2  | 2.19                     | 0.42              |
| 1:A:1161:THR:OG1  | 1:A:1170:ILE:HD11 | 2.20                     | 0.42              |
| 1:A:1242:VAL:CG1  | 1:A:1243:VAL:H    | 2.22                     | 0.42              |
| 2:B:203:PHE:HE1   | 2:B:212:LEU:HD12  | 1.85                     | 0.42              |
| 2:B:482:VAL:O     | 2:B:483:LEU:C     | 2.63                     | 0.42              |
| 2:B:546:SER:OG    | 2:B:631:GLY:N     | 2.52                     | 0.42              |
| 2:B:806:THR:O     | 2:B:808:ALA:N     | 2.53                     | 0.42              |
| 2:B:831:SER:CB    | 2:B:994:TYR:OH    | 2.67                     | 0.42              |
| 2:B:980:PHE:HE1   | 2:B:990:ILE:CD1   | 2.30                     | 0.42              |
| 2:B:1033:LYS:NZ   | 2:B:1070:GLU:OE1  | 2.46                     | 0.42              |
| 2:B:1060:ARG:C    | 2:B:1062:HIS:H    | 2.26                     | 0.42              |
| 2:B:1197:PRO:O    | 2:B:1200:ALA:HB3  | 2.19                     | 0.42              |
| 2:B:1204:PHE:O    | 2:B:1207:LEU:HB2  | 2.19                     | 0.42              |
| 3:C:251:LEU:HG    | 11:K:98:LEU:HD11  | 2.01                     | 0.42              |
| 5:E:168:TYR:CB    | 5:E:170:LEU:HG    | 2.49                     | 0.42              |
| 1:A:88:LYS:HD2    | 1:A:293:GLU:OE1   | 2.20                     | 0.42              |
| 1:A:337:ARG:HH11  | 1:A:839:ARG:HH12  | 1.62                     | 0.42              |
| 1:A:511:ILE:HG12  | 1:A:521:MET:CE    | 2.42                     | 0.42              |
| 1:A:1205:LYS:O    | 1:A:1206:ASP:C    | 2.63                     | 0.42              |
| 1:A:1385:THR:HG22 | 1:A:1386:ARG:N    | 2.34                     | 0.42              |
| 2:B:34:ILE:HG12   | 2:B:542:MET:CE    | 2.49                     | 0.42              |
| 2:B:269:ILE:HB    | 2:B:317:CYS:SG    | 2.60                     | 0.42              |
| 2:B:758:PHE:CE2   | 2:B:1044:ALA:HA   | 2.53                     | 0.42              |
| 2:B:794:ASN:O     | 2:B:795:ILE:HD12  | 2.19                     | 0.42              |
| 3:C:17:ASN:C      | 3:C:18:VAL:HG23   | 2.45                     | 0.42              |
| 5:E:35:VAL:C      | 5:E:37:LEU:N      | 2.78                     | 0.42              |
| 5:E:98:ILE:O      | 5:E:99:HIS:C      | 2.62                     | 0.42              |
| 9:I:101:PHE:HD1   | 9:I:110:PHE:O     | 2.02                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 10:J:53:HIS:CD2   | 10:J:54:VAL:N    | 2.88                     | 0.42              |
| 1:A:35:ILE:HD13   | 1:A:53:LEU:HD23  | 2.01                     | 0.42              |
| 1:A:84:ILE:HG21   | 1:A:239:LEU:HD23 | 2.01                     | 0.42              |
| 1:A:99:ILE:O      | 1:A:102:VAL:HB   | 2.18                     | 0.42              |
| 1:A:451:HIS:HB2   | 1:A:454:SER:OG   | 2.19                     | 0.42              |
| 1:A:568:PRO:CB    | 3:C:221:TYR:CZ   | 3.03                     | 0.42              |
| 1:A:1027:ALA:O    | 1:A:1030:ARG:HB2 | 2.20                     | 0.42              |
| 1:A:1242:VAL:CG1  | 1:A:1243:VAL:N   | 2.83                     | 0.42              |
| 2:B:300:HIS:ND1   | 2:B:376:PHE:CD2  | 2.81                     | 0.42              |
| 2:B:749:LEU:HD22  | 2:B:753:ALA:CB   | 2.49                     | 0.42              |
| 2:B:955:THR:HA    | 12:L:54:ARG:O    | 2.19                     | 0.42              |
| 2:B:1177:HIS:O    | 2:B:1179:GLN:N   | 2.52                     | 0.42              |
| 5:E:16:PHE:CZ     | 5:E:20:LYS:HE2   | 2.54                     | 0.42              |
| 5:E:113:GLN:HG2   | 5:E:137:GLU:OE1  | 2.19                     | 0.42              |
| 8:H:84:ALA:CB     | 8:H:87:ARG:HB2   | 2.49                     | 0.42              |
| 1:A:225:ASN:C     | 1:A:227:VAL:N    | 2.71                     | 0.42              |
| 1:A:383:TYR:O     | 6:F:115:THR:HG22 | 2.20                     | 0.42              |
| 1:A:447:GLN:HA    | 1:A:448:PRO:C    | 2.45                     | 0.42              |
| 1:A:567:LYS:CD    | 8:H:95:TYR:CD1   | 3.00                     | 0.42              |
| 1:A:601:LYS:O     | 1:A:602:ASP:C    | 2.62                     | 0.42              |
| 1:A:751:SER:O     | 1:A:752:LYS:CB   | 2.67                     | 0.42              |
| 1:A:756:ILE:CG2   | 1:A:757:ASN:N    | 2.80                     | 0.42              |
| 1:A:1208:THR:O    | 1:A:1209:MET:C   | 2.62                     | 0.42              |
| 2:B:315:LYS:O     | 2:B:317:CYS:N    | 2.53                     | 0.42              |
| 2:B:556:THR:O     | 2:B:557:PHE:C    | 2.61                     | 0.42              |
| 2:B:1106:ARG:HH12 | 2:B:1118:PRO:CA  | 2.33                     | 0.42              |
| 5:E:28:TYR:CE1    | 5:E:78:LEU:CD1   | 3.03                     | 0.42              |
| 6:F:116:ASP:O     | 6:F:117:PRO:C    | 2.62                     | 0.42              |
| 8:H:5:LEU:O       | 8:H:6:PHE:HB2    | 2.19                     | 0.42              |
| 10:J:52:THR:CG2   | 10:J:52:THR:O    | 2.68                     | 0.42              |
| 10:J:53:HIS:CE1   | 10:J:55:ASP:HA   | 2.54                     | 0.42              |
| 11:K:24:ASP:OD2   | 11:K:74:ARG:NH1  | 2.51                     | 0.42              |
| 1:A:48:ALA:C      | 1:A:49:LYS:HG3   | 2.45                     | 0.42              |
| 1:A:108:MET:O     | 1:A:109:HIS:CB   | 2.66                     | 0.42              |
| 1:A:166:GLY:O     | 1:A:167:CYS:CB   | 2.67                     | 0.42              |
| 1:A:384:ASN:CG    | 1:A:388:LEU:HD12 | 2.45                     | 0.42              |
| 1:A:427:GLN:O     | 1:A:428:TYR:C    | 2.62                     | 0.42              |
| 1:A:458:HIS:CE1   | 1:A:507:VAL:CG2  | 3.00                     | 0.42              |
| 1:A:514:PRO:HB2   | 1:A:875:ALA:HB3  | 2.01                     | 0.42              |
| 1:A:530:GLY:O     | 1:A:532:ARG:N    | 2.53                     | 0.42              |
| 1:A:1015:VAL:HG12 | 1:A:1015:VAL:O   | 2.18                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1129:GLU:O    | 1:A:1130:GLN:C    | 2.61                     | 0.42              |
| 1:A:1329:THR:HG22 | 1:A:1330:ASN:N    | 2.35                     | 0.42              |
| 1:A:1368:MET:O    | 1:A:1369:ALA:C    | 2.62                     | 0.42              |
| 2:B:634:TYR:CD1   | 2:B:692:TYR:HB3   | 2.55                     | 0.42              |
| 2:B:708:GLU:C     | 2:B:710:LEU:N     | 2.72                     | 0.42              |
| 2:B:1023:VAL:O    | 2:B:1024:ALA:C    | 2.62                     | 0.42              |
| 8:H:24:CYS:CB     | 8:H:44:VAL:HG21   | 2.47                     | 0.42              |
| 11:K:96:ASN:O     | 11:K:97:LYS:C     | 2.63                     | 0.42              |
| 12:L:60:ARG:CG    | 12:L:61:THR:N     | 2.62                     | 0.42              |
| 1:A:14:VAL:O      | 1:A:15:LYS:HD3    | 2.20                     | 0.42              |
| 1:A:683:ILE:O     | 1:A:686:ALA:N     | 2.53                     | 0.42              |
| 1:A:760:GLN:CB    | 2:B:1021:MET:HE1  | 2.50                     | 0.42              |
| 1:A:1173:HIS:NE2  | 1:A:1227:ILE:HG23 | 2.35                     | 0.42              |
| 2:B:39:ARG:HG2    | 2:B:39:ARG:HH11   | 1.85                     | 0.42              |
| 2:B:435:THR:O     | 2:B:435:THR:HG22  | 2.20                     | 0.42              |
| 2:B:841:MET:HE3   | 2:B:1010:LEU:HD13 | 2.02                     | 0.42              |
| 2:B:995:ARG:HH11  | 2:B:995:ARG:CB    | 2.33                     | 0.42              |
| 2:B:1115:THR:CG2  | 2:B:1199:ALA:HB2  | 2.50                     | 0.42              |
| 3:C:214:ASN:CB    | 3:C:217:ASP:OD2   | 2.68                     | 0.42              |
| 3:C:261:ALA:O     | 3:C:262:LEU:C     | 2.61                     | 0.42              |
| 6:F:138:LEU:HD23  | 6:F:138:LEU:HA    | 1.83                     | 0.42              |
| 9:I:97:MET:HE3    | 9:I:97:MET:HB2    | 1.87                     | 0.42              |
| 1:A:14:VAL:HB     | 1:A:1430:LEU:HD13 | 2.02                     | 0.42              |
| 1:A:76:GLU:O      | 1:A:78:PRO:CD     | 2.68                     | 0.42              |
| 1:A:113:LEU:C     | 1:A:115:LEU:N     | 2.77                     | 0.42              |
| 1:A:474:VAL:HG13  | 1:A:474:VAL:O     | 2.20                     | 0.42              |
| 1:A:1126:ALA:O    | 1:A:1128:GLN:N    | 2.53                     | 0.42              |
| 1:A:1366:ARG:HG2  | 1:A:1366:ARG:HH11 | 1.84                     | 0.42              |
| 2:B:280:ILE:CG2   | 2:B:285:ILE:HG13  | 2.47                     | 0.42              |
| 2:B:368:GLU:O     | 2:B:371:GLU:OE1   | 2.37                     | 0.42              |
| 2:B:499:ASN:OD1   | 2:B:500:THR:N     | 2.53                     | 0.42              |
| 2:B:640:VAL:HG22  | 2:B:651:LEU:CD2   | 2.50                     | 0.42              |
| 2:B:737:THR:HG23  | 9:I:66:PRO:HB3    | 2.01                     | 0.42              |
| 2:B:911:ILE:HG21  | 2:B:966:VAL:HG11  | 2.01                     | 0.42              |
| 2:B:1148:LYS:O    | 2:B:1152:MET:HB2  | 2.19                     | 0.42              |
| 2:B:1149:GLU:HG3  | 2:B:1153:GLU:OE1  | 2.20                     | 0.42              |
| 3:C:146:LYS:O     | 3:C:147:LEU:HD23  | 2.20                     | 0.42              |
| 3:C:166:GLU:CG    | 11:K:10:PHE:CZ    | 2.96                     | 0.42              |
| 3:C:242:GLN:O     | 3:C:246:ARG:N     | 2.52                     | 0.42              |
| 8:H:138:GLU:HG2   | 8:H:139:ASN:N     | 2.35                     | 0.42              |
| 9:I:63:GLY:O      | 9:I:70:ARG:NH2    | 2.53                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:63:ARG:CA     | 1:A:74:MET:HE2    | 2.49                     | 0.41              |
| 1:A:101:LYS:HG2   | 1:A:139:TRP:CZ2   | 2.55                     | 0.41              |
| 1:A:598:LEU:HD22  | 8:H:25:ARG:CZ     | 2.50                     | 0.41              |
| 1:A:811:GLN:O     | 1:A:812:GLU:C     | 2.61                     | 0.41              |
| 1:A:1168:GLU:O    | 1:A:1172:LEU:HG   | 2.19                     | 0.41              |
| 1:A:1254:ALA:O    | 1:A:1255:GLU:HB2  | 2.19                     | 0.41              |
| 1:A:1394:THR:HG22 | 1:A:1395:GLY:O    | 2.19                     | 0.41              |
| 2:B:167:ILE:O     | 2:B:168:GLY:O     | 2.38                     | 0.41              |
| 2:B:230:ALA:O     | 2:B:232:SER:N     | 2.47                     | 0.41              |
| 2:B:640:VAL:HG22  | 2:B:651:LEU:HD23  | 2.01                     | 0.41              |
| 2:B:707:PRO:HG2   | 2:B:708:GLU:N     | 2.27                     | 0.41              |
| 2:B:1177:HIS:O    | 2:B:1179:GLN:HG3  | 2.19                     | 0.41              |
| 3:C:14:SER:HA     | 11:K:114:LEU:HD22 | 2.02                     | 0.41              |
| 3:C:27:LEU:HD12   | 3:C:27:LEU:O      | 2.20                     | 0.41              |
| 3:C:204:SER:O     | 3:C:205:LYS:C     | 2.63                     | 0.41              |
| 9:I:25:LEU:HD12   | 9:I:26:LEU:N      | 2.35                     | 0.41              |
| 11:K:82:ASP:O     | 11:K:85:ASP:HB2   | 2.20                     | 0.41              |
| 1:A:474:VAL:HG13  | 1:A:478:TYR:HE1   | 1.85                     | 0.41              |
| 1:A:543:LEU:O     | 1:A:544:ASP:C     | 2.63                     | 0.41              |
| 1:A:547:LEU:HD22  | 11:K:58:PHE:HD1   | 1.84                     | 0.41              |
| 1:A:639:PRO:HG2   | 1:A:640:GLN:H     | 1.84                     | 0.41              |
| 1:A:868:TYR:C     | 1:A:870:GLU:N     | 2.76                     | 0.41              |
| 1:A:1223:ASP:C    | 1:A:1243:VAL:HG12 | 2.45                     | 0.41              |
| 1:A:1343:ALA:O    | 1:A:1346:ALA:HB3  | 2.20                     | 0.41              |
| 2:B:92:PHE:HD2    | 2:B:130:VAL:HG11  | 1.85                     | 0.41              |
| 2:B:405:ARG:CZ    | 2:B:632:ARG:HG2   | 2.49                     | 0.41              |
| 2:B:757:PRO:HG2   | 2:B:984:HIS:CE1   | 2.54                     | 0.41              |
| 2:B:901:PRO:O     | 2:B:949:VAL:O     | 2.38                     | 0.41              |
| 2:B:1106:ARG:HH12 | 2:B:1118:PRO:HA   | 1.85                     | 0.41              |
| 2:B:1182:CYS:SG   | 2:B:1185:CYS:HB2  | 2.60                     | 0.41              |
| 6:F:109:VAL:HG12  | 6:F:110:ASP:H     | 1.82                     | 0.41              |
| 9:I:16:PRO:HA     | 9:I:26:LEU:O      | 2.20                     | 0.41              |
| 11:K:65:HIS:HD2   | 11:K:67:PHE:CB    | 2.33                     | 0.41              |
| 1:A:59:GLY:HA2    | 1:A:67:CYS:SG     | 2.60                     | 0.41              |
| 1:A:629:LEU:CD1   | 1:A:645:LEU:HD21  | 2.48                     | 0.41              |
| 1:A:808:LEU:HD12  | 1:A:808:LEU:N     | 2.35                     | 0.41              |
| 1:A:1038:THR:O    | 1:A:1039:LYS:C    | 2.62                     | 0.41              |
| 2:B:745:PRO:C     | 2:B:747:MET:H     | 2.27                     | 0.41              |
| 2:B:1177:HIS:HB2  | 2:B:1179:GLN:HG3  | 2.03                     | 0.41              |
| 8:H:84:ALA:HA     | 8:H:87:ARG:CB     | 2.50                     | 0.41              |
| 12:L:28:LYS:O     | 12:L:29:TYR:CG    | 2.74                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:388:LEU:HD23  | 1:A:388:LEU:HA    | 1.88                     | 0.41              |
| 1:A:871:ASP:CB    | 5:E:204:THR:CG2   | 2.99                     | 0.41              |
| 1:A:913:LEU:CD1   | 1:A:981:LEU:O     | 2.69                     | 0.41              |
| 1:A:1406:VAL:CG1  | 1:A:1410:PHE:CE1  | 3.03                     | 0.41              |
| 2:B:797:TYR:HB3   | 2:B:798:TYR:CD1   | 2.55                     | 0.41              |
| 2:B:879:ARG:O     | 2:B:880:THR:HB    | 2.20                     | 0.41              |
| 2:B:1033:LYS:NZ   | 2:B:1087:PHE:O    | 2.51                     | 0.41              |
| 3:C:252:GLN:HG3   | 11:K:95:ILE:HG23  | 2.03                     | 0.41              |
| 3:C:252:GLN:NE2   | 11:K:99:GLY:N     | 2.68                     | 0.41              |
| 11:K:106:GLU:O    | 11:K:110:ASN:ND2  | 2.54                     | 0.41              |
| 1:A:567:LYS:NZ    | 8:H:95:TYR:CD1    | 2.80                     | 0.41              |
| 1:A:679:ILE:CG2   | 1:A:729:ALA:HB1   | 2.43                     | 0.41              |
| 1:A:738:LYS:HZ1   | 3:C:194:GLU:CA    | 2.34                     | 0.41              |
| 1:A:771:GLU:N     | 1:A:822:GLU:OE1   | 2.53                     | 0.41              |
| 1:A:984:LYS:O     | 1:A:988:LEU:HB2   | 2.19                     | 0.41              |
| 1:A:1026:LEU:HD23 | 1:A:1026:LEU:HA   | 1.90                     | 0.41              |
| 2:B:175:ARG:HH11  | 2:B:175:ARG:CG    | 2.34                     | 0.41              |
| 2:B:276:ILE:HD11  | 2:B:355:ILE:CD1   | 2.50                     | 0.41              |
| 2:B:835:GLN:HE21  | 2:B:835:GLN:HB2   | 1.74                     | 0.41              |
| 2:B:865:LYS:HB3   | 2:B:866:TYR:H     | 1.72                     | 0.41              |
| 2:B:911:ILE:HD11  | 2:B:941:LEU:CB    | 2.51                     | 0.41              |
| 8:H:111:LEU:C     | 8:H:112:ILE:HG13  | 2.45                     | 0.41              |
| 11:K:7:PHE:C      | 11:K:9:LEU:H      | 2.29                     | 0.41              |
| 11:K:107:THR:O    | 11:K:108:GLU:C    | 2.63                     | 0.41              |
| 1:A:38:PRO:CA     | 1:A:270:LEU:HD23  | 2.49                     | 0.41              |
| 1:A:338:GLY:CA    | 2:B:1129:ARG:HH22 | 2.17                     | 0.41              |
| 1:A:339:ASN:HB3   | 2:B:1117:GLN:HE22 | 1.85                     | 0.41              |
| 1:A:407:ARG:HG2   | 1:A:430:TRP:CZ2   | 2.56                     | 0.41              |
| 1:A:531:ILE:CG2   | 1:A:532:ARG:N     | 2.84                     | 0.41              |
| 1:A:960:ILE:HD12  | 1:A:1021:LEU:CD2  | 2.50                     | 0.41              |
| 1:A:1139:GLU:HG3  | 1:A:1280:GLU:O    | 2.20                     | 0.41              |
| 2:B:53:GLN:HG2    | 2:B:547:VAL:HG13  | 2.02                     | 0.41              |
| 2:B:234:ILE:HD12  | 2:B:234:ILE:N     | 2.29                     | 0.41              |
| 2:B:310:MET:O     | 2:B:311:LEU:C     | 2.62                     | 0.41              |
| 2:B:329:THR:O     | 2:B:333:PHE:N     | 2.48                     | 0.41              |
| 2:B:418:LYS:O     | 2:B:420:LEU:N     | 2.54                     | 0.41              |
| 2:B:601:ARG:O     | 2:B:605:ARG:HG3   | 2.19                     | 0.41              |
| 2:B:1053:GLU:C    | 2:B:1055:ILE:N    | 2.79                     | 0.41              |
| 5:E:13:TRP:O      | 5:E:16:PHE:HB3    | 2.21                     | 0.41              |
| 6:F:75:PRO:C      | 6:F:77:ASP:N      | 2.78                     | 0.41              |
| 8:H:4:THR:O       | 8:H:5:LEU:HD23    | 2.20                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:I:40:SER:HB2    | 9:I:41:PRO:HD2    | 2.03                     | 0.41              |
| 9:I:59:VAL:HG12   | 9:I:60:GLN:N      | 2.34                     | 0.41              |
| 9:I:98:VAL:HG12   | 9:I:99:LEU:N      | 2.36                     | 0.41              |
| 10:J:3:VAL:CG2    | 10:J:18:TRP:CG    | 3.02                     | 0.41              |
| 11:K:93:SER:O     | 11:K:97:LYS:HG3   | 2.20                     | 0.41              |
| 1:A:542:GLU:OE1   | 1:A:569:LYS:HE2   | 2.20                     | 0.41              |
| 1:A:579:SER:HG    | 1:A:612:ILE:HG22  | 1.86                     | 0.41              |
| 1:A:675:THR:O     | 1:A:676:MET:C     | 2.64                     | 0.41              |
| 1:A:971:PHE:O     | 1:A:972:HIS:C     | 2.64                     | 0.41              |
| 2:B:54:PHE:O      | 2:B:55:VAL:C      | 2.64                     | 0.41              |
| 2:B:185:THR:N     | 2:B:188:ASP:HB2   | 2.36                     | 0.41              |
| 2:B:702:LEU:HD12  | 2:B:702:LEU:HA    | 1.76                     | 0.41              |
| 2:B:890:TYR:C     | 2:B:892:LYS:N     | 2.78                     | 0.41              |
| 2:B:955:THR:CG2   | 12:L:54:ARG:O     | 2.65                     | 0.41              |
| 5:E:72:PHE:CD2    | 5:E:155:ARG:NH2   | 2.83                     | 0.41              |
| 11:K:35:PHE:O     | 11:K:70:ARG:HB2   | 2.21                     | 0.41              |
| 1:A:209:ASN:O     | 1:A:210:ILE:C     | 2.64                     | 0.41              |
| 1:A:407:ARG:HG2   | 1:A:430:TRP:CE2   | 2.54                     | 0.41              |
| 1:A:515:GLN:CG    | 1:A:516:SER:N     | 2.84                     | 0.41              |
| 1:A:525:GLN:HB2   | 2:B:835:GLN:HG2   | 2.00                     | 0.41              |
| 1:A:1102:LYS:O    | 1:A:1103:GLU:C    | 2.63                     | 0.41              |
| 1:A:1187:GLN:HA   | 1:A:1243:VAL:HG23 | 2.02                     | 0.41              |
| 2:B:105:SER:O     | 2:B:106:ASP:HB2   | 2.20                     | 0.41              |
| 2:B:369:GLY:C     | 2:B:370:PHE:CD1   | 2.99                     | 0.41              |
| 2:B:514:LEU:HD12  | 2:B:514:LEU:C     | 2.45                     | 0.41              |
| 2:B:800:GLN:CB    | 10:J:52:THR:CG2   | 2.89                     | 0.41              |
| 2:B:1104:HIS:HB2  | 2:B:1122:ARG:CB   | 2.51                     | 0.41              |
| 2:B:1152:MET:O    | 2:B:1156:ASP:O    | 2.39                     | 0.41              |
| 2:B:1162:ILE:HG22 | 2:B:1163:CYS:N    | 2.34                     | 0.41              |
| 8:H:126:GLU:N     | 8:H:130:ARG:HH12  | 2.19                     | 0.41              |
| 9:I:92:ARG:CG     | 9:I:93:LYS:N      | 2.84                     | 0.41              |
| 12:L:41:SER:O     | 12:L:44:ASP:HB2   | 2.21                     | 0.41              |
| 1:A:18:GLN:O      | 2:B:1215:ARG:HG3  | 2.21                     | 0.41              |
| 1:A:134:ARG:O     | 1:A:136:ALA:N     | 2.53                     | 0.41              |
| 1:A:289:ILE:C     | 1:A:291:GLU:H     | 2.27                     | 0.41              |
| 1:A:441:PRO:O     | 1:A:441:PRO:HG2   | 2.20                     | 0.41              |
| 1:A:530:GLY:O     | 1:A:533:LYS:N     | 2.53                     | 0.41              |
| 1:A:640:GLN:O     | 1:A:641:VAL:C     | 2.64                     | 0.41              |
| 1:A:815:PHE:O     | 1:A:816:HIS:C     | 2.63                     | 0.41              |
| 1:A:878:ILE:C     | 1:A:879:GLU:CG    | 2.94                     | 0.41              |
| 1:A:909:ASP:OD1   | 1:A:910:PRO:HD2   | 2.21                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1116:LEU:CD2 | 1:A:1316:VAL:HG21 | 2.51                     | 0.41              |
| 1:A:1378:GLN:C   | 1:A:1380:GLY:H    | 2.29                     | 0.41              |
| 2:B:51:PHE:O     | 2:B:54:PHE:N      | 2.54                     | 0.41              |
| 2:B:120:ARG:HH12 | 12:L:54:ARG:NH1   | 2.18                     | 0.41              |
| 2:B:199:MET:SD   | 2:B:199:MET:N     | 2.87                     | 0.41              |
| 2:B:387:LEU:HD23 | 2:B:393:LYS:HD2   | 2.03                     | 0.41              |
| 2:B:591:ARG:O    | 2:B:592:ASN:C     | 2.63                     | 0.41              |
| 2:B:616:ILE:HG12 | 2:B:696:GLU:HG3   | 2.03                     | 0.41              |
| 2:B:784:ASN:HD21 | 2:B:788:ARG:HD2   | 1.84                     | 0.41              |
| 2:B:843:GLN:HB2  | 2:B:993:THR:OG1   | 2.20                     | 0.41              |
| 2:B:872:GLU:CD   | 2:B:914:LYS:CE    | 2.94                     | 0.41              |
| 2:B:872:GLU:HA   | 2:B:915:THR:O     | 2.21                     | 0.41              |
| 2:B:1197:PRO:O   | 2:B:1200:ALA:N    | 2.51                     | 0.41              |
| 3:C:5:GLY:HA3    | 3:C:6:PRO:HD2     | 1.78                     | 0.41              |
| 3:C:46:ILE:CG2   | 3:C:157:CYS:HB3   | 2.51                     | 0.41              |
| 3:C:51:VAL:HG22  | 3:C:155:LEU:CD2   | 2.47                     | 0.41              |
| 3:C:66:ARG:NH2   | 10:J:3:VAL:O      | 2.54                     | 0.41              |
| 3:C:253:LYS:O    | 3:C:254:LYS:C     | 2.64                     | 0.41              |
| 5:E:7:ARG:HG3    | 5:E:8:ASN:N       | 2.36                     | 0.41              |
| 5:E:116:ILE:CG2  | 5:E:117:THR:N     | 2.84                     | 0.41              |
| 5:E:117:THR:O    | 5:E:120:ALA:N     | 2.54                     | 0.41              |
| 8:H:57:VAL:CG1   | 8:H:58:THR:N      | 2.83                     | 0.41              |
| 9:I:6:PHE:HD2    | 9:I:13:MET:HA     | 1.86                     | 0.41              |
| 9:I:99:LEU:HB2   | 9:I:112:SER:OG    | 2.21                     | 0.41              |
| 11:K:49:GLU:C    | 11:K:51:LEU:N     | 2.79                     | 0.41              |
| 11:K:103:THR:O   | 11:K:106:GLU:N    | 2.53                     | 0.41              |
| 12:L:62:LYS:C    | 12:L:64:LEU:N     | 2.79                     | 0.41              |
| 1:A:45:GLN:O     | 1:A:46:THR:C      | 2.63                     | 0.41              |
| 1:A:354:SER:CA   | 1:A:482:PHE:CD2   | 3.03                     | 0.41              |
| 1:A:399:HIS:CB   | 1:A:400:PRO:HD3   | 2.45                     | 0.41              |
| 1:A:401:GLY:N    | 1:A:435:HIS:HD2   | 2.18                     | 0.41              |
| 1:A:577:ILE:O    | 1:A:578:LEU:C     | 2.62                     | 0.41              |
| 1:A:596:THR:C    | 1:A:598:LEU:N     | 2.78                     | 0.41              |
| 1:A:725:ALA:HA   | 1:A:728:LYS:HE2   | 2.02                     | 0.41              |
| 1:A:1352:VAL:O   | 1:A:1353:TYR:C    | 2.64                     | 0.41              |
| 2:B:377:PHE:HE2  | 2:B:381:MET:HE2   | 1.85                     | 0.41              |
| 2:B:530:GLY:O    | 2:B:531:GLN:C     | 2.64                     | 0.41              |
| 2:B:624:LEU:C    | 2:B:624:LEU:HD12  | 2.45                     | 0.41              |
| 2:B:818:PRO:HG3  | 10:J:54:VAL:HG21  | 2.03                     | 0.41              |
| 2:B:850:LEU:HD22 | 2:B:1009:ASP:HB3  | 2.01                     | 0.41              |
| 2:B:941:LEU:HD21 | 2:B:946:ASN:HA    | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1084:GLN:NE2  | 3:C:192:TRP:HB2   | 2.37                     | 0.41              |
| 3:C:178:PHE:C     | 3:C:178:PHE:CD2   | 2.99                     | 0.41              |
| 5:E:72:PHE:CD1    | 5:E:72:PHE:N      | 2.89                     | 0.41              |
| 1:A:15:LYS:HD2    | 2:B:1220:ARG:NE   | 2.35                     | 0.40              |
| 1:A:379:VAL:HG22  | 1:A:431:LYS:HG2   | 2.03                     | 0.40              |
| 1:A:399:HIS:NE2   | 1:A:462:VAL:HG21  | 2.36                     | 0.40              |
| 1:A:738:LYS:CB    | 8:H:19:ARG:HH22   | 2.34                     | 0.40              |
| 1:A:751:SER:OG    | 2:B:1015:HIS:HE1  | 2.03                     | 0.40              |
| 1:A:878:ILE:HG22  | 1:A:879:GLU:N     | 2.37                     | 0.40              |
| 2:B:284:ILE:HG12  | 2:B:324:ILE:HD12  | 2.03                     | 0.40              |
| 2:B:627:PHE:O     | 2:B:632:ARG:NH1   | 2.54                     | 0.40              |
| 2:B:758:PHE:HB2   | 2:B:1024:ALA:HB1  | 2.04                     | 0.40              |
| 2:B:992:ILE:CD1   | 2:B:994:TYR:CE2   | 3.04                     | 0.40              |
| 2:B:1103:ILE:H    | 2:B:1103:ILE:HG13 | 1.52                     | 0.40              |
| 5:E:127:ILE:O     | 5:E:127:ILE:CG1   | 2.63                     | 0.40              |
| 12:L:29:TYR:C     | 12:L:30:ILE:HG13  | 2.45                     | 0.40              |
| 1:A:19:PHE:HB3    | 1:A:1413:GLY:HA2  | 2.03                     | 0.40              |
| 1:A:172:PRO:HB3   | 1:A:185:TRP:CZ2   | 2.56                     | 0.40              |
| 1:A:270:LEU:O     | 1:A:274:ILE:HG13  | 2.21                     | 0.40              |
| 1:A:334:GLY:O     | 1:A:335:ARG:C     | 2.64                     | 0.40              |
| 1:A:384:ASN:O     | 1:A:386:ASP:N     | 2.54                     | 0.40              |
| 1:A:508:PRO:O     | 1:A:511:ILE:HG13  | 2.22                     | 0.40              |
| 1:A:598:LEU:HD22  | 8:H:25:ARG:HH12   | 1.83                     | 0.40              |
| 1:A:1064:VAL:O    | 1:A:1065:GLY:C    | 2.63                     | 0.40              |
| 1:A:1230:GLU:C    | 1:A:1232:ASN:N    | 2.80                     | 0.40              |
| 1:A:1322:ILE:HD12 | 1:A:1327:ILE:HD12 | 2.03                     | 0.40              |
| 1:A:1345:ARG:CG   | 1:A:1372:VAL:HG12 | 2.51                     | 0.40              |
| 1:A:1345:ARG:HH11 | 1:A:1373:ASP:CG   | 2.29                     | 0.40              |
| 2:B:593:PRO:HG2   | 2:B:617:ARG:NH2   | 2.36                     | 0.40              |
| 2:B:801:LYS:HE2   | 10:J:51:LEU:O     | 2.22                     | 0.40              |
| 2:B:1073:TYR:CE2  | 2:B:1080:LYS:HG2  | 2.57                     | 0.40              |
| 5:E:3:GLN:HG3     | 5:E:5:ASN:H       | 1.85                     | 0.40              |
| 5:E:14:ARG:O      | 5:E:15:ALA:C      | 2.65                     | 0.40              |
| 5:E:157:SER:OG    | 5:E:159:ASP:HB2   | 2.22                     | 0.40              |
| 1:A:19:PHE:HA     | 2:B:1213:THR:O    | 2.22                     | 0.40              |
| 1:A:30:ILE:O      | 1:A:31:SER:C      | 2.64                     | 0.40              |
| 1:A:332:LYS:H     | 1:A:337:ARG:CB    | 2.33                     | 0.40              |
| 1:A:403:LYS:O     | 1:A:404:TYR:O     | 2.39                     | 0.40              |
| 1:A:556:TRP:CE2   | 1:A:558:GLY:HA2   | 2.56                     | 0.40              |
| 1:A:1029:ARG:O    | 1:A:1032:LEU:N    | 2.55                     | 0.40              |
| 1:A:1224:LEU:HD11 | 1:A:1240:CYS:HB3  | 2.03                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1316:VAL:O    | 1:A:1322:ILE:HD13 | 2.21                     | 0.40              |
| 1:A:1342:GLU:CD   | 5:E:212:ARG:HH12  | 2.28                     | 0.40              |
| 1:A:1364:ASN:HD21 | 1:A:1366:ARG:NH1  | 2.19                     | 0.40              |
| 2:B:56:ASP:CB     | 2:B:57:TYR:HD1    | 2.33                     | 0.40              |
| 2:B:113:TYR:CE2   | 2:B:192:LEU:HD22  | 2.57                     | 0.40              |
| 2:B:188:ASP:O     | 2:B:192:LEU:HG    | 2.21                     | 0.40              |
| 2:B:233:PRO:HG2   | 2:B:234:ILE:HG13  | 2.03                     | 0.40              |
| 2:B:244:LEU:HB2   | 2:B:249:ARG:HA    | 2.03                     | 0.40              |
| 2:B:288:ALA:HB2   | 2:B:330:ALA:HB1   | 2.04                     | 0.40              |
| 2:B:315:LYS:C     | 2:B:317:CYS:N     | 2.80                     | 0.40              |
| 2:B:345:LYS:N     | 2:B:348:ARG:HE    | 2.15                     | 0.40              |
| 2:B:348:ARG:H     | 2:B:348:ARG:HG2   | 1.67                     | 0.40              |
| 2:B:549:THR:HG22  | 2:B:550:ASP:N     | 2.36                     | 0.40              |
| 2:B:840:ILE:HB    | 2:B:1011:ILE:HB   | 2.03                     | 0.40              |
| 2:B:864:LYS:H     | 2:B:872:GLU:HB2   | 1.87                     | 0.40              |
| 2:B:952:VAL:HG13  | 2:B:966:VAL:HG22  | 2.03                     | 0.40              |
| 2:B:1120:GLU:CG   | 2:B:1121:GLY:N    | 2.84                     | 0.40              |
| 3:C:175:ALA:HB3   | 10:J:43:ARG:CZ    | 2.51                     | 0.40              |
| 5:E:131:THR:HG21  | 5:E:191:LYS:HE2   | 2.02                     | 0.40              |
| 8:H:33:GLN:OE1    | 8:H:129:TYR:HE2   | 2.05                     | 0.40              |
| 9:I:61:ASP:O      | 9:I:62:ILE:C      | 2.63                     | 0.40              |
| 12:L:45:ALA:C     | 12:L:46:VAL:HG23  | 2.45                     | 0.40              |
| 1:A:331:GLY:O     | 1:A:332:LYS:O     | 2.39                     | 0.40              |
| 1:A:336:ILE:CD1   | 1:A:1405:THR:HG21 | 2.45                     | 0.40              |
| 1:A:432:VAL:O     | 1:A:434:ARG:N     | 2.54                     | 0.40              |
| 1:A:553:VAL:HG22  | 1:A:652:VAL:CG2   | 2.51                     | 0.40              |
| 1:A:709:THR:CG2   | 9:I:94:ASP:HA     | 2.52                     | 0.40              |
| 1:A:1283:VAL:O    | 1:A:1306:LEU:HA   | 2.21                     | 0.40              |
| 2:B:283:VAL:HG13  | 2:B:297:ILE:HD12  | 2.03                     | 0.40              |
| 2:B:293:PRO:O     | 2:B:294:ASP:C     | 2.64                     | 0.40              |
| 2:B:365:THR:HG22  | 2:B:367:LEU:H     | 1.87                     | 0.40              |
| 2:B:380:TYR:O     | 2:B:384:ARG:HG2   | 2.21                     | 0.40              |
| 2:B:424:LEU:HD12  | 2:B:424:LEU:HA    | 1.91                     | 0.40              |
| 2:B:446:LEU:O     | 2:B:446:LEU:HG    | 2.21                     | 0.40              |
| 2:B:458:LYS:O     | 2:B:459:TYR:C     | 2.65                     | 0.40              |
| 3:C:114:TYR:CG    | 3:C:140:ASN:HB3   | 2.56                     | 0.40              |
| 8:H:48:PRO:C      | 8:H:49:VAL:HG23   | 2.46                     | 0.40              |
| 8:H:117:SER:HA    | 8:H:122:LEU:HD23  | 2.02                     | 0.40              |
| 9:I:101:PHE:HB2   | 9:I:110:PHE:CE2   | 2.57                     | 0.40              |
| 11:K:46:ILE:CG2   | 11:K:50:LEU:HD12  | 2.51                     | 0.40              |
| 1:A:17:VAL:HA     | 2:B:1215:ARG:O    | 2.22                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:396:PRO:HB3  | 1:A:403:LYS:HG2  | 2.03                     | 0.40              |
| 1:A:768:GLN:HG2  | 1:A:816:HIS:N    | 2.37                     | 0.40              |
| 1:A:783:THR:CG2  | 1:A:815:PHE:CZ   | 2.98                     | 0.40              |
| 1:A:929:LEU:CD2  | 1:A:929:LEU:N    | 2.85                     | 0.40              |
| 1:A:1116:LEU:H   | 1:A:1308:THR:CG2 | 2.35                     | 0.40              |
| 1:A:1378:GLN:O   | 1:A:1380:GLY:N   | 2.55                     | 0.40              |
| 2:B:56:ASP:CB    | 2:B:57:TYR:CD1   | 3.04                     | 0.40              |
| 2:B:121:ASN:HD21 | 2:B:965:LYS:HE3  | 1.86                     | 0.40              |
| 2:B:386:LEU:O    | 2:B:387:LEU:C    | 2.64                     | 0.40              |
| 2:B:418:LYS:O    | 2:B:419:THR:C    | 2.65                     | 0.40              |
| 2:B:637:LEU:O    | 2:B:690:VAL:HG13 | 2.22                     | 0.40              |
| 2:B:1114:LEU:O   | 2:B:1198:TYR:HE2 | 2.04                     | 0.40              |
| 3:C:214:ASN:HB2  | 3:C:217:ASP:OD2  | 2.22                     | 0.40              |
| 5:E:182:ASP:O    | 5:E:186:LEU:HG   | 2.21                     | 0.40              |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1         | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|---------------------|--------------------------|-------------------|
| 1:A:419:LYS:NZ | 3:C:90:ASP:N[4_555] | 1.74                     | 0.46              |

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 1   | A     | 1365/1733 (79%) | 1022 (75%) | 251 (18%) | 92 (7%)  | 1           | 14 |
| 2   | B     | 1077/1224 (88%) | 839 (78%)  | 169 (16%) | 69 (6%)  | 1           | 15 |
| 3   | C     | 264/318 (83%)   | 208 (79%)  | 40 (15%)  | 16 (6%)  | 1           | 15 |
| 5   | E     | 212/215 (99%)   | 170 (80%)  | 33 (16%)  | 9 (4%)   | 2           | 20 |
| 6   | F     | 82/155 (53%)    | 64 (78%)   | 15 (18%)  | 3 (4%)   | 2           | 22 |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 8   | H     | 129/146 (88%)   | 93 (72%)   | 21 (16%)  | 15 (12%) | 0           | 5  |
| 9   | I     | 117/122 (96%)   | 93 (80%)   | 15 (13%)  | 9 (8%)   | 1           | 12 |
| 10  | J     | 63/70 (90%)     | 47 (75%)   | 12 (19%)  | 4 (6%)   | 1           | 15 |
| 11  | K     | 112/120 (93%)   | 96 (86%)   | 15 (13%)  | 1 (1%)   | 14          | 49 |
| 12  | L     | 44/70 (63%)     | 22 (50%)   | 13 (30%)  | 9 (20%)  | 0           | 1  |
| All | All   | 3465/4173 (83%) | 2654 (77%) | 584 (17%) | 227 (7%) | 1           | 14 |

All (227) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 31   | SER  |
| 1   | A     | 48   | ALA  |
| 1   | A     | 55   | ASP  |
| 1   | A     | 56   | PRO  |
| 1   | A     | 74   | MET  |
| 1   | A     | 75   | ASN  |
| 1   | A     | 167  | CYS  |
| 1   | A     | 322  | VAL  |
| 1   | A     | 404  | TYR  |
| 1   | A     | 418  | SER  |
| 1   | A     | 543  | LEU  |
| 1   | A     | 567  | LYS  |
| 1   | A     | 597  | LEU  |
| 1   | A     | 598  | LEU  |
| 1   | A     | 628  | GLY  |
| 1   | A     | 752  | LYS  |
| 1   | A     | 846  | GLU  |
| 1   | A     | 998  | LEU  |
| 1   | A     | 1036 | ARG  |
| 1   | A     | 1127 | ASP  |
| 1   | A     | 1206 | ASP  |
| 1   | A     | 1221 | LYS  |
| 1   | A     | 1223 | ASP  |
| 1   | A     | 1392 | SER  |
| 1   | A     | 1393 | ASN  |
| 1   | A     | 1403 | GLU  |
| 1   | A     | 1406 | VAL  |
| 1   | A     | 1416 | ALA  |
| 2   | B     | 65   | GLU  |
| 2   | B     | 124  | TYR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 174  | LEU  |
| 2   | B     | 175  | ARG  |
| 2   | B     | 200  | GLY  |
| 2   | B     | 229  | ALA  |
| 2   | B     | 364  | ILE  |
| 2   | B     | 367  | LEU  |
| 2   | B     | 531  | GLN  |
| 2   | B     | 708  | GLU  |
| 2   | B     | 709  | ASP  |
| 2   | B     | 731  | VAL  |
| 2   | B     | 751  | VAL  |
| 2   | B     | 958  | GLN  |
| 2   | B     | 959  | ASP  |
| 2   | B     | 1046 | PRO  |
| 2   | B     | 1103 | ILE  |
| 2   | B     | 1167 | GLY  |
| 2   | B     | 1176 | ASN  |
| 2   | B     | 1183 | LYS  |
| 3   | C     | 4    | GLU  |
| 3   | C     | 5    | GLY  |
| 3   | C     | 6    | PRO  |
| 3   | C     | 110  | THR  |
| 3   | C     | 142  | VAL  |
| 3   | C     | 215  | GLU  |
| 6   | F     | 73   | ALA  |
| 8   | H     | 32   | THR  |
| 8   | H     | 81   | PRO  |
| 8   | H     | 140  | ALA  |
| 9   | I     | 8    | ARG  |
| 10  | J     | 2    | ILE  |
| 10  | J     | 55   | ASP  |
| 12  | L     | 27   | LEU  |
| 12  | L     | 38   | LEU  |
| 12  | L     | 64   | LEU  |
| 1   | A     | 35   | ILE  |
| 1   | A     | 54   | ASN  |
| 1   | A     | 62   | ASP  |
| 1   | A     | 87   | ALA  |
| 1   | A     | 109  | HIS  |
| 1   | A     | 135  | PHE  |
| 1   | A     | 168  | GLY  |
| 1   | A     | 332  | LYS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 385  | ILE  |
| 1   | A     | 419  | LYS  |
| 1   | A     | 534  | LEU  |
| 1   | A     | 568  | PRO  |
| 1   | A     | 790  | ASP  |
| 1   | A     | 986  | ILE  |
| 1   | A     | 1114 | PRO  |
| 1   | A     | 1365 | TYR  |
| 1   | A     | 1366 | ARG  |
| 1   | A     | 1379 | GLY  |
| 2   | B     | 55   | VAL  |
| 2   | B     | 168  | GLY  |
| 2   | B     | 275  | TYR  |
| 2   | B     | 346  | GLU  |
| 2   | B     | 410  | GLY  |
| 2   | B     | 480  | SER  |
| 2   | B     | 641  | GLU  |
| 2   | B     | 643  | ASP  |
| 2   | B     | 792  | MET  |
| 2   | B     | 864  | LYS  |
| 2   | B     | 866  | TYR  |
| 2   | B     | 884  | ARG  |
| 2   | B     | 891  | ASP  |
| 2   | B     | 992  | ILE  |
| 2   | B     | 1066 | SER  |
| 2   | B     | 1155 | SER  |
| 3   | C     | 136  | ASP  |
| 6   | F     | 142  | SER  |
| 8   | H     | 61   | SER  |
| 8   | H     | 77   | ARG  |
| 8   | H     | 88   | SER  |
| 8   | H     | 128  | ASN  |
| 9   | I     | 30   | ARG  |
| 9   | I     | 79   | HIS  |
| 12  | L     | 39   | SER  |
| 12  | L     | 52   | GLY  |
| 1   | A     | 6    | TYR  |
| 1   | A     | 45   | GLN  |
| 1   | A     | 59   | GLY  |
| 1   | A     | 67   | CYS  |
| 1   | A     | 69   | THR  |
| 1   | A     | 335  | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 433  | GLU  |
| 1   | A     | 596  | THR  |
| 1   | A     | 737  | LEU  |
| 1   | A     | 775  | ILE  |
| 1   | A     | 830  | LYS  |
| 1   | A     | 920  | LEU  |
| 2   | B     | 28   | GLU  |
| 2   | B     | 249  | ARG  |
| 2   | B     | 277  | LYS  |
| 2   | B     | 447  | ALA  |
| 2   | B     | 629  | ASP  |
| 2   | B     | 735  | ALA  |
| 2   | B     | 880  | THR  |
| 2   | B     | 1017 | ILE  |
| 2   | B     | 1099 | VAL  |
| 2   | B     | 1104 | HIS  |
| 2   | B     | 1178 | ASN  |
| 3   | C     | 48   | SER  |
| 3   | C     | 212  | PRO  |
| 3   | C     | 227  | THR  |
| 5   | E     | 31   | THR  |
| 5   | E     | 102  | GLU  |
| 5   | E     | 103  | LYS  |
| 5   | E     | 122  | LYS  |
| 5   | E     | 139  | ALA  |
| 5   | E     | 206  | GLY  |
| 6   | F     | 128  | LYS  |
| 8   | H     | 8    | ASP  |
| 8   | H     | 17   | PRO  |
| 8   | H     | 82   | PRO  |
| 8   | H     | 135  | LEU  |
| 8   | H     | 139  | ASN  |
| 9   | I     | 9    | ASP  |
| 9   | I     | 33   | SER  |
| 9   | I     | 86   | PHE  |
| 10  | J     | 9    | SER  |
| 12  | L     | 63   | ARG  |
| 1   | A     | 101  | LYS  |
| 1   | A     | 134  | ARG  |
| 1   | A     | 139  | TRP  |
| 1   | A     | 424  | ILE  |
| 1   | A     | 599  | SER  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1067 | LEU  |
| 1   | A     | 1097 | GLY  |
| 1   | A     | 1115 | SER  |
| 1   | A     | 1122 | PRO  |
| 1   | A     | 1405 | THR  |
| 2   | B     | 248  | SER  |
| 2   | B     | 304  | ASP  |
| 2   | B     | 436  | VAL  |
| 2   | B     | 501  | PRO  |
| 2   | B     | 667  | GLN  |
| 2   | B     | 791  | THR  |
| 2   | B     | 807  | ARG  |
| 2   | B     | 1054 | GLY  |
| 2   | B     | 1097 | HIS  |
| 3   | C     | 18   | VAL  |
| 3   | C     | 149  | LYS  |
| 3   | C     | 174  | ALA  |
| 5   | E     | 59   | SER  |
| 10  | J     | 6    | ARG  |
| 12  | L     | 50   | ASP  |
| 12  | L     | 56   | LEU  |
| 1   | A     | 58   | LEU  |
| 1   | A     | 223  | GLY  |
| 1   | A     | 399  | HIS  |
| 1   | A     | 400  | PRO  |
| 1   | A     | 958  | VAL  |
| 1   | A     | 972  | HIS  |
| 1   | A     | 1098 | VAL  |
| 1   | A     | 1130 | GLN  |
| 1   | A     | 1282 | VAL  |
| 1   | A     | 1351 | GLU  |
| 1   | A     | 1378 | GLN  |
| 2   | B     | 419  | THR  |
| 2   | B     | 619  | ILE  |
| 2   | B     | 648  | HIS  |
| 2   | B     | 687  | GLU  |
| 2   | B     | 707  | PRO  |
| 2   | B     | 712  | PRO  |
| 2   | B     | 764  | SER  |
| 2   | B     | 907  | GLY  |
| 2   | B     | 982  | SER  |
| 2   | B     | 1108 | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 5   | E     | 36   | GLU  |
| 8   | H     | 62   | SER  |
| 8   | H     | 89   | LEU  |
| 9   | I     | 47   | GLU  |
| 9   | I     | 88   | SER  |
| 1   | A     | 226  | GLU  |
| 1   | A     | 368  | LYS  |
| 1   | A     | 465  | TYR  |
| 1   | A     | 531  | ILE  |
| 1   | A     | 903  | ASN  |
| 1   | A     | 1014 | ALA  |
| 1   | A     | 1314 | SER  |
| 1   | A     | 1352 | VAL  |
| 2   | B     | 27   | ALA  |
| 5   | E     | 167  | ARG  |
| 8   | H     | 138  | GLU  |
| 9   | I     | 98   | VAL  |
| 11  | K     | 107  | THR  |
| 2   | B     | 247  | GLY  |
| 1   | A     | 336  | ILE  |
| 1   | A     | 1104 | ILE  |
| 12  | L     | 55   | ILE  |
| 1   | A     | 810  | PRO  |
| 1   | A     | 1075 | PRO  |
| 1   | A     | 1242 | VAL  |
| 3   | C     | 172  | PRO  |
| 3   | C     | 216  | GLY  |
| 2   | B     | 511  | PRO  |
| 3   | C     | 218  | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | A     | 1206/1520 (79%) | 1123 (93%) | 83 (7%)  | 14          | 38 |
| 2   | B     | 952/1061 (90%)  | 874 (92%)  | 78 (8%)  | 10          | 33 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 3   | C     | 234/274 (85%)   | 218 (93%)  | 16 (7%)  | 14          | 38 |
| 5   | E     | 196/197 (100%)  | 192 (98%)  | 4 (2%)   | 48          | 66 |
| 6   | F     | 74/137 (54%)    | 68 (92%)   | 6 (8%)   | 11          | 33 |
| 8   | H     | 117/128 (91%)   | 113 (97%)  | 4 (3%)   | 32          | 55 |
| 9   | I     | 113/116 (97%)   | 105 (93%)  | 8 (7%)   | 13          | 37 |
| 10  | J     | 60/65 (92%)     | 54 (90%)   | 6 (10%)  | 7           | 26 |
| 11  | K     | 99/102 (97%)    | 88 (89%)   | 11 (11%) | 6           | 22 |
| 12  | L     | 40/57 (70%)     | 34 (85%)   | 6 (15%)  | 3           | 15 |
| All | All   | 3091/3657 (84%) | 2869 (93%) | 222 (7%) | 13          | 37 |

All (222) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 18  | GLN  |
| 1   | A     | 22  | PHE  |
| 1   | A     | 31  | SER  |
| 1   | A     | 56  | PRO  |
| 1   | A     | 70  | CYS  |
| 1   | A     | 93  | VAL  |
| 1   | A     | 247 | ARG  |
| 1   | A     | 269 | ILE  |
| 1   | A     | 302 | THR  |
| 1   | A     | 322 | VAL  |
| 1   | A     | 326 | ARG  |
| 1   | A     | 351 | THR  |
| 1   | A     | 375 | THR  |
| 1   | A     | 381 | THR  |
| 1   | A     | 385 | ILE  |
| 1   | A     | 397 | ASN  |
| 1   | A     | 434 | ARG  |
| 1   | A     | 443 | LEU  |
| 1   | A     | 445 | ASN  |
| 1   | A     | 450 | LEU  |
| 1   | A     | 451 | HIS  |
| 1   | A     | 461 | LYS  |
| 1   | A     | 466 | SER  |
| 1   | A     | 474 | VAL  |
| 1   | A     | 475 | THR  |
| 1   | A     | 493 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 503  | GLN  |
| 1   | A     | 504  | LEU  |
| 1   | A     | 524  | VAL  |
| 1   | A     | 535  | THR  |
| 1   | A     | 590  | ARG  |
| 1   | A     | 596  | THR  |
| 1   | A     | 597  | LEU  |
| 1   | A     | 598  | LEU  |
| 1   | A     | 618  | GLU  |
| 1   | A     | 629  | LEU  |
| 1   | A     | 666  | ILE  |
| 1   | A     | 682  | THR  |
| 1   | A     | 740  | LEU  |
| 1   | A     | 741  | ASN  |
| 1   | A     | 745  | GLN  |
| 1   | A     | 756  | ILE  |
| 1   | A     | 768  | GLN  |
| 1   | A     | 821  | ARG  |
| 1   | A     | 845  | LEU  |
| 1   | A     | 849  | MET  |
| 1   | A     | 854  | ASN  |
| 1   | A     | 855  | THR  |
| 1   | A     | 858  | ASN  |
| 1   | A     | 904  | THR  |
| 1   | A     | 913  | LEU  |
| 1   | A     | 920  | LEU  |
| 1   | A     | 929  | LEU  |
| 1   | A     | 948  | VAL  |
| 1   | A     | 979  | SER  |
| 1   | A     | 1029 | ARG  |
| 1   | A     | 1035 | TYR  |
| 1   | A     | 1043 | ASP  |
| 1   | A     | 1055 | ARG  |
| 1   | A     | 1057 | VAL  |
| 1   | A     | 1077 | THR  |
| 1   | A     | 1122 | PRO  |
| 1   | A     | 1136 | SER  |
| 1   | A     | 1208 | THR  |
| 1   | A     | 1212 | VAL  |
| 1   | A     | 1222 | ASN  |
| 1   | A     | 1232 | ASN  |
| 1   | A     | 1258 | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1264 | GLU  |
| 1   | A     | 1295 | THR  |
| 1   | A     | 1308 | THR  |
| 1   | A     | 1311 | VAL  |
| 1   | A     | 1318 | THR  |
| 1   | A     | 1332 | PHE  |
| 1   | A     | 1335 | ILE  |
| 1   | A     | 1351 | GLU  |
| 1   | A     | 1355 | VAL  |
| 1   | A     | 1359 | ASP  |
| 1   | A     | 1364 | ASN  |
| 1   | A     | 1375 | MET  |
| 1   | A     | 1376 | THR  |
| 1   | A     | 1425 | SER  |
| 1   | A     | 1442 | ASP  |
| 2   | B     | 43   | LEU  |
| 2   | B     | 57   | TYR  |
| 2   | B     | 63   | ILE  |
| 2   | B     | 98   | THR  |
| 2   | B     | 109  | THR  |
| 2   | B     | 121  | ASN  |
| 2   | B     | 175  | ARG  |
| 2   | B     | 185  | THR  |
| 2   | B     | 194  | GLU  |
| 2   | B     | 232  | SER  |
| 2   | B     | 234  | ILE  |
| 2   | B     | 254  | LEU  |
| 2   | B     | 261  | ARG  |
| 2   | B     | 268  | THR  |
| 2   | B     | 309  | GLN  |
| 2   | B     | 313  | MET  |
| 2   | B     | 317  | CYS  |
| 2   | B     | 320  | ASP  |
| 2   | B     | 331  | LEU  |
| 2   | B     | 361  | LEU  |
| 2   | B     | 387  | LEU  |
| 2   | B     | 396  | ASP  |
| 2   | B     | 408  | LEU  |
| 2   | B     | 453  | ILE  |
| 2   | B     | 484  | ASN  |
| 2   | B     | 485  | ARG  |
| 2   | B     | 498  | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 513  | GLN  |
| 2   | B     | 514  | LEU  |
| 2   | B     | 538  | ASN  |
| 2   | B     | 542  | MET  |
| 2   | B     | 547  | VAL  |
| 2   | B     | 556  | THR  |
| 2   | B     | 563  | MET  |
| 2   | B     | 570  | VAL  |
| 2   | B     | 576  | ASP  |
| 2   | B     | 624  | LEU  |
| 2   | B     | 644  | GLU  |
| 2   | B     | 680  | THR  |
| 2   | B     | 723  | VAL  |
| 2   | B     | 732  | SER  |
| 2   | B     | 737  | THR  |
| 2   | B     | 762  | ASN  |
| 2   | B     | 764  | SER  |
| 2   | B     | 780  | VAL  |
| 2   | B     | 791  | THR  |
| 2   | B     | 835  | GLN  |
| 2   | B     | 839  | MET  |
| 2   | B     | 860  | MET  |
| 2   | B     | 901  | PRO  |
| 2   | B     | 915  | THR  |
| 2   | B     | 944  | THR  |
| 2   | B     | 951  | GLN  |
| 2   | B     | 953  | LEU  |
| 2   | B     | 954  | VAL  |
| 2   | B     | 976  | ILE  |
| 2   | B     | 986  | GLN  |
| 2   | B     | 987  | LYS  |
| 2   | B     | 996  | ARG  |
| 2   | B     | 997  | GLU  |
| 2   | B     | 999  | MET  |
| 2   | B     | 1002 | THR  |
| 2   | B     | 1007 | VAL  |
| 2   | B     | 1017 | ILE  |
| 2   | B     | 1021 | MET  |
| 2   | B     | 1034 | VAL  |
| 2   | B     | 1049 | ASP  |
| 2   | B     | 1065 | GLN  |
| 2   | B     | 1073 | TYR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 1103 | ILE  |
| 2   | B     | 1111 | MET  |
| 2   | B     | 1118 | PRO  |
| 2   | B     | 1132 | GLU  |
| 2   | B     | 1133 | MET  |
| 2   | B     | 1147 | LEU  |
| 2   | B     | 1150 | ARG  |
| 2   | B     | 1151 | LEU  |
| 2   | B     | 1185 | CYS  |
| 3   | C     | 22   | LEU  |
| 3   | C     | 25   | VAL  |
| 3   | C     | 26   | ASP  |
| 3   | C     | 58   | LEU  |
| 3   | C     | 62   | PHE  |
| 3   | C     | 69   | LEU  |
| 3   | C     | 77   | ILE  |
| 3   | C     | 99   | LEU  |
| 3   | C     | 133  | ILE  |
| 3   | C     | 195  | GLN  |
| 3   | C     | 229  | TYR  |
| 3   | C     | 233  | GLU  |
| 3   | C     | 238  | ILE  |
| 3   | C     | 240  | VAL  |
| 3   | C     | 259  | LEU  |
| 3   | C     | 264  | GLN  |
| 5   | E     | 40   | GLU  |
| 5   | E     | 84   | ASP  |
| 5   | E     | 92   | THR  |
| 5   | E     | 183  | PRO  |
| 6   | F     | 79   | ARG  |
| 6   | F     | 90   | ARG  |
| 6   | F     | 103  | MET  |
| 6   | F     | 111  | LEU  |
| 6   | F     | 115  | THR  |
| 6   | F     | 133  | VAL  |
| 8   | H     | 21   | ASN  |
| 8   | H     | 27   | GLU  |
| 8   | H     | 109  | LYS  |
| 8   | H     | 110  | ASP  |
| 9   | I     | 12   | ASN  |
| 9   | I     | 29   | CYS  |
| 9   | I     | 31   | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | I     | 52  | ILE  |
| 9   | I     | 75  | CYS  |
| 9   | I     | 76  | PRO  |
| 9   | I     | 87  | GLN  |
| 9   | I     | 97  | MET  |
| 10  | J     | 1   | MET  |
| 10  | J     | 2   | ILE  |
| 10  | J     | 7   | CYS  |
| 10  | J     | 22  | LEU  |
| 10  | J     | 47  | ARG  |
| 10  | J     | 48  | ARG  |
| 11  | K     | 11  | LEU  |
| 11  | K     | 20  | LYS  |
| 11  | K     | 25  | THR  |
| 11  | K     | 29  | ASN  |
| 11  | K     | 31  | VAL  |
| 11  | K     | 47  | ARG  |
| 11  | K     | 50  | LEU  |
| 11  | K     | 51  | LEU  |
| 11  | K     | 63  | VAL  |
| 11  | K     | 77  | THR  |
| 11  | K     | 114 | LEU  |
| 12  | L     | 50  | ASP  |
| 12  | L     | 54  | ARG  |
| 12  | L     | 55  | ILE  |
| 12  | L     | 65  | VAL  |
| 12  | L     | 68  | GLU  |
| 12  | L     | 70  | ARG  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (93) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 68  | GLN  |
| 1   | A     | 92  | HIS  |
| 1   | A     | 118 | HIS  |
| 1   | A     | 169 | ASN  |
| 1   | A     | 225 | ASN  |
| 1   | A     | 281 | HIS  |
| 1   | A     | 339 | ASN  |
| 1   | A     | 425 | GLN  |
| 1   | A     | 435 | HIS  |
| 1   | A     | 445 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 493  | GLN  |
| 1   | A     | 503  | GLN  |
| 1   | A     | 517  | ASN  |
| 1   | A     | 631  | HIS  |
| 1   | A     | 698  | GLN  |
| 1   | A     | 736  | ASN  |
| 1   | A     | 741  | ASN  |
| 1   | A     | 757  | ASN  |
| 1   | A     | 760  | GLN  |
| 1   | A     | 768  | GLN  |
| 1   | A     | 786  | HIS  |
| 1   | A     | 858  | ASN  |
| 1   | A     | 877  | HIS  |
| 1   | A     | 926  | GLN  |
| 1   | A     | 953  | ASN  |
| 1   | A     | 965  | GLN  |
| 1   | A     | 968  | GLN  |
| 1   | A     | 994  | GLN  |
| 1   | A     | 1011 | GLN  |
| 1   | A     | 1070 | GLN  |
| 1   | A     | 1124 | HIS  |
| 1   | A     | 1130 | GLN  |
| 1   | A     | 1188 | GLN  |
| 1   | A     | 1222 | ASN  |
| 1   | A     | 1364 | ASN  |
| 1   | A     | 1387 | HIS  |
| 1   | A     | 1390 | ASN  |
| 1   | A     | 1432 | GLN  |
| 2   | B     | 46   | GLN  |
| 2   | B     | 47   | GLN  |
| 2   | B     | 53   | GLN  |
| 2   | B     | 121  | ASN  |
| 2   | B     | 215  | GLN  |
| 2   | B     | 236  | HIS  |
| 2   | B     | 309  | GLN  |
| 2   | B     | 325  | GLN  |
| 2   | B     | 363  | HIS  |
| 2   | B     | 415  | GLN  |
| 2   | B     | 465  | ASN  |
| 2   | B     | 484  | ASN  |
| 2   | B     | 513  | GLN  |
| 2   | B     | 515  | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 516  | ASN  |
| 2   | B     | 518  | HIS  |
| 2   | B     | 538  | ASN  |
| 2   | B     | 744  | HIS  |
| 2   | B     | 770  | GLN  |
| 2   | B     | 822  | ASN  |
| 2   | B     | 842  | ASN  |
| 2   | B     | 862  | GLN  |
| 2   | B     | 957  | ASN  |
| 2   | B     | 975  | GLN  |
| 2   | B     | 1015 | HIS  |
| 2   | B     | 1065 | GLN  |
| 2   | B     | 1093 | GLN  |
| 2   | B     | 1117 | GLN  |
| 2   | B     | 1141 | HIS  |
| 2   | B     | 1179 | GLN  |
| 2   | B     | 1193 | GLN  |
| 2   | B     | 1205 | GLN  |
| 3   | C     | 65   | HIS  |
| 3   | C     | 73   | GLN  |
| 3   | C     | 112  | ASN  |
| 3   | C     | 123  | ASN  |
| 3   | C     | 131  | HIS  |
| 3   | C     | 140  | ASN  |
| 3   | C     | 167  | HIS  |
| 3   | C     | 242  | GLN  |
| 3   | C     | 252  | GLN  |
| 5   | E     | 5    | ASN  |
| 5   | E     | 101  | GLN  |
| 5   | E     | 104  | ASN  |
| 5   | E     | 114  | ASN  |
| 5   | E     | 115  | ASN  |
| 5   | E     | 147  | HIS  |
| 6   | F     | 78   | GLN  |
| 8   | H     | 33   | GLN  |
| 9   | I     | 12   | ASN  |
| 10  | J     | 53   | HIS  |
| 11  | K     | 44   | ASN  |
| 11  | K     | 65   | HIS  |
| 11  | K     | 76   | GLN  |
| 11  | K     | 110  | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2                                                                                                                                                                              | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------|-------|
| 1   | A     | 1388/1733 (80%) | 1.11   | 246 (17%)       | 20, 181, 283, 321     | 0     |
| 2   | B     | 1097/1224 (89%) | 1.21   | 208 (18%)       | 74, 189, 297, 321     | 0     |
| 3   | C     | 266/318 (83%)   | 1.06   | 36 (13%)        | 87, 180, 262, 321     | 0     |
| 4   | D     | 0/161           | -      | -                                                                                                                                                                                    | -                     | -     |
| 5   | E     | 214/215 (99%)   | 1.09   | 32 (14%)        | 88, 223, 305, 321     | 0     |
| 6   | F     | 84/155 (54%)    | 0.95   | 14 (16%)        | 90, 163, 254, 321     | 0     |
| 7   | G     | 0/170           | -      | -                                                                                                                                                                                    | -                     | -     |
| 8   | H     | 133/146 (91%)   | 1.59   | 44 (33%)      | 139, 242, 318, 321    | 0     |
| 9   | I     | 119/122 (97%)   | 1.84   | 50 (42%)    | 139, 241, 318, 321    | 0     |
| 10  | J     | 65/70 (92%)     | 0.87   | 6 (9%)      | 68, 173, 284, 313     | 0     |
| 11  | K     | 114/120 (95%)   | 0.78   | 9 (7%)      | 98, 170, 245, 304     | 0     |
| 12  | L     | 46/70 (65%)     | 1.87   | 21 (45%)    | 134, 233, 304, 321    | 0     |
| All | All   | 3526/4504 (78%) | 1.17   | 666 (18%)   | 20, 189, 294, 321     | 0     |

All (666) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 2   | B     | 247  | GLY  | 9.1  |
| 1   | A     | 1449 | SER  | 8.4  |
| 2   | B     | 887  | HIS  | 7.5  |
| 1   | A     | 1256 | GLU  | 7.5  |
| 6   | F     | 104  | ASN  | 7.4  |
| 1   | A     | 1188 | GLN  | 7.3  |
| 1   | A     | 64   | ASN  | 7.2  |
| 1   | A     | 1447 | GLU  | 6.6  |
| 1   | A     | 1448 | GLU  | 6.6  |
| 2   | B     | 869  | SER  | 6.4  |
| 2   | B     | 882  | THR  | 6.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 12  | L     | 46   | VAL  | 5.7  |
| 3   | C     | 106  | GLU  | 5.6  |
| 3   | C     | 4    | GLU  | 5.6  |
| 2   | B     | 446  | LEU  | 5.3  |
| 2   | B     | 734  | HIS  | 5.3  |
| 3   | C     | 211  | ASP  | 5.2  |
| 9   | I     | 23   | ASN  | 5.2  |
| 9   | I     | 34   | TYR  | 5.2  |
| 9   | I     | 72   | ASP  | 5.2  |
| 1   | A     | 593  | GLU  | 5.1  |
| 12  | L     | 60   | ARG  | 5.0  |
| 1   | A     | 1158 | PRO  | 4.9  |
| 2   | B     | 643  | ASP  | 4.9  |
| 2   | B     | 641  | GLU  | 4.9  |
| 2   | B     | 895  | ASP  | 4.9  |
| 2   | B     | 39   | ARG  | 4.8  |
| 2   | B     | 177  | LYS  | 4.8  |
| 2   | B     | 246  | LYS  | 4.7  |
| 1   | A     | 1403 | GLU  | 4.7  |
| 1   | A     | 637  | LYS  | 4.6  |
| 9   | I     | 18   | GLU  | 4.5  |
| 1   | A     | 200  | ARG  | 4.5  |
| 1   | A     | 1161 | THR  | 4.5  |
| 9   | I     | 16   | PRO  | 4.4  |
| 1   | A     | 1127 | ASP  | 4.4  |
| 1   | A     | 1274 | ARG  | 4.4  |
| 1   | A     | 199  | LEU  | 4.4  |
| 5   | E     | 121  | MET  | 4.4  |
| 9   | I     | 2    | THR  | 4.4  |
| 5   | E     | 81   | GLU  | 4.4  |
| 1   | A     | 66   | LYS  | 4.3  |
| 3   | C     | 76   | ASP  | 4.3  |
| 1   | A     | 1257 | ASP  | 4.3  |
| 2   | B     | 427  | ASP  | 4.3  |
| 1   | A     | 1451 | VAL  | 4.3  |
| 8   | H     | 106  | GLU  | 4.2  |
| 2   | B     | 792  | MET  | 4.2  |
| 2   | B     | 810  | GLU  | 4.2  |
| 1   | A     | 590  | ARG  | 4.2  |
| 1   | A     | 1206 | ASP  | 4.2  |
| 2   | B     | 335  | GLY  | 4.1  |
| 11  | K     | 38   | GLU  | 4.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 893  | PHE  | 4.1  |
| 1   | A     | 178  | GLY  | 4.1  |
| 2   | B     | 735  | ALA  | 4.1  |
| 9   | I     | 8    | ARG  | 4.0  |
| 1   | A     | 173  | THR  | 4.0  |
| 2   | B     | 549  | THR  | 4.0  |
| 3   | C     | 79   | GLN  | 4.0  |
| 8   | H     | 139  | ASN  | 4.0  |
| 1   | A     | 249  | SER  | 4.0  |
| 2   | B     | 779  | GLY  | 4.0  |
| 2   | B     | 428  | ILE  | 4.0  |
| 1   | A     | 65   | LEU  | 3.9  |
| 2   | B     | 601  | ARG  | 3.9  |
| 1   | A     | 61   | ILE  | 3.9  |
| 1   | A     | 1109 | LYS  | 3.9  |
| 2   | B     | 249  | ARG  | 3.9  |
| 12  | L     | 70   | ARG  | 3.8  |
| 1   | A     | 2    | VAL  | 3.8  |
| 3   | C     | 28   | ALA  | 3.8  |
| 1   | A     | 911  | SER  | 3.8  |
| 1   | A     | 62   | ASP  | 3.8  |
| 1   | A     | 56   | PRO  | 3.7  |
| 1   | A     | 69   | THR  | 3.7  |
| 5   | E     | 86   | PRO  | 3.7  |
| 8   | H     | 62   | SER  | 3.7  |
| 8   | H     | 6    | PHE  | 3.7  |
| 6   | F     | 128  | LYS  | 3.7  |
| 1   | A     | 496  | GLU  | 3.7  |
| 2   | B     | 294  | ASP  | 3.7  |
| 2   | B     | 325  | GLN  | 3.7  |
| 1   | A     | 626  | ASN  | 3.7  |
| 2   | B     | 834  | ASN  | 3.6  |
| 1   | A     | 896  | ARG  | 3.6  |
| 2   | B     | 730  | ARG  | 3.6  |
| 9   | I     | 9    | ASP  | 3.6  |
| 1   | A     | 1439 | GLY  | 3.6  |
| 2   | B     | 103  | ASN  | 3.6  |
| 2   | B     | 64   | CYS  | 3.6  |
| 1   | A     | 76   | GLU  | 3.6  |
| 2   | B     | 529  | GLU  | 3.6  |
| 2   | B     | 166  | PHE  | 3.6  |
| 1   | A     | 830  | LYS  | 3.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 2   | B     | 1217 | TYR  | 3.5  |
| 2   | B     | 727  | LYS  | 3.5  |
| 1   | A     | 1173 | HIS  | 3.5  |
| 3   | C     | 78   | GLU  | 3.5  |
| 5   | E     | 118  | PRO  | 3.5  |
| 2   | B     | 709  | ASP  | 3.5  |
| 1   | A     | 933  | TYR  | 3.5  |
| 2   | B     | 569  | TYR  | 3.5  |
| 2   | B     | 248  | SER  | 3.5  |
| 8   | H     | 88   | SER  | 3.5  |
| 1   | A     | 170  | THR  | 3.5  |
| 1   | A     | 589  | GLN  | 3.5  |
| 2   | B     | 726  | ALA  | 3.5  |
| 1   | A     | 1236 | LEU  | 3.5  |
| 2   | B     | 295  | GLY  | 3.5  |
| 1   | A     | 1281 | ARG  | 3.5  |
| 1   | A     | 314  | ALA  | 3.4  |
| 9   | I     | 12   | ASN  | 3.4  |
| 2   | B     | 417  | PHE  | 3.4  |
| 9   | I     | 77   | LYS  | 3.4  |
| 3   | C     | 26   | ASP  | 3.4  |
| 8   | H     | 8    | ASP  | 3.4  |
| 1   | A     | 1189 | SER  | 3.4  |
| 2   | B     | 919  | SER  | 3.4  |
| 2   | B     | 1013 | ASN  | 3.4  |
| 3   | C     | 126  | GLY  | 3.4  |
| 11  | K     | 16   | GLU  | 3.4  |
| 1   | A     | 146  | MET  | 3.4  |
| 9   | I     | 119  | THR  | 3.4  |
| 1   | A     | 105  | CYS  | 3.4  |
| 1   | A     | 74   | MET  | 3.4  |
| 2   | B     | 169  | ARG  | 3.3  |
| 2   | B     | 902  | GLY  | 3.3  |
| 8   | H     | 13   | SER  | 3.3  |
| 2   | B     | 875  | GLU  | 3.3  |
| 2   | B     | 958  | GLN  | 3.3  |
| 2   | B     | 267  | ARG  | 3.3  |
| 2   | B     | 1123 | SER  | 3.3  |
| 2   | B     | 250  | PHE  | 3.3  |
| 2   | B     | 1224 | PHE  | 3.3  |
| 8   | H     | 54   | SER  | 3.3  |
| 9   | I     | 43   | VAL  | 3.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 8   | H     | 141  | TYR  | 3.3  |
| 8   | H     | 131  | ASN  | 3.3  |
| 1   | A     | 932  | GLU  | 3.3  |
| 12  | L     | 28   | LYS  | 3.3  |
| 6   | F     | 108  | PHE  | 3.3  |
| 1   | A     | 1145 | SER  | 3.3  |
| 1   | A     | 104  | GLU  | 3.2  |
| 1   | A     | 403  | LYS  | 3.2  |
| 1   | A     | 753  | GLY  | 3.2  |
| 2   | B     | 975  | GLN  | 3.2  |
| 9   | I     | 11   | ASN  | 3.2  |
| 1   | A     | 59   | GLY  | 3.2  |
| 8   | H     | 120  | GLY  | 3.2  |
| 5   | E     | 114  | ASN  | 3.2  |
| 1   | A     | 124  | GLN  | 3.2  |
| 1   | A     | 1159 | ARG  | 3.2  |
| 1   | A     | 1172 | LEU  | 3.2  |
| 2   | B     | 180  | TYR  | 3.2  |
| 9   | I     | 55   | THR  | 3.2  |
| 9   | I     | 56   | ALA  | 3.2  |
| 2   | B     | 302  | CYS  | 3.2  |
| 1   | A     | 1235 | LYS  | 3.2  |
| 1   | A     | 1023 | ARG  | 3.2  |
| 2   | B     | 487  | THR  | 3.2  |
| 5   | E     | 10   | SER  | 3.2  |
| 5   | E     | 172  | GLU  | 3.2  |
| 1   | A     | 50   | ILE  | 3.2  |
| 1   | A     | 903  | ASN  | 3.2  |
| 1   | A     | 461  | LYS  | 3.2  |
| 1   | A     | 321  | PRO  | 3.2  |
| 6   | F     | 113  | GLY  | 3.2  |
| 2   | B     | 815  | ARG  | 3.2  |
| 3   | C     | 175  | ALA  | 3.2  |
| 12  | L     | 32   | ALA  | 3.2  |
| 2   | B     | 523  | CYS  | 3.2  |
| 1   | A     | 97   | ALA  | 3.2  |
| 2   | B     | 871  | THR  | 3.1  |
| 9   | I     | 41   | PRO  | 3.1  |
| 1   | A     | 3    | GLY  | 3.1  |
| 9   | I     | 49   | ILE  | 3.1  |
| 3   | C     | 15   | LYS  | 3.1  |
| 2   | B     | 304  | ASP  | 3.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 2   | B     | 736  | THR  | 3.1  |
| 1   | A     | 591  | PHE  | 3.1  |
| 2   | B     | 617  | ARG  | 3.1  |
| 2   | B     | 298  | LEU  | 3.1  |
| 1   | A     | 1422 | ARG  | 3.1  |
| 2   | B     | 1222 | ARG  | 3.1  |
| 1   | A     | 47   | ARG  | 3.1  |
| 1   | A     | 175  | ARG  | 3.1  |
| 1   | A     | 975  | HIS  | 3.1  |
| 1   | A     | 1124 | HIS  | 3.1  |
| 2   | B     | 262  | GLU  | 3.1  |
| 1   | A     | 168  | GLY  | 3.1  |
| 2   | B     | 259  | TYR  | 3.1  |
| 2   | B     | 413  | LEU  | 3.1  |
| 1   | A     | 1445 | ILE  | 3.1  |
| 3   | C     | 166  | GLU  | 3.1  |
| 1   | A     | 337  | ARG  | 3.0  |
| 9   | I     | 35   | VAL  | 3.0  |
| 1   | A     | 5    | GLN  | 3.0  |
| 2   | B     | 1184 | GLY  | 3.0  |
| 5   | E     | 113  | GLN  | 3.0  |
| 2   | B     | 477  | ALA  | 3.0  |
| 2   | B     | 838  | SER  | 3.0  |
| 1   | A     | 1307 | GLU  | 3.0  |
| 8   | H     | 116  | TYR  | 3.0  |
| 12  | L     | 27   | LEU  | 3.0  |
| 1   | A     | 905  | ASP  | 3.0  |
| 9   | I     | 31   | THR  | 3.0  |
| 10  | J     | 28   | ASP  | 3.0  |
| 12  | L     | 26   | THR  | 3.0  |
| 5   | E     | 17   | ARG  | 3.0  |
| 2   | B     | 725  | PRO  | 3.0  |
| 1   | A     | 914  | GLU  | 3.0  |
| 2   | B     | 60   | GLN  | 3.0  |
| 9   | I     | 114  | GLN  | 3.0  |
| 1   | A     | 1446 | ASP  | 3.0  |
| 8   | H     | 136  | LYS  | 3.0  |
| 12  | L     | 63   | ARG  | 3.0  |
| 1   | A     | 1269 | GLU  | 3.0  |
| 6   | F     | 92   | ARG  | 3.0  |
| 8   | H     | 76   | THR  | 3.0  |
| 12  | L     | 64   | LEU  | 3.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 2   | B     | 610  | ASN  | 3.0  |
| 1   | A     | 1165 | GLU  | 3.0  |
| 2   | B     | 807  | ARG  | 3.0  |
| 2   | B     | 1189 | ILE  | 3.0  |
| 1   | A     | 114  | LEU  | 3.0  |
| 2   | B     | 1009 | ASP  | 3.0  |
| 1   | A     | 383  | TYR  | 3.0  |
| 10  | J     | 65   | PRO  | 3.0  |
| 1   | A     | 892  | ALA  | 3.0  |
| 1   | A     | 1254 | ALA  | 3.0  |
| 1   | A     | 1450 | LEU  | 2.9  |
| 8   | H     | 16   | ASP  | 2.9  |
| 1   | A     | 109  | HIS  | 2.9  |
| 1   | A     | 1204 | ASP  | 2.9  |
| 1   | A     | 1350 | LYS  | 2.9  |
| 1   | A     | 71   | GLN  | 2.9  |
| 1   | A     | 223  | GLY  | 2.9  |
| 1   | A     | 1221 | LYS  | 2.9  |
| 8   | H     | 119  | GLY  | 2.9  |
| 2   | B     | 303  | TYR  | 2.9  |
| 3   | C     | 87   | PHE  | 2.9  |
| 1   | A     | 922  | ASP  | 2.9  |
| 8   | H     | 110  | ASP  | 2.9  |
| 2   | B     | 731  | VAL  | 2.9  |
| 8   | H     | 44   | VAL  | 2.9  |
| 5   | E     | 93   | MET  | 2.9  |
| 2   | B     | 1153 | GLU  | 2.9  |
| 1   | A     | 887  | GLY  | 2.9  |
| 1   | A     | 147  | VAL  | 2.9  |
| 1   | A     | 161  | LEU  | 2.9  |
| 1   | A     | 909  | ASP  | 2.9  |
| 8   | H     | 144  | ILE  | 2.9  |
| 1   | A     | 972  | HIS  | 2.9  |
| 2   | B     | 212  | LEU  | 2.9  |
| 2   | B     | 666  | TYR  | 2.9  |
| 1   | A     | 259  | GLU  | 2.9  |
| 2   | B     | 539  | LEU  | 2.9  |
| 12  | L     | 45   | ALA  | 2.9  |
| 2   | B     | 934  | LYS  | 2.9  |
| 1   | A     | 132  | LYS  | 2.8  |
| 1   | A     | 154  | SER  | 2.8  |
| 2   | B     | 998  | ASP  | 2.8  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 9   | I     | 78   | CYS  | 2.8  |
| 1   | A     | 228  | PHE  | 2.8  |
| 2   | B     | 245  | GLU  | 2.8  |
| 2   | B     | 1121 | GLY  | 2.8  |
| 1   | A     | 897  | TYR  | 2.8  |
| 2   | B     | 762  | ASN  | 2.8  |
| 2   | B     | 1188 | LYS  | 2.8  |
| 12  | L     | 53   | HIS  | 2.8  |
| 1   | A     | 1314 | SER  | 2.8  |
| 2   | B     | 454  | THR  | 2.8  |
| 1   | A     | 402  | ALA  | 2.8  |
| 8   | H     | 63   | LEU  | 2.8  |
| 1   | A     | 412  | ARG  | 2.8  |
| 8   | H     | 19   | ARG  | 2.8  |
| 8   | H     | 117  | SER  | 2.8  |
| 1   | A     | 609  | ASP  | 2.8  |
| 8   | H     | 33   | GLN  | 2.8  |
| 3   | C     | 72   | LEU  | 2.8  |
| 1   | A     | 164  | ARG  | 2.8  |
| 1   | A     | 1194 | ARG  | 2.8  |
| 2   | B     | 434  | ARG  | 2.8  |
| 2   | B     | 744  | HIS  | 2.8  |
| 2   | B     | 933  | SER  | 2.8  |
| 2   | B     | 1223 | ASP  | 2.8  |
| 11  | K     | 114  | LEU  | 2.8  |
| 2   | B     | 305  | VAL  | 2.8  |
| 2   | B     | 243  | ALA  | 2.8  |
| 8   | H     | 105  | GLU  | 2.8  |
| 1   | A     | 1135 | ARG  | 2.7  |
| 2   | B     | 881  | ASN  | 2.7  |
| 2   | B     | 652  | LYS  | 2.7  |
| 5   | E     | 139  | ALA  | 2.7  |
| 9   | I     | 6    | PHE  | 2.7  |
| 2   | B     | 1129 | ARG  | 2.7  |
| 2   | B     | 839  | MET  | 2.7  |
| 2   | B     | 1177 | HIS  | 2.7  |
| 8   | H     | 102  | TYR  | 2.7  |
| 2   | B     | 526  | GLU  | 2.7  |
| 5   | E     | 6    | GLU  | 2.7  |
| 1   | A     | 976  | THR  | 2.7  |
| 2   | B     | 429  | PHE  | 2.7  |
| 8   | H     | 61   | SER  | 2.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 3   | C     | 266  | ASP  | 2.7  |
| 1   | A     | 108  | MET  | 2.7  |
| 1   | A     | 48   | ALA  | 2.7  |
| 1   | A     | 677  | ARG  | 2.7  |
| 5   | E     | 41   | ASP  | 2.7  |
| 1   | A     | 331  | GLY  | 2.7  |
| 2   | B     | 367  | LEU  | 2.7  |
| 5   | E     | 181  | ALA  | 2.7  |
| 9   | I     | 4    | PHE  | 2.7  |
| 1   | A     | 311  | GLN  | 2.7  |
| 5   | E     | 107  | THR  | 2.7  |
| 1   | A     | 51   | GLY  | 2.7  |
| 2   | B     | 196  | PRO  | 2.7  |
| 5   | E     | 201  | LYS  | 2.7  |
| 3   | C     | 249  | ASP  | 2.7  |
| 9   | I     | 91   | ARG  | 2.7  |
| 1   | A     | 520  | CYS  | 2.7  |
| 1   | A     | 980  | ASP  | 2.6  |
| 2   | B     | 462  | ALA  | 2.6  |
| 2   | B     | 663  | ALA  | 2.6  |
| 1   | A     | 1317 | MET  | 2.6  |
| 1   | A     | 68   | GLN  | 2.6  |
| 1   | A     | 670  | ILE  | 2.6  |
| 2   | B     | 962  | LYS  | 2.6  |
| 8   | H     | 94   | ASP  | 2.6  |
| 3   | C     | 40   | GLU  | 2.6  |
| 1   | A     | 135  | PHE  | 2.6  |
| 2   | B     | 548  | GLY  | 2.6  |
| 1   | A     | 1095 | THR  | 2.6  |
| 2   | B     | 125  | SER  | 2.6  |
| 1   | A     | 28   | ARG  | 2.6  |
| 2   | B     | 397  | ASP  | 2.6  |
| 2   | B     | 511  | PRO  | 2.6  |
| 9   | I     | 28   | GLU  | 2.6  |
| 10  | J     | 29   | GLU  | 2.6  |
| 1   | A     | 806  | ARG  | 2.6  |
| 2   | B     | 1113 | VAL  | 2.6  |
| 1   | A     | 1225 | PHE  | 2.6  |
| 2   | B     | 986  | GLN  | 2.6  |
| 8   | H     | 109  | LYS  | 2.6  |
| 1   | A     | 141  | LEU  | 2.6  |
| 2   | B     | 1125 | ASP  | 2.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 3   | C     | 218  | PRO  | 2.6  |
| 11  | K     | 26   | LYS  | 2.6  |
| 1   | A     | 734  | GLU  | 2.6  |
| 1   | A     | 1187 | GLN  | 2.6  |
| 2   | B     | 433  | GLN  | 2.6  |
| 2   | B     | 918  | ILE  | 2.6  |
| 9   | I     | 57   | GLY  | 2.6  |
| 1   | A     | 1205 | LYS  | 2.5  |
| 3   | C     | 192  | TRP  | 2.5  |
| 1   | A     | 171  | GLN  | 2.5  |
| 1   | A     | 510  | GLN  | 2.5  |
| 2   | B     | 241  | ARG  | 2.5  |
| 11  | K     | 64   | GLU  | 2.5  |
| 2   | B     | 449  | ASN  | 2.5  |
| 5   | E     | 131  | THR  | 2.5  |
| 1   | A     | 920  | LEU  | 2.5  |
| 8   | H     | 85   | GLY  | 2.5  |
| 1   | A     | 611  | GLN  | 2.5  |
| 2   | B     | 319  | GLU  | 2.5  |
| 2   | B     | 608  | ASP  | 2.5  |
| 2   | B     | 822  | ASN  | 2.5  |
| 2   | B     | 829  | CYS  | 2.5  |
| 12  | L     | 49   | LYS  | 2.5  |
| 1   | A     | 1169 | ILE  | 2.5  |
| 1   | A     | 1377 | THR  | 2.5  |
| 2   | B     | 1077 | THR  | 2.5  |
| 2   | B     | 754  | SER  | 2.5  |
| 1   | A     | 1259 | MET  | 2.5  |
| 2   | B     | 908  | GLU  | 2.5  |
| 3   | C     | 210  | GLU  | 2.5  |
| 2   | B     | 317  | CYS  | 2.5  |
| 1   | A     | 1243 | VAL  | 2.5  |
| 8   | H     | 57   | VAL  | 2.5  |
| 1   | A     | 786  | HIS  | 2.5  |
| 1   | A     | 277  | GLU  | 2.5  |
| 1   | A     | 1417 | GLU  | 2.5  |
| 2   | B     | 28   | GLU  | 2.5  |
| 1   | A     | 1435 | PRO  | 2.5  |
| 6   | F     | 155  | LEU  | 2.5  |
| 2   | B     | 432  | MET  | 2.5  |
| 9   | I     | 108  | HIS  | 2.5  |
| 5   | E     | 106  | GLN  | 2.5  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 1          | A            | 912        | LEU         | 2.5         |
| 2          | B            | 576        | ASP         | 2.5         |
| 5          | E            | 29         | PHE         | 2.5         |
| 1          | A            | 1333       | ILE         | 2.5         |
| 2          | B            | 605        | ARG         | 2.5         |
| 2          | B            | 599        | THR         | 2.5         |
| 1          | A            | 1404       | GLU         | 2.5         |
| 2          | B            | 431        | TYR         | 2.5         |
| 11         | K            | 14         | GLU         | 2.5         |
| 9          | I            | 70         | ARG         | 2.5         |
| 6          | F            | 112        | GLU         | 2.4         |
| 1          | A            | 949        | ASP         | 2.4         |
| 1          | A            | 399        | HIS         | 2.4         |
| 1          | A            | 220        | THR         | 2.4         |
| 12         | L            | 61         | THR         | 2.4         |
| 1          | A            | 1136       | SER         | 2.4         |
| 2          | B            | 265        | SER         | 2.4         |
| 9          | I            | 120        | GLN         | 2.4         |
| 12         | L            | 41         | SER         | 2.4         |
| 1          | A            | 1223       | ASP         | 2.4         |
| 1          | A            | 1003       | LYS         | 2.4         |
| 2          | B            | 1148       | LYS         | 2.4         |
| 3          | C            | 9          | LYS         | 2.4         |
| 2          | B            | 448        | ILE         | 2.4         |
| 2          | B            | 816        | GLU         | 2.4         |
| 5          | E            | 49         | SER         | 2.4         |
| 1          | A            | 88         | LYS         | 2.4         |
| 2          | B            | 333        | PHE         | 2.4         |
| 2          | B            | 222        | ILE         | 2.4         |
| 8          | H            | 95         | TYR         | 2.4         |
| 1          | A            | 1337       | GLU         | 2.4         |
| 2          | B            | 313        | MET         | 2.4         |
| 2          | B            | 1067       | ARG         | 2.4         |
| 2          | B            | 1183       | LYS         | 2.4         |
| 9          | I            | 105        | SER         | 2.4         |
| 9          | I            | 7          | CYS         | 2.4         |
| 1          | A            | 42         | ASP         | 2.4         |
| 9          | I            | 44         | TYR         | 2.4         |
| 12         | L            | 29         | TYR         | 2.4         |
| 9          | I            | 73         | ARG         | 2.4         |
| 1          | A            | 24         | PRO         | 2.4         |
| 1          | A            | 330        | LYS         | 2.4         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 1151 | GLU  | 2.4  |
| 2   | B     | 296  | GLU  | 2.4  |
| 9   | I     | 67   | THR  | 2.4  |
| 8   | H     | 18   | GLY  | 2.4  |
| 1   | A     | 776  | ALA  | 2.4  |
| 1   | A     | 344  | ARG  | 2.4  |
| 1   | A     | 852  | TYR  | 2.4  |
| 2   | B     | 983  | ARG  | 2.4  |
| 1   | A     | 129  | LYS  | 2.4  |
| 1   | A     | 323  | LYS  | 2.4  |
| 2   | B     | 221  | ASN  | 2.4  |
| 1   | A     | 20   | GLY  | 2.4  |
| 9   | I     | 32   | CYS  | 2.4  |
| 2   | B     | 94   | LYS  | 2.4  |
| 2   | B     | 345  | LYS  | 2.4  |
| 10  | J     | 63   | TYR  | 2.4  |
| 1   | A     | 908  | LEU  | 2.4  |
| 1   | A     | 1122 | PRO  | 2.3  |
| 6   | F     | 106  | PRO  | 2.3  |
| 1   | A     | 149  | GLU  | 2.3  |
| 1   | A     | 206  | GLU  | 2.3  |
| 1   | A     | 628  | GLY  | 2.3  |
| 2   | B     | 216  | GLU  | 2.3  |
| 3   | C     | 52   | GLU  | 2.3  |
| 2   | B     | 777  | ALA  | 2.3  |
| 8   | H     | 107  | VAL  | 2.3  |
| 2   | B     | 553  | PRO  | 2.3  |
| 1   | A     | 360  | GLU  | 2.3  |
| 1   | A     | 801  | GLU  | 2.3  |
| 2   | B     | 263  | GLY  | 2.3  |
| 1   | A     | 1175 | SER  | 2.3  |
| 9   | I     | 13   | MET  | 2.3  |
| 2   | B     | 1049 | ASP  | 2.3  |
| 1   | A     | 660  | ASN  | 2.3  |
| 2   | B     | 172  | ILE  | 2.3  |
| 5   | E     | 199  | ILE  | 2.3  |
| 1   | A     | 1303 | GLU  | 2.3  |
| 1   | A     | 34   | LYS  | 2.3  |
| 1   | A     | 1160 | SER  | 2.3  |
| 2   | B     | 101  | MET  | 2.3  |
| 1   | A     | 287  | HIS  | 2.3  |
| 2   | B     | 1156 | ASP  | 2.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 2   | B     | 70   | ILE  | 2.3  |
| 2   | B     | 1084 | GLN  | 2.3  |
| 8   | H     | 137  | GLN  | 2.3  |
| 8   | H     | 140  | ALA  | 2.3  |
| 1   | A     | 293  | GLU  | 2.3  |
| 1   | A     | 394  | ASN  | 2.3  |
| 1   | A     | 1203 | ASN  | 2.3  |
| 2   | B     | 393  | LYS  | 2.3  |
| 2   | B     | 422  | LYS  | 2.3  |
| 1   | A     | 428  | TYR  | 2.3  |
| 1   | A     | 624  | SER  | 2.3  |
| 1   | A     | 1387 | HIS  | 2.3  |
| 1   | A     | 1027 | ALA  | 2.3  |
| 2   | B     | 752  | ALA  | 2.3  |
| 1   | A     | 768  | GLN  | 2.3  |
| 1   | A     | 1005 | GLU  | 2.3  |
| 1   | A     | 1452 | LYS  | 2.3  |
| 5   | E     | 152  | LYS  | 2.3  |
| 2   | B     | 512  | ARG  | 2.3  |
| 2   | B     | 786  | ASN  | 2.3  |
| 2   | B     | 1187 | ASN  | 2.3  |
| 5   | E     | 162  | ARG  | 2.3  |
| 9   | I     | 24   | ARG  | 2.3  |
| 2   | B     | 1221 | SER  | 2.3  |
| 9   | I     | 46   | HIS  | 2.3  |
| 9   | I     | 94   | ASP  | 2.3  |
| 12  | L     | 43   | THR  | 2.3  |
| 2   | B     | 276  | ILE  | 2.3  |
| 1   | A     | 153  | PRO  | 2.3  |
| 2   | B     | 260  | GLY  | 2.3  |
| 9   | I     | 25   | LEU  | 2.3  |
| 3   | C     | 60   | ASP  | 2.3  |
| 9   | I     | 109  | ILE  | 2.2  |
| 2   | B     | 520  | GLY  | 2.2  |
| 8   | H     | 51   | ALA  | 2.2  |
| 1   | A     | 1407 | GLU  | 2.2  |
| 2   | B     | 513  | GLN  | 2.2  |
| 3   | C     | 195  | GLN  | 2.2  |
| 1   | A     | 46   | THR  | 2.2  |
| 1   | A     | 98   | LYS  | 2.2  |
| 2   | B     | 1057 | LYS  | 2.2  |
| 2   | B     | 424  | LEU  | 2.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 5   | E     | 129  | PRO  | 2.2  |
| 1   | A     | 459  | ARG  | 2.2  |
| 3   | C     | 122  | SER  | 2.2  |
| 2   | B     | 56   | ASP  | 2.2  |
| 2   | B     | 346  | GLU  | 2.2  |
| 3   | C     | 116  | LYS  | 2.2  |
| 1   | A     | 1199 | ARG  | 2.2  |
| 1   | A     | 55   | ASP  | 2.2  |
| 1   | A     | 1119 | TYR  | 2.2  |
| 2   | B     | 61   | ASP  | 2.2  |
| 2   | B     | 320  | ASP  | 2.2  |
| 1   | A     | 165  | GLY  | 2.2  |
| 1   | A     | 1302 | PRO  | 2.2  |
| 3   | C     | 125  | MET  | 2.2  |
| 6   | F     | 122  | MET  | 2.2  |
| 1   | A     | 906  | HIS  | 2.2  |
| 2   | B     | 1062 | HIS  | 2.2  |
| 1   | A     | 45   | GLN  | 2.2  |
| 1   | A     | 1290 | LYS  | 2.2  |
| 2   | B     | 836  | GLU  | 2.2  |
| 2   | B     | 1132 | GLU  | 2.2  |
| 5   | E     | 67   | GLU  | 2.2  |
| 9   | I     | 42   | LEU  | 2.2  |
| 9   | I     | 17   | ARG  | 2.2  |
| 2   | B     | 447  | ALA  | 2.2  |
| 2   | B     | 715  | ALA  | 2.2  |
| 3   | C     | 132  | PRO  | 2.2  |
| 2   | B     | 268  | THR  | 2.2  |
| 2   | B     | 415  | GLN  | 2.2  |
| 10  | J     | 58   | GLU  | 2.2  |
| 1   | A     | 393  | ARG  | 2.2  |
| 6   | F     | 110  | ASP  | 2.2  |
| 8   | H     | 7    | ASP  | 2.2  |
| 11  | K     | 30   | ALA  | 2.2  |
| 2   | B     | 870  | ILE  | 2.2  |
| 9   | I     | 93   | LYS  | 2.2  |
| 8   | H     | 2    | SER  | 2.2  |
| 2   | B     | 705  | MET  | 2.2  |
| 2   | B     | 884  | ARG  | 2.2  |
| 12  | L     | 47   | ARG  | 2.2  |
| 1   | A     | 661  | GLY  | 2.1  |
| 1   | A     | 514  | PRO  | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 2   | B     | 409  | ALA  | 2.1  |
| 2   | B     | 611  | PRO  | 2.1  |
| 3   | C     | 19   | ASP  | 2.1  |
| 8   | H     | 92   | ASP  | 2.1  |
| 1   | A     | 1174 | PHE  | 2.1  |
| 2   | B     | 781  | PHE  | 2.1  |
| 1   | A     | 996  | ASN  | 2.1  |
| 8   | H     | 135  | LEU  | 2.1  |
| 11  | K     | 89   | ASN  | 2.1  |
| 2   | B     | 400  | HIS  | 2.1  |
| 2   | B     | 264  | SER  | 2.1  |
| 3   | C     | 127  | ARG  | 2.1  |
| 5   | E     | 11   | ARG  | 2.1  |
| 8   | H     | 35   | GLN  | 2.1  |
| 10  | J     | 62   | ARG  | 2.1  |
| 3   | C     | 12   | GLU  | 2.1  |
| 2   | B     | 888  | GLY  | 2.1  |
| 3   | C     | 86   | CYS  | 2.1  |
| 1   | A     | 386  | ASP  | 2.1  |
| 1   | A     | 526  | ASP  | 2.1  |
| 1   | A     | 785  | PRO  | 2.1  |
| 2   | B     | 407  | ASP  | 2.1  |
| 1   | A     | 582  | ILE  | 2.1  |
| 1   | A     | 644  | LYS  | 2.1  |
| 2   | B     | 25   | ILE  | 2.1  |
| 1   | A     | 306  | ASN  | 2.1  |
| 2   | B     | 465  | ASN  | 2.1  |
| 2   | B     | 733  | HIS  | 2.1  |
| 2   | B     | 252  | SER  | 2.1  |
| 5   | E     | 126  | SER  | 2.1  |
| 12  | L     | 54   | ARG  | 2.1  |
| 1   | A     | 995  | GLU  | 2.1  |
| 9   | I     | 53   | GLY  | 2.1  |
| 2   | B     | 729  | ILE  | 2.1  |
| 9   | I     | 61   | ASP  | 2.1  |
| 1   | A     | 57   | ARG  | 2.1  |
| 1   | A     | 1267 | MET  | 2.1  |
| 5   | E     | 207  | ARG  | 2.1  |
| 6   | F     | 84   | TYR  | 2.1  |
| 1   | A     | 355  | GLY  | 2.1  |
| 9   | I     | 60   | GLN  | 2.1  |
| 1   | A     | 1280 | GLU  | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 6   | F     | 131  | PRO  | 2.1  |
| 9   | I     | 10   | CYS  | 2.1  |
| 2   | B     | 935  | ARG  | 2.1  |
| 5   | E     | 50   | MET  | 2.1  |
| 5   | E     | 192  | ARG  | 2.1  |
| 8   | H     | 123  | MET  | 2.1  |
| 11  | K     | 29   | ASN  | 2.1  |
| 3   | C     | 102  | GLN  | 2.1  |
| 2   | B     | 116  | GLU  | 2.1  |
| 12  | L     | 57   | LEU  | 2.1  |
| 1   | A     | 1442 | ASP  | 2.1  |
| 2   | B     | 1186 | ASP  | 2.1  |
| 6   | F     | 136  | ARG  | 2.1  |
| 1   | A     | 575  | LYS  | 2.1  |
| 1   | A     | 1081 | LEU  | 2.1  |
| 5   | E     | 44   | ALA  | 2.1  |
| 1   | A     | 26   | GLU  | 2.1  |
| 1   | A     | 486  | GLU  | 2.1  |
| 1   | A     | 639  | PRO  | 2.1  |
| 2   | B     | 183  | GLU  | 2.1  |
| 2   | B     | 33   | VAL  | 2.1  |
| 2   | B     | 373  | ARG  | 2.1  |
| 3   | C     | 185  | LYS  | 2.1  |
| 1   | A     | 292  | ALA  | 2.1  |
| 1   | A     | 772  | GLY  | 2.1  |
| 1   | A     | 1108 | ALA  | 2.1  |
| 2   | B     | 851  | PHE  | 2.1  |
| 12  | L     | 52   | GLY  | 2.1  |
| 1   | A     | 237  | THR  | 2.1  |
| 1   | A     | 1405 | THR  | 2.1  |
| 1   | A     | 226  | GLU  | 2.1  |
| 2   | B     | 665  | GLU  | 2.1  |
| 3   | C     | 83   | SER  | 2.1  |
| 5   | E     | 203  | GLU  | 2.1  |
| 8   | H     | 80   | ARG  | 2.0  |
| 1   | A     | 112  | LYS  | 2.0  |
| 6   | F     | 72   | LYS  | 2.0  |
| 9   | I     | 20   | LYS  | 2.0  |
| 1   | A     | 555  | ASP  | 2.0  |
| 1   | A     | 727  | ASP  | 2.0  |
| 12  | L     | 25   | ALA  | 2.0  |
| 1   | A     | 1222 | ASN  | 2.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 2   | B     | 194  | GLU  | 2.0  |
| 2   | B     | 1004 | GLU  | 2.0  |
| 3   | C     | 152  | GLU  | 2.0  |
| 1   | A     | 1391 | ARG  | 2.0  |
| 8   | H     | 124  | ARG  | 2.0  |
| 9   | I     | 45   | ARG  | 2.0  |
| 2   | B     | 1087 | PHE  | 2.0  |
| 2   | B     | 279  | ASP  | 2.0  |
| 2   | B     | 1101 | ASP  | 2.0  |
| 1   | A     | 994  | GLN  | 2.0  |
| 1   | A     | 1304 | TRP  | 2.0  |
| 1   | A     | 797  | LYS  | 2.0  |
| 1   | A     | 1112 | LYS  | 2.0  |
| 2   | B     | 953  | LEU  | 2.0  |
| 1   | A     | 1154 | TYR  | 2.0  |
| 1   | A     | 1002 | GLY  | 2.0  |
| 1   | A     | 1123 | GLY  | 2.0  |
| 1   | A     | 1321 | GLY  | 2.0  |
| 1   | A     | 144  | THR  | 2.0  |
| 1   | A     | 795  | GLU  | 2.0  |
| 2   | B     | 1185 | CYS  | 2.0  |
| 2   | B     | 1216 | LEU  | 2.0  |
| 1   | A     | 275  | SER  | 2.0  |
| 1   | A     | 466  | SER  | 2.0  |
| 2   | B     | 45   | SER  | 2.0  |

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

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

## 6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 6.4 Ligands ⓘ

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

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 13  | ZN   | I     | 203  | 1/1   | 0.90 | 0.09 | 172,172,172,172             | 0     |
| 13  | ZN   | A     | 1735 | 1/1   | 0.94 | 0.14 | 172,172,172,172             | 0     |
| 13  | ZN   | I     | 204  | 1/1   | 0.96 | 0.05 | 172,172,172,172             | 0     |
| 13  | ZN   | J     | 101  | 1/1   | 0.96 | 0.07 | 172,172,172,172             | 0     |
| 13  | ZN   | B     | 1307 | 1/1   | 0.97 | 0.07 | 172,172,172,172             | 0     |
| 13  | ZN   | A     | 1734 | 1/1   | 0.98 | 0.05 | 172,172,172,172             | 0     |
| 13  | ZN   | C     | 319  | 1/1   | 0.99 | 0.10 | 172,172,172,172             | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.