



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:19 AM GMT

PDB ID : 3DXJ
Title : Crystal structure of thermus thermophilus rna polymerase holoenzyme in complex with the antibiotic myxopyronin
Authors : Das, K.; Arnold, E.
Deposited on : 2008-07-24
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

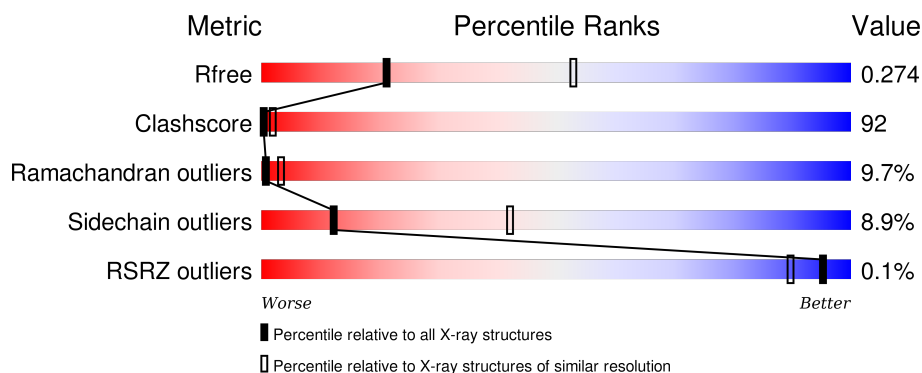
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



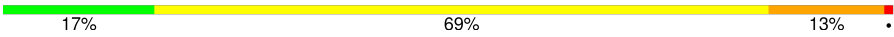
| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 91344 | 1578 (3.00-3.00) |
| Clashscore | 102246 | 1912 (3.00-3.00) |
| Ramachandran outliers | 100387 | 1853 (3.00-3.00) |
| Sidechain outliers | 100360 | 1856 (3.00-3.00) |
| RSRZ outliers | 91569 | 1592 (3.00-3.00) |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 315 | |
| 1 | B | 315 | |
| 1 | K | 315 | |
| 1 | L | 315 | |
| 2 | C | 1119 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 2 | M | 1119 |  |
| 3 | D | 1524 |  |
| 3 | N | 1524 |  |
| 4 | E | 99 |  |
| 4 | O | 99 |  |
| 5 | F | 423 |  |
| 5 | P | 423 |  |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 8 | ZN | D | 1525 | - | - | - | X |
| 8 | ZN | D | 1526 | - | - | - | X |
| 8 | ZN | N | 1525 | - | - | - | X |
| 9 | NE6 | D | 1529 | X | - | - | - |
| 9 | NE6 | N | 1528 | X | - | - | X |

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 56149 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha; CHAIN A, B, K, L.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1 | A | 231 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1816 | 1159 | 315 | 339 | 3 | | | |
| 1 | B | 243 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1902 | 1212 | 328 | 359 | 3 | | | |
| 1 | K | 231 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1816 | 1159 | 315 | 339 | 3 | | | |
| 1 | L | 243 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1902 | 1212 | 328 | 359 | 3 | | | |

- Molecule 2 is a protein called BACTERIAL RNA POLYMERASE BETA SUBUNIT; CHAIN C, M.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 2 | C | 1119 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 8829 | 5581 | 1577 | 1647 | 24 | | | |
| 2 | M | 1119 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 8829 | 5581 | 1577 | 1647 | 24 | | | |

- Molecule 3 is a protein called BACTERIAL RNA POLYMERASE BETA-PRIME SUBUNIT; CHAIN D, N.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 3 | D | 1504 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 11864 | 7518 | 2091 | 2219 | 36 | | | |
| 3 | N | 1504 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 11864 | 7518 | 2091 | 2219 | 36 | | | |

- Molecule 4 is a protein called BACTERIAL RNA POLYMERASE OMEGA SUBUNIT; CHAIN E, O.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4 | E | 95 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 769 | 488 | 133 | 144 | 4 | | | |
| 4 | O | 95 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 769 | 488 | 133 | 144 | 4 | | | |

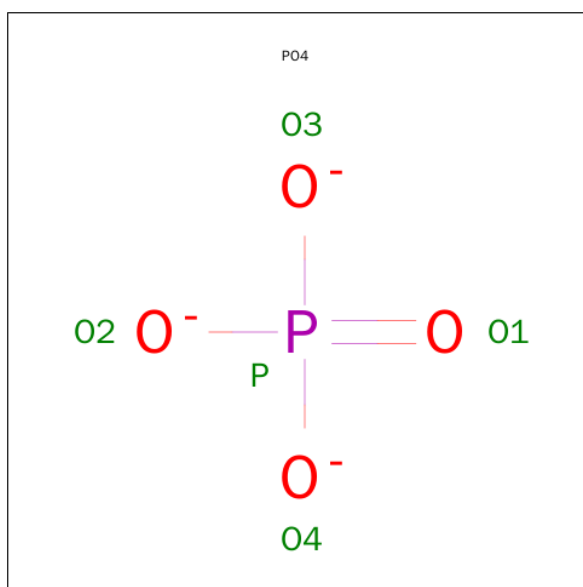
There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------|------------|
| E | 61 | GLU | VAL | VARIANT | UNP Q8RQE7 |
| E | 92 | ILE | LEU | VARIANT | UNP Q8RQE7 |
| E | 95 | GLY | VAL | VARIANT | UNP Q8RQE7 |
| O | 61 | GLU | VAL | VARIANT | UNP Q8RQE7 |
| O | 92 | ILE | LEU | VARIANT | UNP Q8RQE7 |
| O | 95 | GLY | VAL | VARIANT | UNP Q8RQE7 |

- Molecule 5 is a protein called RNA polymerase principal sigma factor (RpoD); CHAIN F, P.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5 | F | 349 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2829 | 1785 | 513 | 527 | 4 | | | |
| 5 | P | 349 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2829 | 1785 | 513 | 527 | 4 | | | |

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 6 | A | 1 | Total O P 5 4 1 | 0 | 0 |
| 6 | D | 1 | Total O P 5 4 1 | 0 | 0 |

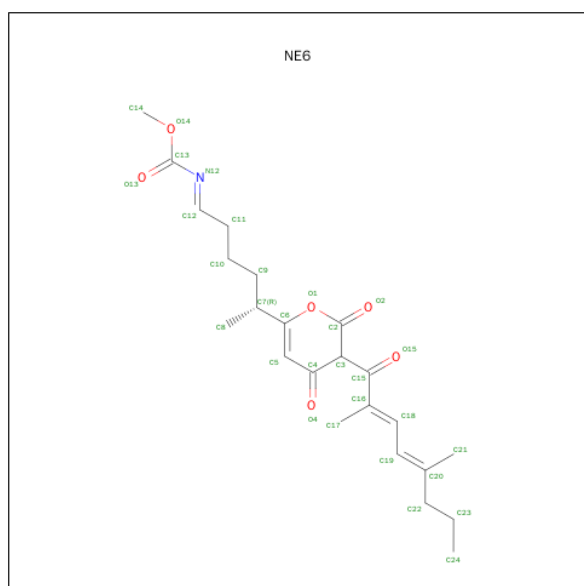
- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 7 | B | 1 | Total Mg 1 1 | 0 | 0 |
| 7 | D | 1 | Total Mg 1 1 | 0 | 0 |
| 7 | N | 1 | Total Mg 1 1 | 0 | 0 |

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

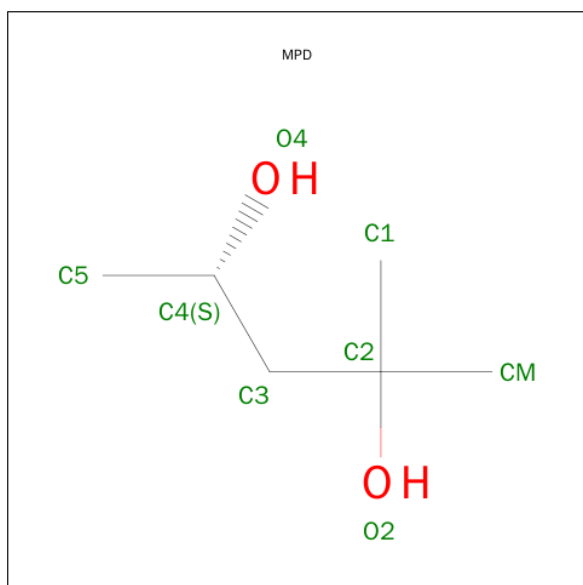
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 8 | D | 2 | Total Zn 2 2 | 0 | 0 |
| 8 | N | 2 | Total Zn 2 2 | 0 | 0 |

- Molecule 9 is METHYL [(1E,5R)-5-{(3S)-3-[(2E,4E)-2,5-DIMETHYLOCTA-2,4-DIENOYL]-2,4-DIOXO-3,4-DIHYDRO-2H-PYRAN-6-YL}HEXYLIDENE]CARBAMATE (three-letter code: NE6) (formula: C₂₃H₃₁NO₆).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 9 | D | 1 | Total | C | N | O | 0 | 0 |
| | | | 30 | 23 | 1 | 6 | | |
| 9 | N | 1 | Total | C | N | O | 0 | 0 |
| | | | 30 | 23 | 1 | 6 | | |

- Molecule 10 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 10 | C | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 10 | C | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 10 | M | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |

- Molecule 11 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 11 | A | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 11 | B | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 11 | C | 7 | Total | O | 0 | 0 |
| | | | 7 | 7 | | |
| 11 | D | 10 | Total | O | 0 | 0 |
| | | | 10 | 10 | | |

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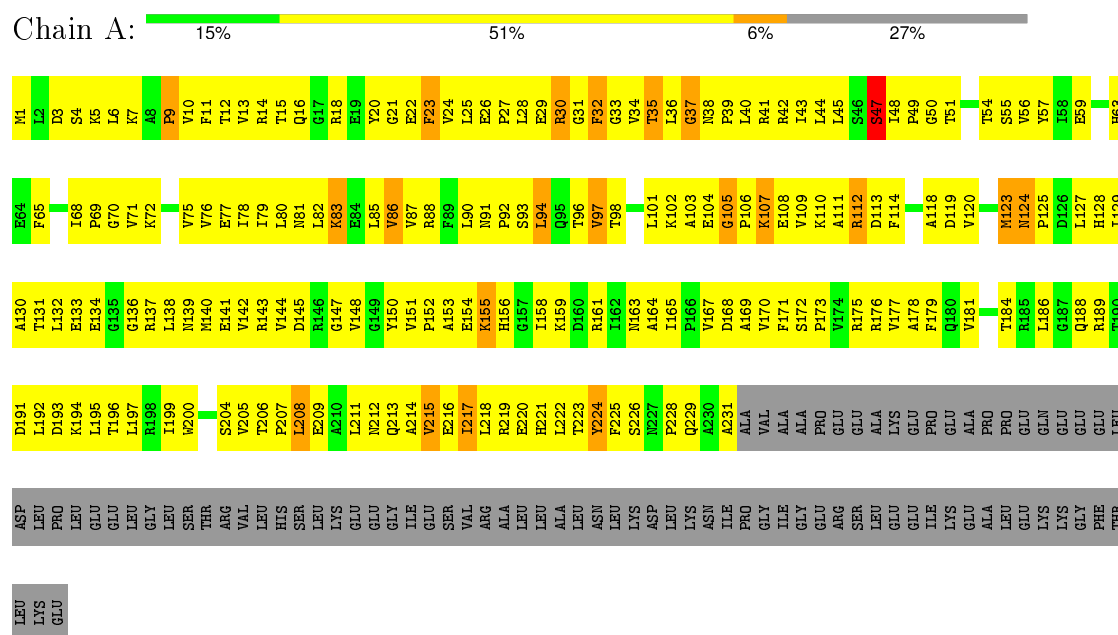
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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|
| 11 | F | 1 | Total 1 | O 1 | 0 | 0 |
| 11 | M | 5 | Total 5 | O 5 | 0 | 0 |
| 11 | N | 4 | Total 4 | O 4 | 0 | 0 |
| 11 | O | 1 | Total 1 | O 1 | 0 | 0 |

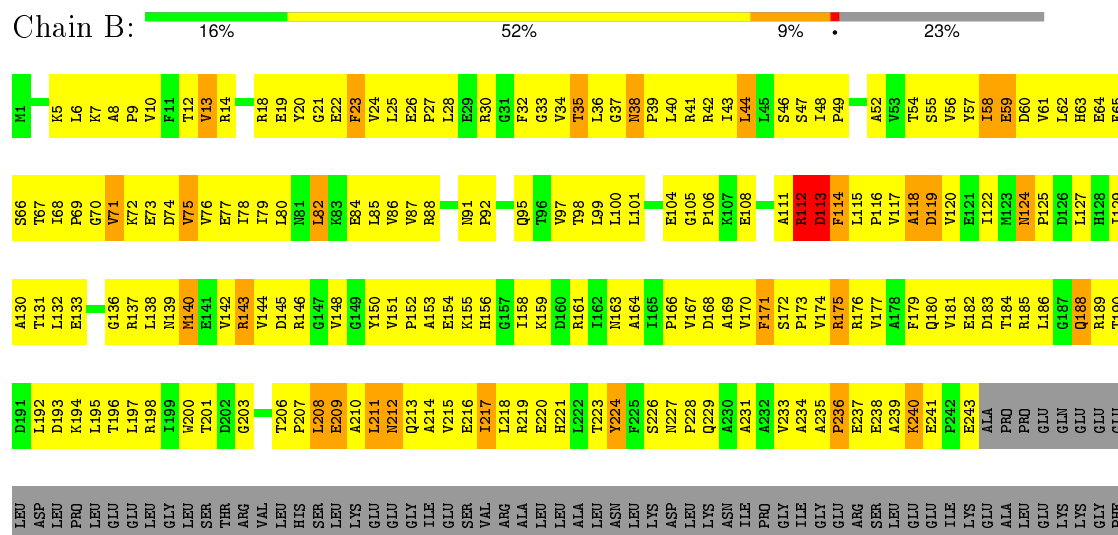
3 Residue-property plots

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

- Molecule 1: DNA-directed RNA polymerase subunit alpha; CHAIN A, B, K, L

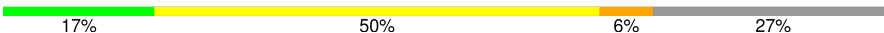


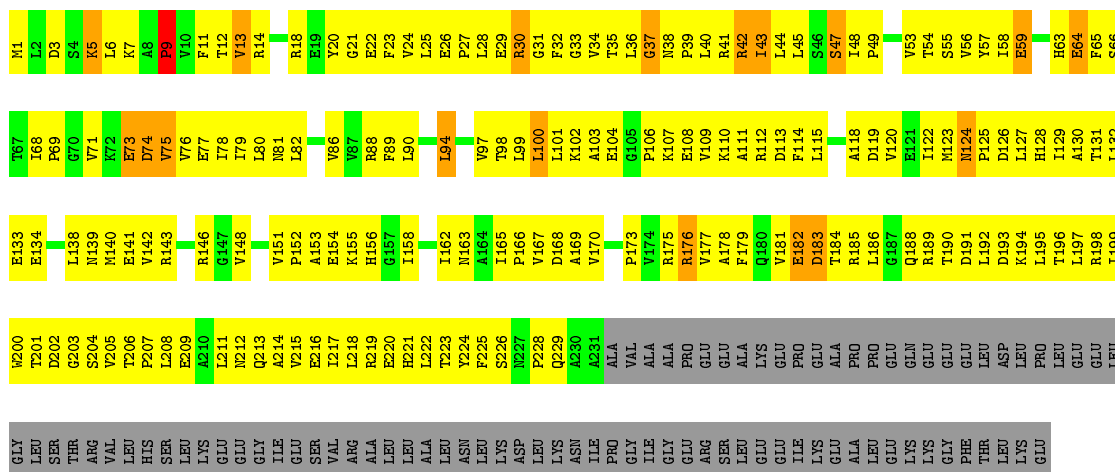
- Molecule 1: DNA-directed RNA polymerase subunit alpha; CHAIN A, B, K, L



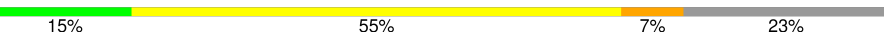
THR
LEU
LYS
GLU

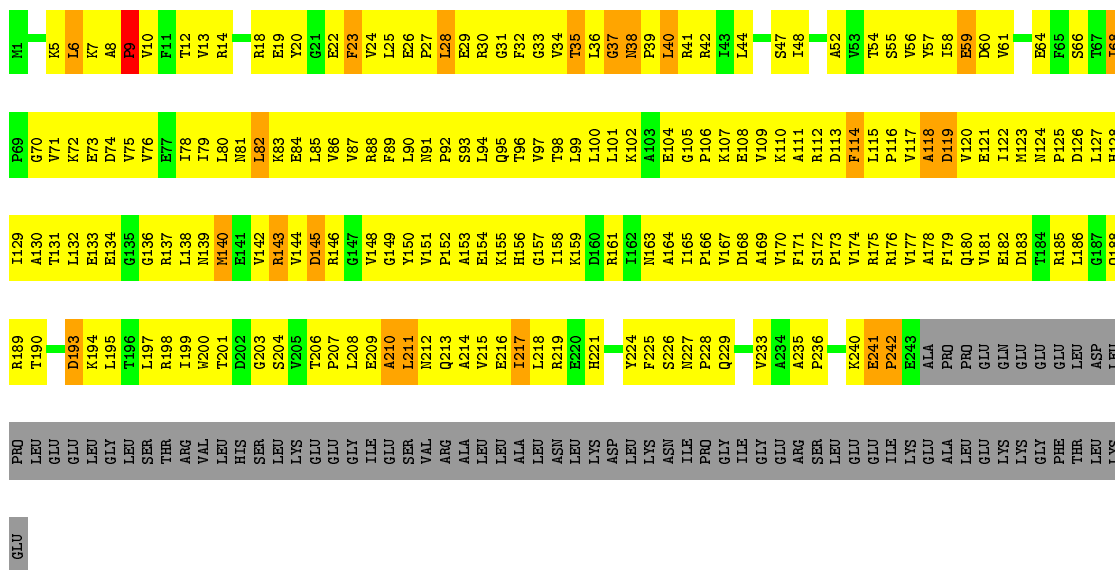
- Molecule 1: DNA-directed RNA polymerase subunit alpha; CHAIN A, B, K, L

Chain K: 



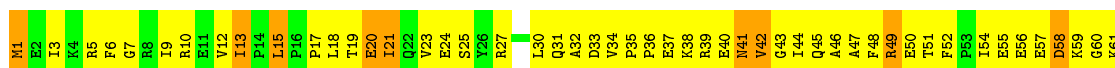
- Molecule 1: DNA-directed RNA polymerase subunit alpha; CHAIN A, B, K, L

Chain L: 



- Molecule 2: BACTERIAL RNA POLYMERASE BETA SUBUNIT; CHAIN C, M

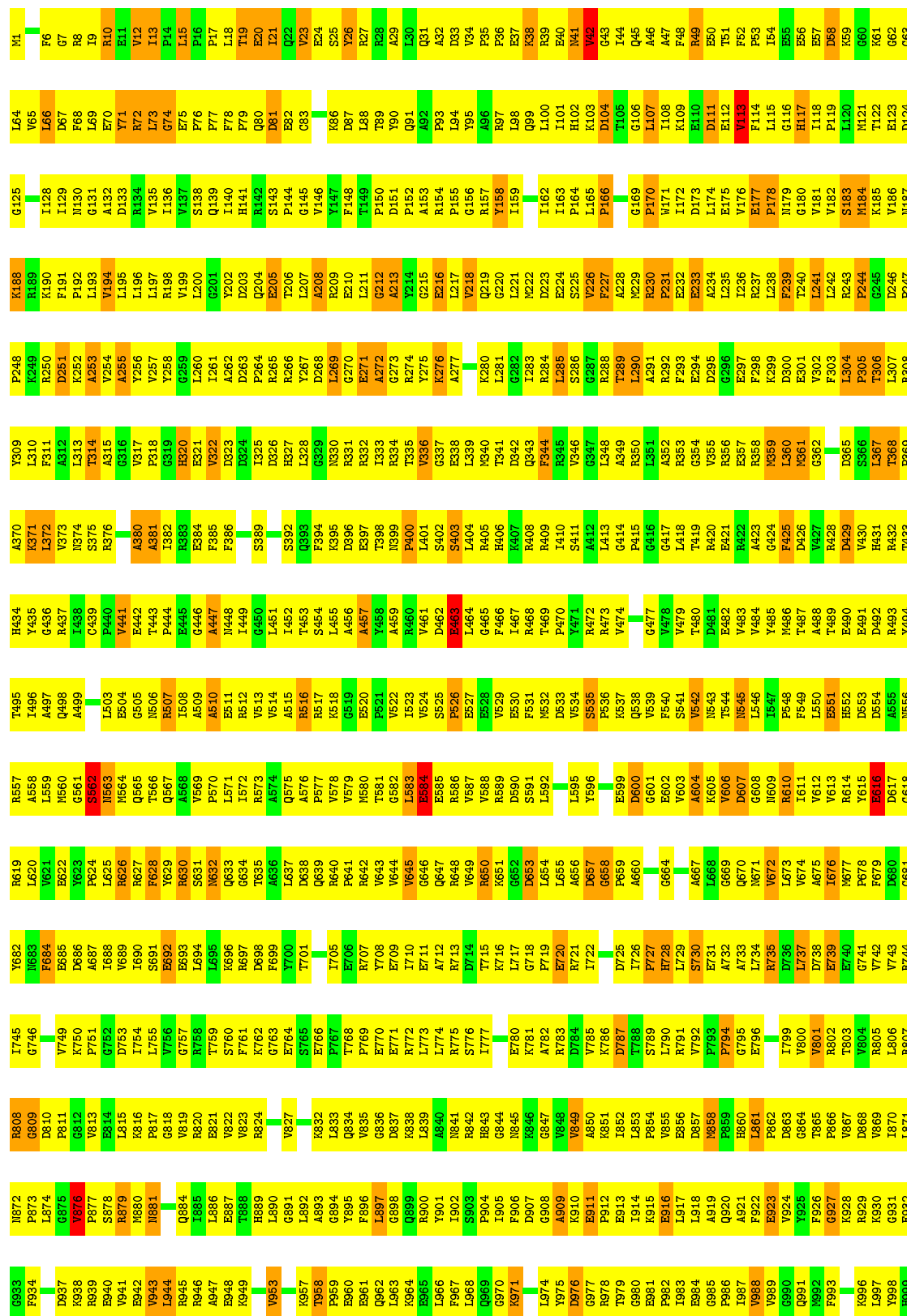
Chain C: 



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| H1064 | K938 | V1001 | H1066 | K939 | E1002 | H1065 | K937 | V1002 | H1067 | K938 | V1003 | H1068 | K939 | E1004 | H1069 | K940 | V1005 | H1070 | K941 | E1006 | H1071 | K942 | V1007 | H1072 | K943 | E1008 | H1073 | K944 | V1009 | H1074 | K945 | E1009 | H1075 | K946 | V1010 | H1076 | K947 | E1011 | H1077 | K948 | V1012 | H1078 | K949 | E1013 | H1079 | K950 | V1014 | H1080 | K951 | E1015 | H1081 | K952 | V1016 | H1082 | K953 | E1017 | H1083 | K954 | V1018 | H1084 | K955 | E1019 | H1085 | K956 | V1020 | H1086 | K957 | E1021 | H1087 | K958 | V1022 | H1088 | K959 | E1023 | H1089 | K960 | V1024 | H1090 | K961 | E1025 | H1091 | K962 | V1026 | H1092 | K963 | E1027 | H1093 | K964 | V1028 | H1094 | K965 | E1029 | H1095 | K966 | V1030 | H1096 | K967 | E1031 | H1097 | K968 | V1032 | H1098 | K969 | E1033 | H1099 | K970 | V1034 | H1100 | K971 | E1035 | H1101 | K972 | V1036 | H1102 | K973 | E1037 | H1103 | K974 | V1038 | H1104 | K975 | E1039 | H1105 | K976 | V1040 | H1106 | K977 | E1041 | H1107 | K978 | V1042 | H1108 | K979 | E1043 | H1109 | K980 | V1044 | H1110 | K981 | E1045 | H1111 | K982 | V1046 | H1112 | K983 | E1047 | H1113 | K984 | V1048 | H1114 | K985 | E1049 | H1115 | K986 | V1050 | H1116 | K987 | E1051 | H1117 | K988 | V1052 | H1118 | K989 | E1053 | H1119 | K990 | V1054 | H1120 | K991 | E1055 | H1121 | K992 | V1056 | H1122 | K993 | E1057 | H1123 | K994 | V1058 | H1124 | K995 | E1059 | H1125 | K996 | V1060 | H1126 | K997 | E1061 | H1127 | K998 | V1062 | H1128 | K999 | E1063 | H1129 | K1000 | V1064 | H1130 | K1001 | E1065 | H1131 | K1002 | V1066 | K1003 | E1067 | H1132 | K1004 | E1068 | H1133 | K1005 | V1069 | H1134 | K1006 | E1069 | H1135 | K1007 | E1070 | H1136 | K1008 | E1071 | H1137 | K1009 | E1072 | H1138 | K1010 | E1073 | H1139 | K1011 | E1074 | H1140 | K1012 | E1075 | H1141 | K1013 | E1076 | H1142 | K1014 | E1077 | H1143 | K1015 | E1078 | H1144 | K1016 | E1079 | H1145 | K1017 | E1080 | H1146 | K1018 | E1081 | H1147 | K1019 | E1082 | H1148 | K1020 | E1083 | H1149 | K1021 | E1084 | H1150 | K1022 | E1085 | H1151 | K1023 | E1086 | H1152 | K1024 | E1087 | H1153 | K1025 | E1088 | H1154 | K1026 | E1089 | H1155 | K1027 | E1090 | H1156 | K1028 | E1091 | H1157 | K1029 | E1092 | H1158 | K1030 | E1093 | H1159 | K1031 | E1094 | H1160 | K1032 | E1095 | H1161 | K1033 | E1096 | H1162 | K1034 | E1097 | H1163 | K1035 | E1098 | H1164 | K1036 | E1099 | H1165 | K1037 | E1100 | H1166 | K1038 | E1101 | H1167 | K1039 | E1102 | H1168 | K1040 | E1103 | H1169 | K1041 | E1104 | H1170 | K1042 | E1105 | H1171 | K1043 | E1106 | H1172 | K1044 | E1107 | H1173 | K1045 | E1108 | H1174 | K1046 | E1109 | H1175 | K1047 | E1110 | H1176 | K1048 | E1111 | H1177 | K1049 | E1112 | H1178 | K1050 | E1113 | H1179 | K1051 | E1114 | H1180 | K1052 | E1115 | H1181 | K1053 | E1116 | H1182 | K1054 | E1117 | H1183 | K1055 | E1118 | H1184 | K1056 | E1119 | H1185 | K1057 | E1120 | H1186 | K1058 | E1121 | H1187 | K1059 | E1122 | H1188 | K1060 | E1123 | H1189 | K1061 | E1124 | H1190 | K1062 | E1125 | H1191 | K1063 | E1126 | H1192 | K1064 | E1127 | H1193 | K1065 | E1128 | H1194 | K1066 | E1129 | H1195 | K1067 | E1130 | H1196 | K1068 | E1131 | H1197 | K1069 | E1132 | H1198 | K1070 | E1133 | H1199 | K1071 | E1134 | H1200 | K1072 | E1135 | H1201 | K1073 | E1136 | H1202 | K1074 | E1137 | H1203 | K1075 | E1138 | H1204 | K1076 | E1139 | H1205 | K1077 | E1140 | H1206 | K1078 | E1141 | H1207 | K1079 | E1142 | H1208 | K1080 | E1143 | H1209 | K1081 | E1144 | H1210 | K1082 | E1145 | H1211 | K1083 | E1146 | H1212 | K1084 | E1147 | H1213 | K1085 | E1148 | H1214 | K1086 | E1149 | H1215 | K1087 | E1150 | H1216 | K1088 | E1151 | H1217 | K1089 | E1152 | H1218 | K1090 | E1153 | H1219 | K1091 | E1154 | H1220 | K1092 | E1155 | H1221 | K1093 | E1156 | H1222 | K1094 | E1157 | H1223 | K1095 | E1158 | H1224 | K1096 | E1159 | H1225 | K1097 | E1160 | H1226 | K1098 | E1161 | H1227 | K1099 | E1162 | H1228 | K1100 | E1163 | H1229 | K1101 | E1164 | H1230 | K1102 | E1165 | H1231 | K1103 | E1166 | H1232 | K1104 | E1167 | H1233 | K1105 | E1168 | H1234 | K1106 | E1169 | H1235 | K1107 | E1170 | H1236 | K1108 | E1171 | H1237 | K1109 | E1172 | H1238 | K1110 | E1173 | H1239 | K1111 | E1174 | H1240 | K1112 | E1175 | H1241 | K1113 | E1176 | H1242 | K1114 | E1177 | H1243 | K1115 | E1178 | H1244 | K1116 | E1179 | H1245 | K1117 | E1180 | H1246 | K1118 | E1181 | H1247 | K1119 | E1182 | H1248 | K1120 | E1183 | H1249 | K1121 | E1184 | H1250 | K1122 | E1185 | H1251 | K1123 | E1186 | H1252 | K1124 | E1187 | H1253 | K1125 | E1188 | H1254 | K1126 | E1189 | H1255 | K1127 | E1190 | H1256 | K1128 | E1191 | H1257 | K1129 | E1192 | H1258 | K1130 | E1193 | H1259 | K1131 | E1194 | H1260 | K1132 | E1195 | H1261 | K1133 | E1196 | H1262 | K1134 | E1197 | H1263 | K1135 | E1198 | H1264 | K1136 | E1199 | H1265 | K1137 | E1200 | H1266 | K1138 | E1201 | H1267 | K1139 | E1202 | H1268 | K1140 | E1203 | H1269 | K1141 | E1204 | H1270 | K1142 | E1205 | H1271 | K1143 | E1206 | H1272 | K1144 | E1207 | H1273 | K1145 | E1208 | H1274 | K1146 | E1209 | H1275 | K1147 | E1210 | H1276 | K1148 | E1211 | H1277 | K1149 | E1212 | H1278 | K1150 | E1213 | H1279 | K1151 | E1214 | H1280 | K1152 | E1215 | H1281 | K1153 | E1216 | H1282 | K1154 | E1217 | H1283 | K1155 | E1218 | H1284 | K1156 | E1219 | H1285 | K1157 | E1220 | H1286 | K1158 | E1221 | H1287 | K1159 | E1222 | H1288 | K1160 | E1223 | H1289 | K1161 | E1224 | H1290 | K1162 | E1225 | H1291 | K1163 | E1226 | H1292 | K1164 | E1227 | H1293 | K1165 | E1228 | H1294 | K1166 | E1229 | H1295 | K1167 | E1230 | H1296 | K1168 | E1231 | H1297 | K1169 | E1232 | H1298 | K1170 | E1233 | H1299 | K1171 | E1234 | H1300 | E1235 | H1301 | E1236 | H1302 | E1237 | H1303 | E1238 | H1304 | E1239 | H1305 | E1240 | H1306 | E1241 | H1307 | E1242 | H1308 | E1243 | H1309 | E1244 | H1310 | E1245 | H1311 | E1246 | H1312 | E1247 | H1313 | E1248 | H1314 | E1249 | H1315 | E1250 | H1316 | E1251 | H1317 | E1252 | H1318 | E1253 | H1319 | E1254 | H1320 | E1255 | H1321 | E1256 | H1322 | E1257 | H1323 | E1258 | H1324 | E1259 | H1325 | E1260 | H1326 | E1261 | H1327 | E1262 | H1328 | E1263 | H1329 | E1264 | H1330 | E1265 | H1331 | E1266 | H1332 | E1267 | H1333 | E1268 | H1334 | E1269 | H1335 | E1270 | H1336 | E1271 | H1337 | E1272 | H1338 | E1273 | H1339 | E1274 | H1340 | E1275 | H1341 | E1276 | H1342 | E1277 | H1343 | E1278 | H1344 | E1279 | H1345 | E1280 | H1346 | E1281 | H1347 | E1282 | H1348 | E1283 | H1349 | E1284 | H1350 | E1285 | H1351 | E1286 | H1352 | E1287 | H1353 | E1288 | H1354 | E1289 | H1355 | E1290 | H1356 | E1291 | H1357 | E1292 | H1358 | E1293 | H1359 | E1294 | H1360 | E1295 | H1361 | E1296 | H1362 | E1297 | H1363 | E1298 | H1364 | E1299 | H1365 | E1300 | H1366 | E1301 | H1367 | E1302 | H1368 | E1303 | H1369 | E1304 | H1370 | E1305 | H1371 | E1306 | H1372 | E1307 | H1373 | E1308 | H1374 | E1309 | H1375 | E1310 | H1376 | E1311 | H1377 | E1312 | H1378 | E1313 | H1379 | E1314 | H1380 | E1315 | H1381 | E1316 | H1382 | E1317 | H1383 | E1318 | H1384 | E1319 | H1385 | E1320 | H1386 | E1321 | H1387 | E1322 | H1388 | E1323 | H1389 | E1324 | H1390 | E1325 | H1391 | E1326 | H1392 | E1327 | H1393 | E1328 | H1394 | E1329 | H1395 | E1330 | H1396 | E1331 | H1397 | E1332 | H1398 | E1333 | H1399 | E1334 | H1400 | E1335 | H1401 | E1336 | H1402 | E1337 | H1403 | E1338 | H1404 | E1339 | H1405 | E1340 | H1406 | E1341 | H1407 | E1342 | H1408 | E1343 | H1409 | E1344 | H1410 | E1345 | H1411 | E1346 | H1412 | E1347 | H1413 | E1348 | H1414 | E1349 | H1415 | E1350 | H1416 | E1351 | H1417 | E1352 | H1418 | E1353 | H1419 | E1354 | H1420 | E1355 | H1421 | E1356 | H1422 | E1357 | H1423 | E1358 | H1424 | E1359 | H1425 | E1360 | H1426 | E1361 | H1427 | E1362 | H1428 | E1363 | H1429 | E1364 | H1430 | E1365 | H1431 | E1366 | H1432 | E1367 | H1433 | E1368 | H1434 | E1369 | H1435 | E1370 | H1436 | E1371 | H1437 | E1372 | H1438 | E1373 | H1439 | E1374 | H1440 | E1375 | H1441 | E1376 | H1442 | E1377 | H1443 | E1378 | H1444 | E1379 | H1445 | E1380 | H1446 | E1381 | H1447 | E1382 | H1448 | E1383 | H1449 | E1384 | H1450 | E1385 | H1451 | E1386 | H1452 | E1387 | H1453 | E1388 | H1454 | E1389 | H1455 | E1390 | H1456 | E1391 | H1457 | E1392 | H1458 | E1393 | H1459 | E1394 | H1460 | E1395 | H1461 | E1396 | H1462 | E1397 | H1463 | E1398 | H1464 | E1399 | H1465 | E1400 | H1466 | E1401 | H1467 | E1402 | H1468 | E1403 | H1469 | E1404 | H1470 | E1405 | H1471 | E1406 | H1472 | E1407 | H1473 | E1408 | H1474 | E1409 | H1475 | E1410 | H1476 | E1411 | H1477 | E1412 | H1478 | E1413 | H1479 | E1414 | H1480 | E1415 | H1481 | E1416 | H1482 | E1417 | H1483 | E1418 | H1484 | E1419 | H1485 | E1420 | H1486 | E1421 | H1487 | E1422 | H1488 | E1423 | H1489 | E1424 | H1490 | E1425 | H1491 | E1426 | H1492 | E1427 | H1493 | E1428 | H1494 | E1429 | H1495 | E1430 | H1496 | E1431 | H1497 | E1432 | H1498 | E1433 | H1499 | E1434 | H1500 | E1435 | H1501 | E1436 | H1502 | E1437 | H1503 | E1438 | H1504 | E1439 | H1505 | E1440 | H1506 | E1441 | H1507 | E1442 | H1508 | E1443 | H1509 | E1444 | H1510 | E1445 | H1511 | E1446 | H1512 | E1447 | H1513 | E1448 | H1514 | E1449 | H1515 | E1450 | H1516 | E1451 | H1517 | E1452 | H1518 | E1453 | H1519 | E1454 | H1520 | E1455 | H1521 | E1456 | H1522 | E1457 | H1523 | E1458 | H1524 | E1459 | H1525 | E1460 | H1526 | E1461 | H1527 | E1462 | H1528 | E1463 | H1529 | E1464 | H1530 | E1465 | H1531 | E1466 | H1532 | E1467 | H1533 | E1468 | H1534 | E1469 | H1535 | E1470 | H1536 | E1471 | H1537 | E1472 | H1538 | E1473 | H1539 | E1474 | H1540 | E1475 | H1541 | E1476 | H1542 | E1477 | H1543 | E1478 | H1544 | E1479 | H1545 | E1480 | H1546 | E1481 | H1547 | E1482 | H1548 | E1483 | H1549 | E1484 | H1550 | E1485 | H1551 | E1486 | H1552 | E1487 | H1553 | E1488 | E1489 | E1490 | E1491 | E1492 | E1493 | E1494 | E1495 | E1496 | E1497 | E1498 | E1499 | E1500 | E1501 | E1502 | E1503 | E1504 | E1505 | E1506 | E1507 | E1508 | E1509 | E1510 | E1511 | E1512 | E1513 | E1514 | E1515 | E1516 | E1517 | E1518 | E1519 | E1520 | E1521 | E1522 | E1523 | E1524 | E1525 | E1526 | E1527 | E1528 | E1529 | E1530 | E1531 | E1532 | E1533 | E1534 | E1535 | E1536 | E1537 | E1538 | E1539 | E1540 | E1541 | E1542 | E1543 | E1544 | E1545 | E1546 | E1547 | E1548 | E1549 | E1550 | E1551 | E1552 | E1553 | E1554 | E1555 | E1556 | E1557 | E1558 | E1559 | E1560 | E1561 | E1562 | E1563 | E1564 | E1565 | E1566 | E1567 | E1568 | E1569 | E1570 | E1571 | E1572 | E1573 | E1574 | E1575 | E1576 | E1577 | E1578 | E1579 | E1580 | E1581 | E1582 | E1583 | E1584 | E1585 | E1586 | E1587 | E1588 | E1589 | E1590 | E1591 | E1592 | E1593 | E1594 | E1595 | E1596 | E1597 | E1598 | E1599 | E1600 | E1601 | E1602 | E1603 | E1604 | E1605 | E1606 | E1607 | E1608 | E1609 | E1610 | E1611 | E1612 | E1613 | E1614 | E1615 | E1616 | E1617 | E1618 | E1619 | E1620 | E1621 | E1622 | E1623 | E1624 | E1625 | E1626 | E1627 | E1628 | E1629 | E1630 | E1631 | E1632 | E1633 | E1634 | E1635 | E1636 | E1637 | E1638 |
|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|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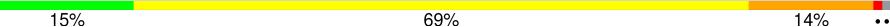
● Molecule 2: BACTERIAL RNA POLYMERASE BETA SUBUNIT; CHAIN C, M

Chain M:  17% 69% 13%



| | | | |
|-------|-------|-------|-------|
| M1000 | G1062 | Q1026 | A1045 |
| V1001 | R1063 | F1027 | A1046 |
| E1002 | M1064 | G1028 | A1047 |
| D1003 | A1065 | G1029 | M1048 |
| K1004 | A1066 | Q1030 | L1049 |
| M1005 | Y1067 | E1031 | Q1050 |
| H1006 | A1068 | L1032 | E1051 |
| A1007 | A1069 | F1033 | M1052 |
| L1008 | I1070 | A1034 | L1053 |
| S1009 | K1071 | E1035 | L1054 |
| T1010 | K1072 | M1036 | L1055 |
| K1011 | G1073 | L1037 | K1056 |
| P1012 | E1074 | V1038 | S1057 |
| T1013 | D1075 | Q1039 | D1058 |
| L1014 | V1076 | T1040 | D1059 |
| L1015 | P1077 | E1041 | I1060 |
| I1016 | E1078 | D1103 | E1061 |
| T1017 | P1079 | A1042 | |
| Q1018 | S1080 | | |
| Q1019 | V1081 | | |
| P1020 | P1082 | | |
| L1021 | E1083 | | |
| G1022 | S1084 | | |
| G1023 | F1085 | | |
| | R1086 | | |
| | V1087 | | |
| | L1088 | | |
| | M1089 | | |
| | K1090 | | |
| | E1091 | | |
| | Q1092 | | |
| | Q1093 | | |
| | A1094 | | |
| | L1095 | | |
| | A1096 | | |
| | L1097 | | |
| | D1098 | | |
| | V1037 | | |
| | V1099 | | |
| | Q1100 | | |
| | T1101 | | |
| | L1102 | | |
| | R41 | | |
| | D1103 | | |
| | E1104 | | |
| | K1105 | | |
| | D1106 | | |
| | M1107 | | |
| | P1108 | | |
| | V1109 | | |
| | D1110 | | |
| | F1111 | | |
| | F1112 | | |
| | E1113 | | |
| | G1114 | | |
| | L1115 | | |
| | K1116 | | |
| | S1117 | | |
| | K1118 | | |
| | R1119 | | |

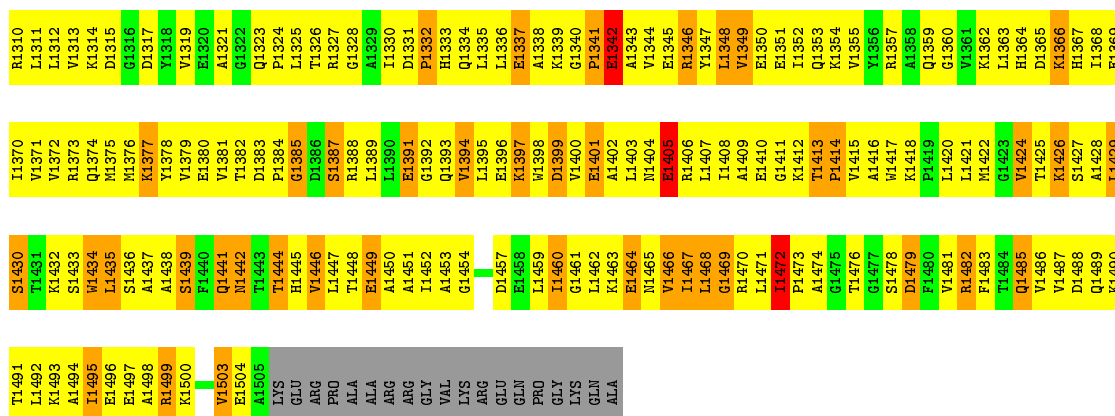
• Molecule 3: BACTERIAL RNA POLYMERASE BETA-PRIME SUBUNIT; CHAIN D, N

Chain D:  15% 69% 14% ..

| | | | | | | | | | | | | | |
|-------|-------|------|------|------|------|------|------|------|------|------|------|------|------|
| WT | G61 | T121 | E183 | E247 | K308 | L371 | R434 | K494 | L554 | R615 | R675 | T737 | K799 |
| R2 | K62 | E122 | E184 | F248 | G309 | D372 | V435 | R495 | K555 | Q616 | M676 | A738 | K800 |
| K3 | Y63 | L123 | V185 | L249 | L310 | P373 | E436 | L496 | K556 | R617 | L677 | A739 | G801 |
| E4 | K64 | E124 | V186 | L250 | L311 | E374 | E437 | E497 | L557 | L618 | E678 | F740 | A802 |
| V5 | R65 | Q125 | K187 | F251 | M313 | E375 | D438 | V498 | L558 | L619 | R679 | D741 | G803 |
| R6 | Q66 | V126 | K188 | R252 | R314 | E376 | L439 | V499 | A559 | G620 | Q680 | G742 | L804 |
| K7 | R67 | L127 | K189 | A253 | R315 | V677 | V440 | R500 | Q560 | K621 | R681 | D743 | E805 |
| L8 | F68 | Y128 | E190 | E254 | Q316 | L378 | R441 | A501 | G561 | K622 | D682 | Q744 | F806 |
| R9 | E69 | F129 | L191 | E255 | V317 | E380 | M442 | F502 | A562 | G623 | L683 | Q745 | A807 |
| T10 | K71 | K130 | A192 | G257 | R318 | E381 | V444 | D504 | P563 | D624 | K684 | V746 | T808 |
| K11 | L12 | R131 | P193 | G257 | R318 | E382 | V445 | S505 | E564 | R625 | D685 | V747 | P809 |
| L12 | L13 | Y132 | G194 | V258 | R319 | V384 | R446 | G506 | I565 | G626 | E686 | H748 | E810 |
| E13 | S14 | V134 | V195 | E260 | V322 | R386 | V447 | R507 | I566 | G627 | V687 | V749 | E811 |
| P15 | R75 | L135 | R198 | L261 | E323 | L387 | E448 | R508 | E567 | R628 | M688 | F750 | A812 |
| E16 | C76 | D136 | L199 | K262 | A324 | E388 | S449 | P509 | R568 | S629 | D689 | L751 | L813 |
| G77 | G77 | P137 | D200 | E263 | E325 | E389 | Y450 | E510 | M569 | Q630 | A690 | S752 | A814 |
| T18 | V78 | K138 | P208 | E264 | E326 | P390 | D451 | M511 | E570 | I631 | L691 | S753 | A815 |
| R19 | E79 | G139 | R209 | L264 | E327 | V396 | G457 | V517 | E571 | G632 | E692 | F754 | H816 |
| S20 | V80 | A140 | R210 | E265 | G328 | A391 | I452 | R512 | R572 | V633 | E693 | A755 | E817 |
| E21 | T81 | I141 | Y205 | E266 | E329 | S392 | D453 | L513 | M573 | Q634 | V694 | Q756 | L818 |
| S22 | S82 | L142 | R206 | G267 | T330 | L394 | R455 | E515 | L574 | P635 | L695 | A757 | E819 |
| S83 | S83 | J143 | F207 | F269 | V331 | V397 | M456 | A516 | Q575 | Q636 | H696 | E758 | E820 |
| G24 | G24 | G144 | P208 | L270 | V332 | V396 | G457 | A517 | E576 | L637 | E697 | A759 | V821 |
| R85 | V85 | V145 | R209 | V271 | L333 | K397 | A458 | P518 | A577 | K638 | K698 | R760 | A822 |
| V86 | R86 | P146 | R210 | L272 | T334 | A398 | E459 | V519 | D579 | H640 | V700 | V761 | L823 |
| V1087 | E27 | V147 | V211 | R273 | L335 | R399 | A460 | L520 | A580 | Q641 | L701 | L764 | A825 |
| L1088 | K28 | E148 | R212 | R274 | F336 | V400 | I461 | P521 | L581 | C642 | L702 | S765 | P826 |
| G1029 | R89 | K149 | R89 | E213 | L337 | V401 | Q462 | P522 | L582 | G643 | N703 | A766 | L827 |
| Q1030 | E90 | R150 | N90 | E214 | E338 | P402 | Q463 | D523 | L583 | L644 | R704 | H767 | K828 |
| R1031 | L1092 | G91 | T31 | Y215 | K339 | F403 | L464 | L524 | M584 | P645 | A705 | N768 | V829 |
| F1032 | Q1093 | L152 | H82 | V216 | T340 | E404 | L465 | R525 | G585 | K646 | V706 | L769 | A830 |
| G1033 | A1094 | L153 | I93 | K217 | E341 | D405 | K466 | P526 | R586 | R647 | T707 | L770 | E831 |
| E1034 | L1095 | T154 | E94 | T282 | P342 | V406 | E467 | M527 | R587 | M648 | L708 | S771 | E832 |
| M1035 | L95 | D155 | E219 | Y283 | D343 | V407 | L468 | Q529 | P594 | A649 | H709 | F772 | E833 |
| E1036 | L1097 | E156 | A96 | F283 | D344 | E408 | D469 | V530 | G533 | L650 | R710 | A773 | T834 |
| V1037 | L1098 | E157 | T37 | L284 | R346 | V409 | L470 | V531 | G534 | E651 | L711 | S774 | S835 |
| M1038 | V1099 | Y158 | P98 | G222 | R347 | S410 | E471 | D531 | P535 | L852 | G712 | G775 | V836 |
| A1039 | Q1100 | R159 | A99 | L223 | V347 | T411 | A472 | G532 | G536 | F653 | L713 | F776 | G837 |
| L1040 | T1101 | E160 | A100 | R224 | Q348 | G412 | L473 | G533 | P594 | K654 | I714 | P777 | R838 |
| E1041 | L1102 | L161 | H01 | L225 | P349 | D413 | E474 | R534 | G595 | L655 | A715 | L778 | L839 |
| A1042 | D1103 | R162 | I102 | P226 | M288 | R414 | K475 | P535 | S596 | F656 | F716 | A779 | K840 |
| | E1104 | Y163 | V103 | L227 | K351 | V415 | E476 | A536 | D597 | L657 | Q717 | K780 | Y841 |
| | K1105 | L164 | F104 | | N352 | A416 | L477 | T537 | R598 | L658 | L720 | S781 | F842 |
| | D1106 | K165 | V105 | | V353 | P417 | L478 | S533 | P599 | K659 | V721 | S782 | F843 |
| | M1107 | Q166 | K106 | | V354 | G418 | E479 | D539 | L600 | M661 | | D784 | A844 |
| | P1108 | E167 | D107 | | V355 | | E480 | R601 | L540 | E662 | Q724 | I785 | N845 |
| | V1109 | T168 | V108 | | P356 | | M481 | N541 | S602 | E663 | S725 | I786 | P846 |
| | D1110 | Y169 | P109 | | E357 | | K482 | D542 | L603 | E664 | L726 | L787 | D847 |
| | F1111 | P170 | S110 | | G358 | | H483 | L543 | T604 | K665 | Q727 | G788 | E848 |
| | F1112 | P171 | K111 | | A359 | | P484 | Y544 | D605 | Q665 | | | A849 |
| | E1113 | P172 | I112 | | R360 | | S485 | R545 | L606 | I666 | L728 | | L850 |
| | G1114 | G113 | T114 | | K300 | | R486 | R546 | L607 | A667 | H729 | Y791 | L851 |
| | L1115 | E54 | R54 | | P238 | | V427 | L547 | S608 | Q668 | F730 | I792 | A852 |
| | K1116 | D55 | L116 | | I241 | | R488 | I548 | G609 | N669 | L731 | T793 | V853 |
| | S1117 | V56 | L117 | | L242 | | E489 | K610 | N549 | K670 | V732 | Q794 | A854 |
| | K1118 | E57 | D117 | | A243 | | A480 | R550 | Q611 | K671 | C733 | V795 | E855 |
| | R1119 | C58 | L118 | | E244 | | R491 | N551 | G612 | A672 | E734 | R796 | G856 |
| | | S119 | S119 | | L245 | | A492 | N552 | R613 | A673 | T857 | R797 | H857 |
| | | A120 | G182 | | P246 | | R493 | R553 | F614 | R674 | F736 | E798 | V858 |

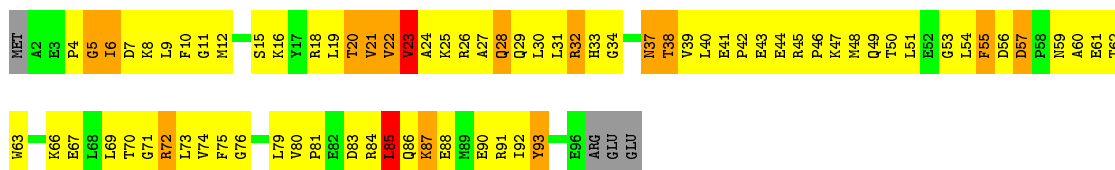
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|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------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| P1048 | P1049 | P1050 | P1051 | P1052 | P1053 | P1054 | P1055 | P1056 | P1057 | P1058 | P1059 | P1060 | P1061 | P1062 | L1065 | L1066 | L1067 | L1068 | L1069 | L1070 | L1071 | L1072 | L1073 | L1074 | L1075 | L1076 | L1077 | L1078 | L1079 | L1080 | L1081 | L1082 | L1083 | L1084 | L1085 | L1086 | L1087 | L1088 | L1089 | L1090 | L1091 | L1092 | L1093 | L1094 | L1095 | L1096 | L1097 | L1098 | L1099 | L1100 | L1101 | L1102 | L1103 | L1104 | L1105 | L1106 | L1107 | L1108 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| S1049 | G1050 | E1051 | T1052 | F1053 | E1054 | V1055 | P1056 | V1057 | R1058 | S1059 | S1060 | F1061 | R1062 | L1065 | T1066 | V1067 | L1068 | E1069 | F1070 | C1071 | L1072 | S1073 | S1074 | H1075 | G1076 | A1077 | R1078 | K1079 | G1080 | L1081 | A1082 | D1083 | T1084 | A1085 | L1086 | R1087 | T1088 | A1089 | D1090 | S1091 | G1092 | L1093 | L1094 | T1095 | R1096 | K1097 | L1098 | V1099 | D1100 | V1101 | T1102 | L1103 | R1104 | E1105 | V1106 | V1107 | L1108 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| T1114 | N1115 | N1116 | Y1117 | F1118 | E1119 | V1120 | P1121 | P1122 | F1123 | Q1124 | P1125 | D1126 | E1127 | L1128 | T1129 | S1130 | S1131 | L1132 | L1133 | L1134 | L1135 | K1136 | L1137 | A1138 | L1139 | L1140 | A1141 | A1142 | L1143 | L1144 | G1145 | L1146 | L1147 | V1148 | L1149 | A1150 | A1151 | E1152 | V1153 | E1154 | V1155 | L1156 | G1157 | V1158 | R1159 | L1160 | E1161 | L1162 | G1163 | Y1165 | L1166 | T1167 | L1168 | D1169 | D1170 | V1171 | H1172 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| L1173 | L1174 | K1175 | A1177 | A1178 | L1179 | A1180 | G1181 | E1182 | L1183 | Q1184 | P1185 | V1186 | P1187 | V1188 | L1189 | S1190 | P1191 | L1192 | L1193 | C1194 | Q1195 | T1196 | L1197 | Y1198 | G1199 | K1203 | C1204 | Y1205 | G1206 | L1207 | D1208 | L1209 | L1210 | L1211 | A1212 | R1213 | P1214 | V1215 | S1216 | L1217 | G1218 | E1219 | A1220 | V1221 | G1222 | L1223 | V1224 | Q1227 | S1228 | L1229 | G1230 | E1231 | P1232 | G1233 | T1234 | Q1235 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| L1236 | T1237 | R1238 | G1239 | G1240 | V1241 | A1242 | L1243 | T1244 | L1245 | P1246 | P1247 | L1248 | L1249 | L1250 | R1251 | L1252 | L1253 | Q1254 | G1255 | P1256 | P1257 | L1258 | R1259 | L1260 | E1261 | L1262 | L1263 | L1264 | K1265 | A1266 | L1267 | L1268 | L1269 | L1270 | L1271 | L1272 | L1273 | L1274 | L1275 | L1276 | L1277 | L1278 | G1279 | L1280 | L1281 | L1282 | L1283 | E1284 | L1285 | L1286 | L1287 | L1288 | K1289 | L1290 | S1291 | L1292 | F1293 | L1294 | E1295 | G1296 | E1297 | G1298 | F1299 | L1300 | K1301 | L1302 | L1303 | L1304 | L1305 | P1306 | K1307 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| R1310 | L1311 | L1312 | L1313 | L1314 | D1315 | G1316 | L1317 | L1318 | L1319 | Q1320 | P1321 | L1322 | R1323 | L1324 | L1325 | L1326 | R1327 | L1328 | L1329 | L1330 | D1331 | P1332 | H1333 | Q1334 | L1335 | L1336 | E1337 | L1338 | L1339 | L1340 | L1341 | L1342 | L1343 | L1344 | L1345 | L1346 | Y1347 | L1348 | L1349 | E1350 | L1351 | L1352 | Q1353 | K1354 | V1355 | L1356 | R1357 | A1358 | Q1359 | L1360 | V1361 | K1362 | L1363 | H1364 | L1365 | L1366 | L1367 | L1368 | L1369 | L1370 | L1371 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| V1372 | R1373 | M1374 | M1375 | L1376 | L1377 | L1378 | L1379 | E1380 | L1381 | T1382 | L1383 | P1384 | S1387 | L1388 | L1389 | L1390 | E1391 | L1392 | Q1393 | L1394 | L1395 | E1396 | K1397 | L1398 | L1399 | L1400 | L1401 | L1402 | L1403 | L1404 | E1405 | L1406 | L1407 | G1408 | L1409 | L1410 | L1411 | K1412 | L1413 | P1414 | V1415 | A1416 | L1417 | L1418 | F1419 | V1420 | L1421 | M1422 | G1423 | L1424 | T1425 | L1426 | L1427 | L1428 | L1429 | S1430 | T1431 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| V1434 | L1435 | S1436 | A1437 | A1438 | L1439 | F1440 | Q1441 | M1442 | T1443 | T1444 | H1445 | L1446 | L1447 | T1448 | E1449 | A1450 | A1451 | L1452 | A1453 | G1454 | K1455 | K1456 | D1457 | E1458 | L1459 | L1460 | G1461 | L1462 | K1463 | E1464 | L1465 | V1466 | L1467 | G1468 | G1469 | R1470 | L1471 | L1472 | P1473 | A1474 | G1475 | L1476 | G1477 | S1478 | D1479 | F1480 | V1481 | R1482 | F1483 | T1484 | Q1485 | V1486 | L1487 | D1488 | Q1489 | K1490 | T1491 | L1492 | K1493 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| A1494 | L1495 | E1496 | E1497 | A1498 | R1499 | K1500 | E1501 | A1502 | V1503 | E1504 | A1505 | L1506 | L1507 | L1508 | L1509 | L1510 | L1511 | L1512 | L1513 | L1514 | L1515 | L1516 | L1517 | L1518 | L1519 | L1520 | L1521 | L1522 | L1523 | L1524 | L1525 | L1526 | L1527 | L1528 | L1529 | L1530 | L1531 | L1532 | L1533 | L1534 | L1535 | L1536 | L1537 | L1538 | L1539 | L1540 | L1541 | L1542 | L1543 | L1544 | L1545 | L1546 | L1547 | L1548 | L1549 | L1550 | L1551 | L1552 | L1553 | L1554 | L1555 | L1556 | L1557 | L1558 | L1559 | L1560 | L1561 | L1562 | L1563 | L1564 | L1565 | L1566 | L1567 | L1568 | L1569 | L1570 | L1571 | L1572 | L1573 | L1574 | L1575 | L1576 | L1577 | L1578 | L1579 | L1580 | L1581 | L1582 | L1583 | L1584 | L1585 | L1586 | L1587 | L1588 | L1589 | L1590 | L1591 | L1592 | L1593 | L1594 | L1595 | L1596 | L1597 | L1598 | L1599 | L1600 | L1601 | L1602 | L1603 | L1604 | L1605 | L1606 | L1607 | L1608 | L1609 | L1610 | L1611 | L1612 | L1613 | L1614 | L1615 | L1616 | L1617 | L1618 | L1619 | L1620 | L1621 | L1622 | L1623 | L1624 | L1625 | L1626 | L1627 | L1628 | L1629 | L1630 | L1631 | L1632 | L1633 | L1634 | L1635 | L1636 | L1637 | L1638 | L1639 | L1640 | L1641 | L1642 | L1643 | L1644 | L1645 | L1646 | L1647 | L1648 | L1649 | L1650 | L1651 | L1652 | L1653 | L1654 | L1655 | L1656 | L1657 | L1658 | L1659 | L1660 | L1661 | L1662 | L1663 | L1664 | L1665 | L1666 | L1667 | L1668 | L1669 | L1670 | L1671 | L1672 | L1673 | L1674 | L1675 | L1676 | L1677 | L1678 | L1679 | L1680 | L1681 | L1682 | L1683 | L1684 | L1685 | L1686 | L1687 | L1688 | L1689 | L1690 | L1691 | L1692 | L1693 | L1694 | L1695 | L1696 | L1697 | L1698 | L1699 | L1700 | L1701 | L1702 | L1703 | L1704 | L1705 | L1706 | L1707 | L1708 | L1709 | L1710 | L1711 | L1712 | L1713 | L1714 | L1715 | L1716 | L1717 | L1718 | L1719 | L1720 | L1721 | L1722 | L1723 | L1724 | L1725 | L1726 | L1727 | L1728 | L1729 | L1730 | L1731 | L1732 | L1733 | L1734 | L1735 | L1736 | L1737 | L1738 | L1739 | L1740 | L1741 | L1742 | L1743 | L1744 | L1745 | L1746 | L1747 | L1748 | L1749 | L1750 | L1751 | L1752 | L1753 | L1754 | L1755 | L1756 | L1757 | L1758 | L1759 | L1760 | L1761 | L1762 | L1763 | L1764 | L1765 | L1766 | L1767 | L1768 | L1769 | L1770 | L1771 | L1772 | L1773 | L1774 | L1775 | L1776 | L1777 | L1778 | L1779 | L1780 | L1781 | L1782 | L1783 | L1784 | L1785 | L1786 | L1787 | L1788 | L1789 | L1790 | L1791 | L1792 | L1793 | L1794 | L1795 | L1796 | L1797 | L1798 | L1799 | L1800 | L1801 | L1802 | L1803 | L1804 | L1805 | L1806 | L1807 | L1808 | L1809 | L1810 | L1811 | L1812 | L1813 | L1814 | L1815 | L1816 | L1817 | L1818 | L1819 | L1820 | L1821 | L1822 | L1823 | L1824 | L1825 | L1826 | L1827 | L1828 | L1829 | L1830 | L1831 | L1832 | L1833 | L1834 | L1835 | L1836 | L1837 | L1838 | L1839 | L1840 | L1841 | L1842 | L1843 | L1844 | L1845 | L1846 | L1847 | L1848 | L1849 | L1850 | L1851 | L1852 | L1853 | L1854 | L1855 | L1856 | L1857 | L1858 | L1859 | L1860 | L1861 | L1862 | L1863 | L1864 | L1865 | L1866 | L1867 | L1868 | L1869 | L1870 | L1871 | L1872 | L1873 | L1874 | L1875 | L1876 | L1877 | L1878 | L1879 | L1880 | L1881 | L1882 | L1883 | L1884 | L1885 | L1886 | L1887 | L1888 | L1889 | L1890 | L1891 | L1892 | L1893 | L1894 | L1895 | L1896 | L1897 | L1898 | L1899 | L1900 | L1901 | L1902 | L1903 | L1904 | L1905 | L1906 | L1907 | L1908 | L1909 | L1910 | L1911 | L1912 | L1913 | L1914 | L1915 | L1916 | L1917 | L1918 | L1919 | L1920 | L1921 | L1922 | L1923 | L1924 | L1925 | L1926 | L1927 | L1928 | L1929 | L1930 | L1931 | L1932 | L1933 | L1934 | L1935 | L1936 | L1937 | L1938 | L1939 | L1940 | L1941 | L1942 | L1943 | L1944 | L1945 | L1946 | L1947 | L1948 | L1949 | L1950 | L1951 | L1952 | L1953 | L1954 | L1955 | L1956 | L1957 | L1958 | L1959 | L1960 | L1961 | L1962 | L1963 | L1964 | L1965 | L1966 | L1967 | L1968 | L1969 | L1970 | L1971 | L1972 | L1973 | L1974 | L1975 | L1976 | L1977 | L1978 | L1979 | L1980 | L1981 | L1982 | L1983 | L1984 | L1985 | L1986 | L1987 | L1988 | L1989 | L1990 | L1991 | L1992 | L1993 | L1994 | L1995 | L1996 | L1997 | L1998 | L1999 | L2000 | L2001 | L2002 | L2003 | L2004 | L2005 | L2006 | L2007 | L2008 | L2009 | L2010 | L2011 | L2012 | L2013 | L2014 | L2015 | L2016 | L2017 | L2018 | L2019 | L2020 | L2021 | L2022 | L2023 | L2024 | L2025 | L2026 | L2027 | L2028 | L2029 | L2030 | L2031 | L2032 | L2033 | L2034 | L2035 | L2036 | L2037 | L2038 | L2039 | L2040 | L2041 | L2042 | L2043 | L2044 | L2045 | L2046 | L2047 | L2048 | L2049 | L2050 | L2051 | L2052 | L2053 | L2054 | L2055 | L2056 | L2057 | L2058 | L2059 | L2060 | L2061 | L2062 | L2063 | L2064 | L2065 | L2066 | L2067 | L2068 | L2069 | L2070 | L2071 | L2072 | L2073 | L2074 | L2075 | L2076 | L2077 | L2078 | L2079 | L2080 | L2081 | L2082 | L2083 | L2084 | L2085 | L2086 | L2087 | L2088 | L2089 | L2090 | L2091 | L2092 | L2093 | L2094 | L2095 | L2096 | L2097 | L2098 | L2099 | L2100 | L2101 | L2102 | L2103 | L2104 | L2105 | L2106 | L2107 | L2108 | L2109 | L2110 | L2111 | L2112 | L2113 | L2114 | L2115 | L2116 | L2117 | L2118 | L2119 | L2120 | L2121 | L2122 | L2123 | L2124 | L2125 | L2126 | L2127 | L2128 | L2129 | L2130 | L2131 | L2132 | L2133 | L2134 | L2135 | L2136 | L2137 | L2138 | L2139 | L2140 | L2141 | L2142 | L2143 | L2144 | L2145 | L2146 | L2147 | L2148 | L2149 | L2150 | L2151 | L2152 | L2153 | L2154 | L2155 | L2156 | L2157 | L2158 | L2159 | L2160 | L2161 | L2162 | L2163 | L2164 | L2165 | L2166 | L2167 | L2168 | L2169 | L2170 | L2171 | L2172 | L2173 | L2174 | L2175 | L2176 | L2177 | L2178 | L2179 | L2180 | L2181 | L2182 | L2183 | L2184 | L2185 | L2186 | L2187 | L2188 | L2189 | L2190 | L2191 | L2192 | L2193 | L2194 | L2195 | L2196 | L2197 | L2198 | L2199 | L2200 | L2201 | L2202 | L2203 | L2204 | L2205 | L2206 | L2207 | L2208 | L2209 | L2210 | L2211 | L2212 | L2213 | L2214 | L2215 | L2216 | L2217 | L2218 | L2219 | L2220 | L2221 | L2222 | L2223 | L2224 | L2225 | L2226 | L2227 | L2228 | L2229 | L2230 | L2231 | L2232 | L2233 | L2234 | L2235 | L2236 | L2237 | L2238 | L2239 | L2240 | L2241 | L2242 | L2243 | L2244 | L2245 | L2246 | L2247 | L2248 | L2249 | L2250 | L2251 | L2252 | L2253 | L2254 | L2255 | L2256 | L2257 | L2258 | L2259 | L2260 | L2261 | L2262 | L2263 | L2264 | L2265 | L2266 | L2267 | L2268 | L2269 | L2270 | L2271 | L2272 | L2273 | L2274 | L2275 | L2276 | L2277 | L2278 | L2279 | L2280 | L2281 | L2282 | L2283 | L2284 | L2285 | L2286 | L2287 | L2288 | L2289 | L2290 | L2291 | L2292 | L2293 | L2294 | L2295 | L2296 | L2297 | L2298 | L2299 | L2300 | L2301 | L2302 | L2303 | L2304 | L2305 | L2306 | L2307 | L2308 | L2309 | L2310 | L2311 | L2312 | L2313 | L2314 | L2315 | L2316 | L2317 | L2318 | L2319 | L2320 | L2321 | L2322 | L2323 | L2324 | L2325 | L2326 | L2327 | L2328 | L2329 | L2330 | L2331 | L2332 | L2333 | L2334 | L2335 | L2336 | L2337 | L2338 | L2339 | L2340 | L2341 | L2342 | L2343 | L2344 | L2345 | L2346 | L2347 | L2348 | L2349 | L2350 | L2351 | L2352 | L2353 | L2354 | L2355 | L2356 | L2357 | L2358 | L2359 | L2360 | L2361 | L2362 | L23 |

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|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|
| G1248 | D1251 | T1253 | Q1254 | G1255 | L1256 | P1257 | R1258 | V1259 | E1260 | L1261 | L1262 | F1263 | E1264 | A1265 | R1266 | R1267 | T1268 | K1269 | A1270 | K1271 | A1272 | V1273 | L1274 | S1275 | E1276 | L1277 | D1278 | E1285 | L1286 | E1287 | K1288 | K1289 | L1290 | S1291 | L1292 | F1293 | S1296 | E1297 | L1298 | S1300 | E1301 | E1302 | Y1303 | K1304 | M1305 | R1306 | G1307 | E1308 | E1309 | E1310 | E1311 | E1312 | E1313 | E1314 | E1315 | E1316 | E1317 | E1318 | E1319 | E1320 | E1321 | E1322 | E1323 | E1324 | E1325 | E1326 | E1327 | E1328 | E1329 | E1330 | E1331 | E1332 | E1333 | E1334 | E1335 | E1336 | E1337 | E1338 | E1339 | E1340 | E1341 | E1342 | E1343 | E1344 | E1345 | E1346 | E1347 | E1348 | E1349 | E1350 | E1351 | E1352 | E1353 | E1354 | E1355 | E1356 | E1357 | E1358 | E1359 | E1360 | E1361 | E1362 | E1363 | E1364 | E1365 | E1366 | E1367 | E1368 | E1369 | E1370 | E1371 | E1372 | E1373 | E1374 | E1375 | E1376 | E1377 | E1378 | E1379 | E1380 | E1381 | E1382 | E1383 | E1384 | E1385 | E1386 | E1387 | E1388 | E1389 | E1390 | E1391 | E1392 | E1393 | E1394 | E1395 | E1396 | E1397 | E1398 | E1399 | E1400 | E1401 | E1402 | E1403 | E1404 | E1405 | E1406 | E1407 | E1408 | E1409 | E1410 | E1411 | E1412 | E1413 | E1414 | E1415 | E1416 | E1417 | E1418 | E1419 | E1420 | E1421 | E1422 | E1423 | E1424 | E1425 | E1426 | E1427 | E1428 | E1429 | E1430 | E1431 | E1432 | E1433 | E1434 | E1435 | E1436 | E1437 | E1438 | E1439 | E1440 | E1441 | E1442 | E1443 | E1444 | E1445 | E1446 | E1447 | E1448 | E1449 | E1450 | E1451 | E1452 | E1453 | E1454 | E1455 | E1456 | E1457 | E1458 | E1459 | E1460 | E1461 | E1462 | E1463 | E1464 | E1465 | E1466 | E1467 | E1468 | E1469 | E1470 | E1471 | E1472 | E1473 | E1474 | E1475 | E1476 | E1477 | E1478 | E1479 | E1480 | E1481 | E1482 | E1483 | E1484 | E1485 | E1486 | E1487 | E1488 | E1489 | E1490 | E1491 | E1492 | E1493 | E1494 | E1495 | E1496 | E1497 | E1498 | E1499 | E1500 | E1501 | E1502 | E1503 | E1504 | E1505 | E1506 | E1507 | E1508 | E1509 | E1510 | E1511 | E1512 | E1513 | E1514 | E1515 | E1516 | E1517 | E1518 | E1519 | E1520 | E1521 | E1522 | E1523 | E1524 | E1525 | E1526 | E1527 | E1528 | E1529 | E1530 | E1531 | E1532 | E1533 | E1534 | E1535 | E1536 | E1537 | E1538 | E1539 | E1540 | E1541 | E1542 | E1543 | E1544 | E1545 | E1546 | E1547 | E1548 | E1549 | E1550 | E1551 | E1552 | E1553 | E1554 | E1555 | E1556 | E1557 | E1558 | E1559 | E1560 | E1561 | E1562 | E1563 | E1564 | E1565 | E1566 | E1567 | E1568 | E1569 | E1570 | E1571 | E1572 | E1573 | E1574 | E1575 | E1576 | E1577 | E1578 | E1579 | E1580 | E1581 | E1582 | E1583 | E1584 | E1585 | E1586 | E1587 | E1588 | E1589 | E1590 | E1591 | E1592 | E1593 | E1594 | E1595 | E1596 | E1597 | E1598 | E1599 | E1600 | E1601 | E1602 | E1603 | E1604 | E1605 | E1606 | E1607 | E1608 | E1609 | E1610 | E1611 | E1612 | E1613 | E1614 | E1615 | E1616 | E1617 | E1618 | E1619 | E1620 | E1621 | E1622 | E1623 | E1624 | E1625 | E1626 | E1627 | E1628 | E1629 | E1630 | E1631 | E1632 | E1633 | E1634 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| E1885 | E1886 | E1887 | E1888 | E1889 | E1890 | E1891 | E1892 | E1893 | E1894 | E1895 | E1896 | E1897 | E1898 | E1899 | E1900 | E1901 | E1902 | E1903 | E1904 | E1905 | E1906 | E1907 | E1908 | E1909 | E1910 | E1911 | E1912 | E1913 | E1914 | E1915 | E1916 | E1917 | E1918 | E1919 | E1920 | E1921 | E1922 | E1923 | E1924 | E1925 | E1926 | E1927 | E1928 | E1929 | E1930 | E1931 | E1932 | E1933 | E1934 | E1935 | E1936 | E1937 | E1938 | E1939 | E1940 | E1941 | E1942 | E1943 | E1944 | E1945 | E1946 | E1947 | E1948 | E1949 | E1950 | E1951 | E1952 | E1953 | E1954 | E1955 | E1956 | E1957 | E1958 | E1959 | E1960 | E1961 | E1962 | E1963 | E1964 | E1965 | E1966 | E1967 | E1968 | E1969 | E1970 | E1971 | E1972 | E1973 | E1974 | E1975 | E1976 | E1977 | E1978 | E1979 | E1980 | E1981 | E1982 | E1983 | E1984 | E1985 | E1986 | E1987 | E1988 | E1989 | E1990 | E1991 | E1992 | E1993 | E1994 | E1995 | E1996 | E1997 | E1998 | E1999 | E2000 | E2001 | E2002 | E2003 | E2004 | E2005 | E2006 | E2007 | E2008 | E2009 | E2010 | E2011 | E2012 | E2013 | E2014 | E2015 | E2016 | E2017 | E2018 | E2019 | E2020 | E2021 | E2022 | E2023 | E2024 | E2025 | E2026 | E2027 | E2028 | E2029 | E2030 | E2031 | E2032 | E2033 | E2034 | E2035 | E2036 | E2037 | E2038 | E2039 | E2040 | E2041 | E2042 | E2043 | E2044 | E2045 | E2046 | E2047 | E2048 | E2049 | E2050 | E2051 | E2052 | E2053 | E2054 | E2055 | E2056 | E2057 | E2058 | E2059 | E2060 | E2061 | E2062 | E2063 | E2064 | E2065 | E2066 | E2067 | E2068 | E2069 | E2070 | E2071 | E2072 | E2073 | E2074 | E2075 | E2076 | E2077 | E2078 | E2079 | E2080 | E2081 | E2082 | E2083 | E2084 | E2085 | E2086 | E2087 | E2088 | E2089 | E2090 | E2091 | E2092 | E2093 | E2094 | E2095 | E2096 | E2097 | E2098 | E2099 | E2100 | E2101 | E2102 | E2103 | E2104 | E2105 | E2106 | E2107 | E2108 | E2109 | E2110 | E2111 | E2112 | E2113 | E2114 | E2115 | E2116 | E2117 | E2118 | E2119 | E2120 | E2121 | E2122 | E2123 | E2124 | E2125 | E2126 | E2127 | E2128 | E2129 | E2130 | E2131 | E2132 | E2133 | E2134 | E2135 | E2136 | E2137 | E2138 | E2139 | E2140 | E2141 | E2142 | E2143 | E2144 | E2145 | E2146 | E2147 | E2148 | E2149 | E2150 | E2151 | E2152 | E2153 | E2154 | E2155 | E2156 | E2157 | E2158 | E2159 | E2160 | E2161 | E2162 | E2163 | E2164 | E2165 | E2166 | E2167 | E2168 | E2169 | E2170 | E2171 | E2172 | E2173 | E2174 | E2175 | E2176 | E2177 | E2178 | E2179 | E2180 | E2181 | E2182 | E2183 | E2184 | E2185 | E2186 | E2187 | E2188 | E2189 | E2190 | E2191 | E2192 | E2193 | E2194 | E2195 | E2196 | E2197 | E2198 | E2199 | E2200 | E2201 | E2202 | E2203 | E2204 | E2205 | E2206 | E2207 | E2208 | E2209 | E2210 | E2211 | E2212 | E2213 | E2214 | E2215 | E2216 | E2217 | E2218 | E2219 | E2220 | E2221 | E2222 | E2223 | E2224 | E2225 | E2226 | E2227 | E2228 | E2229 | E2230 | E2231 | E2232 | E2233 | E2234 | E2235 | E2236 | E2237 | E2238 | E2239 | E2240 | E2241 | E2242 | E2243 | E2244 | E2245 | E2246 | E2247 | E2248 | E2249 | E2250 | E2251 | E2252 | E2253 | E2254 | E2255 | E2256 | E2257 | E2258 | E2259 | E2260 | E2261 | E2262 | E2263 | E2264 | E2265 | E2266 | E2267 | E2268 | E2269 | E2270 | E2271 | E2272 | E2273 | E2274 | E2275 | E2276 | E2277 | E2278 | E2279 | E2280 | E2281 | E2282 | E2283 | E2284 | E2285 | E2286 | E2287 | E2288 | E2289 | E2290 | E2291 | E2292 | E2293 | E2294 | E2295 | E2296 | E2297 | E2298 | E2299 | E2300 | E2301 | E2302 | E2303 | E2304 | E2305 | E2306 | E2307 | E2308 | E2309 | E2310 | E2311 | E2312 | E2313 | E2314 | E2315 | E2316 | E2317 | E2318 | E2319 | E2320 | E2321 | E2322 | E2323 | E2324 | E2325 | E2326 | E2327 | E2328 | E2329 | E2330 | E2331 | E2332 | E2333 | E2334 | E2335 | E2336 | E2337 | E2338 | E2339 | E2340 | E2341 | E2342 | E2343 | E2344 | E2345 | E2346 | E2347 | E2348 | E2349 | E2350 | E2351 | E2352 | E2353 | E2354 | E2355 | E2356 | E2357 | E2358 | E2359 | E2360 | E2361 | E2362 | E2363 | E2364 | E2365 | E2366 | E2367 | E2368 | E2369 | E2370 | E2371 | E2372 | E2373 | E2374 | E2375 | E2376 | E2377 | E2378 | E2379 | E2380 | E2381 | E2382 | E2383 | E2384 | E2385 | E2386 | E2387 | E2388 | E2389 | E2390 | E2391 | E2392 | E2393 | E2394 | E2395 | E2396 | E2397 | E2398 | E2399 | E2400 | E2401 | E2402 | E2403 | E2404 | E2405 | E2406 | E2407 | E2408 | E2409 | E2410 | E2411 | E2412 | E2413 | E2414 | E2415 | E2416 | E2417 | E2418 | E2419 | E2420 | E2421 | E2422 | E2423 | E2424 | E2425 | E2426 | E2427 | E2428 | E2429 | E2430 | E2431 | E2432 | E2433 | E2434 | E2435 | E2436 | E2437 | E2438 | E2439 | E2440 | E2441 | E2442 | E2443 | E2444 | E2445 | E2446 | E2447 | E2448 | E2449 | E2450 | E2451 | E2452 | E2453 | E2454 | E2455 | E2456 | E2457 | E2458 | E2459 | E2460 | E2461 | E2462 | E2463 | E2464 | E2465 | E2466 | E2467 | E2468 | E2469 | E2470 | E2471 | E2472 | E2473 | E2474 | E2475 | E2476 | E2477 | E2478 | E2479 | E2480 | E2481 | E2482 | E2483 | E2484 | E2485 | E2486 | E2487 | E2488 | E2489 | E2490 | E2491 | E2492 | E2493 | E2494 | E2495 | E2496 | E2497 | E2498 | E2499 | E2500 | E2501 | E2502 | E2503 | E2504 | E2505 | E2506 | E2507 | E2508 | E2509 | E2510 | E2511 | E2512 | E2513 | E2514 | E2515 | E2516 | E2517 | E2518 | E2519 | E2520 | E2521 | E2522 | E2523 | E2524 | E2525 | E2526 | E2527 | E252 |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------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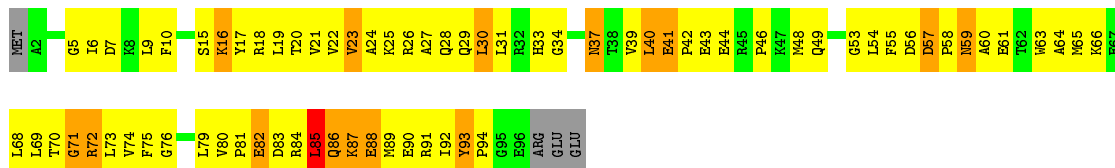
• Molecule 4: BACTERIAL RNA POLYMERASE OMEGA SUBUNIT; CHAIN E, O

Chain E: 19% 61% 14%



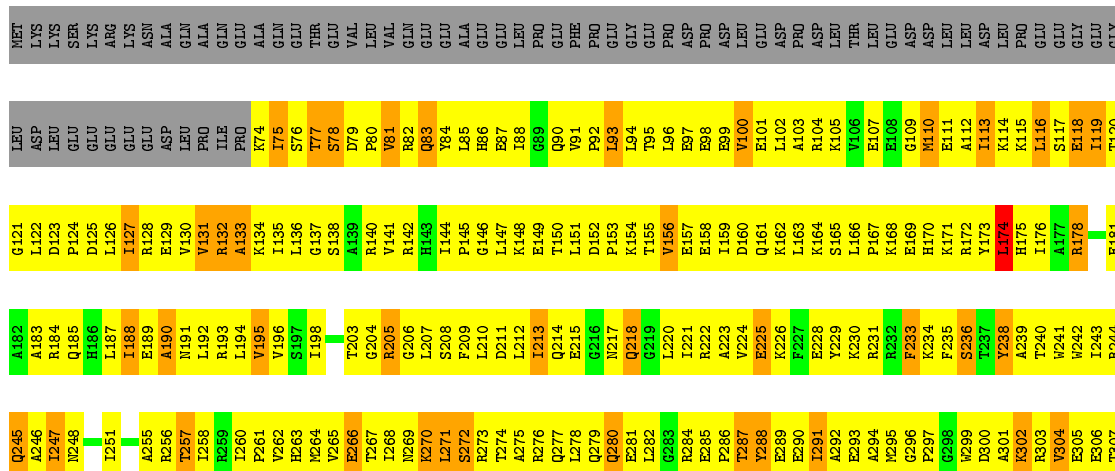
• Molecule 4: BACTERIAL RNA POLYMERASE OMEGA SUBUNIT; CHAIN E, O

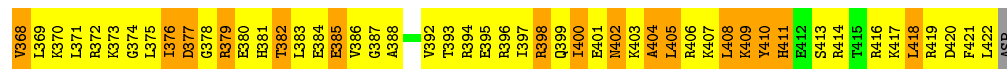
Chain O: 23% 57% 15%



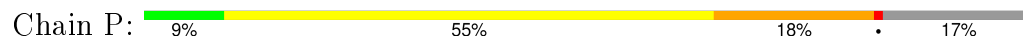
• Molecule 5: RNA polymerase principal sigma factor (RpoD); CHAIN F, P

Chain F: 9% 57% 16% 17%





- Molecule 5: RNA polymerase principal sigma factor (RpoD); CHAIN F, P



4 Data and refinement statistics

| Property | Value | Source |
|---|--|------------------|
| Space group | P 32 | Depositor |
| Cell constants a, b, c, α , β , γ | 235.09 Å 235.09 Å 250.88 Å 90.00° 90.00° 120.00° | Depositor |
| Resolution (Å) | 50.00 – 3.00 46.80 – 3.00 | Depositor EDS |
| % Data completeness (in resolution range) | 96.3 (50.00-3.00) 96.0 (46.80-3.00) | Depositor EDS |
| R_{merge} | 0.11 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.52 (at 3.01 Å) | Xtriage |
| Refinement program | CNS 1.0 | Depositor |
| R, R_{free} | 0.235 , 0.289 0.221 , 0.274 | Depositor DCC |
| R_{free} test set | 2351 reflections (0.79%) | DCC |
| Wilson B-factor (Å ²) | 83.8 | Xtriage |
| Anisotropy | 0.053 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | (Not available) , (Not available) | EDS |
| Estimated twinning fraction | 0.499 for -h,-k,l 0.047 for h,-h-k,-l 0.047 for -k,-h,-l | Xtriage |
| L-test for twinning ² | $\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$ | Xtriage |
| Outliers | 0 of 299146 reflections | Xtriage |
| F_o, F_c correlation | 0.95 | EDS |
| Total number of atoms | 56149 | wwPDB-VP |
| Average B, all atoms (Å ²) | 81.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: PO4, ZN, MPD, NE6, MG

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|-----------------|
| | | RMSZ | # $ Z > 5$ | RMSZ | # $ Z > 5$ |
| 1 | A | 0.43 | 0/1848 | 0.73 | 0/2512 |
| 1 | B | 0.39 | 0/1936 | 0.68 | 0/2633 |
| 1 | K | 0.43 | 0/1848 | 0.72 | 1/2512 (0.0%) |
| 1 | L | 0.41 | 0/1936 | 0.70 | 0/2633 |
| 2 | C | 0.43 | 0/8997 | 0.73 | 8/12164 (0.1%) |
| 2 | M | 0.43 | 0/8997 | 0.73 | 3/12164 (0.0%) |
| 3 | D | 0.44 | 0/12073 | 0.77 | 11/16324 (0.1%) |
| 3 | N | 0.46 | 2/12073 (0.0%) | 0.76 | 9/16324 (0.1%) |
| 4 | E | 0.40 | 0/783 | 0.69 | 0/1054 |
| 4 | O | 0.41 | 0/783 | 0.65 | 0/1054 |
| 5 | F | 0.40 | 0/2874 | 0.72 | 1/3866 (0.0%) |
| 5 | P | 0.40 | 0/2874 | 0.69 | 1/3866 (0.0%) |
| All | All | 0.43 | 2/57022 (0.0%) | 0.74 | 34/77106 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 3 | N | 0 | 1 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3 | N | 58 | CYS | CB-SG | -5.87 | 1.72 | 1.81 |
| 3 | N | 60 | CYS | CB-SG | -5.42 | 1.73 | 1.81 |

All (34) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 3 | D | 831 | GLY | N-CA-C | -12.95 | 80.74 | 113.10 |
| 3 | N | 831 | GLY | N-CA-C | -11.03 | 85.51 | 113.10 |
| 2 | C | 177 | GLU | N-CA-C | -8.93 | 86.88 | 111.00 |
| 5 | F | 313 | GLU | N-CA-C | 8.15 | 133.01 | 111.00 |
| 2 | M | 58 | ASP | N-CA-C | -8.08 | 89.18 | 111.00 |
| 3 | D | 803 | GLY | N-CA-C | -7.75 | 93.74 | 113.10 |
| 2 | M | 177 | GLU | N-CA-C | -7.54 | 90.65 | 111.00 |
| 3 | N | 803 | GLY | N-CA-C | -7.53 | 94.27 | 113.10 |
| 5 | P | 313 | GLU | N-CA-C | 7.14 | 130.27 | 111.00 |
| 2 | C | 58 | ASP | N-CA-C | -6.66 | 93.03 | 111.00 |
| 3 | D | 1128 | VAL | N-CA-C | -6.34 | 93.87 | 111.00 |
| 2 | C | 177 | GLU | C-N-CD | -6.19 | 106.98 | 120.60 |
| 3 | D | 798 | GLU | N-CA-C | 6.16 | 127.63 | 111.00 |
| 3 | N | 1128 | VAL | N-CA-C | -6.03 | 94.72 | 111.00 |
| 3 | D | 799 | LYS | N-CA-C | 5.89 | 126.90 | 111.00 |
| 3 | N | 1125 | PRO | N-CA-C | 5.87 | 127.37 | 112.10 |
| 3 | N | 199 | LEU | CA-CB-CG | -5.65 | 102.30 | 115.30 |
| 3 | D | 131 | LYS | N-CA-C | 5.54 | 125.95 | 111.00 |
| 3 | N | 799 | LYS | N-CA-C | 5.35 | 125.44 | 111.00 |
| 2 | C | 182 | VAL | N-CA-C | -5.29 | 96.72 | 111.00 |
| 3 | D | 807 | ALA | N-CA-C | -5.28 | 96.74 | 111.00 |
| 2 | M | 1092 | LEU | CA-CB-CG | -5.27 | 103.19 | 115.30 |
| 3 | D | 410 | SER | N-CA-C | 5.23 | 125.13 | 111.00 |
| 3 | N | 798 | GLU | N-CA-C | 5.20 | 125.04 | 111.00 |
| 3 | N | 807 | ALA | N-CA-C | -5.19 | 96.99 | 111.00 |
| 3 | D | 830 | ALA | N-CA-C | 5.17 | 124.96 | 111.00 |
| 2 | C | 675 | ALA | N-CA-C | -5.10 | 97.23 | 111.00 |
| 3 | N | 144 | GLY | N-CA-C | -5.09 | 100.37 | 113.10 |
| 2 | C | 165 | LEU | N-CA-C | 5.08 | 124.72 | 111.00 |
| 2 | C | 178 | PRO | N-CA-C | 5.06 | 125.26 | 112.10 |
| 3 | D | 717 | GLN | N-CA-C | -5.06 | 97.35 | 111.00 |
| 1 | K | 47 | SER | N-CA-C | 5.03 | 124.57 | 111.00 |
| 2 | C | 9 | ILE | N-CA-C | -5.02 | 97.44 | 111.00 |
| 3 | D | 1286 | THR | N-CA-C | -5.00 | 97.50 | 111.00 |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|-----------|
| 3 | N | 1117 | TYR | Sidechain |

5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 1816 | 0 | 1871 | 279 | 0 |
| 1 | B | 1902 | 0 | 1951 | 321 | 0 |
| 1 | K | 1816 | 0 | 1871 | 296 | 0 |
| 1 | L | 1902 | 0 | 1951 | 318 | 0 |
| 2 | C | 8829 | 0 | 8933 | 1694 | 0 |
| 2 | M | 8829 | 0 | 8933 | 1598 | 0 |
| 3 | D | 11864 | 0 | 12094 | 2489 | 0 |
| 3 | N | 11864 | 0 | 12094 | 2441 | 0 |
| 4 | E | 769 | 0 | 775 | 163 | 0 |
| 4 | O | 769 | 0 | 775 | 123 | 0 |
| 5 | F | 2829 | 0 | 2914 | 587 | 0 |
| 5 | P | 2829 | 0 | 2914 | 671 | 0 |
| 6 | A | 5 | 0 | 0 | 0 | 0 |
| 6 | D | 5 | 0 | 0 | 1 | 0 |
| 7 | B | 1 | 0 | 0 | 0 | 0 |
| 7 | D | 1 | 0 | 0 | 0 | 0 |
| 7 | N | 1 | 0 | 0 | 0 | 0 |
| 8 | D | 2 | 0 | 0 | 0 | 0 |
| 8 | N | 2 | 0 | 0 | 0 | 0 |
| 9 | D | 30 | 0 | 30 | 8 | 0 |
| 9 | N | 30 | 0 | 30 | 7 | 0 |
| 10 | C | 16 | 0 | 26 | 0 | 0 |
| 10 | M | 8 | 0 | 13 | 0 | 0 |
| 11 | A | 1 | 0 | 0 | 1 | 0 |
| 11 | B | 1 | 0 | 0 | 1 | 0 |
| 11 | C | 7 | 0 | 0 | 2 | 0 |
| 11 | D | 10 | 0 | 0 | 0 | 0 |
| 11 | F | 1 | 0 | 0 | 1 | 0 |
| 11 | M | 5 | 0 | 0 | 1 | 0 |
| 11 | N | 4 | 0 | 0 | 0 | 0 |
| 11 | O | 1 | 0 | 0 | 0 | 0 |
| All | All | 56149 | 0 | 57175 | 10419 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 92.

All (10419) 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) |
|-------------------|------------------|--------------------------|-------------------|
| 2:M:283:ILE:HG22 | 2:M:284:ARG:H | 1.03 | 1.17 |
| 3:D:416:ALA:HB2 | 3:D:432:TYR:HA | 1.19 | 1.17 |
| 3:D:1489:GLN:HA | 3:D:1492:LEU:HG | 1.23 | 1.17 |
| 3:N:272:LEU:HD12 | 3:N:280:ALA:HB3 | 1.23 | 1.16 |
| 3:N:322:VAL:HA | 3:N:335:LEU:HG | 1.20 | 1.16 |
| 1:A:14:ARG:HB2 | 1:B:233:VAL:HA | 1.27 | 1.16 |
| 2:C:178:PRO:O | 2:C:220:GLY:HA2 | 1.40 | 1.15 |
| 2:M:264:PRO:HB2 | 2:M:289:THR:HG21 | 1.24 | 1.15 |
| 3:N:416:ALA:HB2 | 3:N:432:TYR:HA | 1.16 | 1.15 |
| 3:D:237:LYS:HB3 | 3:D:238:PRO:HD2 | 1.25 | 1.15 |
| 3:D:1481:VAL:HG11 | 4:E:18:ARG:HA | 1.18 | 1.15 |
| 2:C:304:LEU:HB3 | 2:C:305:PRO:HD3 | 1.24 | 1.15 |
| 3:D:297:ILE:HD13 | 3:D:298:VAL:HG23 | 1.24 | 1.14 |
| 2:C:267:TYR:HB2 | 2:C:272:ALA:HB2 | 1.25 | 1.14 |
| 3:N:421:LEU:HG | 3:N:428:LYS:HA | 1.20 | 1.14 |
| 3:D:353:VAL:HA | 3:D:368:VAL:HG22 | 1.17 | 1.14 |
| 3:D:258:VAL:HB | 3:D:273:ARG:HB2 | 1.15 | 1.14 |
| 3:N:353:VAL:HA | 3:N:368:VAL:HG22 | 1.22 | 1.13 |
| 2:M:72:ARG:HG2 | 2:M:95:TYR:HB2 | 1.27 | 1.13 |
| 3:N:244:GLU:O | 3:N:246:PRO:HD3 | 1.49 | 1.13 |
| 3:D:249:TYR:HB3 | 3:D:307:ALA:HB3 | 1.14 | 1.13 |
| 3:D:931:LEU:HA | 3:D:934:LEU:HD12 | 1.30 | 1.12 |
| 2:C:580:MET:HB3 | 2:C:584:GLU:OE2 | 1.50 | 1.12 |
| 5:P:418:LEU:H | 5:P:418:LEU:HD12 | 1.08 | 1.12 |
| 3:N:1494:ALA:HA | 3:N:1497:GLU:HG2 | 1.16 | 1.12 |
| 3:D:274:ARG:HB3 | 3:D:279:VAL:HG21 | 1.26 | 1.11 |
| 2:M:15:LEU:H | 2:M:15:LEU:HD12 | 1.02 | 1.11 |
| 1:B:137:ARG:HH12 | 1:B:139:ASN:HB2 | 1.07 | 1.11 |
| 3:D:534:ARG:NH2 | 5:F:313:GLU:HB2 | 1.66 | 1.11 |
| 3:D:368:VAL:HB | 3:D:377:VAL:HG21 | 1.33 | 1.11 |
| 1:B:206:THR:HB | 1:B:209:GLU:HG3 | 1.32 | 1.10 |
| 1:L:76:VAL:HA | 1:L:79:ILE:HD12 | 1.33 | 1.10 |
| 2:M:150:PRO:HA | 2:M:158:TYR:HB3 | 1.26 | 1.10 |
| 3:D:1217:ILE:HD12 | 3:D:1217:ILE:H | 1.15 | 1.10 |
| 3:D:119:SER:HB3 | 3:D:123:LEU:H | 1.13 | 1.10 |
| 3:D:582:LEU:HA | 3:D:603:LEU:HD12 | 1.24 | 1.10 |
| 3:D:804:LEU:HB2 | 3:D:809:PRO:HG3 | 1.11 | 1.10 |
| 3:D:188:GLY:H | 3:D:198:ARG:HA | 0.99 | 1.10 |
| 2:C:31:GLN:HG2 | 2:C:35:PRO:HB3 | 1.25 | 1.10 |
| 3:N:548:ILE:HG22 | 3:N:552:ASN:HD21 | 1.11 | 1.09 |
| 5:F:413:SER:HA | 5:F:416:ARG:CZ | 1.81 | 1.09 |
| 2:C:72:ARG:HG2 | 2:C:95:TYR:HB2 | 1.31 | 1.09 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:34:VAL:HB | 1:B:42:ARG:HH12 | 1.02 | 1.09 |
| 2:M:230:ARG:HE | 2:M:233:GLU:HG2 | 1.06 | 1.09 |
| 3:N:237:LYS:HB3 | 3:N:238:PRO:HD2 | 1.28 | 1.09 |
| 3:D:530:VAL:HG23 | 3:D:531:ASP:H | 1.10 | 1.09 |
| 2:M:650:ARG:HE | 2:M:650:ARG:N | 1.50 | 1.09 |
| 3:D:658:LEU:HA | 3:D:661:MET:HE3 | 1.25 | 1.09 |
| 2:C:59:LYS:HD2 | 2:C:59:LYS:H | 1.18 | 1.09 |
| 1:A:206:THR:HB | 1:A:209:GLU:HG3 | 1.33 | 1.09 |
| 3:N:227:LEU:HA | 3:N:331:VAL:HG23 | 1.18 | 1.08 |
| 5:F:113:ILE:HA | 5:F:116:LEU:HD12 | 1.35 | 1.08 |
| 3:N:1101:VAL:HG22 | 3:N:1428:ALA:HB2 | 1.30 | 1.08 |
| 2:C:115:LEU:HD11 | 2:C:373:VAL:CG1 | 1.83 | 1.08 |
| 2:M:192:PRO:O | 2:M:195:LEU:HG | 1.53 | 1.08 |
| 5:P:302:LYS:HD2 | 5:P:303:ARG:N | 1.68 | 1.08 |
| 3:N:148:GLU:HB3 | 3:N:151:GLN:HB2 | 1.34 | 1.08 |
| 3:D:33:ASN:HD21 | 3:D:35:ARG:HG2 | 0.91 | 1.08 |
| 3:N:245:LEU:HA | 3:N:309:GLY:H | 1.19 | 1.07 |
| 3:N:675:ARG:HH22 | 5:P:420:ASP:HB3 | 1.11 | 1.07 |
| 5:P:368:VAL:HG23 | 5:P:369:LEU:H | 1.12 | 1.07 |
| 2:C:230:ARG:HG2 | 2:C:233:GLU:HG3 | 1.35 | 1.07 |
| 2:M:762:LYS:HG2 | 2:M:763:GLY:H | 1.19 | 1.07 |
| 1:K:12:THR:HA | 1:L:229:GLN:HB3 | 1.29 | 1.07 |
| 3:N:36:THR:HB | 3:N:38:LYS:HG2 | 1.36 | 1.07 |
| 3:N:407:VAL:HG22 | 3:N:408:GLU:H | 1.17 | 1.07 |
| 2:C:776:SER:HA | 2:C:780:GLU:HB2 | 1.10 | 1.07 |
| 3:D:356:PRO:HB3 | 3:D:440:VAL:HB | 1.37 | 1.07 |
| 3:N:361:VAL:HG13 | 3:N:365:ASP:HB3 | 1.28 | 1.07 |
| 5:F:280:GLN:HG3 | 5:F:281:GLU:H | 1.09 | 1.07 |
| 2:M:250:ARG:HB3 | 2:M:253:ALA:HB2 | 1.36 | 1.06 |
| 5:F:210:LEU:HA | 5:F:213:ILE:HD12 | 1.23 | 1.06 |
| 3:N:567:ILE:HG22 | 3:N:571:LYS:HE3 | 1.37 | 1.06 |
| 3:D:182:GLY:HA2 | 3:D:203:ALA:HB3 | 1.31 | 1.06 |
| 2:C:368:THR:HB | 2:C:369:PRO:HD3 | 1.37 | 1.06 |
| 3:D:812:ALA:HA | 3:D:816:HIS:HB2 | 1.37 | 1.06 |
| 1:A:14:ARG:HD2 | 1:B:234:ALA:H | 1.14 | 1.06 |
| 5:P:210:LEU:HA | 5:P:213:ILE:HD12 | 1.38 | 1.05 |
| 4:O:41:GLU:HB2 | 4:O:42:PRO:HD2 | 1.35 | 1.05 |
| 3:N:1286:THR:HG22 | 3:N:1288:GLU:H | 1.10 | 1.05 |
| 3:N:1486:VAL:HG21 | 4:O:22:VAL:HG13 | 1.39 | 1.05 |
| 3:D:1152:GLU:N | 3:D:1162:GLU:HB3 | 1.72 | 1.05 |
| 3:N:266:GLU:HB3 | 3:N:286:VAL:CG2 | 1.87 | 1.05 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:1217:ILE:H | 3:N:1217:ILE:HD12 | 1.21 | 1.05 |
| 5:P:278:LEU:HB2 | 5:P:286:PRO:HG3 | 1.36 | 1.05 |
| 3:N:133:ILE:HG23 | 3:N:456:MET:HE1 | 1.39 | 1.05 |
| 3:D:47:GLU:HB2 | 3:D:51:GLY:O | 1.57 | 1.05 |
| 2:M:772:ARG:HE | 5:P:373:LYS:HG3 | 1.17 | 1.05 |
| 3:D:437:VAL:HG11 | 5:F:175:HIS:HB3 | 1.37 | 1.04 |
| 3:D:227:LEU:HA | 3:D:331:VAL:HG23 | 1.06 | 1.04 |
| 2:C:150:PRO:HA | 2:C:158:TYR:HB3 | 1.07 | 1.04 |
| 2:C:192:PRO:HB2 | 2:C:195:LEU:HD21 | 1.40 | 1.04 |
| 2:C:195:LEU:HD23 | 2:C:195:LEU:H | 1.22 | 1.04 |
| 3:N:1412:LYS:O | 3:N:1414:PRO:HD3 | 1.57 | 1.04 |
| 3:D:253:ALA:H | 3:D:301:GLY:HA3 | 1.21 | 1.04 |
| 2:M:650:ARG:H | 2:M:650:ARG:NE | 1.55 | 1.04 |
| 3:D:1101:VAL:HG21 | 3:D:1424:VAL:HB | 1.36 | 1.04 |
| 3:D:33:ASN:ND2 | 3:D:35:ARG:HG2 | 1.73 | 1.04 |
| 2:C:776:SER:CA | 2:C:780:GLU:HB2 | 1.86 | 1.04 |
| 2:C:100:LEU:HD23 | 2:C:368:THR:HA | 1.05 | 1.03 |
| 2:M:197:LEU:HB3 | 2:M:207:LEU:HD13 | 1.41 | 1.03 |
| 3:D:804:LEU:HB2 | 3:D:809:PRO:CG | 1.89 | 1.03 |
| 1:B:179:PHE:HB3 | 1:B:197:LEU:HD13 | 1.40 | 1.03 |
| 1:L:101:LEU:HD13 | 1:L:114:PHE:HA | 1.40 | 1.03 |
| 2:C:15:LEU:HD12 | 2:C:15:LEU:H | 1.19 | 1.03 |
| 2:C:166:PRO:HG2 | 2:C:169:GLY:HA3 | 1.39 | 1.03 |
| 4:E:6:ILE:HA | 4:E:9:LEU:HD12 | 1.35 | 1.03 |
| 1:L:104:GLU:HB3 | 1:L:137:ARG:HG3 | 1.41 | 1.03 |
| 2:M:6:PHE:HB3 | 2:M:908:GLY:HA2 | 1.41 | 1.03 |
| 3:N:1267:ARG:NH1 | 3:N:1267:ARG:HB2 | 1.73 | 1.03 |
| 3:D:951:ILE:HD11 | 3:D:1062:ARG:HG3 | 1.41 | 1.03 |
| 2:C:1115:LEU:HB3 | 3:D:85:VAL:HG23 | 1.39 | 1.03 |
| 3:N:121:THR:HG23 | 3:N:122:GLU:H | 1.19 | 1.02 |
| 3:N:142:LEU:HB3 | 3:N:146:PRO:HA | 1.38 | 1.02 |
| 2:M:274:ARG:HH21 | 2:M:284:ARG:HB3 | 1.22 | 1.02 |
| 3:N:417:PRO:HB3 | 3:N:430:ASP:HA | 1.38 | 1.02 |
| 3:D:957:PRO:HG3 | 3:D:1010:ASN:HD22 | 1.19 | 1.02 |
| 3:D:820:GLU:HG3 | 3:D:836:VAL:HG11 | 1.40 | 1.02 |
| 3:N:965:GLU:HG3 | 3:N:969:ARG:HH21 | 1.20 | 1.02 |
| 5:P:136:LEU:HB3 | 5:P:140:ARG:HD3 | 1.36 | 1.02 |
| 1:B:188:GLN:HG2 | 1:B:189:ARG:H | 1.18 | 1.02 |
| 3:D:534:ARG:HH21 | 5:F:313:GLU:HB2 | 1.18 | 1.02 |
| 3:D:660:LYS:HG3 | 3:D:694:VAL:HG22 | 1.37 | 1.02 |
| 3:D:295:GLY:HA2 | 3:D:302:GLN:HB3 | 1.37 | 1.02 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:101:LEU:HD13 | 1:B:114:PHE:HA | 1.37 | 1.02 |
| 2:C:65:VAL:O | 2:C:100:LEU:HA | 1.56 | 1.02 |
| 2:M:108:ILE:HB | 2:M:368:THR:HG21 | 1.40 | 1.02 |
| 2:C:988:VAL:HG12 | 3:D:948:THR:HB | 1.42 | 1.02 |
| 3:D:433:GLY:HA2 | 3:D:449:SER:H | 1.20 | 1.02 |
| 3:D:1171:VAL:HA | 3:D:1174:LEU:HD12 | 1.42 | 1.02 |
| 3:N:60:CYS:SG | 3:N:62:LYS:HG2 | 1.99 | 1.02 |
| 3:D:1128:VAL:CG2 | 3:D:1131:SER:HB3 | 1.88 | 1.02 |
| 2:M:1101:THR:HB | 3:N:5:VAL:HG21 | 1.37 | 1.02 |
| 3:D:554:LEU:HA | 3:D:557:LEU:HD12 | 1.40 | 1.01 |
| 2:C:904:PRO:HB2 | 2:C:907:ASP:HB3 | 1.42 | 1.01 |
| 2:C:195:LEU:HB2 | 2:C:238:LEU:HD21 | 1.41 | 1.01 |
| 3:D:127:LEU:HD23 | 3:D:128:TYR:N | 1.76 | 1.01 |
| 3:D:411:THR:HB | 3:D:437:VAL:HB | 1.39 | 1.01 |
| 3:N:490:ALA:HA | 3:N:493:ARG:HE | 1.25 | 1.01 |
| 3:D:534:ARG:HE | 5:F:314:PRO:HA | 1.26 | 1.01 |
| 2:C:910:LYS:HG3 | 2:C:912:PRO:HD2 | 1.39 | 1.01 |
| 3:N:1033:GLN:H | 3:N:1033:GLN:CD | 1.63 | 1.01 |
| 2:M:751:PRO:HB3 | 2:M:794:PRO:HA | 1.42 | 1.01 |
| 2:C:283:ILE:HG22 | 2:C:284:ARG:H | 1.20 | 1.00 |
| 2:C:542:VAL:HG23 | 2:C:543:ASN:H | 1.24 | 1.00 |
| 3:D:355:VAL:HG11 | 3:D:385:VAL:HG21 | 1.41 | 1.00 |
| 3:D:284:LEU:HD12 | 3:D:290:PRO:HB3 | 1.43 | 1.00 |
| 2:C:41:ASN:HA | 2:C:45:GLN:HB3 | 1.42 | 1.00 |
| 3:N:253:ALA:H | 3:N:301:GLY:HA3 | 1.26 | 1.00 |
| 3:N:411:THR:HG21 | 5:P:179:GLU:HG3 | 1.40 | 1.00 |
| 2:M:260:LEU:HD13 | 2:M:291:ALA:HB2 | 1.41 | 1.00 |
| 2:M:580:MET:HB3 | 2:M:584:GLU:CD | 1.81 | 1.00 |
| 5:F:214:GLN:HA | 5:F:217:ASN:HD22 | 1.26 | 1.00 |
| 3:D:440:VAL:HG23 | 3:D:441:ARG:H | 1.26 | 1.00 |
| 1:K:188:GLN:HG3 | 1:K:189:ARG:H | 1.23 | 1.00 |
| 3:N:147:VAL:HG22 | 3:N:148:GLU:H | 1.23 | 1.00 |
| 2:M:175:GLU:HG2 | 2:M:176:VAL:H | 1.24 | 1.00 |
| 2:M:230:ARG:NH2 | 2:M:237:ARG:HH22 | 1.58 | 1.00 |
| 3:N:1098:LEU:HD12 | 3:N:1098:LEU:H | 1.24 | 1.00 |
| 2:M:194:VAL:HA | 2:M:197:LEU:HG | 1.44 | 0.99 |
| 2:C:1115:LEU:HD13 | 3:D:85:VAL:HB | 1.44 | 0.99 |
| 2:M:413:LEU:HA | 2:M:419:THR:HG21 | 1.40 | 0.99 |
| 3:N:118:LEU:HA | 3:N:123:LEU:HD12 | 1.40 | 0.99 |
| 3:D:148:GLU:HB3 | 3:D:151:GLN:HB2 | 1.44 | 0.99 |
| 3:N:843:PHE:HE2 | 3:N:864:VAL:HG11 | 1.26 | 0.99 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:D:206:ARG:HE | 3:D:394:LEU:HB2 | 1.26 | 0.99 |
| 2:M:470:PRO:HG3 | 2:M:485:TYR:CZ | 1.97 | 0.99 |
| 2:M:230:ARG:HH21 | 2:M:237:ARG:NH2 | 1.58 | 0.99 |
| 3:D:249:TYR:CE1 | 3:D:330:THR:HG21 | 1.97 | 0.99 |
| 5:F:418:LEU:H | 5:F:418:LEU:HD12 | 1.27 | 0.99 |
| 2:C:100:LEU:CD2 | 2:C:368:THR:HA | 1.93 | 0.99 |
| 2:M:186:VAL:HG13 | 2:M:187:ASN:H | 1.28 | 0.99 |
| 1:L:161:ARG:HB2 | 1:L:164:ALA:HB2 | 1.45 | 0.99 |
| 2:M:909:ALA:HB1 | 2:M:914:ILE:HD11 | 1.42 | 0.99 |
| 3:D:361:VAL:HG13 | 3:D:379:ALA:HB1 | 1.44 | 0.99 |
| 3:D:483:HIS:HB2 | 3:D:484:PRO:HD3 | 1.41 | 0.99 |
| 2:C:694:LEU:HD21 | 2:C:868:ASP:HB3 | 1.44 | 0.99 |
| 3:N:254:GLU:O | 3:N:299:GLU:HB2 | 1.61 | 0.99 |
| 2:C:737:LEU:HA | 2:C:743:VAL:HA | 1.45 | 0.99 |
| 2:M:301:GLU:HA | 2:M:304:LEU:HD22 | 1.41 | 0.99 |
| 3:D:1383:ASP:HB3 | 3:D:1416:ALA:H | 1.24 | 0.99 |
| 3:N:826:PRO:O | 3:N:829:VAL:HG22 | 1.63 | 0.99 |
| 1:L:241:GLU:H | 1:L:242:PRO:HD2 | 1.27 | 0.99 |
| 1:B:104:GLU:HB3 | 1:B:137:ARG:HG3 | 1.41 | 0.98 |
| 3:D:206:ARG:HH21 | 3:D:394:LEU:HD13 | 1.24 | 0.98 |
| 2:M:542:VAL:HG23 | 2:M:543:ASN:H | 1.26 | 0.98 |
| 3:D:257:GLY:HA2 | 3:D:274:ARG:HA | 1.43 | 0.98 |
| 2:M:987:ILE:HG23 | 3:N:948:THR:HG21 | 1.45 | 0.98 |
| 3:N:274:ARG:HB3 | 3:N:279:VAL:HG21 | 1.45 | 0.98 |
| 2:C:56:GLU:OE2 | 2:C:356:ARG:HA | 1.61 | 0.98 |
| 2:M:243:ARG:HG3 | 2:M:244:PRO:HA | 1.44 | 0.98 |
| 3:D:1161:GLU:HG3 | 3:D:1164:ARG:HB2 | 1.43 | 0.98 |
| 2:C:257:VAL:HA | 2:C:261:ILE:HD12 | 1.39 | 0.98 |
| 1:A:41:ARG:HA | 1:A:44:LEU:HD12 | 1.45 | 0.98 |
| 5:P:75:ILE:HG13 | 5:P:76:SER:H | 1.27 | 0.97 |
| 3:D:227:LEU:HD11 | 3:D:326:GLU:HA | 1.46 | 0.97 |
| 3:N:584:ASN:OD1 | 3:N:590:PRO:HD2 | 1.61 | 0.97 |
| 4:E:40:LEU:HD12 | 4:E:41:GLU:H | 1.30 | 0.97 |
| 2:M:226:VAL:HG23 | 2:M:227:PHE:HD1 | 1.30 | 0.97 |
| 2:M:304:LEU:HB3 | 2:M:305:PRO:HD3 | 1.44 | 0.97 |
| 5:P:208:SER:HB3 | 5:P:211:ASP:OD2 | 1.65 | 0.97 |
| 2:M:690:ILE:HG22 | 2:M:852:ILE:HG23 | 1.46 | 0.97 |
| 3:N:1171:VAL:HA | 3:N:1174:LEU:HD12 | 1.45 | 0.97 |
| 5:F:81:VAL:HG23 | 5:F:82:ARG:H | 1.28 | 0.97 |
| 1:L:73:GLU:HG3 | 1:L:130:ALA:HB1 | 1.47 | 0.97 |
| 2:M:1056:LYS:HE2 | 3:N:625:TYR:HB2 | 1.46 | 0.97 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:P:343:ASP:HB3 | 5:P:347:GLN:HE22 | 1.30 | 0.97 |
| 5:F:385:GLU:HA | 5:F:388:ALA:HB3 | 1.42 | 0.96 |
| 1:B:76:VAL:HA | 1:B:79:ILE:HD12 | 1.44 | 0.96 |
| 3:D:1277:ILE:HG22 | 3:D:1278:ASP:H | 1.29 | 0.96 |
| 2:C:238:LEU:O | 2:C:241:LEU:HG | 1.64 | 0.96 |
| 2:M:257:VAL:HA | 2:M:261:ILE:HD12 | 1.46 | 0.96 |
| 3:D:227:LEU:HA | 3:D:331:VAL:CG2 | 1.94 | 0.96 |
| 2:M:600:ASP:HB3 | 2:M:650:ARG:HA | 1.45 | 0.96 |
| 3:N:133:ILE:HB | 3:N:454:ALA:HB1 | 1.46 | 0.96 |
| 2:C:650:ARG:H | 2:C:650:ARG:NE | 1.63 | 0.96 |
| 2:C:267:TYR:HB2 | 2:C:272:ALA:CB | 1.95 | 0.96 |
| 5:P:214:GLN:HA | 5:P:217:ASN:HD22 | 1.28 | 0.96 |
| 2:C:363:SER:HB2 | 2:C:366:SER:HB3 | 1.43 | 0.96 |
| 3:D:137:PRO:HD2 | 3:D:453:ASP:HB3 | 1.48 | 0.96 |
| 1:B:185:ARG:HA | 1:B:190:THR:HA | 1.47 | 0.96 |
| 3:D:843:PHE:HE2 | 3:D:864:VAL:HG11 | 1.29 | 0.96 |
| 3:D:245:LEU:H | 3:D:309:GLY:CA | 1.77 | 0.96 |
| 2:C:625:LEU:HD11 | 2:C:639:GLN:HB2 | 1.45 | 0.96 |
| 2:C:926:PHE:HE2 | 2:C:960:GLU:HG3 | 1.31 | 0.96 |
| 3:N:249:TYR:HB3 | 3:N:307:ALA:HB3 | 1.46 | 0.95 |
| 5:P:368:VAL:HG23 | 5:P:369:LEU:HG | 1.47 | 0.95 |
| 2:M:59:LYS:HD2 | 2:M:59:LYS:N | 1.81 | 0.95 |
| 1:L:206:THR:HB | 1:L:209:GLU:HG3 | 1.47 | 0.95 |
| 3:N:22:SER:HA | 3:N:90:MET:O | 1.66 | 0.95 |
| 3:D:139:GLY:O | 3:D:147:VAL:HB | 1.65 | 0.95 |
| 2:C:650:ARG:N | 2:C:650:ARG:HE | 1.63 | 0.95 |
| 3:N:540:LEU:HA | 3:N:543:LEU:HD12 | 1.47 | 0.95 |
| 3:N:1267:ARG:HH21 | 3:N:1271:LYS:HZ1 | 0.99 | 0.95 |
| 3:N:1341:PRO:HG2 | 3:N:1342:GLU:OE2 | 1.67 | 0.95 |
| 2:M:839:LEU:HD23 | 2:M:996:LYS:HA | 1.45 | 0.95 |
| 3:N:542:ASP:O | 3:N:546:ARG:HG2 | 1.66 | 0.95 |
| 3:D:223:LEU:O | 3:D:332:TYR:HA | 1.67 | 0.95 |
| 2:C:881:ASN:HD22 | 2:C:881:ASN:H | 0.98 | 0.95 |
| 3:N:827:ILE:HA | 3:N:836:VAL:HB | 1.48 | 0.95 |
| 2:M:93:PRO:HA | 2:M:117:HIS:HB3 | 1.49 | 0.95 |
| 3:N:485:SER:O | 3:N:489:ARG:HD3 | 1.66 | 0.95 |
| 3:N:217:LYS:HB2 | 3:N:339:TRP:HE1 | 1.30 | 0.95 |
| 2:M:21:ILE:HD12 | 2:M:21:ILE:H | 1.29 | 0.95 |
| 3:D:543:LEU:HA | 3:D:546:ARG:HD3 | 1.47 | 0.95 |
| 2:M:368:THR:H | 2:M:369:PRO:CD | 1.80 | 0.94 |
| 3:D:30:GLU:HB3 | 3:D:40:GLU:HG2 | 1.48 | 0.94 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:417:PRO:HB2 | 3:D:428:LYS:HG2 | 1.49 | 0.94 |
| 3:D:249:TYR:CB | 3:D:307:ALA:HB3 | 1.97 | 0.94 |
| 3:D:248:PRO:HA | 3:D:308:LYS:HZ3 | 1.31 | 0.94 |
| 2:M:474:VAL:HG12 | 2:M:530:GLU:O | 1.66 | 0.94 |
| 5:F:215:GLU:O | 5:F:218:GLN:HG3 | 1.67 | 0.94 |
| 3:D:408:GLU:OE2 | 3:D:421:LEU:HG | 1.68 | 0.94 |
| 1:A:39:PRO:HG3 | 1:B:39:PRO:HG3 | 1.49 | 0.94 |
| 3:N:654:LYS:HB3 | 3:N:655:PRO:HD3 | 1.46 | 0.94 |
| 3:D:147:VAL:HG22 | 3:D:148:GLU:H | 1.32 | 0.94 |
| 3:D:187:LYS:HG3 | 3:D:198:ARG:HG3 | 1.50 | 0.94 |
| 2:C:31:GLN:HG2 | 2:C:35:PRO:CB | 1.97 | 0.94 |
| 2:C:38:LYS:HG3 | 2:C:39:ARG:H | 1.32 | 0.94 |
| 3:D:485:SER:O | 3:D:489:ARG:HD3 | 1.67 | 0.94 |
| 3:N:349:PRO:HB2 | 5:P:232:ARG:HH22 | 1.32 | 0.94 |
| 5:F:392:VAL:HG11 | 5:F:396:ARG:HD3 | 1.49 | 0.94 |
| 1:A:76:VAL:HA | 1:A:79:ILE:HD12 | 1.49 | 0.94 |
| 1:L:235:ALA:HB3 | 1:L:236:PRO:HD3 | 1.50 | 0.94 |
| 3:D:421:LEU:HD23 | 3:D:427:VAL:HG12 | 1.47 | 0.94 |
| 3:D:631:ILE:HG21 | 3:D:745:MET:HG3 | 1.48 | 0.94 |
| 3:D:1353:GLN:O | 3:D:1357:ARG:HG2 | 1.68 | 0.94 |
| 3:N:127:LEU:HD23 | 3:N:128:TYR:N | 1.83 | 0.93 |
| 3:D:928:ALA:HA | 3:D:931:LEU:HD12 | 1.50 | 0.93 |
| 1:K:110:LYS:HB2 | 1:K:112:ARG:HG2 | 1.48 | 0.93 |
| 2:M:230:ARG:NE | 2:M:233:GLU:HG2 | 1.83 | 0.93 |
| 3:D:188:GLY:N | 3:D:198:ARG:HA | 1.82 | 0.93 |
| 3:N:15:PRO:HA | 3:N:18:ILE:HD12 | 1.50 | 0.93 |
| 2:M:1058:ASP:OD2 | 2:M:1084:SER:HB3 | 1.69 | 0.93 |
| 2:M:31:GLN:HG2 | 2:M:35:PRO:HB3 | 1.48 | 0.93 |
| 3:N:906:GLN:HB3 | 3:N:911:LEU:HD21 | 1.47 | 0.93 |
| 2:M:1047:HIS:O | 2:M:1051:GLU:HG2 | 1.68 | 0.93 |
| 2:C:503:LEU:HD12 | 2:C:508:ILE:HA | 1.50 | 0.93 |
| 2:C:21:ILE:HD12 | 2:C:21:ILE:H | 1.30 | 0.93 |
| 3:D:543:LEU:O | 3:D:546:ARG:HG3 | 1.67 | 0.93 |
| 5:F:379:ARG:HD3 | 5:F:380:GLU:HB2 | 1.50 | 0.93 |
| 5:F:282:LEU:HG | 5:F:284:ARG:HG2 | 1.49 | 0.93 |
| 3:N:931:LEU:HA | 3:N:934:LEU:HD12 | 1.49 | 0.93 |
| 2:C:654:LEU:HD12 | 2:C:655:LEU:H | 1.33 | 0.92 |
| 2:C:751:PRO:HB3 | 2:C:794:PRO:HA | 1.51 | 0.92 |
| 3:N:535:PHE:O | 5:P:314:PRO:HB2 | 1.69 | 0.92 |
| 2:M:397:GLU:H | 2:M:633:GLN:HE21 | 1.18 | 0.92 |
| 2:C:182:VAL:HB | 2:C:193:LEU:H | 1.34 | 0.92 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:128:TYR:HD1 | 3:D:457:GLY:HA2 | 1.35 | 0.92 |
| 1:B:112:ARG:NH1 | 1:B:112:ARG:HB3 | 1.84 | 0.92 |
| 2:C:115:LEU:HD11 | 2:C:373:VAL:HG12 | 1.49 | 0.92 |
| 3:D:954:ALA:HB3 | 3:D:1062:ARG:HD2 | 1.52 | 0.92 |
| 2:C:909:ALA:HB1 | 2:C:914:ILE:HD11 | 1.48 | 0.92 |
| 1:K:122:ILE:HG22 | 1:K:124:ASN:H | 1.30 | 0.92 |
| 3:D:1172:HIS:HA | 3:D:1175:ILE:HD12 | 1.48 | 0.92 |
| 3:N:348:GLN:H | 3:N:351:MET:HE2 | 1.30 | 0.92 |
| 3:N:1498:ALA:HB3 | 4:O:84:ARG:CZ | 2.00 | 0.92 |
| 3:N:699:VAL:HG12 | 3:N:717:GLN:HG2 | 1.49 | 0.92 |
| 1:B:41:ARG:HA | 1:B:44:LEU:HD12 | 1.49 | 0.92 |
| 3:D:957:PRO:HG2 | 3:D:1007:VAL:HA | 1.52 | 0.92 |
| 3:D:1128:VAL:HG21 | 3:D:1131:SER:HB3 | 1.48 | 0.92 |
| 2:M:1101:THR:HB | 3:N:5:VAL:CG2 | 1.99 | 0.92 |
| 2:C:166:PRO:HG2 | 2:C:169:GLY:CA | 2.00 | 0.92 |
| 3:N:553:ARG:HH12 | 5:P:211:ASP:HA | 1.33 | 0.92 |
| 3:N:358:GLY:HA2 | 3:N:385:VAL:HB | 1.51 | 0.92 |
| 2:M:503:LEU:HD12 | 2:M:508:ILE:HA | 1.50 | 0.92 |
| 3:N:297:ILE:HG23 | 3:N:298:VAL:H | 1.35 | 0.92 |
| 3:N:806:PHE:HA | 3:N:809:PRO:HD2 | 1.49 | 0.92 |
| 3:N:131:LYS:HA | 3:N:456:MET:HG3 | 1.52 | 0.92 |
| 3:N:82:LYS:HB2 | 3:N:84:ILE:HG22 | 1.50 | 0.92 |
| 3:D:118:LEU:HA | 3:D:123:LEU:HD12 | 1.52 | 0.92 |
| 3:D:1405:GLU:O | 3:D:1412:LYS:HA | 1.70 | 0.92 |
| 1:K:152:PRO:HG2 | 1:K:155:LYS:HB2 | 1.50 | 0.92 |
| 1:B:38:ASN:HB3 | 1:B:39:PRO:HD3 | 1.51 | 0.91 |
| 1:L:137:ARG:HH12 | 1:L:139:ASN:HB2 | 1.33 | 0.91 |
| 2:M:1058:ASP:O | 2:M:1083:GLU:HG2 | 1.70 | 0.91 |
| 2:M:325:ILE:HD12 | 2:M:325:ILE:H | 1.34 | 0.91 |
| 3:D:253:ALA:H | 3:D:301:GLY:CA | 1.84 | 0.91 |
| 3:D:930:LEU:HG | 3:D:934:LEU:HD11 | 1.53 | 0.91 |
| 3:N:138:LYS:HB3 | 3:N:450:TYR:OH | 1.67 | 0.91 |
| 3:N:565:ILE:HG23 | 3:N:566:ILE:H | 1.33 | 0.91 |
| 3:N:368:VAL:HB | 3:N:377:VAL:HG21 | 1.50 | 0.91 |
| 2:C:1104:GLU:HA | 3:D:7:LYS:NZ | 1.86 | 0.91 |
| 3:N:408:GLU:HB3 | 3:N:422:ALA:HB2 | 1.50 | 0.91 |
| 1:L:197:LEU:HD12 | 1:L:198:ARG:H | 1.33 | 0.91 |
| 2:M:185:LYS:HG2 | 2:M:190:LYS:HD3 | 1.50 | 0.91 |
| 2:C:305:PRO:HA | 2:C:308:ARG:NE | 1.86 | 0.91 |
| 3:D:313:MET:SD | 3:D:314:PRO:HD2 | 2.10 | 0.91 |
| 2:M:238:LEU:O | 2:M:241:LEU:HG | 1.71 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:M:264:PRO:HB2 | 2:M:289:THR:CG2 | 2.01 | 0.91 |
| 1:L:233:VAL:O | 1:L:236:PRO:HD2 | 1.69 | 0.91 |
| 3:N:800:LYS:HD2 | 3:N:800:LYS:C | 1.91 | 0.91 |
| 1:A:34:VAL:HB | 1:B:42:ARG:NH1 | 1.85 | 0.91 |
| 3:N:1345:GLU:HA | 3:N:1348:LEU:HD12 | 1.51 | 0.91 |
| 2:C:317:VAL:N | 2:C:318:PRO:HD3 | 1.85 | 0.91 |
| 3:D:133:ILE:HG23 | 3:D:456:MET:HG3 | 1.50 | 0.91 |
| 3:D:610:LYS:NZ | 3:D:1442:ASN:H | 1.68 | 0.91 |
| 4:E:37:ASN:N | 4:E:37:ASN:HD22 | 1.69 | 0.91 |
| 3:D:245:LEU:H | 3:D:309:GLY:HA2 | 1.34 | 0.91 |
| 5:P:343:ASP:HB3 | 5:P:347:GLN:NE2 | 1.86 | 0.91 |
| 2:C:72:ARG:CG | 2:C:95:TYR:HB2 | 2.01 | 0.91 |
| 5:F:189:GLU:HA | 5:F:192:LEU:HG | 1.50 | 0.91 |
| 2:M:628:PHE:HD1 | 2:M:628:PHE:H | 1.17 | 0.91 |
| 3:N:484:PRO:O | 3:N:489:ARG:HB2 | 1.71 | 0.91 |
| 3:D:417:PRO:HB3 | 3:D:430:ASP:N | 1.85 | 0.91 |
| 3:D:137:PRO:CD | 3:D:453:ASP:HB3 | 2.01 | 0.90 |
| 2:C:910:LYS:HG2 | 2:C:913:GLU:HG3 | 1.50 | 0.90 |
| 1:K:76:VAL:HA | 1:K:79:ILE:HD12 | 1.52 | 0.90 |
| 3:D:416:ALA:HB2 | 3:D:432:TYR:CA | 2.00 | 0.90 |
| 2:M:1038:TRP:HA | 2:M:1041:GLU:OE1 | 1.70 | 0.90 |
| 2:C:150:PRO:HA | 2:C:158:TYR:CB | 1.98 | 0.90 |
| 2:C:186:VAL:HG23 | 2:C:187:ASN:H | 1.33 | 0.90 |
| 2:M:585:GLU:O | 2:M:588:VAL:HG22 | 1.71 | 0.90 |
| 1:K:206:THR:HB | 1:K:209:GLU:HG3 | 1.52 | 0.90 |
| 2:C:759:THR:HB | 2:C:785:VAL:HG12 | 1.53 | 0.90 |
| 2:C:776:SER:HA | 2:C:780:GLU:CB | 2.00 | 0.90 |
| 1:L:73:GLU:HG3 | 1:L:130:ALA:CB | 2.01 | 0.90 |
| 3:D:1489:GLN:HA | 3:D:1492:LEU:CG | 2.01 | 0.90 |
| 2:C:415:PRO:HB2 | 2:C:418:LEU:HB2 | 1.51 | 0.90 |
| 2:M:679:PHE:HA | 3:N:943:THR:HG23 | 1.52 | 0.90 |
| 1:B:235:ALA:HB3 | 1:B:236:PRO:HD3 | 1.53 | 0.90 |
| 3:D:243:ALA:HB3 | 3:D:311:LEU:HD12 | 1.52 | 0.90 |
| 1:B:212:ASN:O | 1:B:215:VAL:HG22 | 1.72 | 0.90 |
| 3:D:820:GLU:HG3 | 3:D:836:VAL:CG1 | 2.00 | 0.90 |
| 3:N:217:LYS:HB2 | 3:N:339:TRP:NE1 | 1.86 | 0.90 |
| 3:N:241:ILE:HD13 | 3:N:310:LEU:HD22 | 1.52 | 0.90 |
| 3:N:147:VAL:HG22 | 3:N:148:GLU:N | 1.86 | 0.90 |
| 2:M:15:LEU:N | 2:M:15:LEU:HD12 | 1.87 | 0.90 |
| 2:C:115:LEU:HD11 | 2:C:373:VAL:HG11 | 1.53 | 0.90 |
| 5:P:367:MET:HB2 | 5:P:371:LEU:HG | 1.53 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:58:ILE:HG12 | 1:L:140:MET:CB | 2.02 | 0.90 |
| 1:L:36:LEU:O | 1:L:39:PRO:HD2 | 1.72 | 0.90 |
| 3:N:219:GLU:HG2 | 3:N:220:ARG:H | 1.35 | 0.90 |
| 3:N:52:PRO:O | 3:N:86:ARG:HD2 | 1.71 | 0.90 |
| 3:D:367:ILE:HB | 3:D:377:VAL:HG12 | 1.53 | 0.90 |
| 2:M:15:LEU:H | 2:M:15:LEU:CD1 | 1.78 | 0.90 |
| 1:A:226:SER:O | 1:A:228:PRO:HD3 | 1.72 | 0.90 |
| 3:N:249:TYR:CB | 3:N:307:ALA:HB3 | 2.01 | 0.90 |
| 3:N:322:VAL:HA | 3:N:335:LEU:CG | 2.01 | 0.90 |
| 5:F:265:VAL:HA | 5:F:268:ILE:HD12 | 1.54 | 0.90 |
| 2:C:290:LEU:HD22 | 2:C:302:VAL:HG21 | 1.51 | 0.90 |
| 3:D:368:VAL:HB | 3:D:377:VAL:CG2 | 2.01 | 0.90 |
| 2:M:958:THR:HG23 | 2:M:961:GLU:HB2 | 1.53 | 0.90 |
| 3:D:1481:VAL:CG1 | 4:E:18:ARG:HA | 2.02 | 0.89 |
| 1:L:143:ARG:HD3 | 1:L:144:VAL:N | 1.85 | 0.89 |
| 2:C:1000:MET:HB3 | 2:C:1002:GLU:HG3 | 1.53 | 0.89 |
| 4:E:41:GLU:HB2 | 4:E:42:PRO:HD2 | 1.53 | 0.89 |
| 3:N:410:SER:HB3 | 5:P:175:HIS:ND1 | 1.88 | 0.89 |
| 2:C:676:ILE:HG23 | 2:C:988:VAL:HG13 | 1.55 | 0.89 |
| 1:B:151:VAL:HB | 1:B:169:ALA:HB3 | 1.53 | 0.89 |
| 2:C:59:LYS:N | 2:C:59:LYS:HD2 | 1.88 | 0.89 |
| 5:P:321:ILE:HG13 | 5:P:332:PHE:CE1 | 2.08 | 0.89 |
| 2:M:230:ARG:O | 2:M:233:GLU:HG3 | 1.70 | 0.89 |
| 2:C:516:ARG:HA | 2:C:520:GLU:O | 1.72 | 0.89 |
| 3:D:266:GLU:HB2 | 3:D:314:PRO:HG3 | 1.55 | 0.89 |
| 5:P:413:SER:HA | 5:P:416:ARG:CZ | 2.03 | 0.89 |
| 1:A:86:VAL:HG12 | 1:A:124:ASN:HD21 | 1.35 | 0.89 |
| 2:C:151:ASP:H | 2:C:158:TYR:HA | 1.38 | 0.89 |
| 5:P:265:VAL:HA | 5:P:268:ILE:HD12 | 1.54 | 0.89 |
| 1:K:9:PRO:HG3 | 1:K:27:PRO:O | 1.70 | 0.89 |
| 3:D:387:LEU:H | 3:D:387:LEU:HD12 | 1.36 | 0.89 |
| 3:N:322:VAL:CA | 3:N:335:LEU:HG | 2.03 | 0.89 |
| 3:D:227:LEU:CA | 3:D:331:VAL:HG23 | 2.01 | 0.89 |
| 3:D:811:GLU:O | 3:D:815:ALA:HB3 | 1.72 | 0.89 |
| 2:C:150:PRO:CA | 2:C:158:TYR:HB3 | 1.98 | 0.89 |
| 3:D:136:ASP:HB3 | 3:D:137:PRO:HD3 | 1.54 | 0.89 |
| 1:B:161:ARG:HB2 | 1:B:164:ALA:HB2 | 1.55 | 0.89 |
| 3:D:230:TRP:HE1 | 3:D:233:LYS:HG3 | 1.37 | 0.89 |
| 2:M:41:ASN:HA | 2:M:45:GLN:HB3 | 1.55 | 0.89 |
| 2:M:267:TYR:HB2 | 2:M:272:ALA:HB3 | 1.54 | 0.89 |
| 2:C:504:GLU:O | 2:C:507:ARG:HD2 | 1.72 | 0.89 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:79:GLU:HG2 | 3:D:80:VAL:N | 1.88 | 0.89 |
| 1:L:214:ALA:HA | 1:L:217:ILE:HD12 | 1.53 | 0.89 |
| 3:N:285:PRO:HB2 | 3:N:312:ARG:O | 1.72 | 0.89 |
| 2:C:325:ILE:HD12 | 2:C:325:ILE:H | 1.38 | 0.89 |
| 2:M:698:ASP:HA | 2:M:832:LYS:HE3 | 1.53 | 0.89 |
| 3:N:1277:ILE:HG22 | 3:N:1278:ASP:H | 1.35 | 0.89 |
| 2:M:283:ILE:CG2 | 2:M:284:ARG:H | 1.86 | 0.88 |
| 5:F:101:GLU:HA | 5:F:104:ARG:NH1 | 1.87 | 0.88 |
| 3:D:1407:LEU:O | 3:D:1410:GLU:HG2 | 1.73 | 0.88 |
| 3:N:826:PRO:HD2 | 3:N:829:VAL:HG11 | 1.55 | 0.88 |
| 2:M:958:THR:HG23 | 2:M:961:GLU:CB | 2.02 | 0.88 |
| 2:M:283:ILE:HG22 | 2:M:284:ARG:N | 1.86 | 0.88 |
| 3:N:1267:ARG:HE | 3:N:1271:LYS:HZ2 | 1.19 | 0.88 |
| 3:N:483:HIS:HB2 | 3:N:484:PRO:CD | 2.03 | 0.88 |
| 5:F:368:VAL:HG23 | 5:F:369:LEU:H | 1.39 | 0.88 |
| 3:D:1095:THR:O | 3:D:1099:VAL:HG23 | 1.73 | 0.88 |
| 3:D:79:GLU:HG2 | 3:D:80:VAL:H | 1.37 | 0.88 |
| 3:D:530:VAL:HG23 | 3:D:531:ASP:N | 1.88 | 0.88 |
| 3:D:584:ASN:OD1 | 3:D:590:PRO:HD2 | 1.73 | 0.88 |
| 2:C:626:ARG:HG3 | 2:C:629:TYR:HD1 | 1.37 | 0.88 |
| 2:C:269:LEU:HD12 | 2:C:288:ARG:HB3 | 1.55 | 0.88 |
| 2:C:304:LEU:HB3 | 2:C:305:PRO:CD | 2.03 | 0.88 |
| 3:D:237:LYS:HB3 | 3:D:238:PRO:CD | 2.03 | 0.88 |
| 2:M:413:LEU:HA | 2:M:419:THR:CG2 | 2.02 | 0.88 |
| 3:N:845:ASN:HB2 | 3:N:848:GLU:HB2 | 1.56 | 0.88 |
| 2:C:23:VAL:HA | 2:C:121:MET:CE | 2.04 | 0.88 |
| 2:M:44:ILE:HG23 | 2:M:344:PHE:HE1 | 1.37 | 0.88 |
| 2:M:781:LYS:HA | 2:M:781:LYS:HE2 | 1.53 | 0.88 |
| 3:N:130:SER:HB3 | 3:N:132:TYR:CE1 | 2.08 | 0.88 |
| 3:D:238:PRO:HB3 | 3:D:317:VAL:O | 1.73 | 0.88 |
| 2:M:603:VAL:HG23 | 2:M:647:GLN:O | 1.74 | 0.88 |
| 3:N:1495:ILE:O | 3:N:1499:ARG:HB2 | 1.72 | 0.88 |
| 2:C:762:LYS:HG2 | 2:C:763:GLY:H | 1.39 | 0.88 |
| 2:C:157:ARG:HG3 | 2:C:158:TYR:H | 1.39 | 0.88 |
| 3:N:416:ALA:HB2 | 3:N:432:TYR:CA | 2.02 | 0.88 |
| 3:D:260:GLU:HB2 | 3:D:271:VAL:HB | 1.55 | 0.88 |
| 1:L:58:ILE:HG23 | 1:L:139:ASN:O | 1.74 | 0.88 |
| 3:D:806:PHE:HA | 3:D:809:PRO:HD2 | 1.53 | 0.88 |
| 2:M:277:ALA:HB1 | 2:M:281:LEU:HD12 | 1.56 | 0.88 |
| 3:D:249:TYR:HB3 | 3:D:307:ALA:CB | 2.00 | 0.88 |
| 3:N:805:GLU:HA | 3:N:831:GLY:HA2 | 1.55 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:N:592:THR:HG23 | 3:N:600:LEU:HD21 | 1.56 | 0.88 |
| 2:M:38:LYS:HG3 | 2:M:39:ARG:H | 1.37 | 0.88 |
| 2:M:1056:LYS:HD3 | 3:N:623:VAL:HG13 | 1.55 | 0.87 |
| 2:C:185:LYS:HG2 | 2:C:190:LYS:HD3 | 1.54 | 0.87 |
| 3:N:79:GLU:HG2 | 3:N:80:VAL:H | 1.38 | 0.87 |
| 2:C:401:LEU:HD11 | 2:C:543:ASN:HB3 | 1.55 | 0.87 |
| 3:N:136:ASP:HB2 | 3:N:137:PRO:HD3 | 1.53 | 0.87 |
| 3:D:552:ASN:HA | 3:D:555:LYS:HD2 | 1.54 | 0.87 |
| 1:B:32:PHE:HA | 1:B:35:THR:HB | 1.56 | 0.87 |
| 5:F:261:PRO:O | 5:F:264:MET:HB2 | 1.74 | 0.87 |
| 2:M:317:VAL:N | 2:M:318:PRO:HD3 | 1.89 | 0.87 |
| 5:F:280:GLN:HG3 | 5:F:281:GLU:N | 1.87 | 0.87 |
| 3:N:864:VAL:HG12 | 3:N:865:THR:H | 1.38 | 0.87 |
| 3:N:912:LYS:HB3 | 3:N:912:LYS:HZ3 | 1.38 | 0.87 |
| 3:N:349:PRO:HB2 | 5:P:232:ARG:NH2 | 1.88 | 0.87 |
| 3:N:1394:VAL:HB | 3:N:1397:LYS:HD2 | 1.54 | 0.87 |
| 3:N:227:LEU:HA | 3:N:331:VAL:CG2 | 2.03 | 0.87 |
| 3:D:223:LEU:HG | 3:D:224:ARG:H | 1.37 | 0.87 |
| 2:M:352:ALA:HA | 2:M:355:VAL:HG12 | 1.56 | 0.87 |
| 1:K:152:PRO:HB2 | 1:K:154:GLU:OE1 | 1.73 | 0.87 |
| 5:F:80:PRO:HA | 5:F:83:GLN:HE21 | 1.39 | 0.87 |
| 5:F:263:HIS:HA | 5:F:266:GLU:OE2 | 1.73 | 0.87 |
| 2:C:186:VAL:HG23 | 2:C:187:ASN:N | 1.86 | 0.87 |
| 2:M:776:SER:HB3 | 5:P:379:ARG:HH22 | 1.38 | 0.87 |
| 3:D:1031:ASN:H | 3:D:1034:GLN:NE2 | 1.72 | 0.87 |
| 3:N:119:SER:H | 3:N:123:LEU:CG | 1.87 | 0.87 |
| 4:E:37:ASN:ND2 | 4:E:37:ASN:H | 1.70 | 0.87 |
| 5:P:373:LYS:HD2 | 5:P:374:GLY:N | 1.90 | 0.87 |
| 2:C:603:VAL:HG23 | 2:C:647:GLN:O | 1.75 | 0.87 |
| 3:N:1213:ARG:HH11 | 3:N:1213:ARG:HG2 | 1.40 | 0.87 |
| 1:L:106:PRO:HA | 1:L:133:GLU:HA | 1.54 | 0.87 |
| 3:N:288:MET:HE1 | 3:N:307:ALA:HB2 | 1.56 | 0.87 |
| 3:N:553:ARG:HH11 | 5:P:214:GLN:HB2 | 1.40 | 0.87 |
| 3:D:548:ILE:HG22 | 3:D:552:ASN:HD21 | 1.38 | 0.87 |
| 3:D:1494:ALA:HB1 | 4:E:88:GLU:HB3 | 1.57 | 0.87 |
| 2:M:250:ARG:CB | 2:M:253:ALA:HB2 | 2.05 | 0.87 |
| 3:D:1307:LYS:H | 3:D:1307:LYS:HE3 | 1.38 | 0.87 |
| 3:D:1372:VAL:HA | 3:D:1375:MET:CE | 2.05 | 0.87 |
| 1:B:58:ILE:HG12 | 1:B:139:ASN:O | 1.75 | 0.86 |
| 1:B:188:GLN:HG2 | 1:B:189:ARG:N | 1.90 | 0.86 |
| 3:D:433:GLY:HA2 | 3:D:449:SER:N | 1.90 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:694:LEU:HD21 | 2:M:868:ASP:HB3 | 1.54 | 0.86 |
| 3:N:1353:GLN:O | 3:N:1357:ARG:HG2 | 1.74 | 0.86 |
| 1:L:108:GLU:HG3 | 1:L:131:THR:HG22 | 1.57 | 0.86 |
| 3:N:237:LYS:HB3 | 3:N:238:PRO:CD | 2.04 | 0.86 |
| 3:D:127:LEU:HD22 | 3:D:461:ILE:HD11 | 1.57 | 0.86 |
| 2:M:302:VAL:O | 2:M:305:PRO:HD2 | 1.74 | 0.86 |
| 3:D:259:VAL:HA | 3:D:270:LEU:HD11 | 1.54 | 0.86 |
| 3:N:843:PHE:CE2 | 3:N:864:VAL:HG11 | 2.10 | 0.86 |
| 3:N:1312:LEU:HB3 | 3:N:1325:LEU:O | 1.75 | 0.86 |
| 3:D:188:GLY:H | 3:D:198:ARG:CA | 1.86 | 0.86 |
| 2:M:368:THR:H | 2:M:369:PRO:HD3 | 1.40 | 0.86 |
| 3:N:257:GLY:HA2 | 3:N:274:ARG:HA | 1.56 | 0.86 |
| 3:N:356:PRO:HB3 | 3:N:440:VAL:HB | 1.58 | 0.86 |
| 5:P:352:GLU:HA | 5:P:355:GLU:OE2 | 1.74 | 0.86 |
| 3:D:417:PRO:HB3 | 3:D:430:ASP:HA | 1.58 | 0.86 |
| 2:C:243:ARG:HG3 | 2:C:244:PRO:HA | 1.55 | 0.86 |
| 5:F:289:GLU:CD | 5:F:289:GLU:H | 1.79 | 0.86 |
| 2:M:1085:PHE:O | 2:M:1088:LEU:HB3 | 1.75 | 0.86 |
| 3:N:808:THR:H | 3:N:809:PRO:CD | 1.88 | 0.86 |
| 3:N:411:THR:HG21 | 5:P:179:GLU:CG | 2.04 | 0.86 |
| 5:P:282:LEU:HG | 5:P:284:ARG:CG | 2.03 | 0.86 |
| 3:N:10:ILE:O | 3:N:1454:GLY:HA2 | 1.75 | 0.86 |
| 2:M:1005:MET:HG2 | 3:N:629:SER:HB2 | 1.57 | 0.86 |
| 3:N:243:ALA:HB3 | 3:N:311:LEU:HD12 | 1.57 | 0.86 |
| 2:C:157:ARG:HD2 | 2:C:314:THR:HG22 | 1.55 | 0.86 |
| 3:D:210:ARG:HB2 | 3:D:389:GLU:HG3 | 1.54 | 0.86 |
| 3:D:438:ASP:OD1 | 3:D:440:VAL:HG22 | 1.75 | 0.86 |
| 2:C:93:PRO:HG3 | 2:C:117:HIS:HD2 | 1.40 | 0.86 |
| 3:N:1099:VAL:HG12 | 9:N:1528:NE6:H14 | 1.58 | 0.86 |
| 2:M:226:VAL:HG23 | 2:M:227:PHE:CD1 | 2.10 | 0.86 |
| 3:N:1406:ARG:HD3 | 3:N:1412:LYS:NZ | 1.90 | 0.86 |
| 3:N:1267:ARG:HH11 | 3:N:1267:ARG:HB2 | 1.41 | 0.86 |
| 2:C:23:VAL:HA | 2:C:121:MET:HE1 | 1.58 | 0.86 |
| 2:C:605:LYS:HB3 | 2:C:610:ARG:NH2 | 1.88 | 0.86 |
| 2:M:1051:GLU:HG3 | 2:M:1052:MET:H | 1.40 | 0.85 |
| 3:N:1341:PRO:O | 3:N:1344:VAL:HG12 | 1.74 | 0.85 |
| 3:N:441:ARG:HG3 | 3:N:443:VAL:HG23 | 1.59 | 0.85 |
| 3:D:1029:ARG:HH11 | 3:D:1029:ARG:HG3 | 1.40 | 0.85 |
| 3:D:521:PRO:HD2 | 3:D:524:LEU:HD12 | 1.57 | 0.85 |
| 3:D:295:GLY:CA | 3:D:302:GLN:HB3 | 2.06 | 0.85 |
| 3:D:348:GLN:H | 3:D:351:MET:HE2 | 1.40 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:138:LEU:HD12 | 1:A:139:ASN:H | 1.41 | 0.85 |
| 1:A:38:ASN:HB3 | 1:A:39:PRO:HD3 | 1.57 | 0.85 |
| 2:M:1088:LEU:HA | 2:M:1091:GLU:OE1 | 1.76 | 0.85 |
| 2:C:352:ALA:HA | 2:C:355:VAL:HG12 | 1.58 | 0.85 |
| 5:P:367:MET:HB3 | 5:P:370:LYS:HE2 | 1.58 | 0.85 |
| 2:M:878:SER:HA | 3:N:1034:GLN:OE1 | 1.76 | 0.85 |
| 3:N:1404:ASN:HA | 3:N:1408:ILE:HB | 1.56 | 0.85 |
| 5:P:138:SER:O | 5:P:141:VAL:HG22 | 1.76 | 0.85 |
| 3:D:1489:GLN:CA | 3:D:1492:LEU:HG | 2.06 | 0.85 |
| 3:D:658:LEU:CA | 3:D:661:MET:HE3 | 2.06 | 0.85 |
| 2:C:1064:ASN:HA | 5:F:341:PRO:HB3 | 1.56 | 0.85 |
| 2:C:881:ASN:H | 2:C:881:ASN:ND2 | 1.75 | 0.85 |
| 3:D:95:LEU:HB2 | 3:D:515:GLU:HA | 1.58 | 0.85 |
| 3:N:1018:ASN:O | 3:N:1022:VAL:HG23 | 1.76 | 0.85 |
| 2:M:230:ARG:HG2 | 2:M:233:GLU:CG | 2.07 | 0.85 |
| 3:D:367:ILE:HB | 3:D:377:VAL:CG1 | 2.06 | 0.85 |
| 2:M:649:VAL:HA | 2:M:650:ARG:HH21 | 1.41 | 0.85 |
| 3:N:1400:VAL:HG12 | 3:N:1404:ASN:HD21 | 1.42 | 0.85 |
| 1:B:106:PRO:HA | 1:B:133:GLU:HA | 1.58 | 0.85 |
| 1:B:36:LEU:O | 1:B:39:PRO:HD2 | 1.77 | 0.85 |
| 2:C:737:LEU:HD12 | 2:C:743:VAL:N | 1.91 | 0.85 |
| 3:N:106:LYS:HE2 | 3:N:106:LYS:HA | 1.58 | 0.85 |
| 3:D:352:ASN:C | 3:D:368:VAL:HG13 | 1.97 | 0.85 |
| 2:C:1071:ILE:O | 3:D:659:LYS:HD3 | 1.76 | 0.85 |
| 3:D:860:LEU:HA | 3:D:877:PRO:HB2 | 1.58 | 0.85 |
| 2:M:146:VAL:HG22 | 2:M:162:ILE:HG12 | 1.58 | 0.85 |
| 2:M:264:PRO:CB | 2:M:289:THR:HG21 | 2.06 | 0.84 |
| 5:P:132:ARG:NH2 | 5:P:184:ARG:HH12 | 1.74 | 0.84 |
| 3:N:826:PRO:HB2 | 3:N:829:VAL:HG13 | 1.57 | 0.84 |
| 2:C:640:ARG:HD2 | 2:C:642:ARG:HH22 | 1.41 | 0.84 |
| 1:K:90:LEU:HD12 | 1:K:119:ASP:HA | 1.58 | 0.84 |
| 2:M:448:ASN:HA | 2:M:451:LEU:HD12 | 1.59 | 0.84 |
| 3:N:565:ILE:HD13 | 5:P:192:LEU:HD13 | 1.58 | 0.84 |
| 3:D:261:LEU:HA | 3:D:269:PHE:O | 1.76 | 0.84 |
| 5:F:355:GLU:HA | 5:F:358:LEU:HB3 | 1.56 | 0.84 |
| 3:D:417:PRO:HB3 | 3:D:430:ASP:CA | 2.07 | 0.84 |
| 3:N:806:PHE:CG | 3:N:809:PRO:HB2 | 2.12 | 0.84 |
| 3:N:168:THR:HG21 | 5:P:93:LEU:HD22 | 1.59 | 0.84 |
| 3:N:135:LEU:HD21 | 3:N:153:LEU:HB2 | 1.59 | 0.84 |
| 3:N:819:GLY:CA | 3:N:824:ASN:HD22 | 1.90 | 0.84 |
| 5:P:101:GLU:HA | 5:P:104:ARG:NH1 | 1.92 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:137:PRO:HG2 | 3:N:138:LYS:H | 1.40 | 0.84 |
| 3:D:406:ASP:HB2 | 3:D:424:GLY:N | 1.91 | 0.84 |
| 2:M:373:VAL:HG12 | 2:M:374:ASN:H | 1.41 | 0.84 |
| 5:F:87:GLU:O | 5:F:90:GLN:HB2 | 1.77 | 0.84 |
| 2:C:535:SER:O | 2:C:538:GLN:HG2 | 1.76 | 0.84 |
| 1:B:137:ARG:NH1 | 1:B:139:ASN:HB2 | 1.91 | 0.84 |
| 2:C:370:ALA:HA | 2:C:373:VAL:HG23 | 1.60 | 0.84 |
| 2:M:1092:LEU:HA | 2:M:1095:LEU:HD12 | 1.58 | 0.84 |
| 3:D:57:GLU:HG3 | 3:D:64:LYS:HA | 1.59 | 0.84 |
| 3:N:1494:ALA:CA | 3:N:1497:GLU:HG2 | 2.04 | 0.84 |
| 5:P:373:LYS:NZ | 5:P:373:LYS:HB3 | 1.90 | 0.84 |
| 2:C:233:GLU:CD | 2:C:234:ALA:H | 1.80 | 0.84 |
| 2:C:71:TYR:H | 2:C:71:TYR:HD2 | 1.26 | 0.84 |
| 1:K:111:ALA:HA | 1:K:129:ILE:HD11 | 1.59 | 0.84 |
| 2:M:535:SER:O | 2:M:538:GLN:HG2 | 1.77 | 0.84 |
| 2:M:881:ASN:H | 2:M:881:ASN:HD22 | 1.20 | 0.84 |
| 2:M:194:VAL:HA | 2:M:197:LEU:CG | 2.07 | 0.84 |
| 2:C:193:LEU:HD12 | 2:C:196:LEU:HD12 | 1.57 | 0.84 |
| 3:N:133:ILE:HD13 | 3:N:133:ILE:H | 1.42 | 0.84 |
| 3:N:562:ALA:HB3 | 3:N:567:ILE:HD11 | 1.59 | 0.84 |
| 3:N:771:SER:HB2 | 3:N:778:LEU:HD22 | 1.60 | 0.84 |
| 1:K:100:LEU:HB3 | 1:K:115:LEU:HD12 | 1.57 | 0.84 |
| 2:C:186:VAL:CG2 | 2:C:187:ASN:H | 1.89 | 0.84 |
| 2:M:41:ASN:C | 2:M:41:ASN:HD22 | 1.81 | 0.84 |
| 2:C:643:VAL:HG23 | 2:C:647:GLN:NE2 | 1.93 | 0.84 |
| 2:M:175:GLU:HG2 | 2:M:176:VAL:N | 1.93 | 0.83 |
| 3:N:322:VAL:HG23 | 3:N:335:LEU:HD11 | 1.60 | 0.83 |
| 3:N:510:GLU:O | 3:N:513:ILE:HG22 | 1.78 | 0.83 |
| 1:L:57:TYR:CE1 | 1:L:163:ASN:HB2 | 2.13 | 0.83 |
| 3:N:141:ILE:HB | 3:N:450:TYR:HD2 | 1.41 | 0.83 |
| 3:D:569:ASN:O | 3:D:572:ARG:HB3 | 1.79 | 0.83 |
| 3:N:420:VAL:O | 3:N:421:LEU:HD23 | 1.77 | 0.83 |
| 3:N:368:VAL:HB | 3:N:377:VAL:CG2 | 2.07 | 0.83 |
| 2:M:762:LYS:HG2 | 2:M:763:GLY:N | 1.93 | 0.83 |
| 3:N:1459:LEU:HD12 | 3:N:1470:ARG:HH11 | 1.42 | 0.83 |
| 1:B:175:ARG:HG3 | 1:B:201:THR:O | 1.78 | 0.83 |
| 2:C:838:LYS:HG3 | 2:C:997:LEU:HB2 | 1.60 | 0.83 |
| 2:C:44:ILE:HG23 | 2:C:344:PHE:HE1 | 1.40 | 0.83 |
| 1:B:108:GLU:HG3 | 1:B:131:THR:HG22 | 1.61 | 0.83 |
| 2:M:285:LEU:HG | 2:M:286:SER:N | 1.92 | 0.83 |
| 3:N:323:GLU:O | 3:N:333:LEU:HA | 1.78 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:M:1102:LEU:N | 3:N:5:VAL:HG13 | 1.94 | 0.83 |
| 2:C:175:GLU:O | 2:C:176:VAL:HG13 | 1.79 | 0.83 |
| 3:N:543:LEU:O | 3:N:546:ARG:HG3 | 1.77 | 0.83 |
| 2:C:1100:GLN:HG3 | 2:C:1102:LEU:HD21 | 1.60 | 0.83 |
| 3:N:295:GLY:HA2 | 3:N:302:GLN:HB3 | 1.59 | 0.83 |
| 3:D:206:ARG:HB2 | 3:D:392:SER:O | 1.78 | 0.83 |
| 3:D:706:PRO:HB2 | 3:D:708:LEU:HD21 | 1.58 | 0.83 |
| 3:N:119:SER:H | 3:N:123:LEU:HG | 1.43 | 0.83 |
| 2:C:881:ASN:HD22 | 2:C:881:ASN:N | 1.73 | 0.83 |
| 2:M:1100:GLN:HG3 | 2:M:1102:LEU:HD21 | 1.60 | 0.83 |
| 3:N:882:PHE:HA | 3:N:885:ILE:HD12 | 1.60 | 0.83 |
| 1:B:9:PRO:HG3 | 1:B:27:PRO:O | 1.79 | 0.83 |
| 2:M:334:ARG:HA | 2:M:338:GLU:OE1 | 1.77 | 0.83 |
| 3:N:1147:ARG:HB2 | 3:N:1166:LEU:HD12 | 1.60 | 0.83 |
| 1:L:179:PHE:HB3 | 1:L:197:LEU:HD13 | 1.61 | 0.83 |
| 2:M:91:GLN:HB2 | 2:M:118:ILE:O | 1.78 | 0.83 |
| 2:M:631:SER:HB3 | 2:M:635:THR:H | 1.42 | 0.83 |
| 1:B:185:ARG:HH22 | 3:D:692:GLU:HG3 | 1.41 | 0.83 |
| 3:D:820:GLU:HG2 | 3:D:825:ALA:O | 1.79 | 0.83 |
| 3:N:167:GLU:O | 3:N:394:LEU:HD12 | 1.77 | 0.83 |
| 3:N:407:VAL:HG22 | 3:N:408:GLU:N | 1.92 | 0.83 |
| 3:D:209:ARG:O | 3:D:346:ARG:HA | 1.79 | 0.83 |
| 5:P:305:GLU:HG3 | 5:P:309:LYS:HE3 | 1.59 | 0.83 |
| 3:N:192:ALA:HB3 | 3:N:195:VAL:HG23 | 1.60 | 0.83 |
| 5:P:329:TYR:CD1 | 5:P:333:ILE:HD11 | 2.14 | 0.83 |
| 3:N:207:PHE:O | 3:N:390:PRO:HA | 1.78 | 0.83 |
| 2:C:266:ARG:HD2 | 2:C:273:GLY:H | 1.43 | 0.82 |
| 3:N:124:GLU:HG3 | 3:N:128:TYR:CE2 | 2.13 | 0.82 |
| 3:D:565:ILE:HG12 | 3:D:566:ILE:N | 1.92 | 0.82 |
| 3:D:259:VAL:HG11 | 3:D:293:VAL:HA | 1.61 | 0.82 |
| 3:N:675:ARG:HH22 | 5:P:420:ASP:CB | 1.92 | 0.82 |
| 2:C:197:LEU:HD11 | 2:C:221:LEU:HD11 | 1.61 | 0.82 |
| 3:D:408:GLU:HG3 | 3:D:421:LEU:C | 2.00 | 0.82 |
| 5:F:171:LYS:O | 5:F:174:LEU:HB3 | 1.80 | 0.82 |
| 3:N:1069:GLU:HA | 3:N:1072:ILE:HD12 | 1.60 | 0.82 |
| 3:D:317:VAL:HG23 | 3:D:338:GLU:O | 1.79 | 0.82 |
| 5:F:207:LEU:HB3 | 5:F:212:LEU:HD21 | 1.60 | 0.82 |
| 1:A:5:LYS:NZ | 1:A:192:LEU:HD22 | 1.93 | 0.82 |
| 2:C:755:LEU:HD21 | 2:C:792:VAL:HG22 | 1.61 | 0.82 |
| 1:A:14:ARG:HD2 | 1:B:234:ALA:N | 1.94 | 0.82 |
| 3:N:154:THR:HG22 | 3:N:157:GLU:CG | 2.08 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:575:GLN:O | 3:D:578:VAL:HB | 1.78 | 0.82 |
| 5:P:418:LEU:HD12 | 5:P:418:LEU:N | 1.93 | 0.82 |
| 5:P:280:GLN:HG3 | 5:P:281:GLU:H | 1.45 | 0.82 |
| 3:N:1399:ASP:O | 3:N:1403:LEU:HB2 | 1.80 | 0.82 |
| 3:D:142:LEU:HB3 | 3:D:146:PRO:HA | 1.58 | 0.82 |
| 2:C:517:ARG:HB2 | 2:C:520:GLU:HB2 | 1.61 | 0.82 |
| 3:D:119:SER:H | 3:D:123:LEU:HD12 | 1.44 | 0.82 |
| 3:D:1388:ARG:NH2 | 3:D:1390:LEU:HD23 | 1.94 | 0.82 |
| 3:D:1378:TYR:HB2 | 3:D:1422:MET:HE3 | 1.61 | 0.82 |
| 1:L:212:ASN:O | 1:L:215:VAL:HG22 | 1.80 | 0.82 |
| 1:K:42:ARG:NH1 | 1:L:34:VAL:HB | 1.95 | 0.82 |
| 3:D:1372:VAL:HA | 3:D:1375:MET:HE3 | 1.61 | 0.82 |
| 1:L:91:ASN:HB3 | 1:L:94:LEU:HG | 1.61 | 0.82 |
| 3:D:147:VAL:HG22 | 3:D:148:GLU:N | 1.94 | 0.82 |
| 3:D:353:VAL:CA | 3:D:368:VAL:HG22 | 2.06 | 0.82 |
| 2:M:609:ASN:O | 2:M:625:LEU:HB3 | 1.80 | 0.82 |
| 3:D:207:PHE:O | 3:D:390:PRO:HA | 1.79 | 0.82 |
| 3:N:16:GLU:H | 3:N:16:GLU:CD | 1.83 | 0.82 |
| 1:K:102:LYS:HG2 | 1:K:139:ASN:OD1 | 1.79 | 0.82 |
| 3:D:1094:LEU:HD23 | 3:D:1230:GLY:HA2 | 1.62 | 0.82 |
| 2:C:1102:LEU:HD11 | 3:D:9:ARG:HD2 | 1.62 | 0.82 |
| 5:F:413:SER:HB3 | 5:F:414:ARG:HH21 | 1.43 | 0.82 |
| 3:N:1176:LYS:HA | 3:N:1179:GLU:OE1 | 1.80 | 0.82 |
| 3:D:884:ARG:O | 3:D:888:GLU:HG2 | 1.78 | 0.82 |
| 3:D:1238:MET:HE2 | 3:D:1239:ARG:HB3 | 1.59 | 0.82 |
| 3:D:295:GLY:HA2 | 3:D:302:GLN:CB | 2.10 | 0.82 |
| 3:D:355:VAL:CG1 | 3:D:385:VAL:HG21 | 2.08 | 0.82 |
| 2:C:52:PHE:CD2 | 2:C:68:PHE:HB2 | 2.15 | 0.82 |
| 3:N:60:CYS:HB2 | 3:N:62:LYS:HE2 | 1.61 | 0.82 |
| 3:N:658:LEU:HA | 3:N:661:MET:HE3 | 1.61 | 0.82 |
| 2:C:477:GLY:HA2 | 2:C:508:ILE:HD12 | 1.61 | 0.82 |
| 2:C:227:PHE:HA | 2:C:237:ARG:HH12 | 1.43 | 0.82 |
| 3:D:1397:LYS:HB2 | 3:D:1398:TRP:CZ3 | 2.15 | 0.82 |
| 5:F:278:LEU:CB | 5:F:286:PRO:HG3 | 2.10 | 0.82 |
| 3:N:772:PRO:HG3 | 3:N:1210:SER:HB3 | 1.62 | 0.82 |
| 5:P:102:LEU:CD1 | 5:P:183:ALA:HB1 | 2.09 | 0.82 |
| 2:C:1085:PHE:O | 2:C:1088:LEU:HB3 | 1.80 | 0.82 |
| 2:M:809:GLY:C | 2:M:811:PRO:HD2 | 1.98 | 0.82 |
| 2:M:328:LEU:HD12 | 2:M:437:ARG:HD2 | 1.61 | 0.82 |
| 2:M:194:VAL:HG22 | 2:M:221:LEU:HG | 1.59 | 0.81 |
| 3:D:1231:GLU:HB3 | 3:D:1232:PRO:HD3 | 1.61 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:D:241:ILE:HA | 3:D:312:ARG:HA | 1.62 | 0.81 |
| 5:P:353:GLU:O | 5:P:356:LYS:HB2 | 1.79 | 0.81 |
| 2:M:51:THR:HG21 | 2:M:348:LEU:HG | 1.59 | 0.81 |
| 2:C:1012:PRO:HD3 | 2:C:1026:GLN:HG2 | 1.62 | 0.81 |
| 2:C:166:PRO:CG | 2:C:169:GLY:HA3 | 2.10 | 0.81 |
| 3:N:433:GLY:HA3 | 3:N:447:VAL:O | 1.80 | 0.81 |
| 3:N:127:LEU:HD22 | 3:N:461:ILE:HD11 | 1.60 | 0.81 |
| 3:D:806:PHE:CG | 3:D:809:PRO:HB2 | 2.15 | 0.81 |
| 5:P:368:VAL:HG23 | 5:P:369:LEU:N | 1.94 | 0.81 |
| 3:N:1472:ILE:CG2 | 3:N:1474:ALA:H | 1.92 | 0.81 |
| 2:M:1037:VAL:O | 2:M:1041:GLU:HG3 | 1.79 | 0.81 |
| 3:N:207:PHE:CZ | 5:P:98:GLU:HG3 | 2.14 | 0.81 |
| 2:C:841:ASN:ND2 | 2:C:845:ASN:HB3 | 1.95 | 0.81 |
| 3:D:1213:ARG:HB2 | 3:D:1214:PRO:HD2 | 1.62 | 0.81 |
| 2:M:322:VAL:HG12 | 2:M:323:ASP:H | 1.45 | 0.81 |
| 3:N:292:VAL:HG23 | 3:N:293:VAL:H | 1.45 | 0.81 |
| 3:N:141:ILE:HB | 3:N:450:TYR:CD2 | 2.15 | 0.81 |
| 3:N:458:ALA:HB1 | 3:N:513:ILE:HD11 | 1.60 | 0.81 |
| 3:D:135:LEU:HD23 | 3:D:135:LEU:N | 1.95 | 0.81 |
| 3:D:149:LYS:HE3 | 3:D:150:ARG:HE | 1.43 | 0.81 |
| 5:P:418:LEU:CD1 | 5:P:418:LEU:H | 1.85 | 0.81 |
| 1:B:138:LEU:HD12 | 1:B:139:ASN:H | 1.46 | 0.81 |
| 5:P:274:THR:O | 5:P:278:LEU:HG | 1.79 | 0.81 |
| 5:F:371:LEU:HA | 5:F:375:LEU:HG | 1.62 | 0.81 |
| 3:N:252:ARG:HE | 3:N:300:LYS:HA | 1.44 | 0.81 |
| 3:N:610:LYS:HZ1 | 3:N:1442:ASN:H | 1.26 | 0.81 |
| 1:K:100:LEU:HD23 | 1:K:101:LEU:H | 1.44 | 0.81 |
| 3:D:264:LEU:HD22 | 3:D:316:GLN:NE2 | 1.96 | 0.81 |
| 3:N:402:PRO:HG3 | 3:N:443:VAL:HG22 | 1.61 | 0.81 |
| 3:N:494:LYS:HA | 3:N:1388:ARG:HH12 | 1.45 | 0.81 |
| 3:N:820:GLU:HG2 | 3:N:825:ALA:O | 1.81 | 0.81 |
| 2:C:958:THR:HG23 | 2:C:961:GLU:HB3 | 1.63 | 0.81 |
| 2:M:230:ARG:HG2 | 2:M:233:GLU:HG3 | 1.62 | 0.81 |
| 2:M:397:GLU:N | 2:M:633:GLN:HE21 | 1.78 | 0.81 |
| 2:C:542:VAL:HG23 | 2:C:543:ASN:N | 1.94 | 0.81 |
| 3:D:225:LEU:HB3 | 3:D:226:PRO:CD | 2.11 | 0.81 |
| 5:P:402:ASN:HB3 | 5:P:406:ARG:CZ | 2.10 | 0.81 |
| 5:P:370:LYS:HG3 | 5:P:371:LEU:N | 1.94 | 0.81 |
| 1:L:206:THR:HB | 1:L:209:GLU:CG | 2.09 | 0.81 |
| 2:M:164:PRO:HD3 | 2:M:266:ARG:NH2 | 1.94 | 0.81 |
| 2:C:194:VAL:HA | 2:C:197:LEU:HG | 1.61 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:119:SER:HB3 | 3:N:123:LEU:H | 1.45 | 0.81 |
| 3:D:525:ARG:N | 3:D:526:PRO:HD3 | 1.95 | 0.81 |
| 3:D:1495:ILE:HG13 | 4:E:84:ARG:NH1 | 1.95 | 0.81 |
| 2:C:115:LEU:HB2 | 2:C:375:SER:HB3 | 1.62 | 0.81 |
| 3:N:1152:GLU:N | 3:N:1162:GLU:HB3 | 1.96 | 0.81 |
| 2:M:170:PRO:HD3 | 2:M:263:ASP:HB3 | 1.61 | 0.81 |
| 2:C:69:LEU:HD23 | 2:C:70:GLU:HG3 | 1.62 | 0.81 |
| 3:D:30:GLU:CB | 3:D:40:GLU:HG2 | 2.09 | 0.81 |
| 1:A:78:ILE:O | 1:A:81:ASN:HB2 | 1.81 | 0.81 |
| 3:N:1372:VAL:HA | 3:N:1375:MET:CE | 2.10 | 0.81 |
| 2:C:149:THR:HG23 | 2:C:159:ILE:HG13 | 1.63 | 0.81 |
| 3:N:133:ILE:HG23 | 3:N:456:MET:CE | 2.11 | 0.81 |
| 5:P:417:LYS:HB2 | 5:P:418:LEU:HD12 | 1.62 | 0.81 |
| 2:C:101:ILE:HG22 | 2:C:102:HIS:N | 1.95 | 0.81 |
| 5:P:282:LEU:HG | 5:P:284:ARG:HG2 | 1.63 | 0.81 |
| 2:C:876:VAL:H | 2:C:877:PRO:HD2 | 1.45 | 0.81 |
| 3:N:642:CYS:SG | 3:N:716:PHE:HB2 | 2.21 | 0.81 |
| 3:N:1130:ARG:HH22 | 3:N:1323:GLN:HE22 | 1.27 | 0.81 |
| 3:D:1311:LEU:HD12 | 3:D:1312:LEU:H | 1.46 | 0.81 |
| 1:A:90:LEU:HD12 | 1:A:119:ASP:HA | 1.61 | 0.81 |
| 2:M:198:ARG:HH21 | 2:M:231:PRO:HD3 | 1.46 | 0.81 |
| 3:D:411:THR:HA | 3:D:435:VAL:HG12 | 1.62 | 0.81 |
| 2:M:774:LEU:HA | 2:M:777:ILE:HD12 | 1.62 | 0.81 |
| 3:N:483:HIS:HB2 | 3:N:484:PRO:HD2 | 1.61 | 0.81 |
| 2:C:226:VAL:HG23 | 2:C:227:PHE:HD1 | 1.46 | 0.81 |
| 3:D:1151:ARG:C | 3:D:1162:GLU:HB3 | 2.01 | 0.81 |
| 3:N:1267:ARG:HH21 | 3:N:1271:LYS:NZ | 1.78 | 0.81 |
| 3:N:796:ARG:HE | 3:N:861:GLN:HB2 | 1.45 | 0.81 |
| 3:D:387:LEU:N | 3:D:387:LEU:HD12 | 1.96 | 0.81 |
| 3:D:988:ARG:HG2 | 3:D:992:ILE:HD11 | 1.62 | 0.81 |
| 3:D:562:ALA:HB3 | 3:D:567:ILE:HD11 | 1.63 | 0.80 |
| 5:P:288:TYR:O | 5:P:291:ILE:HG23 | 1.81 | 0.80 |
| 2:C:689:VAL:CG2 | 2:C:870:ILE:HB | 2.10 | 0.80 |
| 2:C:21:ILE:H | 2:C:21:ILE:CD1 | 1.93 | 0.80 |
| 5:P:152:ASP:O | 5:P:156:VAL:HG21 | 1.82 | 0.80 |
| 2:C:810:ASP:N | 2:C:811:PRO:HD2 | 1.96 | 0.80 |
| 3:N:433:GLY:HA2 | 3:N:449:SER:N | 1.97 | 0.80 |
| 3:N:458:ALA:CB | 3:N:513:ILE:HD11 | 2.11 | 0.80 |
| 5:P:217:ASN:O | 5:P:220:LEU:HB3 | 1.81 | 0.80 |
| 3:D:678:GLU:HG3 | 3:D:679:ARG:HG3 | 1.62 | 0.80 |
| 2:C:626:ARG:HG3 | 2:C:629:TYR:CD1 | 2.17 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:347:GLY:HA2 | 2:C:350:ARG:HD2 | 1.63 | 0.80 |
| 1:K:12:THR:HG22 | 1:L:229:GLN:HG2 | 1.63 | 0.80 |
| 2:C:666:LEU:HD11 | 2:C:668:LEU:HG | 1.63 | 0.80 |
| 2:C:346:VAL:HG23 | 2:C:347:GLY:H | 1.46 | 0.80 |
| 2:C:632:ASN:HB3 | 2:C:633:GLN:NE2 | 1.96 | 0.80 |
| 3:D:644:LEU:HD12 | 3:D:645:PRO:HD2 | 1.61 | 0.80 |
| 2:M:23:VAL:HG23 | 2:M:24:GLU:H | 1.46 | 0.80 |
| 2:M:631:SER:HB3 | 2:M:635:THR:N | 1.95 | 0.80 |
| 2:C:162:ILE:HD12 | 2:C:172:ILE:HD12 | 1.64 | 0.80 |
| 2:C:492:ASP:HB3 | 2:C:518:LYS:HE3 | 1.62 | 0.80 |
| 3:D:113:GLY:C | 3:D:115:LEU:H | 1.83 | 0.80 |
| 3:N:25:GLU:OE1 | 3:N:27:GLU:HG2 | 1.81 | 0.80 |
| 3:N:1490:LYS:HD2 | 4:O:39:VAL:HG13 | 1.63 | 0.80 |
| 5:F:378:GLY:HA3 | 5:F:381:HIS:CE1 | 2.15 | 0.80 |
| 2:M:904:PRO:HB2 | 2:M:907:ASP:HB3 | 1.63 | 0.80 |
| 3:D:1018:ASN:O | 3:D:1022:VAL:HG23 | 1.80 | 0.80 |
| 3:D:1031:ASN:H | 3:D:1034:GLN:HE21 | 1.29 | 0.80 |
| 1:A:151:VAL:HB | 1:A:169:ALA:HB3 | 1.62 | 0.80 |
| 1:L:38:ASN:HB3 | 1:L:39:PRO:HD3 | 1.62 | 0.80 |
| 3:N:1048:PRO:HG3 | 3:N:1075:HIS:HD2 | 1.45 | 0.80 |
| 2:C:801:VAL:HG22 | 2:C:826:TYR:O | 1.81 | 0.80 |
| 3:D:149:LYS:HG3 | 3:D:150:ARG:HG2 | 1.63 | 0.80 |
| 3:D:582:LEU:O | 3:D:603:LEU:HB2 | 1.82 | 0.80 |
| 3:D:272:LEU:HD12 | 3:D:282:TYR:HE1 | 1.47 | 0.80 |
| 3:N:408:GLU:HB3 | 3:N:422:ALA:CB | 2.10 | 0.80 |
| 2:M:772:ARG:NE | 5:P:373:LYS:HG3 | 1.95 | 0.80 |
| 3:N:847:ASP:O | 3:N:851:LEU:HG | 1.82 | 0.80 |
| 1:K:86:VAL:HG12 | 1:K:124:ASN:HD21 | 1.46 | 0.80 |
| 3:N:174:GLY:HA2 | 3:N:389:GLU:HG2 | 1.63 | 0.80 |
| 4:O:7:ASP:HA | 4:O:10:PHE:HD1 | 1.47 | 0.80 |
| 3:D:244:GLU:HA | 3:D:309:GLY:O | 1.82 | 0.80 |
| 3:D:245:LEU:N | 3:D:309:GLY:HA2 | 1.95 | 0.80 |
| 5:P:111:GLU:HG3 | 5:P:114:LYS:HZ2 | 1.46 | 0.80 |
| 2:M:415:PRO:HB2 | 2:M:418:LEU:HB2 | 1.64 | 0.80 |
| 3:N:238:PRO:HB3 | 3:N:317:VAL:O | 1.81 | 0.80 |
| 2:C:303:PHE:H | 2:C:303:PHE:HD1 | 1.26 | 0.80 |
| 2:M:108:ILE:CB | 2:M:368:THR:HG21 | 2.11 | 0.80 |
| 3:N:1381:VAL:HG13 | 3:N:1389:LEU:O | 1.81 | 0.80 |
| 5:F:278:LEU:HB2 | 5:F:286:PRO:HG3 | 1.64 | 0.80 |
| 3:N:261:LEU:HA | 3:N:269:PHE:O | 1.81 | 0.80 |
| 3:N:268:ALA:HB3 | 3:N:290:PRO:HG3 | 1.63 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:N:325:GLU:HG2 | 3:N:332:TYR:HB3 | 1.62 | 0.80 |
| 3:N:153:LEU:HD11 | 3:N:157:GLU:HB3 | 1.64 | 0.80 |
| 3:N:141:ILE:HD12 | 3:N:450:TYR:HB3 | 1.63 | 0.80 |
| 3:D:128:TYR:HA | 3:D:457:GLY:HA2 | 1.64 | 0.80 |
| 2:C:341:THR:O | 2:C:344:PHE:HB3 | 1.82 | 0.80 |
| 3:D:1264:GLU:OE1 | 3:D:1423:GLY:HA3 | 1.81 | 0.80 |
| 5:F:81:VAL:HG23 | 5:F:82:ARG:N | 1.96 | 0.80 |
| 2:C:274:ARG:HH21 | 2:C:284:ARG:HB3 | 1.47 | 0.80 |
| 3:N:445:ARG:H | 3:N:445:ARG:HD2 | 1.47 | 0.80 |
| 2:C:101:ILE:HG23 | 2:C:107:LEU:HD23 | 1.63 | 0.80 |
| 3:N:1486:VAL:HG22 | 4:O:75:PHE:CB | 2.12 | 0.80 |
| 1:B:237:GLU:OE2 | 1:B:239:ALA:HB2 | 1.82 | 0.79 |
| 3:D:1083:ASP:HB2 | 3:D:1239:ARG:NH2 | 1.96 | 0.79 |
| 3:N:555:LYS:HA | 3:N:558:LEU:HD12 | 1.61 | 0.79 |
| 3:N:1494:ALA:HA | 3:N:1497:GLU:CG | 2.07 | 0.79 |
| 1:B:97:VAL:HG12 | 1:B:98:THR:H | 1.47 | 0.79 |
| 2:C:101:ILE:HG22 | 2:C:102:HIS:H | 1.46 | 0.79 |
| 3:D:33:ASN:HD21 | 3:D:35:ARG:CG | 1.85 | 0.79 |
| 1:K:45:LEU:HD21 | 1:K:177:VAL:HB | 1.62 | 0.79 |
| 5:P:253:ASP:HA | 5:P:259:ARG:NH1 | 1.97 | 0.79 |
| 3:N:400:VAL:HG23 | 3:N:443:VAL:HG13 | 1.62 | 0.79 |
| 2:M:98:LEU:HD11 | 2:M:113:VAL:HG21 | 1.64 | 0.79 |
| 5:F:372:ARG:HG3 | 5:F:378:GLY:O | 1.82 | 0.79 |
| 2:M:654:LEU:HD12 | 2:M:655:LEU:H | 1.45 | 0.79 |
| 1:L:28:LEU:HB3 | 1:L:193:ASP:HB2 | 1.61 | 0.79 |
| 2:M:23:VAL:HA | 2:M:121:MET:HE1 | 1.64 | 0.79 |
| 5:P:94:LEU:HG | 5:P:190:ALA:HB1 | 1.64 | 0.79 |
| 5:P:219:GLY:HA3 | 5:P:246:ALA:HB2 | 1.64 | 0.79 |
| 2:C:230:ARG:HG2 | 2:C:233:GLU:CG | 2.10 | 0.79 |
| 5:F:270:LYS:HE3 | 5:F:295:MET:SD | 2.22 | 0.79 |
| 3:N:1170:ASP:O | 3:N:1173:LEU:HB3 | 1.83 | 0.79 |
| 1:K:35:THR:O | 1:K:39:PRO:HG2 | 1.83 | 0.79 |
| 2:C:290:LEU:CD2 | 2:C:302:VAL:HG21 | 2.12 | 0.79 |
| 3:N:837:GLY:HA2 | 3:N:841:TYR:HD1 | 1.45 | 0.79 |
| 3:D:230:TRP:NE1 | 3:D:233:LYS:HG3 | 1.98 | 0.79 |
| 3:D:25:GLU:HB2 | 3:D:92:HIS:CE1 | 2.16 | 0.79 |
| 2:C:197:LEU:HB3 | 2:C:207:LEU:HD13 | 1.64 | 0.79 |
| 3:N:158:TYR:CE1 | 3:N:454:ALA:HB3 | 2.17 | 0.79 |
| 2:M:72:ARG:O | 2:M:94:LEU:HD12 | 1.81 | 0.79 |
| 3:D:207:PHE:HB2 | 3:D:391:ALA:HB3 | 1.64 | 0.79 |
| 2:C:382:ILE:O | 2:C:385:PHE:HB3 | 1.81 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:154:THR:HG22 | 3:D:157:GLU:CG | 2.12 | 0.79 |
| 3:N:441:ARG:HG3 | 3:N:443:VAL:CG2 | 2.13 | 0.79 |
| 2:C:100:LEU:HD23 | 2:C:368:THR:CA | 2.01 | 0.79 |
| 3:D:1394:VAL:HB | 3:D:1397:LYS:HE2 | 1.65 | 0.79 |
| 2:C:571:LEU:HD22 | 2:C:701:THR:H | 1.47 | 0.79 |
| 3:N:806:PHE:HA | 3:N:809:PRO:CD | 2.11 | 0.79 |
| 2:M:292:ARG:HG2 | 2:M:297:GLU:O | 1.83 | 0.79 |
| 2:M:543:ASN:HA | 2:M:546:LEU:HD12 | 1.64 | 0.79 |
| 3:D:1472:ILE:HD13 | 3:D:1473:PRO:HD2 | 1.65 | 0.79 |
| 3:D:412:GLY:H | 3:D:435:VAL:HB | 1.47 | 0.79 |
| 3:D:1405:GLU:OE2 | 3:D:1407:LEU:HG | 1.83 | 0.79 |
| 3:N:147:VAL:CG2 | 3:N:148:GLU:H | 1.94 | 0.79 |
| 2:M:72:ARG:CG | 2:M:95:TYR:HB2 | 2.12 | 0.79 |
| 3:N:675:ARG:NH2 | 5:P:420:ASP:HB3 | 1.95 | 0.79 |
| 3:N:693:GLU:HA | 4:O:48:MET:HE3 | 1.64 | 0.79 |
| 2:M:479:VAL:H | 2:M:506:ASN:HB3 | 1.47 | 0.79 |
| 5:P:333:ILE:HD12 | 5:P:333:ILE:N | 1.97 | 0.79 |
| 1:L:112:ARG:NH1 | 1:L:125:PRO:HB2 | 1.98 | 0.79 |
| 2:M:165:LEU:HD23 | 2:M:165:LEU:O | 1.83 | 0.79 |
| 3:N:387:LEU:H | 3:N:387:LEU:HD12 | 1.48 | 0.79 |
| 2:C:414:GLY:H | 2:C:419:THR:HG21 | 1.47 | 0.79 |
| 3:D:535:PHE:O | 5:F:314:PRO:HB2 | 1.83 | 0.79 |
| 5:F:396:ARG:HA | 5:F:399:GLN:HE21 | 1.46 | 0.79 |
| 1:A:15:THR:HB | 1:A:21:GLY:HA3 | 1.65 | 0.79 |
| 3:D:14:SER:HB2 | 3:D:17:LYS:H | 1.48 | 0.79 |
| 2:M:197:LEU:HB3 | 2:M:207:LEU:CD1 | 2.11 | 0.79 |
| 3:N:227:LEU:HD11 | 3:N:327:GLU:H | 1.47 | 0.79 |
| 3:D:1232:PRO:O | 3:D:1235:GLN:HG2 | 1.82 | 0.79 |
| 3:D:655:PRO:HA | 3:D:658:LEU:HD12 | 1.65 | 0.79 |
| 3:D:799:LYS:HB3 | 3:D:800:LYS:CE | 2.13 | 0.79 |
| 1:L:219:ARG:HG2 | 1:L:219:ARG:HH11 | 1.48 | 0.79 |
| 3:D:1472:ILE:O | 3:D:1477:GLY:HA3 | 1.82 | 0.78 |
| 1:K:206:THR:HB | 1:K:209:GLU:CG | 2.12 | 0.78 |
| 3:D:1183:ILE:HG13 | 3:D:1184:GLN:N | 1.97 | 0.78 |
| 2:M:715:THR:HG22 | 2:M:717:LEU:H | 1.48 | 0.78 |
| 2:M:737:LEU:HA | 2:M:743:VAL:HA | 1.64 | 0.78 |
| 3:D:658:LEU:HD23 | 3:D:661:MET:HE1 | 1.66 | 0.78 |
| 2:C:47:ALA:HA | 2:C:50:GLU:OE2 | 1.83 | 0.78 |
| 3:D:82:LYS:HB2 | 3:D:84:ILE:HG22 | 1.65 | 0.78 |
| 3:N:676:MET:HG3 | 3:N:677:LEU:HD23 | 1.65 | 0.78 |
| 2:C:720:GLU:HB3 | 2:C:760:SER:HB3 | 1.63 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:1307:LYS:H | 3:D:1307:LYS:CE | 1.95 | 0.78 |
| 2:C:949:LYS:HZ2 | 3:D:796:ARG:HH12 | 1.32 | 0.78 |
| 2:M:512:ARG:HD2 | 2:M:523:ILE:HG12 | 1.65 | 0.78 |
| 2:C:1:MET:HB2 | 2:C:899:GLN:HA | 1.65 | 0.78 |
| 3:N:288:MET:CE | 3:N:307:ALA:HB2 | 2.13 | 0.78 |
| 3:N:416:ALA:CB | 3:N:432:TYR:HA | 2.08 | 0.78 |
| 3:D:98:PRO:HA | 3:D:514:LEU:O | 1.83 | 0.78 |
| 3:N:1486:VAL:HG22 | 4:O:75:PHE:HB3 | 1.65 | 0.78 |
| 1:L:58:ILE:HG12 | 1:L:140:MET:HB3 | 1.65 | 0.78 |
| 3:D:162:ARG:NH1 | 3:D:434:ARG:HH22 | 1.82 | 0.78 |
| 3:N:711:LEU:HB3 | 3:N:735:ALA:HB1 | 1.65 | 0.78 |
| 3:N:841:TYR:HB2 | 3:N:864:VAL:HG13 | 1.64 | 0.78 |
| 5:P:173:TYR:HA | 5:P:176:ILE:HD12 | 1.63 | 0.78 |
| 2:M:290:LEU:HD22 | 2:M:302:VAL:HG21 | 1.64 | 0.78 |
| 3:N:433:GLY:CA | 3:N:449:SER:H | 1.96 | 0.78 |
| 3:D:537:THR:O | 5:F:317:LEU:HG | 1.82 | 0.78 |
| 2:M:773:LEU:HG | 2:M:774:LEU:N | 1.99 | 0.78 |
| 3:D:843:PHE:CE2 | 3:D:864:VAL:HG11 | 2.16 | 0.78 |
| 2:M:265:ARG:HB2 | 2:M:267:TYR:O | 1.84 | 0.78 |
| 3:D:252:ARG:CZ | 3:D:300:LYS:HG2 | 2.14 | 0.78 |
| 2:M:157:ARG:HD2 | 2:M:314:THR:HG22 | 1.63 | 0.78 |
| 3:N:875:THR:HG22 | 3:N:879:ARG:HG3 | 1.64 | 0.78 |
| 5:F:234:LYS:HE2 | 5:F:236:SER:HB3 | 1.64 | 0.78 |
| 2:M:834:GLN:HG3 | 2:M:837:ASP:OD2 | 1.84 | 0.78 |
| 2:M:208:ALA:HB2 | 2:M:221:LEU:HD22 | 1.63 | 0.78 |
| 3:D:542:ASP:O | 3:D:546:ARG:HG2 | 1.83 | 0.78 |
| 2:M:600:ASP:CB | 2:M:650:ARG:HA | 2.14 | 0.78 |
| 3:D:799:LYS:HB3 | 3:D:800:LYS:HE3 | 1.66 | 0.78 |
| 3:N:610:LYS:NZ | 3:N:1442:ASN:H | 1.80 | 0.78 |
| 2:C:689:VAL:HG22 | 2:C:870:ILE:HB | 1.66 | 0.78 |
| 5:F:90:GLN:O | 5:F:92:PRO:HD3 | 1.83 | 0.78 |
| 1:B:13:VAL:HG22 | 1:B:14:ARG:H | 1.49 | 0.78 |
| 2:M:755:LEU:HD21 | 2:M:792:VAL:HG22 | 1.66 | 0.78 |
| 3:N:135:LEU:O | 3:N:150:ARG:HA | 1.84 | 0.78 |
| 5:P:209:PHE:CD2 | 5:P:213:ILE:HD11 | 2.18 | 0.78 |
| 2:C:367:LEU:HG | 2:C:372:LEU:HD21 | 1.64 | 0.78 |
| 2:C:649:VAL:HA | 2:C:650:ARG:HH21 | 1.49 | 0.78 |
| 2:M:1071:ILE:O | 3:N:659:LYS:HD3 | 1.83 | 0.78 |
| 3:N:230:TRP:HE1 | 3:N:233:LYS:HG3 | 1.49 | 0.78 |
| 4:E:49:GLN:HA | 4:E:53:GLY:O | 1.83 | 0.78 |
| 3:N:238:PRO:HG3 | 3:N:318:ARG:HG2 | 1.66 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:526:PRO:O | 3:N:537:THR:HG22 | 1.84 | 0.78 |
| 3:D:1103:HIS:CD2 | 3:D:1463:LYS:H | 2.01 | 0.78 |
| 5:P:353:GLU:HA | 5:P:356:LYS:HD2 | 1.66 | 0.78 |
| 5:P:264:MET:HA | 5:P:264:MET:HE2 | 1.65 | 0.78 |
| 2:C:15:LEU:HD12 | 2:C:15:LEU:N | 1.99 | 0.78 |
| 3:N:858:VAL:HG12 | 3:N:859:ASP:N | 1.99 | 0.78 |
| 3:N:85:VAL:HG21 | 3:N:89:ARG:CZ | 2.14 | 0.78 |
| 3:N:1267:ARG:CB | 3:N:1267:ARG:HH11 | 1.97 | 0.78 |
| 3:N:782:SER:H | 3:N:785:ILE:HD12 | 1.48 | 0.78 |
| 1:L:241:GLU:N | 1:L:242:PRO:HD2 | 1.99 | 0.78 |
| 1:L:111:ALA:HB3 | 1:L:125:PRO:HA | 1.65 | 0.78 |
| 2:M:1031:ARG:HB2 | 3:N:622:ARG:HH12 | 1.48 | 0.78 |
| 3:D:225:LEU:HD12 | 3:D:333:LEU:HD11 | 1.65 | 0.77 |
| 3:D:225:LEU:HD11 | 3:D:242:LEU:HD11 | 1.64 | 0.77 |
| 3:D:808:THR:H | 3:D:809:PRO:HD2 | 1.50 | 0.77 |
| 3:D:417:PRO:HA | 3:D:429:SER:O | 1.83 | 0.77 |
| 1:K:39:PRO:HG3 | 1:L:39:PRO:HG3 | 1.66 | 0.77 |
| 4:E:76:GLY:HA3 | 4:E:79:LEU:HD21 | 1.65 | 0.77 |
| 3:D:421:LEU:HD23 | 3:D:427:VAL:CG1 | 2.14 | 0.77 |
| 2:C:600:ASP:HB3 | 2:C:650:ARG:HA | 1.66 | 0.77 |
| 2:C:606:VAL:HG12 | 2:C:611:ILE:HG23 | 1.66 | 0.77 |
| 2:M:21:ILE:CD1 | 2:M:21:ILE:H | 1.96 | 0.77 |
| 3:D:258:VAL:HB | 3:D:273:ARG:CB | 2.07 | 0.77 |
| 3:N:352:ASN:C | 3:N:368:VAL:HG13 | 2.05 | 0.77 |
| 2:M:773:LEU:HD23 | 5:P:354:LEU:HD22 | 1.67 | 0.77 |
| 1:L:78:ILE:HG22 | 1:L:82:LEU:HD21 | 1.66 | 0.77 |
| 3:D:36:THR:HB | 3:D:38:LYS:HG2 | 1.65 | 0.77 |
| 3:N:1496:GLU:HA | 3:N:1499:ARG:HB3 | 1.67 | 0.77 |
| 3:N:1286:THR:HG22 | 3:N:1288:GLU:N | 1.95 | 0.77 |
| 3:D:1380:GLU:HG2 | 3:D:1381:VAL:H | 1.48 | 0.77 |
| 3:D:827:ILE:HA | 3:D:836:VAL:HB | 1.64 | 0.77 |
| 2:C:575:GLN:N | 2:C:667:ALA:HB1 | 1.99 | 0.77 |
| 3:D:989:TYR:HA | 3:D:992:ILE:HD12 | 1.66 | 0.77 |
| 2:M:837:ASP:O | 2:M:849:VAL:HG23 | 1.83 | 0.77 |
| 2:C:91:GLN:HA | 2:C:120:LEU:HG | 1.65 | 0.77 |
| 3:N:387:LEU:N | 3:N:387:LEU:HD12 | 2.00 | 0.77 |
| 2:C:266:ARG:HB2 | 2:C:272:ALA:HB3 | 1.65 | 0.77 |
| 2:C:413:LEU:HA | 2:C:419:THR:HG21 | 1.65 | 0.77 |
| 3:N:407:VAL:CG2 | 3:N:408:GLU:H | 1.96 | 0.77 |
| 3:D:804:LEU:O | 3:D:805:GLU:HG2 | 1.83 | 0.77 |
| 3:D:945:SER:OG | 3:D:947:ILE:HG22 | 1.84 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:1102:LEU:H | 3:N:5:VAL:HG13 | 1.48 | 0.77 |
| 2:C:21:ILE:HD12 | 2:C:21:ILE:N | 1.98 | 0.77 |
| 1:B:13:VAL:HG22 | 1:B:14:ARG:N | 1.99 | 0.77 |
| 5:P:156:VAL:HG23 | 5:P:157:GLU:OE1 | 1.84 | 0.77 |
| 3:N:241:ILE:HA | 3:N:312:ARG:HA | 1.64 | 0.77 |
| 2:C:141:HIS:CE1 | 2:C:332:ARG:HB3 | 2.19 | 0.77 |
| 5:F:350:LEU:HG | 5:F:354:LEU:HD11 | 1.66 | 0.77 |
| 4:O:40:LEU:HD13 | 4:O:72:ARG:HH12 | 1.49 | 0.77 |
| 3:D:853:VAL:HG13 | 3:D:858:VAL:O | 1.85 | 0.77 |
| 3:N:800:LYS:HD2 | 3:N:801:GLY:N | 1.99 | 0.77 |
| 5:F:368:VAL:HG23 | 5:F:369:LEU:N | 2.00 | 0.77 |
| 2:C:605:LYS:HB3 | 2:C:610:ARG:HH21 | 1.48 | 0.77 |
| 3:N:1048:PRO:HG3 | 3:N:1075:HIS:CD2 | 2.20 | 0.77 |
| 2:M:516:ARG:HA | 2:M:520:GLU:O | 1.84 | 0.77 |
| 1:A:211:LEU:O | 1:A:215:VAL:HG23 | 1.85 | 0.77 |
| 2:M:397:GLU:H | 2:M:633:GLN:NE2 | 1.80 | 0.77 |
| 3:N:433:GLY:HA2 | 3:N:449:SER:H | 1.48 | 0.77 |
| 5:P:367:MET:HB2 | 5:P:371:LEU:CG | 2.15 | 0.77 |
| 3:D:841:TYR:HB2 | 3:D:864:VAL:HG13 | 1.65 | 0.77 |
| 3:N:476:GLU:O | 3:N:479:GLU:HB2 | 1.84 | 0.77 |
| 1:K:14:ARG:HD2 | 1:L:233:VAL:HA | 1.64 | 0.77 |
| 2:C:759:THR:HB | 2:C:785:VAL:CG1 | 2.13 | 0.77 |
| 4:E:61:GLU:H | 4:E:61:GLU:CD | 1.87 | 0.77 |
| 3:D:1048:PRO:HG3 | 3:D:1075:HIS:HD2 | 1.48 | 0.77 |
| 1:L:181:VAL:HG22 | 1:L:195:LEU:HD13 | 1.67 | 0.77 |
| 1:B:153:ALA:HA | 1:B:156:HIS:CE1 | 2.19 | 0.77 |
| 3:N:921:ARG:NH1 | 3:N:921:ARG:HB3 | 1.99 | 0.77 |
| 1:B:104:GLU:HA | 1:B:132:LEU:HD13 | 1.66 | 0.77 |
| 2:M:625:LEU:HD11 | 2:M:639:GLN:HB2 | 1.66 | 0.77 |
| 3:D:1380:GLU:HG2 | 3:D:1381:VAL:N | 1.99 | 0.77 |
| 3:N:297:ILE:HG12 | 3:N:298:VAL:HG23 | 1.67 | 0.77 |
| 1:A:154:GLU:H | 1:A:154:GLU:CD | 1.88 | 0.77 |
| 2:M:325:ILE:N | 2:M:325:ILE:HD12 | 1.98 | 0.77 |
| 1:K:38:ASN:HB3 | 1:K:39:PRO:HD3 | 1.65 | 0.77 |
| 3:N:815:ALA:HA | 3:N:818:ARG:HD2 | 1.67 | 0.77 |
| 5:P:102:LEU:HD12 | 5:P:183:ALA:HB1 | 1.67 | 0.77 |
| 2:M:74:GLY:O | 2:M:76:PRO:HD3 | 1.84 | 0.77 |
| 2:M:580:MET:HB3 | 2:M:584:GLU:OE2 | 1.84 | 0.77 |
| 2:C:413:LEU:HA | 2:C:419:THR:CG2 | 2.13 | 0.77 |
| 3:N:548:ILE:HG22 | 3:N:552:ASN:ND2 | 1.96 | 0.77 |
| 2:M:355:VAL:HA | 2:M:358:ARG:HG3 | 1.67 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:N:490:ALA:HA | 3:N:493:ARG:NE | 2.00 | 0.77 |
| 3:N:1472:ILE:HG23 | 3:N:1474:ALA:H | 1.50 | 0.77 |
| 2:M:1051:GLU:HG3 | 2:M:1052:MET:N | 1.99 | 0.77 |
| 1:K:86:VAL:HG13 | 1:K:123:MET:HB2 | 1.64 | 0.77 |
| 3:N:734:GLU:OE1 | 3:N:734:GLU:HA | 1.85 | 0.77 |
| 5:P:333:ILE:HD12 | 5:P:333:ILE:H | 1.48 | 0.77 |
| 1:A:86:VAL:HG12 | 1:A:124:ASN:ND2 | 2.00 | 0.77 |
| 3:D:1286:THR:HG22 | 3:D:1288:GLU:H | 1.49 | 0.77 |
| 3:D:440:VAL:HG23 | 3:D:441:ARG:N | 1.99 | 0.76 |
| 3:N:761:ILE:HG22 | 3:N:762:GLN:N | 1.98 | 0.76 |
| 2:C:1051:GLU:HG3 | 2:C:1052:MET:N | 1.98 | 0.76 |
| 2:M:193:LEU:HG | 2:M:197:LEU:HD21 | 1.67 | 0.76 |
| 2:M:194:VAL:CA | 2:M:197:LEU:HG | 2.13 | 0.76 |
| 3:N:119:SER:HB3 | 3:N:123:LEU:HG | 1.67 | 0.76 |
| 2:M:93:PRO:CA | 2:M:117:HIS:HB3 | 2.15 | 0.76 |
| 1:B:58:ILE:CG2 | 1:B:61:VAL:HB | 2.15 | 0.76 |
| 2:M:780:GLU:HG2 | 5:P:379:ARG:NH2 | 2.00 | 0.76 |
| 3:D:793:THR:HG21 | 3:D:906:GLN:HG2 | 1.68 | 0.76 |
| 3:N:1380:GLU:HG2 | 3:N:1381:VAL:H | 1.48 | 0.76 |
| 4:O:7:ASP:HA | 4:O:10:PHE:CD1 | 2.20 | 0.76 |
| 3:N:1041:LEU:CD1 | 3:N:1058:ARG:HA | 2.15 | 0.76 |
| 1:K:224:TYR:CE1 | 1:L:9:PRO:HD2 | 2.19 | 0.76 |
| 1:B:152:PRO:HG2 | 1:B:155:LYS:CB | 2.16 | 0.76 |
| 3:N:612:GLY:O | 3:N:615:ARG:HG2 | 1.85 | 0.76 |
| 3:N:646:LYS:HG2 | 3:N:720:LEU:HB3 | 1.66 | 0.76 |
| 2:C:184:MET:HG3 | 2:C:193:LEU:HD13 | 1.66 | 0.76 |
| 2:C:264:PRO:HB2 | 2:C:289:THR:HG21 | 1.66 | 0.76 |
| 3:D:140:ALA:N | 3:D:450:TYR:CE2 | 2.52 | 0.76 |
| 3:N:367:ILE:HB | 3:N:377:VAL:CG1 | 2.14 | 0.76 |
| 3:D:654:LYS:HB3 | 3:D:655:PRO:HD3 | 1.65 | 0.76 |
| 2:C:100:LEU:HD21 | 2:C:367:LEU:HD23 | 1.67 | 0.76 |
| 2:M:37:GLU:HG2 | 2:M:71:TYR:CE2 | 2.20 | 0.76 |
| 3:N:1253:THR:HG22 | 3:N:1254:GLN:H | 1.46 | 0.76 |
| 3:N:160:GLU:CD | 3:N:165:LYS:HE2 | 2.06 | 0.76 |
| 2:C:309:TYR:CE2 | 2:C:321:GLU:HG3 | 2.20 | 0.76 |
| 3:N:119:SER:H | 3:N:123:LEU:HB2 | 1.50 | 0.76 |
| 3:D:253:ALA:N | 3:D:301:GLY:HA3 | 2.00 | 0.76 |
| 3:N:421:LEU:HG | 3:N:428:LYS:CA | 2.10 | 0.76 |
| 1:B:206:THR:HB | 1:B:209:GLU:CG | 2.13 | 0.76 |
| 2:M:101:ILE:HG22 | 2:M:102:HIS:N | 2.01 | 0.76 |
| 3:N:671:LYS:HA | 3:N:674:ARG:HB2 | 1.64 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:253:ALA:N | 3:N:301:GLY:HA3 | 1.99 | 0.76 |
| 1:A:152:PRO:HG2 | 1:A:155:LYS:HB2 | 1.67 | 0.76 |
| 5:F:156:VAL:HG23 | 5:F:157:GLU:H | 1.49 | 0.76 |
| 3:D:1213:ARG:HG2 | 3:D:1213:ARG:HH11 | 1.50 | 0.76 |
| 2:C:631:SER:HB3 | 2:C:635:THR:N | 2.00 | 0.76 |
| 5:F:353:GLU:O | 5:F:356:LYS:HB2 | 1.84 | 0.76 |
| 3:N:219:GLU:O | 3:N:337:LEU:HG | 1.84 | 0.76 |
| 2:C:468:ARG:HA | 2:C:486:MET:O | 1.85 | 0.76 |
| 1:B:32:PHE:HA | 1:B:35:THR:CB | 2.14 | 0.76 |
| 2:C:988:VAL:HG12 | 3:D:948:THR:CB | 2.14 | 0.76 |
| 2:M:1100:GLN:O | 3:N:8:VAL:HA | 1.85 | 0.76 |
| 3:N:1095:THR:HG23 | 3:N:1230:GLY:HA3 | 1.66 | 0.76 |
| 3:D:1345:GLU:O | 3:D:1349:VAL:HG23 | 1.85 | 0.76 |
| 4:E:46:PRO:HB2 | 4:E:57:ASP:HB3 | 1.66 | 0.76 |
| 2:M:385:PHE:CD1 | 2:M:389:SER:HB2 | 2.21 | 0.76 |
| 5:F:276:ARG:O | 5:F:280:GLN:HG2 | 1.85 | 0.76 |
| 2:M:428:ARG:NE | 2:M:451:LEU:HD21 | 2.01 | 0.76 |
| 5:F:353:GLU:HG3 | 5:F:356:LYS:HD2 | 1.67 | 0.76 |
| 3:D:1114:THR:HB | 3:D:1195:GLN:HG3 | 1.68 | 0.76 |
| 3:N:285:PRO:HB3 | 3:N:313:MET:SD | 2.25 | 0.76 |
| 3:D:119:SER:HB3 | 3:D:123:LEU:HG | 1.66 | 0.76 |
| 3:D:1099:VAL:HG12 | 9:D:1529:NE6:C14 | 2.16 | 0.76 |
| 3:D:361:VAL:CG1 | 3:D:379:ALA:HB1 | 2.16 | 0.76 |
| 5:F:380:GLU:HA | 5:F:385:GLU:OE1 | 1.84 | 0.76 |
| 2:C:17:PRO:HB2 | 2:C:20:GLU:HB2 | 1.68 | 0.76 |
| 3:N:1213:ARG:HB2 | 3:N:1214:PRO:HD2 | 1.67 | 0.76 |
| 3:N:165:LYS:O | 3:N:396:VAL:HA | 1.84 | 0.76 |
| 3:D:1216:SER:HB2 | 4:E:15:SER:HA | 1.68 | 0.76 |
| 2:C:167:LYS:HE2 | 2:C:168:ARG:HE | 1.50 | 0.76 |
| 3:N:553:ARG:NH1 | 5:P:214:GLN:HB2 | 2.00 | 0.76 |
| 3:D:322:VAL:HA | 3:D:335:LEU:HG | 1.66 | 0.76 |
| 4:E:6:ILE:HG13 | 4:E:10:PHE:CE1 | 2.20 | 0.76 |
| 2:C:1064:ASN:HA | 5:F:341:PRO:CB | 2.15 | 0.76 |
| 5:F:261:PRO:HD2 | 5:F:264:MET:HG3 | 1.66 | 0.76 |
| 3:D:801:GLY:HA2 | 3:D:830:ALA:O | 1.86 | 0.76 |
| 1:L:176:ARG:HG2 | 1:L:177:VAL:N | 2.01 | 0.76 |
| 1:L:18:ARG:HH12 | 1:L:88:ARG:HH22 | 1.30 | 0.76 |
| 2:C:958:THR:HG23 | 2:C:961:GLU:CB | 2.15 | 0.76 |
| 5:F:302:LYS:HD2 | 5:F:303:ARG:N | 2.00 | 0.76 |
| 1:L:150:TYR:OH | 1:L:168:ASP:HB3 | 1.85 | 0.76 |
| 2:C:226:VAL:HG23 | 2:C:227:PHE:CD1 | 2.20 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:285:LEU:HG | 2:C:286:SER:N | 2.00 | 0.76 |
| 3:N:409:VAL:HG12 | 3:N:413:ASP:OD2 | 1.84 | 0.76 |
| 3:D:1480:PHE:CD2 | 3:D:1481:VAL:HG23 | 2.20 | 0.76 |
| 3:D:931:LEU:CA | 3:D:934:LEU:HD12 | 2.13 | 0.76 |
| 3:D:1398:TRP:N | 3:D:1398:TRP:HE3 | 1.84 | 0.76 |
| 3:D:65:ARG:CG | 3:D:67:ARG:HG2 | 2.16 | 0.76 |
| 3:D:875:THR:HG22 | 3:D:876:SER:H | 1.51 | 0.76 |
| 3:D:1211:MET:HB2 | 3:D:1213:ARG:HH11 | 1.51 | 0.76 |
| 5:P:242:TRP:HA | 5:P:245:GLN:HG2 | 1.66 | 0.76 |
| 2:C:84:ARG:HA | 2:C:131:GLY:HA2 | 1.68 | 0.76 |
| 3:D:960:LYS:HE3 | 3:D:964:LEU:HD11 | 1.67 | 0.76 |
| 3:N:1119:SER:HA | 3:N:1186:VAL:O | 1.86 | 0.76 |
| 3:N:566:ILE:HG22 | 5:P:84:TYR:OH | 1.85 | 0.76 |
| 5:F:113:ILE:HD13 | 5:F:128:ARG:HB3 | 1.66 | 0.76 |
| 1:B:104:GLU:HB3 | 1:B:137:ARG:CG | 2.13 | 0.76 |
| 1:B:112:ARG:HH12 | 1:B:125:PRO:HB2 | 1.49 | 0.76 |
| 2:C:1067:TYR:CE2 | 5:F:342:VAL:HA | 2.21 | 0.76 |
| 3:N:1161:GLU:HG3 | 3:N:1164:ARG:HB2 | 1.68 | 0.76 |
| 1:A:228:PRO:O | 1:A:229:GLN:HG3 | 1.85 | 0.76 |
| 3:D:992:ILE:O | 3:D:995:LEU:HB3 | 1.85 | 0.76 |
| 3:D:191:LEU:HD23 | 3:D:195:VAL:HG11 | 1.67 | 0.76 |
| 4:O:46:PRO:CB | 4:O:57:ASP:HB3 | 2.15 | 0.76 |
| 3:N:406:ASP:HB2 | 3:N:423:ASP:HA | 1.67 | 0.76 |
| 3:N:1105:ILE:HD11 | 3:N:1374:GLN:CD | 2.05 | 0.76 |
| 3:N:329:GLU:HG2 | 3:N:330:THR:HG23 | 1.68 | 0.75 |
| 2:C:195:LEU:N | 2:C:195:LEU:HD23 | 1.97 | 0.75 |
| 2:M:807:ARG:HB3 | 2:M:807:ARG:NH1 | 2.01 | 0.75 |
| 3:N:793:THR:O | 3:N:905:PRO:HA | 1.87 | 0.75 |
| 2:C:599:GLU:HB3 | 2:C:615:TYR:CD2 | 2.21 | 0.75 |
| 2:M:431:HIS:CE1 | 2:M:432:ARG:HG2 | 2.21 | 0.75 |
| 3:D:192:ALA:HB3 | 3:D:195:VAL:HG23 | 1.68 | 0.75 |
| 3:N:530:VAL:HG23 | 3:N:531:ASP:H | 1.49 | 0.75 |
| 3:N:57:GLU:HG3 | 3:N:64:LYS:HG2 | 1.68 | 0.75 |
| 3:N:318:ARG:HB2 | 3:N:338:GLU:OE2 | 1.86 | 0.75 |
| 3:N:400:VAL:HG23 | 3:N:443:VAL:CG1 | 2.16 | 0.75 |
| 3:D:438:ASP:HB3 | 3:D:443:VAL:O | 1.85 | 0.75 |
| 4:O:40:LEU:HD12 | 4:O:41:GLU:N | 2.00 | 0.75 |
| 3:N:711:LEU:HD22 | 3:N:778:LEU:HD23 | 1.68 | 0.75 |
| 2:M:691:SER:HB2 | 2:M:858:MET:SD | 2.26 | 0.75 |
| 3:D:206:ARG:NH2 | 3:D:394:LEU:HD13 | 2.01 | 0.75 |
| 3:N:1208:ASP:O | 3:N:1209:LEU:HB2 | 1.87 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:607:ASP:HB3 | 2:C:610:ARG:HH12 | 1.51 | 0.75 |
| 2:C:396:ASP:O | 2:C:403:SER:HA | 1.86 | 0.75 |
| 4:E:46:PRO:CB | 4:E:57:ASP:HB3 | 2.15 | 0.75 |
| 2:M:443:THR:OG1 | 2:M:444:PRO:HD2 | 1.86 | 0.75 |
| 3:N:244:GLU:HG2 | 3:N:245:LEU:H | 1.50 | 0.75 |
| 3:N:122:GLU:O | 3:N:126:VAL:HB | 1.87 | 0.75 |
| 3:D:567:ILE:HG22 | 3:D:571:LYS:HE3 | 1.68 | 0.75 |
| 5:P:416:ARG:NH1 | 5:P:419:ARG:HD3 | 2.00 | 0.75 |
| 3:D:675:ARG:O | 3:D:678:GLU:HG2 | 1.85 | 0.75 |
| 1:B:5:LYS:C | 1:B:7:LYS:H | 1.89 | 0.75 |
| 3:N:1117:TYR:C | 3:N:1193:THR:HG21 | 2.07 | 0.75 |
| 1:K:1:MET:H1 | 1:K:6:LEU:HD13 | 1.49 | 0.75 |
| 3:N:323:GLU:HB2 | 3:N:334:THR:HB | 1.68 | 0.75 |
| 2:C:189:ARG:NH2 | 2:C:242:LEU:HA | 2.02 | 0.75 |
| 3:N:417:PRO:HA | 3:N:429:SER:O | 1.85 | 0.75 |
| 3:D:808:THR:H | 3:D:809:PRO:CD | 2.00 | 0.75 |
| 3:D:1404:ASN:HA | 3:D:1408:ILE:HB | 1.67 | 0.75 |
| 1:K:186:LEU:C | 1:K:188:GLN:H | 1.90 | 0.75 |
| 1:B:76:VAL:HA | 1:B:79:ILE:CD1 | 2.15 | 0.75 |
| 3:N:819:GLY:HA2 | 3:N:824:ASN:HD22 | 1.50 | 0.75 |
| 2:C:762:LYS:HG2 | 2:C:763:GLY:N | 1.99 | 0.75 |
| 2:C:266:ARG:HG3 | 2:C:266:ARG:HH11 | 1.52 | 0.75 |
| 3:D:610:LYS:HZ1 | 3:D:1442:ASN:H | 1.33 | 0.75 |
| 5:F:349:LEU:HA | 5:F:352:GLU:OE2 | 1.86 | 0.75 |
| 3:N:769:LEU:N | 3:N:769:LEU:HD12 | 2.01 | 0.75 |
| 2:M:873:PRO:O | 2:M:876:VAL:HG23 | 1.85 | 0.75 |
| 3:N:1476:THR:HB | 4:O:21:VAL:HG23 | 1.69 | 0.75 |
| 2:C:185:LYS:HA | 2:C:190:LYS:HB3 | 1.68 | 0.75 |
| 2:C:1014:SER:HA | 2:C:1021:LEU:HD22 | 1.68 | 0.75 |
| 2:C:349:ALA:O | 2:C:353:ARG:HG3 | 1.85 | 0.75 |
| 1:A:132:LEU:HD13 | 1:A:136:GLY:O | 1.86 | 0.75 |
| 2:M:401:LEU:HD11 | 2:M:543:ASN:HB3 | 1.67 | 0.75 |
| 2:C:358:ARG:HD2 | 2:C:372:LEU:HA | 1.68 | 0.75 |
| 2:C:57:GLU:HG3 | 2:C:62:GLY:O | 1.86 | 0.75 |
| 3:N:676:MET:HG3 | 3:N:677:LEU:CD2 | 2.17 | 0.75 |
| 2:M:834:GLN:N | 2:M:837:ASP:OD2 | 2.20 | 0.75 |
| 3:D:1119:SER:HA | 3:D:1186:VAL:O | 1.87 | 0.75 |
| 2:M:300:ASP:O | 2:M:304:LEU:HD13 | 1.86 | 0.75 |
| 3:D:136:ASP:CB | 3:D:137:PRO:HD3 | 2.17 | 0.75 |
| 2:C:93:PRO:N | 2:C:117:HIS:HB3 | 2.01 | 0.75 |
| 3:N:1335:LEU:CD2 | 3:N:1344:VAL:HA | 2.16 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:425:PHE:HE2 | 3:N:1239:ARG:HH21 | 1.34 | 0.75 |
| 3:D:1281:VAL:HG23 | 3:D:1317:ASP:O | 1.86 | 0.75 |
| 2:M:122:THR:HB | 2:M:124:ASP:OD1 | 1.86 | 0.75 |
| 4:O:76:GLY:HA3 | 4:O:79:LEU:HD21 | 1.68 | 0.75 |
| 2:C:79:PRO:HG2 | 2:C:82:GLU:HB2 | 1.68 | 0.75 |
| 3:N:284:LEU:HD13 | 3:N:288:MET:HG3 | 1.67 | 0.75 |
| 2:C:325:ILE:HD12 | 2:C:325:ILE:N | 2.01 | 0.75 |
| 3:D:358:GLY:HA2 | 3:D:385:VAL:HB | 1.67 | 0.75 |
| 3:N:365:ASP:O | 3:N:379:ALA:HB2 | 1.87 | 0.75 |
| 2:M:101:ILE:HG22 | 2:M:102:HIS:H | 1.52 | 0.75 |
| 2:C:15:LEU:H | 2:C:15:LEU:CD1 | 1.95 | 0.75 |
| 2:M:676:ILE:HG23 | 2:M:988:VAL:HG13 | 1.69 | 0.75 |
| 1:L:208:LEU:HG | 1:L:209:GLU:N | 1.99 | 0.75 |
| 3:N:1335:LEU:HD23 | 3:N:1344:VAL:HA | 1.68 | 0.75 |
| 2:M:939:ARG:HD2 | 2:M:982:PRO:HD3 | 1.69 | 0.75 |
| 3:N:808:THR:H | 3:N:809:PRO:HD2 | 1.50 | 0.75 |
| 2:C:91:GLN:HB2 | 2:C:118:ILE:O | 1.87 | 0.75 |
| 1:K:195:LEU:HD12 | 1:K:196:THR:H | 1.50 | 0.75 |
| 2:C:431:HIS:CE1 | 2:C:432:ARG:HG2 | 2.22 | 0.75 |
| 3:N:1424:VAL:HG23 | 3:N:1425:THR:H | 1.51 | 0.75 |
| 3:D:1001:GLU:HA | 3:D:1001:GLU:OE2 | 1.87 | 0.75 |
| 2:M:737:LEU:HD11 | 2:M:741:GLY:O | 1.86 | 0.75 |
| 3:D:1496:GLU:OE2 | 3:D:1500:LYS:HB2 | 1.87 | 0.75 |
| 2:M:304:LEU:CB | 2:M:305:PRO:HD3 | 2.17 | 0.74 |
| 3:N:135:LEU:HD12 | 3:N:148:GLU:HB2 | 1.67 | 0.74 |
| 3:D:112:ILE:O | 3:D:115:LEU:HB3 | 1.87 | 0.74 |
| 3:D:548:ILE:HG22 | 3:D:552:ASN:ND2 | 2.00 | 0.74 |
| 3:D:567:ILE:HG21 | 5:F:140:ARG:HH12 | 1.52 | 0.74 |
| 4:E:25:LYS:HA | 4:E:28:GLN:NE2 | 2.02 | 0.74 |
| 2:C:984:GLU:OE1 | 3:D:945:SER:HA | 1.86 | 0.74 |
| 3:D:1339:LYS:HB3 | 3:D:1343:ALA:HB2 | 1.69 | 0.74 |
| 1:A:138:LEU:HD21 | 1:A:140:MET:HE3 | 1.68 | 0.74 |
| 3:N:1085:ALA:HA | 3:N:1088:THR:HG22 | 1.69 | 0.74 |
| 3:N:1372:VAL:HA | 3:N:1375:MET:HE3 | 1.68 | 0.74 |
| 2:C:709:GLU:HG2 | 2:C:824:ARG:HG2 | 1.66 | 0.74 |
| 3:D:411:THR:HB | 3:D:437:VAL:CB | 2.16 | 0.74 |
| 3:D:523:ASP:HA | 3:D:526:PRO:HG3 | 1.68 | 0.74 |
| 5:F:115:LYS:O | 5:F:119:ILE:HG13 | 1.87 | 0.74 |
| 5:F:123:ASP:O | 5:F:126:LEU:HB3 | 1.87 | 0.74 |
| 3:D:811:GLU:HB2 | 3:D:816:HIS:CE1 | 2.22 | 0.74 |
| 2:C:101:ILE:HA | 2:C:106:GLY:O | 1.87 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:L:101:LEU:HB3 | 1:L:140:MET:SD | 2.27 | 0.74 |
| 1:L:58:ILE:HG12 | 1:L:140:MET:HB2 | 1.68 | 0.74 |
| 3:N:1095:THR:O | 3:N:1099:VAL:HG23 | 1.87 | 0.74 |
| 1:A:178:ALA:HB2 | 2:C:864:GLY:HA3 | 1.69 | 0.74 |
| 3:N:775:GLY:HA2 | 3:N:1209:LEU:O | 1.87 | 0.74 |
| 1:A:42:ARG:HH12 | 1:B:34:VAL:HB | 1.52 | 0.74 |
| 2:C:264:PRO:C | 2:C:289:THR:HG21 | 2.08 | 0.74 |
| 3:D:119:SER:H | 3:D:123:LEU:CD1 | 2.00 | 0.74 |
| 5:F:386:VAL:HG23 | 5:F:387:GLY:N | 2.03 | 0.74 |
| 2:C:344:PHE:O | 2:C:348:LEU:HB2 | 1.85 | 0.74 |
| 3:N:252:ARG:HG3 | 3:N:300:LYS:C | 2.08 | 0.74 |
| 1:A:5:LYS:HZ1 | 1:A:192:LEU:HD22 | 1.50 | 0.74 |
| 1:K:86:VAL:HG12 | 1:K:124:ASN:ND2 | 2.01 | 0.74 |
| 3:N:1394:VAL:HG21 | 3:N:1397:LYS:HZ1 | 1.52 | 0.74 |
| 5:P:113:ILE:HA | 5:P:116:LEU:HD12 | 1.69 | 0.74 |
| 3:N:264:LEU:HD12 | 3:N:267:GLY:HA3 | 1.67 | 0.74 |
| 2:M:194:VAL:HA | 2:M:197:LEU:CD1 | 2.16 | 0.74 |
| 2:C:300:ASP:OD2 | 2:C:302:VAL:HB | 1.87 | 0.74 |
| 2:C:31:GLN:O | 2:C:35:PRO:HB2 | 1.88 | 0.74 |
| 3:D:82:LYS:CB | 3:D:84:ILE:HG22 | 2.18 | 0.74 |
| 3:N:1098:LEU:CD1 | 3:N:1098:LEU:H | 2.00 | 0.74 |
| 5:F:155:THR:HA | 5:F:158:GLU:OE2 | 1.87 | 0.74 |
| 3:D:16:GLU:H | 3:D:16:GLU:CD | 1.91 | 0.74 |
| 2:M:626:ARG:HG3 | 2:M:629:TYR:HD1 | 1.52 | 0.74 |
| 2:M:199:VAL:HG21 | 2:M:238:LEU:HD11 | 1.70 | 0.74 |
| 1:L:100:LEU:HD12 | 1:L:140:MET:O | 1.88 | 0.74 |
| 3:N:1381:VAL:HG12 | 3:N:1391:GLU:O | 1.87 | 0.74 |
| 5:F:321:ILE:HG13 | 5:F:332:PHE:CE1 | 2.22 | 0.74 |
| 3:D:700:VAL:O | 3:D:715:ALA:HA | 1.87 | 0.74 |
| 2:M:163:ILE:O | 2:M:266:ARG:HG3 | 1.87 | 0.74 |
| 2:M:439:CYS:HB2 | 2:M:541:SER:HB3 | 1.69 | 0.74 |
| 3:N:119:SER:H | 3:N:123:LEU:CB | 2.01 | 0.74 |
| 3:D:119:SER:HB3 | 3:D:123:LEU:N | 1.98 | 0.74 |
| 2:M:95:TYR:CD2 | 2:M:114:PHE:HB3 | 2.23 | 0.74 |
| 1:B:68:ILE:HG13 | 1:B:71:VAL:O | 1.87 | 0.74 |
| 1:L:55:SER:HB2 | 1:L:165:ILE:O | 1.88 | 0.74 |
| 3:N:1201:CYS:SG | 3:N:1203:LYS:HB2 | 2.28 | 0.74 |
| 3:N:812:ALA:HA | 3:N:816:HIS:HB2 | 1.69 | 0.74 |
| 2:M:325:ILE:CD1 | 2:M:325:ILE:H | 2.00 | 0.74 |
| 2:C:353:ARG:HG2 | 2:C:353:ARG:HH11 | 1.52 | 0.74 |
| 1:A:91:ASN:HD21 | 1:A:93:SER:HB2 | 1.53 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:P:81:VAL:HG23 | 5:P:82:ARG:H | 1.52 | 0.74 |
| 3:N:432:TYR:O | 3:N:448:GLU:HA | 1.86 | 0.74 |
| 3:D:119:SER:CB | 3:D:123:LEU:HG | 2.18 | 0.74 |
| 3:D:534:ARG:NE | 5:F:314:PRO:HA | 2.02 | 0.74 |
| 3:D:241:ILE:HG13 | 3:D:312:ARG:NH1 | 2.02 | 0.74 |
| 3:N:1290:LEU:HD23 | 3:N:1307:LYS:HA | 1.68 | 0.74 |
| 3:D:1394:VAL:HB | 3:D:1397:LYS:CE | 2.16 | 0.74 |
| 3:N:252:ARG:NH2 | 3:N:300:LYS:HG2 | 2.03 | 0.74 |
| 2:M:575:GLN:HG3 | 2:M:670:GLN:HG2 | 1.69 | 0.74 |
| 3:N:192:ALA:HB3 | 3:N:195:VAL:CG2 | 2.17 | 0.74 |
| 5:F:157:GLU:HA | 5:F:160:ASP:OD2 | 1.88 | 0.74 |
| 2:M:1055:LEU:HD11 | 2:M:1079:PRO:HG3 | 1.70 | 0.74 |
| 3:N:890:VAL:HG23 | 3:N:892:ASP:H | 1.52 | 0.74 |
| 2:C:325:ILE:H | 2:C:325:ILE:CD1 | 2.01 | 0.74 |
| 4:E:7:ASP:HA | 4:E:10:PHE:HD1 | 1.51 | 0.74 |
| 2:C:115:LEU:H | 2:C:115:LEU:HD23 | 1.53 | 0.74 |
| 3:D:65:ARG:HG3 | 3:D:67:ARG:HG2 | 1.68 | 0.74 |
| 3:D:864:VAL:HG12 | 3:D:865:THR:N | 2.01 | 0.74 |
| 3:N:371:ILE:HD13 | 5:P:232:ARG:HD3 | 1.70 | 0.74 |
| 3:N:1080:GLY:O | 3:N:1084:THR:HG22 | 1.88 | 0.74 |
| 2:C:678:PRO:O | 3:D:943:THR:HA | 1.87 | 0.74 |
| 2:M:764:GLU:O | 2:M:766:GLU:HG3 | 1.87 | 0.74 |
| 3:D:1269:LYS:HE2 | 3:D:1270:ALA:H | 1.53 | 0.74 |
| 2:C:232:GLU:HA | 2:C:235:LEU:HD13 | 1.69 | 0.74 |
| 2:C:278:GLU:OE2 | 2:C:284:ARG:HG2 | 1.87 | 0.74 |
| 3:D:610:LYS:NZ | 3:D:1441:GLN:HG3 | 2.02 | 0.74 |
| 5:P:271:LEU:HD11 | 5:P:307:THR:HG21 | 1.70 | 0.74 |
| 2:C:889:HIS:HE1 | 3:D:951:ILE:H | 1.36 | 0.74 |
| 3:D:1029:ARG:NH1 | 3:D:1029:ARG:HG3 | 2.01 | 0.74 |
| 5:F:192:LEU:O | 5:F:195:VAL:HB | 1.88 | 0.74 |
| 3:D:119:SER:H | 3:D:123:LEU:CG | 2.00 | 0.74 |
| 3:D:519:VAL:HA | 3:D:544:TYR:OH | 1.87 | 0.74 |
| 5:F:386:VAL:HG23 | 5:F:387:GLY:H | 1.53 | 0.74 |
| 2:M:628:PHE:HD1 | 2:M:628:PHE:N | 1.85 | 0.74 |
| 2:C:712:ALA:O | 2:C:820:ARG:HG3 | 1.87 | 0.74 |
| 2:C:918:LEU:HD12 | 2:C:968:LEU:HA | 1.70 | 0.74 |
| 3:N:133:ILE:CD1 | 3:N:456:MET:HE1 | 2.19 | 0.73 |
| 3:N:1267:ARG:NH2 | 3:N:1271:LYS:HZ1 | 1.82 | 0.73 |
| 2:M:276:LYS:HB3 | 2:M:280:LYS:NZ | 2.03 | 0.73 |
| 3:D:1066:THR:HB | 3:D:1069:GLU:H | 1.51 | 0.73 |
| 2:C:774:LEU:HA | 2:C:777:ILE:HD12 | 1.70 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:1406:ARG:HB3 | 3:N:1412:LYS:HE2 | 1.70 | 0.73 |
| 2:C:674:VAL:HG21 | 2:C:871:LEU:HD12 | 1.70 | 0.73 |
| 3:N:1464:GLU:HG2 | 3:N:1465:ASN:H | 1.51 | 0.73 |
| 1:L:18:ARG:HH12 | 1:L:88:ARG:NH2 | 1.86 | 0.73 |
| 3:N:810:GLU:O | 3:N:813:LEU:HG | 1.87 | 0.73 |
| 3:D:1311:LEU:HD21 | 3:D:1313:VAL:O | 1.86 | 0.73 |
| 3:D:191:LEU:HD23 | 3:D:195:VAL:CG1 | 2.18 | 0.73 |
| 5:P:392:VAL:HG11 | 5:P:396:ARG:HD3 | 1.69 | 0.73 |
| 4:E:31:LEU:HD21 | 4:E:60:ALA:HB2 | 1.69 | 0.73 |
| 3:D:249:TYR:HE1 | 3:D:330:THR:HG21 | 1.53 | 0.73 |
| 2:C:913:GLU:O | 2:C:916:GLU:HB3 | 1.89 | 0.73 |
| 1:K:64:GLU:HG3 | 1:K:76:VAL:HG22 | 1.70 | 0.73 |
| 2:M:673:LEU:HD21 | 2:M:895:TYR:CE1 | 2.23 | 0.73 |
| 2:C:1005:MET:HG2 | 3:D:629:SER:HB2 | 1.71 | 0.73 |
| 3:N:990:ASP:HA | 3:N:993:LEU:HD12 | 1.70 | 0.73 |
| 2:M:456:ALA:HB3 | 2:M:459:ALA:HB2 | 1.70 | 0.73 |
| 2:C:1037:VAL:O | 2:C:1041:GLU:HG3 | 1.88 | 0.73 |
| 3:D:227:LEU:HD11 | 3:D:327:GLU:H | 1.51 | 0.73 |
| 3:N:853:VAL:HG13 | 3:N:858:VAL:O | 1.88 | 0.73 |
| 3:N:701:LEU:HB2 | 3:N:748:HIS:HB2 | 1.68 | 0.73 |
| 2:C:91:GLN:HB2 | 2:C:118:ILE:C | 2.07 | 0.73 |
| 2:M:267:TYR:HB2 | 2:M:272:ALA:CB | 2.18 | 0.73 |
| 2:C:425:PHE:HZ | 3:D:1239:ARG:HH21 | 1.35 | 0.73 |
| 3:N:551:ASN:O | 3:N:554:LEU:HB3 | 1.88 | 0.73 |
| 3:N:86:ARG:HB3 | 3:N:523:ASP:OD2 | 1.89 | 0.73 |
| 3:D:269:PHE:HD1 | 3:D:283:PHE:HB2 | 1.53 | 0.73 |
| 1:B:112:ARG:HB3 | 1:B:112:ARG:HH11 | 1.54 | 0.73 |
| 2:C:55:GLU:HG2 | 2:C:57:GLU:H | 1.53 | 0.73 |
| 1:B:86:VAL:HG12 | 1:B:124:ASN:ND2 | 2.04 | 0.73 |
| 3:N:478:LEU:O | 3:N:481:MET:HB3 | 1.89 | 0.73 |
| 2:M:836:GLY:H | 2:M:849:VAL:HB | 1.53 | 0.73 |
| 1:B:153:ALA:HA | 1:B:156:HIS:HE1 | 1.51 | 0.73 |
| 2:M:136:ILE:HD13 | 2:M:392:SER:HA | 1.71 | 0.73 |
| 3:N:260:GLU:HB2 | 3:N:271:VAL:HB | 1.71 | 0.73 |
| 2:C:261:ILE:O | 2:C:264:PRO:HD2 | 1.88 | 0.73 |
| 2:C:439:CYS:HB2 | 2:C:541:SER:HB2 | 1.69 | 0.73 |
| 3:N:119:SER:N | 3:N:123:LEU:HG | 2.02 | 0.73 |
| 3:N:462:GLN:HG3 | 3:N:513:ILE:HG21 | 1.68 | 0.73 |
| 2:M:15:LEU:HD13 | 2:M:586:ARG:HH11 | 1.53 | 0.73 |
| 3:D:806:PHE:H | 3:D:809:PRO:HG2 | 1.53 | 0.73 |
| 3:N:266:GLU:HB3 | 3:N:286:VAL:HG23 | 1.71 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:490:ALA:O | 3:D:494:LYS:HG2 | 1.88 | 0.73 |
| 2:M:479:VAL:HG23 | 2:M:506:ASN:O | 1.87 | 0.73 |
| 5:F:245:GLN:HA | 5:F:245:GLN:HE21 | 1.54 | 0.73 |
| 2:M:861:LEU:HB3 | 2:M:862:PRO:HD2 | 1.70 | 0.73 |
| 3:N:618:LEU:HD22 | 5:P:326:ASP:HB2 | 1.70 | 0.73 |
| 5:P:235:PHE:O | 5:P:238:TYR:HB3 | 1.88 | 0.73 |
| 2:C:334:ARG:HH11 | 2:C:418:LEU:CD1 | 2.01 | 0.73 |
| 3:N:139:GLY:C | 3:N:147:VAL:HB | 2.08 | 0.73 |
| 3:N:399:ARG:HB3 | 3:N:401:TYR:HE1 | 1.51 | 0.73 |
| 3:D:285:PRO:HB2 | 3:D:312:ARG:O | 1.88 | 0.73 |
| 5:P:416:ARG:HD2 | 5:P:419:ARG:HG2 | 1.71 | 0.73 |
| 3:D:48:ARG:HA | 3:D:78:VAL:HG22 | 1.69 | 0.73 |
| 2:M:1086:ARG:HB3 | 2:M:1112:PHE:HE2 | 1.52 | 0.73 |
| 5:F:159:ILE:O | 5:F:162:LYS:HB2 | 1.88 | 0.73 |
| 3:N:284:LEU:HD22 | 3:N:288:MET:HG2 | 1.71 | 0.73 |
| 5:P:181:GLU:OE2 | 5:P:184:ARG:HD3 | 1.89 | 0.73 |
| 5:P:383:LEU:CD2 | 5:P:394:ARG:HD3 | 2.19 | 0.73 |
| 3:D:806:PHE:HA | 3:D:809:PRO:CD | 2.18 | 0.73 |
| 5:F:383:LEU:HD11 | 5:F:394:ARG:NH1 | 2.04 | 0.73 |
| 1:A:206:THR:HG22 | 1:A:208:LEU:HB3 | 1.71 | 0.73 |
| 3:N:1495:ILE:HG23 | 3:N:1496:GLU:N | 2.03 | 0.73 |
| 2:M:986:PRO:O | 2:M:987:ILE:HD13 | 1.88 | 0.73 |
| 3:D:28:LYS:HG2 | 3:D:42:ASP:HB3 | 1.71 | 0.73 |
| 2:M:626:ARG:HG3 | 2:M:629:TYR:CD1 | 2.24 | 0.73 |
| 3:D:1208:ASP:O | 3:D:1209:LEU:HB2 | 1.89 | 0.73 |
| 2:M:234:ALA:O | 2:M:238:LEU:HG | 1.89 | 0.73 |
| 4:E:40:LEU:HD12 | 4:E:41:GLU:N | 2.01 | 0.73 |
| 5:P:185:GLN:HA | 5:P:188:ILE:HD12 | 1.70 | 0.73 |
| 1:B:138:LEU:HD12 | 1:B:139:ASN:N | 2.04 | 0.73 |
| 2:C:93:PRO:CA | 2:C:117:HIS:HB3 | 2.19 | 0.73 |
| 2:C:987:ILE:HA | 3:D:948:THR:HG21 | 1.70 | 0.73 |
| 3:N:301:GLY:C | 3:N:303:PRO:HD2 | 2.09 | 0.73 |
| 2:M:413:LEU:CA | 2:M:419:THR:HG21 | 2.19 | 0.73 |
| 2:M:21:ILE:HD12 | 2:M:21:ILE:N | 2.02 | 0.73 |
| 2:C:1008:ARG:NH1 | 3:D:624:ASP:OD1 | 2.22 | 0.73 |
| 3:D:983:LEU:HD22 | 3:D:987:GLU:HB3 | 1.71 | 0.73 |
| 5:P:111:GLU:HA | 5:P:114:LYS:CD | 2.18 | 0.73 |
| 3:N:984:THR:HG22 | 3:N:987:GLU:CG | 2.18 | 0.73 |
| 3:N:182:GLY:HA2 | 3:N:203:ALA:HB3 | 1.71 | 0.73 |
| 1:A:13:VAL:O | 1:B:231:ALA:HB3 | 1.89 | 0.72 |
| 2:C:176:VAL:HG12 | 2:C:183:SER:H | 1.53 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:199:VAL:HG21 | 2:C:238:LEU:HD12 | 1.71 | 0.72 |
| 3:N:121:THR:HG23 | 3:N:122:GLU:N | 2.01 | 0.72 |
| 3:D:283:PHE:O | 3:D:284:LEU:HD23 | 1.89 | 0.72 |
| 5:P:355:GLU:O | 5:P:358:LEU:HB3 | 1.88 | 0.72 |
| 5:P:422:LEU:N | 5:P:422:LEU:HD23 | 2.04 | 0.72 |
| 1:L:80:LEU:HB3 | 3:N:844:ALA:HB2 | 1.69 | 0.72 |
| 3:N:1085:ALA:HA | 3:N:1088:THR:CG2 | 2.19 | 0.72 |
| 5:F:142:ARG:HD2 | 5:F:145:PRO:HA | 1.71 | 0.72 |
| 2:M:293:PHE:HD1 | 2:M:294:GLU:HG3 | 1.52 | 0.72 |
| 2:M:289:THR:C | 2:M:290:LEU:HD23 | 2.09 | 0.72 |
| 3:D:1238:MET:CE | 3:D:1239:ARG:HB3 | 2.19 | 0.72 |
| 3:N:410:SER:HB2 | 5:P:178:ARG:HG3 | 1.71 | 0.72 |
| 2:M:606:VAL:HG12 | 2:M:611:ILE:HG23 | 1.70 | 0.72 |
| 5:P:282:LEU:HG | 5:P:284:ARG:HG3 | 1.71 | 0.72 |
| 5:F:267:THR:O | 5:F:270:LYS:HB3 | 1.89 | 0.72 |
| 3:N:1380:GLU:HG2 | 3:N:1381:VAL:N | 2.04 | 0.72 |
| 2:M:896:PHE:C | 2:M:898:GLY:H | 1.89 | 0.72 |
| 3:N:500:ARG:O | 3:N:504:ASP:HB2 | 1.88 | 0.72 |
| 3:D:1041:LEU:HG | 3:D:1043:GLY:N | 2.03 | 0.72 |
| 1:A:1:MET:H1 | 1:A:6:LEU:HB2 | 1.54 | 0.72 |
| 2:M:281:LEU:HB3 | 2:M:305:PRO:HB3 | 1.71 | 0.72 |
| 3:N:241:ILE:HG12 | 3:N:312:ARG:HG3 | 1.70 | 0.72 |
| 2:C:180:GLY:HA2 | 2:C:223:ASP:OD2 | 1.89 | 0.72 |
| 2:C:1104:GLU:HA | 3:D:7:LYS:HZ2 | 1.50 | 0.72 |
| 3:D:108:VAL:HA | 3:D:109:PRO:C | 2.07 | 0.72 |
| 3:D:100:ALA:HB3 | 3:D:128:TYR:CE2 | 2.23 | 0.72 |
| 3:D:530:VAL:CG2 | 3:D:531:ASP:H | 1.94 | 0.72 |
| 2:C:93:PRO:HG3 | 2:C:117:HIS:CD2 | 2.23 | 0.72 |
| 3:N:806:PHE:CD1 | 3:N:809:PRO:HB2 | 2.24 | 0.72 |
| 3:N:644:LEU:HD12 | 3:N:645:PRO:HD2 | 1.71 | 0.72 |
| 3:D:499:VAL:O | 3:D:503:LEU:N | 2.22 | 0.72 |
| 3:N:148:GLU:CB | 3:N:151:GLN:HB2 | 2.18 | 0.72 |
| 3:N:550:ARG:NH1 | 3:N:573:MET:HB3 | 2.04 | 0.72 |
| 3:D:351:MET:HG3 | 3:D:370:ALA:HB2 | 1.71 | 0.72 |
| 3:N:361:VAL:CG1 | 3:N:365:ASP:HB3 | 2.14 | 0.72 |
| 2:C:112:GLU:O | 2:C:113:VAL:HG13 | 1.89 | 0.72 |
| 2:M:1067:TYR:O | 2:M:1071:ILE:HG12 | 1.89 | 0.72 |
| 2:M:628:PHE:CD1 | 2:M:628:PHE:N | 2.57 | 0.72 |
| 1:K:118:ALA:O | 1:K:120:VAL:HG23 | 1.88 | 0.72 |
| 3:D:972:LEU:CD2 | 3:D:972:LEU:H | 2.02 | 0.72 |
| 3:N:1197:ARG:HG2 | 3:N:1198:TYR:CE2 | 2.25 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:334:ARG:HB2 | 2:C:339:LEU:HD21 | 1.72 | 0.72 |
| 5:F:181:GLU:O | 5:F:184:ARG:HB3 | 1.90 | 0.72 |
| 1:B:97:VAL:HG12 | 1:B:98:THR:N | 2.04 | 0.72 |
| 5:F:382:THR:O | 5:F:386:VAL:HG13 | 1.89 | 0.72 |
| 2:M:599:GLU:HB3 | 2:M:615:TYR:CD2 | 2.24 | 0.72 |
| 2:M:1100:GLN:HG3 | 2:M:1102:LEU:CD2 | 2.19 | 0.72 |
| 3:N:1130:ARG:NH2 | 3:N:1323:GLN:HE22 | 1.87 | 0.72 |
| 5:F:169:GLU:O | 5:F:172:ARG:HG2 | 1.90 | 0.72 |
| 3:D:245:LEU:H | 3:D:309:GLY:N | 1.87 | 0.72 |
| 3:D:248:PRO:HB3 | 3:D:308:LYS:HZ1 | 1.53 | 0.72 |
| 4:E:6:ILE:HG23 | 4:E:7:ASP:N | 2.04 | 0.72 |
| 2:M:101:ILE:HG12 | 2:M:107:LEU:HA | 1.70 | 0.72 |
| 5:P:280:GLN:HG3 | 5:P:281:GLU:N | 2.05 | 0.72 |
| 1:B:74:ASP:O | 1:B:77:GLU:HB3 | 1.89 | 0.72 |
| 3:N:804:LEU:O | 3:N:809:PRO:HG2 | 1.90 | 0.72 |
| 3:D:192:ALA:HB3 | 3:D:195:VAL:CG2 | 2.19 | 0.72 |
| 3:D:1083:ASP:HB2 | 3:D:1239:ARG:HH22 | 1.52 | 0.72 |
| 3:D:355:VAL:CG2 | 3:D:367:ILE:HG23 | 2.20 | 0.72 |
| 5:F:402:ASN:HB3 | 5:F:406:ARG:CZ | 2.19 | 0.72 |
| 3:D:1172:HIS:O | 3:D:1175:ILE:HB | 1.88 | 0.72 |
| 2:M:676:ILE:HG12 | 2:M:873:PRO:HG3 | 1.72 | 0.72 |
| 3:N:274:ARG:HE | 3:N:279:VAL:HG11 | 1.55 | 0.72 |
| 1:B:74:ASP:HB3 | 1:B:77:GLU:HB2 | 1.70 | 0.72 |
| 1:A:152:PRO:HB2 | 1:A:154:GLU:OE1 | 1.89 | 0.72 |
| 2:M:1007:ALA:CB | 3:N:648:MET:HG3 | 2.18 | 0.72 |
| 2:M:881:ASN:N | 2:M:881:ASN:HD22 | 1.85 | 0.72 |
| 2:M:512:ARG:HG3 | 2:M:523:ILE:HD11 | 1.71 | 0.72 |
| 1:K:182:GLU:HG3 | 1:K:194:LYS:HD3 | 1.70 | 0.72 |
| 2:M:224:GLU:HB3 | 2:M:227:PHE:HB2 | 1.72 | 0.72 |
| 3:N:525:ARG:HG2 | 3:N:525:ARG:HH11 | 1.54 | 0.72 |
| 5:P:213:ILE:HG22 | 5:P:217:ASN:HD21 | 1.55 | 0.72 |
| 3:D:462:GLN:HG3 | 3:D:513:ILE:HG21 | 1.70 | 0.72 |
| 5:F:208:SER:O | 5:F:212:LEU:HG | 1.90 | 0.72 |
| 3:D:358:GLY:HA2 | 3:D:385:VAL:O | 1.89 | 0.72 |
| 3:D:368:VAL:H | 3:D:377:VAL:HB | 1.55 | 0.72 |
| 3:D:441:ARG:O | 3:D:441:ARG:HG2 | 1.90 | 0.72 |
| 3:D:803:GLY:C | 3:D:805:GLU:H | 1.92 | 0.72 |
| 2:C:1063:ARG:O | 2:C:1066:ALA:HB3 | 1.89 | 0.72 |
| 5:F:351:SER:HA | 5:F:354:LEU:HD12 | 1.72 | 0.72 |
| 3:N:1114:THR:HB | 3:N:1195:GLN:CD | 2.10 | 0.72 |
| 3:D:30:GLU:HB3 | 3:D:40:GLU:CG | 2.20 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:841:ASN:HD21 | 2:C:845:ASN:HB3 | 1.54 | 0.72 |
| 2:C:631:SER:HA | 2:C:637:LEU:HD11 | 1.71 | 0.72 |
| 3:N:1001:GLU:OE2 | 3:N:1001:GLU:HA | 1.88 | 0.72 |
| 2:C:182:VAL:HG22 | 2:C:220:GLY:O | 1.89 | 0.72 |
| 3:D:1479:ASP:HA | 3:D:1482:ARG:HE | 1.55 | 0.72 |
| 5:F:265:VAL:HG12 | 5:F:269:ASN:HD21 | 1.52 | 0.72 |
| 3:N:297:ILE:HG23 | 3:N:298:VAL:N | 2.05 | 0.72 |
| 3:D:1500:LYS:C | 3:D:1502:ALA:H | 1.92 | 0.72 |
| 1:K:176:ARG:CZ | 2:M:865:THR:HG22 | 2.20 | 0.72 |
| 2:M:309:TYR:CE2 | 2:M:321:GLU:HG3 | 2.25 | 0.72 |
| 2:C:204:GLN:O | 2:C:209:ARG:HD3 | 1.89 | 0.72 |
| 3:N:89:ARG:HH11 | 3:N:89:ARG:HG2 | 1.55 | 0.72 |
| 3:D:154:THR:HG22 | 3:D:157:GLU:CD | 2.10 | 0.72 |
| 3:N:367:ILE:HB | 3:N:377:VAL:HG12 | 1.71 | 0.72 |
| 3:D:927:THR:O | 3:D:930:LEU:HB3 | 1.90 | 0.72 |
| 3:D:204:LEU:O | 3:D:393:ILE:HG23 | 1.90 | 0.72 |
| 5:F:274:THR:O | 5:F:278:LEU:HG | 1.90 | 0.72 |
| 1:K:5:LYS:HE3 | 1:K:29:GLU:OE1 | 1.90 | 0.72 |
| 1:A:9:PRO:HG3 | 1:A:27:PRO:O | 1.89 | 0.72 |
| 3:N:1074:SER:O | 3:N:1077:ALA:HB3 | 1.90 | 0.72 |
| 3:N:563:PRO:O | 3:N:566:ILE:HG12 | 1.90 | 0.71 |
| 3:D:140:ALA:H | 3:D:450:TYR:HE2 | 1.33 | 0.71 |
| 1:B:112:ARG:NH1 | 1:B:125:PRO:HB2 | 2.05 | 0.71 |
| 3:D:187:LYS:HA | 3:D:198:ARG:O | 1.89 | 0.71 |
| 3:D:1428:ALA:O | 3:D:1431:THR:HG23 | 1.90 | 0.71 |
| 3:D:916:TYR:CE2 | 3:D:920:LEU:HD11 | 2.25 | 0.71 |
| 3:N:828:LYS:N | 3:N:828:LYS:HD3 | 2.05 | 0.71 |
| 2:C:654:LEU:O | 2:C:655:LEU:HD23 | 1.89 | 0.71 |
| 3:D:704:ARG:HB2 | 3:D:745:MET:SD | 2.29 | 0.71 |
| 2:C:679:PHE:HA | 3:D:943:THR:HG23 | 1.72 | 0.71 |
| 1:K:49:PRO:HA | 1:K:148:VAL:HG12 | 1.72 | 0.71 |
| 2:M:398:THR:CA | 2:M:633:GLN:HG3 | 2.21 | 0.71 |
| 3:N:149:LYS:N | 3:N:149:LYS:HD3 | 2.05 | 0.71 |
| 3:N:128:TYR:HA | 3:N:457:GLY:HA2 | 1.71 | 0.71 |
| 3:N:463:GLN:HB3 | 3:N:467:GLU:OE2 | 1.91 | 0.71 |
| 2:M:810:ASP:N | 2:M:811:PRO:HD2 | 2.05 | 0.71 |
| 1:K:12:THR:HG22 | 1:L:229:GLN:CG | 2.20 | 0.71 |
| 3:N:1405:GLU:OE1 | 3:N:1406:ARG:HG3 | 1.91 | 0.71 |
| 3:D:827:ILE:HG23 | 3:D:837:GLY:HA3 | 1.72 | 0.71 |
| 1:K:189:ARG:HB3 | 1:K:192:LEU:HD21 | 1.72 | 0.71 |
| 3:N:1461:GLY:O | 3:N:1473:PRO:HG2 | 1.89 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1499:ARG:HG3 | 3:D:1499:ARG:HH11 | 1.54 | 0.71 |
| 3:N:1159:ARG:C | 3:N:1160:LEU:HD23 | 2.11 | 0.71 |
| 3:D:181:ASP:C | 3:D:183:GLU:H | 1.93 | 0.71 |
| 3:N:224:ARG:HB3 | 3:N:249:TYR:HH | 1.55 | 0.71 |
| 2:C:328:LEU:HG | 2:C:433:THR:OG1 | 1.89 | 0.71 |
| 3:D:1066:THR:H | 3:D:1069:GLU:HB2 | 1.55 | 0.71 |
| 5:F:208:SER:HB3 | 5:F:211:ASP:OD2 | 1.90 | 0.71 |
| 2:C:44:ILE:HG23 | 2:C:344:PHE:CE1 | 2.24 | 0.71 |
| 4:O:41:GLU:CB | 4:O:42:PRO:HD2 | 2.19 | 0.71 |
| 2:C:987:ILE:HD11 | 3:D:946:GLY:HA2 | 1.72 | 0.71 |
| 1:K:5:LYS:HE3 | 1:K:29:GLU:CD | 2.11 | 0.71 |
| 5:F:158:GLU:O | 5:F:162:LYS:HG3 | 1.89 | 0.71 |
| 3:N:992:ILE:O | 3:N:995:LEU:HB3 | 1.90 | 0.71 |
| 2:M:274:ARG:NH2 | 2:M:284:ARG:HB3 | 2.02 | 0.71 |
| 2:C:368:THR:CB | 2:C:369:PRO:HD3 | 2.19 | 0.71 |
| 3:N:807:ALA:HA | 3:N:833:GLU:CG | 2.21 | 0.71 |
| 2:C:211:LEU:C | 2:C:213:ALA:H | 1.89 | 0.71 |
| 2:M:463:GLU:CD | 2:M:463:GLU:N | 2.43 | 0.71 |
| 3:D:1217:ILE:CD1 | 3:D:1217:ILE:H | 1.93 | 0.71 |
| 3:D:127:LEU:HD23 | 3:D:128:TYR:CA | 2.19 | 0.71 |
| 3:N:357:GLU:CD | 3:N:357:GLU:H | 1.94 | 0.71 |
| 4:O:40:LEU:HD13 | 4:O:72:ARG:NH1 | 2.04 | 0.71 |
| 3:D:85:VAL:HG21 | 3:D:89:ARG:NE | 2.06 | 0.71 |
| 5:F:358:LEU:HD21 | 5:F:370:LYS:HZ2 | 1.55 | 0.71 |
| 2:C:595:LEU:O | 2:C:654:LEU:HD12 | 1.89 | 0.71 |
| 2:M:976:ASP:OD2 | 2:M:978:ARG:HB2 | 1.91 | 0.71 |
| 1:A:111:ALA:HA | 1:A:129:ILE:HD11 | 1.72 | 0.71 |
| 3:D:887:ALA:HB1 | 3:D:893:GLU:HA | 1.72 | 0.71 |
| 2:C:346:VAL:HG23 | 2:C:347:GLY:N | 2.04 | 0.71 |
| 3:N:48:ARG:HA | 3:N:78:VAL:HG22 | 1.70 | 0.71 |
| 3:D:250:LEU:HD11 | 3:D:304:LEU:HD22 | 1.71 | 0.71 |
| 2:C:1060:ILE:O | 2:C:1063:ARG:HG2 | 1.91 | 0.71 |
| 3:N:1495:ILE:HG23 | 3:N:1496:GLU:H | 1.55 | 0.71 |
| 3:N:274:ARG:HB3 | 3:N:279:VAL:CG2 | 2.20 | 0.71 |
| 3:N:1149:LEU:HD23 | 3:N:1161:GLU:O | 1.90 | 0.71 |
| 2:C:477:GLY:HA2 | 2:C:508:ILE:CD1 | 2.21 | 0.71 |
| 3:N:806:PHE:CA | 3:N:809:PRO:HD2 | 2.20 | 0.71 |
| 2:C:760:SER:O | 2:C:785:VAL:HA | 1.90 | 0.71 |
| 2:M:304:LEU:HB3 | 2:M:305:PRO:CD | 2.17 | 0.71 |
| 3:N:272:LEU:HD12 | 3:N:280:ALA:CB | 2.13 | 0.71 |
| 2:C:208:ALA:HB2 | 2:C:221:LEU:CD2 | 2.21 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:P:78:SER:C | 5:P:80:PRO:HD3 | 2.11 | 0.71 |
| 3:D:408:GLU:CD | 3:D:422:ALA:HB2 | 2.11 | 0.71 |
| 3:D:221:ALA:O | 3:D:334:THR:HA | 1.91 | 0.71 |
| 1:A:206:THR:CG2 | 1:A:208:LEU:HB3 | 2.20 | 0.71 |
| 5:P:264:MET:HA | 5:P:264:MET:CE | 2.19 | 0.71 |
| 3:D:826:PRO:HD2 | 3:D:829:VAL:HG21 | 1.71 | 0.71 |
| 2:C:672:VAL:CG2 | 2:C:868:ASP:HB2 | 2.21 | 0.71 |
| 3:N:209:ARG:HA | 3:N:347:VAL:HB | 1.71 | 0.71 |
| 5:P:90:GLN:O | 5:P:92:PRO:HD3 | 1.90 | 0.71 |
| 3:D:699:VAL:HG12 | 3:D:717:GLN:HG2 | 1.71 | 0.71 |
| 2:M:199:VAL:HG21 | 2:M:238:LEU:CD1 | 2.20 | 0.71 |
| 3:N:224:ARG:HB3 | 3:N:249:TYR:OH | 1.90 | 0.71 |
| 3:D:120:ALA:HA | 3:D:124:GLU:OE2 | 1.90 | 0.71 |
| 3:D:508:ARG:HB3 | 3:D:510:GLU:OE1 | 1.90 | 0.71 |
| 5:F:409:LYS:HD2 | 5:F:410:TYR:N | 2.05 | 0.71 |
| 1:L:61:VAL:HG23 | 1:L:163:ASN:HB3 | 1.72 | 0.71 |
| 2:M:480:THR:HG22 | 2:M:482:GLU:H | 1.56 | 0.71 |
| 2:M:537:LYS:HA | 2:M:545:ASN:OD1 | 1.91 | 0.71 |
| 3:N:307:ALA:HB1 | 3:N:311:LEU:HD11 | 1.72 | 0.71 |
| 2:C:302:VAL:O | 2:C:305:PRO:HD2 | 1.91 | 0.71 |
| 2:C:305:PRO:HA | 2:C:308:ARG:HE | 1.53 | 0.71 |
| 3:D:138:LYS:HB3 | 3:D:450:TYR:OH | 1.91 | 0.71 |
| 3:D:1486:VAL:HG21 | 4:E:22:VAL:HG13 | 1.73 | 0.71 |
| 5:F:214:GLN:O | 5:F:217:ASN:HB2 | 1.91 | 0.71 |
| 3:D:252:ARG:HG3 | 3:D:300:LYS:HA | 1.73 | 0.71 |
| 3:D:407:VAL:HG22 | 3:D:408:GLU:H | 1.56 | 0.71 |
| 3:D:284:LEU:HB3 | 3:D:288:MET:HB3 | 1.72 | 0.71 |
| 2:C:31:GLN:HA | 2:C:35:PRO:HG2 | 1.70 | 0.71 |
| 5:P:295:MET:HG3 | 5:P:299:TRP:CE2 | 2.26 | 0.71 |
| 3:D:1152:GLU:HG2 | 3:D:1153:VAL:N | 2.05 | 0.71 |
| 3:D:1155:VAL:HG12 | 3:D:1156:LEU:HG | 1.73 | 0.71 |
| 3:N:1217:ILE:H | 3:N:1217:ILE:CD1 | 1.96 | 0.71 |
| 3:D:1378:TYR:HB2 | 3:D:1422:MET:CE | 2.20 | 0.71 |
| 5:F:81:VAL:CG2 | 5:F:82:ARG:H | 2.03 | 0.71 |
| 1:A:224:TYR:N | 1:A:224:TYR:CD2 | 2.59 | 0.71 |
| 1:B:87:VAL:HG12 | 1:B:122:ILE:HG12 | 1.71 | 0.71 |
| 1:L:47:SER:O | 1:L:48:ILE:HD12 | 1.91 | 0.71 |
| 2:C:1043:TYR:CE1 | 3:D:710:ARG:HB2 | 2.26 | 0.71 |
| 3:N:563:PRO:O | 3:N:567:ILE:HG12 | 1.91 | 0.71 |
| 3:D:148:GLU:CB | 3:D:151:GLN:HB2 | 2.20 | 0.71 |
| 3:D:358:GLY:CA | 3:D:385:VAL:HB | 2.21 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:406:ASP:HB2 | 3:D:423:ASP:HA | 1.73 | 0.71 |
| 3:D:1388:ARG:HH21 | 3:D:1390:LEU:HD23 | 1.52 | 0.71 |
| 1:A:49:PRO:HA | 1:A:148:VAL:HG12 | 1.70 | 0.71 |
| 5:P:81:VAL:HG23 | 5:P:82:ARG:N | 2.05 | 0.71 |
| 3:D:680:GLN:HA | 3:D:683:ILE:CD1 | 2.21 | 0.71 |
| 2:M:175:GLU:HB3 | 2:M:185:LYS:HE3 | 1.73 | 0.70 |
| 3:N:237:LYS:CB | 3:N:238:PRO:HD2 | 2.16 | 0.70 |
| 3:N:153:LEU:CD1 | 3:N:157:GLU:HB3 | 2.21 | 0.70 |
| 5:P:210:LEU:CA | 5:P:213:ILE:HD12 | 2.19 | 0.70 |
| 3:D:610:LYS:HZ1 | 3:D:1441:GLN:HG3 | 1.54 | 0.70 |
| 3:D:540:LEU:HA | 3:D:543:LEU:HD12 | 1.73 | 0.70 |
| 5:F:101:GLU:O | 5:F:105:LYS:HG3 | 1.90 | 0.70 |
| 5:P:373:LYS:HZ2 | 5:P:373:LYS:HB3 | 1.56 | 0.70 |
| 2:M:889:HIS:HD1 | 2:M:970:GLY:HA3 | 1.55 | 0.70 |
| 3:N:591:VAL:HG12 | 3:N:599:PRO:HA | 1.71 | 0.70 |
| 1:B:19:GLU:HA | 1:B:201:THR:OG1 | 1.91 | 0.70 |
| 5:P:151:LEU:HD13 | 5:P:154:LYS:HD2 | 1.72 | 0.70 |
| 3:D:777:PRO:O | 3:D:780:LYS:HD3 | 1.91 | 0.70 |
| 2:C:266:ARG:HD2 | 2:C:273:GLY:N | 2.06 | 0.70 |
| 3:N:119:SER:CB | 3:N:123:LEU:HG | 2.20 | 0.70 |
| 3:N:135:LEU:N | 3:N:135:LEU:HD23 | 2.07 | 0.70 |
| 5:P:175:HIS:O | 5:P:178:ARG:HB2 | 1.91 | 0.70 |
| 5:P:383:LEU:O | 5:P:386:VAL:HG22 | 1.90 | 0.70 |
| 2:M:100:LEU:HD23 | 2:M:368:THR:HG23 | 1.73 | 0.70 |
| 3:D:1153:VAL:HB | 3:D:1160:LEU:HB2 | 1.72 | 0.70 |
| 1:L:57:TYR:HE1 | 1:L:163:ASN:HB2 | 1.54 | 0.70 |
| 1:B:5:LYS:C | 1:B:7:LYS:N | 2.42 | 0.70 |
| 3:N:632:VAL:O | 3:N:728:LEU:N | 2.22 | 0.70 |
| 2:C:192:PRO:O | 2:C:195:LEU:HG | 1.91 | 0.70 |
| 3:N:563:PRO:HD2 | 3:N:566:ILE:HD11 | 1.72 | 0.70 |
| 5:P:214:GLN:CA | 5:P:217:ASN:HD22 | 2.03 | 0.70 |
| 3:D:800:LYS:HE3 | 3:D:826:PRO:CD | 2.20 | 0.70 |
| 3:N:490:ALA:O | 3:N:494:LYS:HG2 | 1.90 | 0.70 |
| 5:F:94:LEU:HG | 5:F:190:ALA:HB1 | 1.74 | 0.70 |
| 1:A:195:LEU:HD12 | 1:A:196:THR:N | 2.05 | 0.70 |
| 1:K:9:PRO:HG2 | 1:K:28:LEU:HD21 | 1.73 | 0.70 |
| 3:N:191:LEU:HD23 | 3:N:195:VAL:CG1 | 2.22 | 0.70 |
| 3:D:1496:GLU:HA | 3:D:1499:ARG:HB3 | 1.73 | 0.70 |
| 2:C:839:LEU:HD23 | 2:C:996:LYS:HA | 1.73 | 0.70 |
| 2:M:299:LYS:HE2 | 2:M:301:GLU:HG3 | 1.73 | 0.70 |
| 3:N:327:GLU:HG3 | 3:N:327:GLU:O | 1.91 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:N:522:PRO:HA | 3:N:525:ARG:NH1 | 2.06 | 0.70 |
| 3:N:82:LYS:CB | 3:N:84:ILE:HG22 | 2.22 | 0.70 |
| 3:D:807:ALA:HA | 3:D:833:GLU:HG2 | 1.73 | 0.70 |
| 3:D:185:VAL:HA | 3:D:189:GLN:NE2 | 2.06 | 0.70 |
| 2:M:643:VAL:HG23 | 2:M:647:GLN:CD | 2.12 | 0.70 |
| 2:C:37:GLU:HG2 | 2:C:71:TYR:HE2 | 1.56 | 0.70 |
| 2:M:89:THR:HA | 2:M:128:ILE:O | 1.91 | 0.70 |
| 3:N:1496:GLU:OE2 | 3:N:1500:LYS:HG3 | 1.91 | 0.70 |
| 3:N:1155:VAL:HG12 | 3:N:1156:LEU:HG | 1.72 | 0.70 |
| 3:N:178:LEU:HG | 3:N:181:ASP:HB2 | 1.71 | 0.70 |
| 2:M:398:THR:HA | 2:M:633:GLN:HG3 | 1.72 | 0.70 |
| 3:D:118:LEU:HD22 | 3:D:123:LEU:HB3 | 1.72 | 0.70 |
| 3:N:441:ARG:O | 3:N:441:ARG:NE | 2.24 | 0.70 |
| 2:M:15:LEU:HD13 | 2:M:586:ARG:NH1 | 2.07 | 0.70 |
| 5:P:260:ILE:HG13 | 5:P:261:PRO:HD2 | 1.72 | 0.70 |
| 2:M:808:ARG:HG2 | 2:M:820:ARG:O | 1.91 | 0.70 |
| 3:N:1307:LYS:H | 3:N:1307:LYS:HE3 | 1.55 | 0.70 |
| 1:B:5:LYS:HE2 | 1:B:189:ARG:NH1 | 2.05 | 0.70 |
| 3:D:864:VAL:HG12 | 3:D:865:THR:H | 1.56 | 0.70 |
| 2:C:640:ARG:HD2 | 2:C:642:ARG:NH2 | 2.05 | 0.70 |
| 2:C:503:LEU:HG | 2:C:504:GLU:H | 1.57 | 0.70 |
| 3:N:800:LYS:O | 3:N:830:ALA:HB3 | 1.91 | 0.70 |
| 2:M:50:GLU:C | 2:M:52:PHE:H | 1.93 | 0.70 |
| 2:C:892:LEU:O | 2:C:895:TYR:HB3 | 1.91 | 0.70 |
| 2:M:261:ILE:HG22 | 2:M:262:ALA:N | 2.07 | 0.70 |
| 2:C:175:GLU:O | 2:C:183:SER:HB2 | 1.91 | 0.70 |
| 2:C:283:ILE:HG22 | 2:C:284:ARG:N | 2.01 | 0.70 |
| 4:E:88:GLU:O | 4:E:92:ILE:HG13 | 1.91 | 0.70 |
| 5:F:207:LEU:HB3 | 5:F:212:LEU:CD2 | 2.20 | 0.70 |
| 3:D:676:MET:HG3 | 3:D:677:LEU:HD23 | 1.73 | 0.70 |
| 5:P:289:GLU:H | 5:P:289:GLU:CD | 1.95 | 0.70 |
| 5:F:306:GLU:O | 5:F:310:ILE:HG13 | 1.92 | 0.70 |
| 2:C:904:PRO:HD2 | 2:C:908:GLY:CA | 2.21 | 0.70 |
| 2:C:185:LYS:HE2 | 2:C:190:LYS:HZ2 | 1.57 | 0.70 |
| 3:N:206:ARG:HG2 | 3:N:392:SER:O | 1.90 | 0.70 |
| 2:M:334:ARG:HB2 | 2:M:339:LEU:HD21 | 1.74 | 0.70 |
| 2:C:257:VAL:HA | 2:C:261:ILE:CD1 | 2.19 | 0.70 |
| 3:D:833:GLU:CD | 3:D:833:GLU:H | 1.93 | 0.70 |
| 3:N:142:LEU:HD13 | 3:N:144:GLY:N | 2.07 | 0.70 |
| 3:N:966:GLU:O | 3:N:969:ARG:HG2 | 1.92 | 0.70 |
| 2:M:693:GLU:HG3 | 2:M:697:ARG:NH1 | 2.07 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:626:ARG:HG3 | 2:C:626:ARG:HH11 | 1.55 | 0.70 |
| 3:N:669:ASN:OD1 | 3:N:672:ALA:HB2 | 1.92 | 0.70 |
| 3:N:525:ARG:N | 3:N:526:PRO:HD3 | 2.05 | 0.70 |
| 3:D:690:ALA:O | 3:D:693:GLU:HB3 | 1.92 | 0.70 |
| 5:F:288:TYR:HB3 | 5:F:301:ALA:HA | 1.73 | 0.70 |
| 2:C:910:LYS:HG2 | 2:C:913:GLU:CG | 2.21 | 0.70 |
| 3:N:820:GLU:HG3 | 3:N:836:VAL:HG11 | 1.74 | 0.70 |
| 3:N:882:PHE:CE1 | 3:N:906:GLN:HG3 | 2.26 | 0.70 |
| 2:M:470:PRO:HB2 | 2:M:534:VAL:HG21 | 1.73 | 0.70 |
| 3:N:1481:VAL:HG13 | 4:O:18:ARG:HA | 1.73 | 0.70 |
| 1:A:76:VAL:HG12 | 1:A:80:LEU:HD21 | 1.73 | 0.70 |
| 3:N:932:ASP:O | 3:N:935:LYS:HB3 | 1.92 | 0.70 |
| 3:N:209:ARG:NH2 | 3:N:391:ALA:HA | 2.07 | 0.70 |
| 3:D:264:LEU:HD22 | 3:D:316:GLN:HE21 | 1.57 | 0.70 |
| 4:O:6:ILE:HG13 | 4:O:10:PHE:CE1 | 2.27 | 0.70 |
| 5:P:219:GLY:CA | 5:P:246:ALA:HB2 | 2.22 | 0.70 |
| 5:P:234:LYS:HE2 | 5:P:236:SER:HB3 | 1.74 | 0.70 |
| 3:D:1074:SER:O | 3:D:1077:ALA:HB3 | 1.92 | 0.70 |
| 2:M:75:GLU:O | 2:M:77:PRO:HD3 | 1.91 | 0.70 |
| 2:C:1103:ASP:O | 3:D:7:LYS:HD2 | 1.92 | 0.70 |
| 3:D:408:GLU:HG3 | 3:D:421:LEU:O | 1.92 | 0.70 |
| 2:C:115:LEU:CD1 | 2:C:373:VAL:HG12 | 2.21 | 0.70 |
| 5:P:330:GLY:HA2 | 5:P:333:ILE:HD13 | 1.72 | 0.70 |
| 5:F:234:LYS:HE2 | 5:F:236:SER:CB | 2.21 | 0.70 |
| 3:N:245:LEU:HD23 | 3:N:309:GLY:N | 2.05 | 0.70 |
| 2:C:151:ASP:H | 2:C:158:TYR:CA | 2.05 | 0.70 |
| 2:C:266:ARG:NH1 | 2:C:266:ARG:HG3 | 2.07 | 0.70 |
| 3:N:47:GLU:HB2 | 3:N:51:GLY:O | 1.91 | 0.70 |
| 3:D:147:VAL:CG2 | 3:D:148:GLU:H | 2.05 | 0.70 |
| 3:D:1173:LEU:O | 3:D:1176:LYS:HB3 | 1.92 | 0.70 |
| 1:K:214:ALA:HA | 1:K:217:ILE:HD12 | 1.73 | 0.70 |
| 2:C:808:ARG:HG2 | 2:C:815:LEU:HD12 | 1.73 | 0.70 |
| 4:O:46:PRO:HB2 | 4:O:57:ASP:HB3 | 1.74 | 0.70 |
| 3:N:325:GLU:CG | 3:N:332:TYR:HB3 | 2.21 | 0.69 |
| 3:N:32:ILE:HG22 | 3:N:33:ASN:O | 1.91 | 0.69 |
| 3:D:761:ILE:HD12 | 4:E:20:THR:HG23 | 1.73 | 0.69 |
| 5:F:210:LEU:CA | 5:F:213:ILE:HD12 | 2.12 | 0.69 |
| 5:F:214:GLN:CA | 5:F:217:ASN:HD22 | 2.04 | 0.69 |
| 3:D:805:GLU:HA | 3:D:831:GLY:HA2 | 1.72 | 0.69 |
| 5:F:189:GLU:HA | 5:F:192:LEU:CG | 2.20 | 0.69 |
| 1:L:197:LEU:HD12 | 1:L:198:ARG:N | 2.06 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:948:GLU:HB3 | 2:M:953:VAL:HG23 | 1.74 | 0.69 |
| 5:P:329:TYR:HD1 | 5:P:333:ILE:HD11 | 1.55 | 0.69 |
| 3:D:760:ARG:NH1 | 4:E:61:GLU:HB2 | 2.07 | 0.69 |
| 3:N:998:GLU:O | 3:N:1001:GLU:HB3 | 1.91 | 0.69 |
| 5:P:184:ARG:HG2 | 5:P:188:ILE:HD11 | 1.73 | 0.69 |
| 2:C:676:ILE:O | 3:D:948:THR:HG22 | 1.91 | 0.69 |
| 2:C:861:LEU:N | 2:C:861:LEU:HD23 | 2.07 | 0.69 |
| 3:D:882:PHE:HA | 3:D:885:ILE:HD12 | 1.73 | 0.69 |
| 3:N:419:ASP:O | 3:N:428:LYS:HE2 | 1.91 | 0.69 |
| 5:P:386:VAL:HG23 | 5:P:387:GLY:N | 2.07 | 0.69 |
| 5:F:288:TYR:HB2 | 5:F:289:GLU:OE2 | 1.91 | 0.69 |
| 2:C:737:LEU:HD12 | 2:C:742:VAL:C | 2.11 | 0.69 |
| 1:K:101:LEU:HD12 | 1:K:102:LYS:H | 1.57 | 0.69 |
| 5:P:322:GLY:O | 5:P:324:GLU:HG3 | 1.91 | 0.69 |
| 2:M:41:ASN:ND2 | 2:M:46:ALA:HB2 | 2.07 | 0.69 |
| 3:N:1081:GLY:O | 3:N:1084:THR:HG23 | 1.92 | 0.69 |
| 2:C:939:ARG:NH2 | 2:C:981:GLU:HG2 | 2.07 | 0.69 |
| 2:M:177:GLU:O | 2:M:181:VAL:HB | 1.93 | 0.69 |
| 2:C:182:VAL:HG21 | 2:C:194:VAL:HG23 | 1.75 | 0.69 |
| 3:D:135:LEU:HD12 | 3:D:148:GLU:O | 1.92 | 0.69 |
| 5:F:115:LYS:HA | 5:F:118:GLU:OE2 | 1.92 | 0.69 |
| 1:B:185:ARG:NH2 | 3:D:692:GLU:HG3 | 2.08 | 0.69 |
| 3:N:1381:VAL:HG11 | 3:N:1391:GLU:HB2 | 1.75 | 0.69 |
| 3:N:860:LEU:HA | 3:N:877:PRO:HB2 | 1.74 | 0.69 |
| 2:M:71:TYR:HD2 | 2:M:71:TYR:H | 1.40 | 0.69 |
| 2:M:448:ASN:HB3 | 2:M:452:ILE:HD12 | 1.75 | 0.69 |
| 5:P:312:GLN:HA | 5:P:312:GLN:OE1 | 1.92 | 0.69 |
| 5:P:220:LEU:O | 5:P:224:VAL:HG23 | 1.93 | 0.69 |
| 3:D:1472:ILE:HD13 | 3:D:1473:PRO:CD | 2.23 | 0.69 |
| 3:D:322:VAL:HG23 | 3:D:335:LEU:HD11 | 1.74 | 0.69 |
| 2:M:368:THR:N | 2:M:369:PRO:CD | 2.55 | 0.69 |
| 2:M:373:VAL:HG12 | 2:M:374:ASN:N | 2.07 | 0.69 |
| 3:N:1288:GLU:O | 3:N:1307:LYS:HD3 | 1.92 | 0.69 |
| 1:B:86:VAL:HG12 | 1:B:124:ASN:HD21 | 1.57 | 0.69 |
| 1:L:185:ARG:HA | 1:L:190:THR:HA | 1.72 | 0.69 |
| 3:N:658:LEU:HD23 | 3:N:661:MET:HE1 | 1.73 | 0.69 |
| 1:K:39:PRO:HG3 | 1:L:39:PRO:CG | 2.21 | 0.69 |
| 1:K:29:GLU:HA | 1:K:29:GLU:OE1 | 1.91 | 0.69 |
| 1:A:11:PHE:O | 1:B:229:GLN:HB3 | 1.92 | 0.69 |
| 3:D:212:ARG:HA | 3:D:343:LYS:O | 1.92 | 0.69 |
| 2:C:492:ASP:HA | 2:C:518:LYS:HB3 | 1.74 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:N:545:ARG:NE | 5:P:257:THR:HA | 2.07 | 0.69 |
| 5:P:75:ILE:HG13 | 5:P:76:SER:N | 2.04 | 0.69 |
| 3:D:103:TRP:HZ2 | 3:D:604:THR:HG23 | 1.58 | 0.69 |
| 3:D:225:LEU:HB3 | 3:D:226:PRO:HD2 | 1.73 | 0.69 |
| 5:P:373:LYS:HB2 | 5:P:378:GLY:C | 2.13 | 0.69 |
| 1:L:58:ILE:HB | 1:L:61:VAL:HG11 | 1.75 | 0.69 |
| 1:K:183:ASP:OD2 | 2:M:938:LYS:HE3 | 1.92 | 0.69 |
| 2:M:419:THR:O | 2:M:420:ARG:HG3 | 1.93 | 0.69 |
| 1:L:206:THR:HB | 1:L:209:GLU:CD | 2.12 | 0.69 |
| 3:N:1122:LEU:O | 3:N:1135:ARG:HG3 | 1.91 | 0.69 |
| 3:N:1396:GLU:O | 3:N:1398:TRP:N | 2.23 | 0.69 |
| 1:A:70:GLY:H | 2:C:607:ASP:HB2 | 1.57 | 0.69 |
| 1:B:70:GLY:O | 1:B:136:GLY:HA3 | 1.92 | 0.69 |
| 2:M:139:GLN:O | 2:M:333:ILE:HD12 | 1.92 | 0.69 |
| 3:N:324:ALA:HB1 | 3:N:331:VAL:HG11 | 1.74 | 0.69 |
| 2:M:599:GLU:HA | 2:M:651:LYS:HB2 | 1.74 | 0.69 |
| 2:C:101:ILE:CG2 | 2:C:102:HIS:H | 2.06 | 0.69 |
| 1:L:161:ARG:H | 1:L:164:ALA:CB | 2.06 | 0.69 |
| 3:N:1267:ARG:HE | 3:N:1271:LYS:NZ | 1.90 | 0.69 |
| 3:D:1038:LEU:HA | 3:D:1061:PHE:HB2 | 1.75 | 0.69 |
| 3:N:529:GLN:HB2 | 3:N:535:PHE:CD2 | 2.28 | 0.69 |
| 3:N:173:PRO:HA | 3:N:209:ARG:NH1 | 2.07 | 0.69 |
| 1:L:92:PRO:C | 1:L:146:ARG:HH22 | 1.96 | 0.69 |
| 5:F:321:ILE:HB | 5:F:327:SER:OG | 1.93 | 0.69 |
| 1:L:9:PRO:HG3 | 1:L:27:PRO:O | 1.93 | 0.69 |
| 2:M:182:VAL:HB | 2:M:193:LEU:H | 1.57 | 0.69 |
| 2:M:232:GLU:HA | 2:M:235:LEU:HD13 | 1.72 | 0.69 |
| 2:M:408:ARG:HG2 | 2:M:455:LEU:HB3 | 1.75 | 0.69 |
| 3:N:241:ILE:CD1 | 3:N:310:LEU:HD22 | 2.23 | 0.69 |
| 2:C:334:ARG:HH11 | 2:C:418:LEU:HD11 | 1.58 | 0.69 |
| 2:C:260:LEU:HD13 | 2:C:291:ALA:HB2 | 1.75 | 0.69 |
| 2:C:414:GLY:N | 2:C:419:THR:HG21 | 2.08 | 0.69 |
| 2:C:443:THR:O | 2:C:559:LEU:HD11 | 1.92 | 0.69 |
| 3:N:522:PRO:N | 3:N:525:ARG:HH12 | 1.91 | 0.69 |
| 3:D:1229:ILE:O | 3:D:1232:PRO:HD2 | 1.93 | 0.69 |
| 3:D:1494:ALA:HB1 | 4:E:88:GLU:CB | 2.22 | 0.69 |
| 3:N:358:GLY:CA | 3:N:385:VAL:HB | 2.23 | 0.69 |
| 3:D:353:VAL:HA | 3:D:368:VAL:CG2 | 2.10 | 0.69 |
| 1:B:217:ILE:HG22 | 1:B:221:HIS:CD2 | 2.27 | 0.69 |
| 3:D:819:GLY:HA2 | 3:D:824:ASN:HD22 | 1.56 | 0.69 |
| 1:B:5:LYS:HD3 | 1:B:7:LYS:HD2 | 1.72 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:949:LYS:NZ | 3:D:796:ARG:HH12 | 1.90 | 0.69 |
| 3:N:769:LEU:N | 3:N:769:LEU:CD1 | 2.56 | 0.69 |
| 2:M:672:VAL:O | 2:M:991:GLN:HA | 1.93 | 0.69 |
| 3:N:1176:LYS:O | 3:N:1179:GLU:HB2 | 1.92 | 0.69 |
| 3:N:1118:ILE:CD1 | 3:N:1190:SER:HB2 | 2.22 | 0.69 |
| 2:M:1052:MET:SD | 2:M:1056:LYS:HD2 | 2.33 | 0.69 |
| 3:N:1481:VAL:CG1 | 4:O:18:ARG:HA | 2.23 | 0.69 |
| 1:A:33:GLY:O | 1:A:195:LEU:HD22 | 1.92 | 0.69 |
| 3:N:660:LYS:HD2 | 3:N:693:GLU:OE2 | 1.91 | 0.69 |
| 3:N:807:ALA:HA | 3:N:833:GLU:HG2 | 1.74 | 0.69 |
| 5:F:365:GLU:HA | 5:F:368:VAL:HG13 | 1.72 | 0.69 |
| 1:A:69:PRO:HA | 2:C:607:ASP:OD1 | 1.93 | 0.69 |
| 3:D:60:CYS:HB2 | 3:D:62:LYS:HE2 | 1.75 | 0.69 |
| 2:M:553:ASP:HA | 2:M:881:ASN:HA | 1.74 | 0.69 |
| 3:N:1196:THR:HB | 3:N:1199:GLY:O | 1.91 | 0.69 |
| 3:N:680:GLN:HA | 3:N:683:ILE:HD12 | 1.74 | 0.69 |
| 3:N:1127:GLU:HG3 | 3:N:1128:VAL:H | 1.58 | 0.69 |
| 5:P:123:ASP:O | 5:P:126:LEU:HB3 | 1.93 | 0.69 |
| 2:M:178:PRO:O | 2:M:220:GLY:HA2 | 1.93 | 0.69 |
| 2:C:197:LEU:HB3 | 2:C:207:LEU:CD1 | 2.22 | 0.69 |
| 2:C:276:LYS:HA | 2:C:280:LYS:HE3 | 1.74 | 0.69 |
| 3:N:87:ARG:HG3 | 3:N:88:TYR:CD2 | 2.28 | 0.69 |
| 3:N:367:ILE:HG22 | 3:N:368:VAL:HG23 | 1.74 | 0.69 |
| 5:P:276:ARG:O | 5:P:280:GLN:HG2 | 1.91 | 0.69 |
| 3:D:65:ARG:HG3 | 3:D:67:ARG:H | 1.58 | 0.69 |
| 2:C:949:LYS:NZ | 3:D:796:ARG:NH1 | 2.40 | 0.69 |
| 2:M:575:GLN:HE21 | 2:M:670:GLN:HB3 | 1.58 | 0.69 |
| 3:N:845:ASN:HB2 | 3:N:848:GLU:CB | 2.22 | 0.69 |
| 5:P:321:ILE:HG13 | 5:P:332:PHE:HE1 | 1.56 | 0.69 |
| 3:D:1344:VAL:HG13 | 3:D:1345:GLU:N | 2.07 | 0.69 |
| 3:D:61:GLY:O | 3:D:64:LYS:HE3 | 1.92 | 0.69 |
| 1:B:152:PRO:HG2 | 1:B:155:LYS:HB2 | 1.73 | 0.69 |
| 1:L:5:LYS:HZ3 | 1:L:189:ARG:CZ | 2.06 | 0.69 |
| 2:M:1046:ALA:HB1 | 3:N:1471:LEU:HD11 | 1.74 | 0.69 |
| 2:M:230:ARG:HE | 2:M:233:GLU:CG | 1.95 | 0.69 |
| 2:M:439:CYS:CB | 2:M:541:SER:HB3 | 2.22 | 0.69 |
| 3:D:119:SER:N | 3:D:123:LEU:HD12 | 2.07 | 0.69 |
| 3:D:527:MET:SD | 3:D:537:THR:HG23 | 2.34 | 0.69 |
| 3:D:930:LEU:O | 3:D:934:LEU:HG | 1.92 | 0.69 |
| 2:M:774:LEU:HD13 | 2:M:775:ARG:N | 2.07 | 0.69 |
| 2:C:72:ARG:O | 2:C:94:LEU:HD12 | 1.93 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:1405:GLU:CD | 3:N:1406:ARG:H | 1.96 | 0.69 |
| 3:D:1377:LYS:HE2 | 3:D:1394:VAL:HG22 | 1.75 | 0.69 |
| 3:D:916:TYR:CZ | 3:D:920:LEU:HD11 | 2.28 | 0.69 |
| 3:N:858:VAL:HG12 | 3:N:859:ASP:H | 1.55 | 0.69 |
| 2:C:926:PHE:CE2 | 2:C:960:GLU:HG3 | 2.21 | 0.69 |
| 5:P:321:ILE:HD11 | 5:P:329:TYR:N | 2.08 | 0.69 |
| 2:M:41:ASN:HD22 | 2:M:46:ALA:HB2 | 1.58 | 0.69 |
| 2:M:327:HIS:HB3 | 2:M:330:ASN:HD22 | 1.58 | 0.69 |
| 3:D:264:LEU:HB2 | 3:D:267:GLY:N | 2.07 | 0.69 |
| 5:P:159:ILE:HG22 | 5:P:163:LEU:HD11 | 1.74 | 0.69 |
| 3:N:647:ARG:O | 3:N:650:LEU:HB3 | 1.92 | 0.69 |
| 2:C:3:ILE:HG13 | 2:C:3:ILE:O | 1.93 | 0.68 |
| 2:C:512:ARG:HH11 | 2:C:524:VAL:HA | 1.58 | 0.68 |
| 3:N:127:LEU:CD2 | 3:N:461:ILE:HD11 | 2.22 | 0.68 |
| 5:F:291:ILE:HA | 5:F:294:ALA:HB3 | 1.75 | 0.68 |
| 3:N:298:VAL:HB | 3:N:300:LYS:HE3 | 1.75 | 0.68 |
| 3:N:1114:THR:HG21 | 3:N:1193:THR:O | 1.93 | 0.68 |
| 2:M:1060:ILE:HG22 | 2:M:1061:GLU:N | 2.08 | 0.68 |
| 2:M:1096:ALA:O | 2:M:1097:LEU:HD23 | 1.93 | 0.68 |
| 3:N:673:ALA:HA | 3:N:676:MET:HB3 | 1.74 | 0.68 |
| 1:B:10:VAL:HG22 | 1:B:26:GLU:O | 1.93 | 0.68 |
| 1:L:112:ARG:HB3 | 1:L:112:ARG:NH1 | 2.08 | 0.68 |
| 2:M:722:ILE:HD11 | 2:M:805:ARG:NH2 | 2.08 | 0.68 |
| 2:M:230:ARG:N | 2:M:230:ARG:HD3 | 2.08 | 0.68 |
| 2:C:145:GLY:HA3 | 2:C:276:LYS:HD2 | 1.74 | 0.68 |
| 2:C:164:PRO:HD2 | 2:C:170:PRO:O | 1.92 | 0.68 |
| 2:C:1101:THR:O | 2:C:1102:LEU:HD23 | 1.93 | 0.68 |
| 3:D:640:HIS:HB2 | 3:D:764:LEU:HD11 | 1.76 | 0.68 |
| 2:M:1091:GLU:O | 2:M:1094:ALA:HB3 | 1.92 | 0.68 |
| 5:F:364:ARG:O | 5:F:368:VAL:HG13 | 1.93 | 0.68 |
| 2:C:1009:SER:HB3 | 3:D:651:GLU:OE2 | 1.93 | 0.68 |
| 1:B:143:ARG:HD3 | 1:B:144:VAL:N | 2.09 | 0.68 |
| 3:D:1367:HIS:HA | 3:D:1370:ILE:HD12 | 1.74 | 0.68 |
| 2:M:144:PRO:HB3 | 2:M:163:ILE:O | 1.93 | 0.68 |
| 2:M:260:LEU:HD12 | 2:M:288:ARG:HG2 | 1.75 | 0.68 |
| 2:M:299:LYS:HE2 | 2:M:301:GLU:CG | 2.23 | 0.68 |
| 2:C:139:GLN:O | 2:C:333:ILE:HD12 | 1.93 | 0.68 |
| 2:C:269:LEU:HA | 2:C:288:ARG:HB2 | 1.75 | 0.68 |
| 2:C:438:ILE:HG23 | 2:C:453:THR:OG1 | 1.94 | 0.68 |
| 3:D:107:ASP:O | 3:D:110:SER:HA | 1.94 | 0.68 |
| 3:D:127:LEU:HD23 | 3:D:128:TYR:H | 1.56 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:F:373:LYS:HD3 | 5:F:379:ARG:HB3 | 1.74 | 0.68 |
| 2:M:904:PRO:HD2 | 2:M:908:GLY:CA | 2.23 | 0.68 |
| 3:D:907:GLU:O | 3:D:911:LEU:HG | 1.93 | 0.68 |
| 2:M:1096:ALA:HB1 | 3:N:13:ALA:HB3 | 1.75 | 0.68 |
| 2:M:944:LEU:HD21 | 2:M:963:LEU:HD23 | 1.75 | 0.68 |
| 1:K:5:LYS:NZ | 1:K:28:LEU:C | 2.47 | 0.68 |
| 2:M:838:LYS:HG3 | 2:M:997:LEU:HB2 | 1.74 | 0.68 |
| 3:N:990:ASP:HA | 3:N:993:LEU:CD1 | 2.23 | 0.68 |
| 3:D:680:GLN:HA | 3:D:683:ILE:HD12 | 1.75 | 0.68 |
| 3:N:470:LEU:HB2 | 3:N:503:LEU:HD21 | 1.74 | 0.68 |
| 2:M:739:GLU:OE1 | 2:M:739:GLU:HA | 1.93 | 0.68 |
| 2:C:289:THR:HG22 | 2:C:290:LEU:HG | 1.75 | 0.68 |
| 2:C:304:LEU:CB | 2:C:305:PRO:HD3 | 2.16 | 0.68 |
| 3:D:1099:VAL:HG12 | 9:D:1529:NE6:H14B | 1.75 | 0.68 |
| 4:E:19:LEU:O | 4:E:23:VAL:HG23 | 1.93 | 0.68 |
| 3:D:210:ARG:HB2 | 3:D:389:GLU:CG | 2.24 | 0.68 |
| 2:C:54:ILE:HD13 | 2:C:355:VAL:HG11 | 1.75 | 0.68 |
| 3:D:794:GLN:OE1 | 3:D:794:GLN:HA | 1.93 | 0.68 |
| 3:N:1147:ARG:HB3 | 3:N:1188:VAL:HG21 | 1.76 | 0.68 |
| 3:N:1311:LEU:HD12 | 3:N:1312:LEU:H | 1.57 | 0.68 |
| 2:M:292:ARG:HE | 2:M:295:ASP:CB | 2.05 | 0.68 |
| 1:L:85:LEU:HD12 | 1:L:86:VAL:H | 1.57 | 0.68 |
| 3:N:583:ASP:HB2 | 3:N:604:THR:OG1 | 1.93 | 0.68 |
| 3:N:260:GLU:OE1 | 3:N:273:ARG:HG3 | 1.93 | 0.68 |
| 2:C:409:ARG:NH2 | 2:C:452:ILE:HG21 | 2.07 | 0.68 |
| 2:C:471:TYR:CZ | 2:C:496:ILE:HD13 | 2.28 | 0.68 |
| 3:D:227:LEU:CD1 | 3:D:326:GLU:HA | 2.21 | 0.68 |
| 1:K:12:THR:CA | 1:L:229:GLN:HB3 | 2.16 | 0.68 |
| 2:C:773:LEU:HG | 2:C:774:LEU:N | 2.07 | 0.68 |
| 3:N:1460:ILE:HG13 | 3:N:1461:GLY:H | 1.57 | 0.68 |
| 3:N:864:VAL:HG12 | 3:N:865:THR:N | 2.07 | 0.68 |
| 2:C:690:ILE:HG23 | 2:C:694:LEU:HD12 | 1.75 | 0.68 |
| 3:N:1126:ASP:CG | 3:N:1129:THR:HA | 2.13 | 0.68 |
| 3:N:1041:LEU:HD11 | 3:N:1058:ARG:HA | 1.76 | 0.68 |
| 3:N:188:GLY:H | 3:N:198:ARG:HA | 1.57 | 0.68 |
| 2:C:178:PRO:O | 2:C:180:GLY:N | 2.26 | 0.68 |
| 2:C:545:ASN:O | 2:C:581:THR:HG21 | 1.93 | 0.68 |
| 3:N:132:TYR:N | 3:N:456:MET:HE3 | 2.09 | 0.68 |
| 3:N:137:PRO:CD | 3:N:453:ASP:HB3 | 2.24 | 0.68 |
| 3:N:29:PRO:HG3 | 3:N:548:ILE:HB | 1.76 | 0.68 |
| 3:N:96:ALA:HB3 | 3:N:554:LEU:CD2 | 2.24 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:P:78:SER:O | 5:P:80:PRO:HD3 | 1.94 | 0.68 |
| 3:D:548:ILE:CG2 | 3:D:552:ASN:HD21 | 2.07 | 0.68 |
| 3:D:546:ARG:HH21 | 3:D:577:ALA:HA | 1.57 | 0.68 |
| 2:M:72:ARG:HG2 | 2:M:95:TYR:CB | 2.17 | 0.68 |
| 1:B:100:LEU:HD12 | 1:B:140:MET:O | 1.94 | 0.68 |
| 3:D:812:ALA:O | 3:D:814:ALA:N | 2.27 | 0.68 |
| 3:N:8:VAL:HG13 | 3:N:1434:TRP:CH2 | 2.29 | 0.68 |
| 3:D:1122:LEU:O | 3:D:1134:LEU:HD12 | 1.94 | 0.68 |
| 3:N:1009:LYS:O | 3:N:1013:GLU:HG2 | 1.93 | 0.68 |
| 2:C:205:GLU:N | 2:C:209:ARG:HH11 | 1.92 | 0.68 |
| 2:C:454:SER:HB3 | 2:C:541:SER:HB2 | 1.76 | 0.68 |
| 2:C:1058:ASP:OD2 | 2:C:1084:SER:HB3 | 1.93 | 0.68 |
| 3:D:301:GLY:C | 3:D:303:PRO:HD2 | 2.14 | 0.68 |
| 3:N:400:VAL:HG22 | 3:N:402:PRO:HD3 | 1.74 | 0.68 |
| 3:D:407:VAL:HG22 | 3:D:408:GLU:N | 2.09 | 0.68 |
| 2:M:889:HIS:ND1 | 2:M:970:GLY:HA3 | 2.08 | 0.68 |
| 3:N:701:LEU:O | 3:N:702:LEU:HD23 | 1.94 | 0.68 |
| 2:M:430:VAL:CG1 | 3:N:1075:HIS:HA | 2.24 | 0.68 |
| 2:M:380:ALA:O | 2:M:384:GLU:N | 2.26 | 0.68 |
| 5:F:118:GLU:C | 5:F:120:THR:H | 1.97 | 0.68 |
| 2:M:773:LEU:HD11 | 2:M:777:ILE:HD11 | 1.76 | 0.68 |
| 1:B:58:ILE:HD13 | 1:B:60:ASP:H | 1.58 | 0.68 |
| 2:C:768:THR:HG22 | 2:C:770:GLU:H | 1.58 | 0.68 |
| 1:K:68:ILE:HG23 | 1:K:69:PRO:HD2 | 1.76 | 0.68 |
| 3:N:142:LEU:HB3 | 3:N:146:PRO:CA | 2.21 | 0.68 |
| 3:D:554:LEU:CA | 3:D:557:LEU:HD12 | 2.20 | 0.68 |
| 1:L:28:LEU:HD11 | 1:L:36:LEU:HD12 | 1.74 | 0.68 |
| 2:M:964:LYS:O | 2:M:968:LEU:HG | 1.94 | 0.68 |
| 5:P:142:ARG:CD | 5:P:145:PRO:HA | 2.24 | 0.68 |
| 3:D:1216:SER:CB | 4:E:16:LYS:H | 2.06 | 0.68 |
| 3:N:181:ASP:C | 3:N:183:GLU:H | 1.97 | 0.68 |
| 2:C:153:ALA:O | 2:C:155:PRO:HD3 | 1.94 | 0.68 |
| 2:M:230:ARG:HG2 | 2:M:233:GLU:HG2 | 1.76 | 0.68 |
| 2:C:264:PRO:HB2 | 2:C:289:THR:CG2 | 2.23 | 0.68 |
| 2:C:1046:ALA:CB | 3:D:1472:ILE:HB | 2.24 | 0.68 |
| 5:F:265:VAL:CA | 5:F:268:ILE:HD12 | 2.23 | 0.68 |
| 5:F:292:ALA:O | 5:F:299:TRP:HB2 | 1.93 | 0.68 |
| 3:D:482:LYS:HA | 3:D:489:ARG:HD2 | 1.75 | 0.68 |
| 3:D:796:ARG:C | 3:D:797:LYS:HG2 | 2.13 | 0.68 |
| 3:N:837:GLY:HA2 | 3:N:841:TYR:CD1 | 2.29 | 0.68 |
| 3:D:204:LEU:HD12 | 3:D:205:TYR:H | 1.58 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:1006:HIS:HA | 2:C:1027:PHE:CZ | 2.29 | 0.68 |
| 2:M:341:THR:O | 2:M:344:PHE:HB3 | 1.93 | 0.68 |
| 3:D:128:TYR:CE2 | 3:D:575:GLN:NE2 | 2.62 | 0.68 |
| 2:C:59:LYS:CD | 2:C:59:LYS:H | 2.01 | 0.68 |
| 5:P:300:ASP:O | 5:P:304:VAL:HG23 | 1.93 | 0.68 |
| 2:C:774:LEU:HD11 | 5:F:422:LEU:HD23 | 1.76 | 0.68 |
| 3:N:965:GLU:HG3 | 3:N:969:ARG:NH2 | 2.01 | 0.68 |
| 2:M:1014:SER:HB3 | 2:M:1017:THR:OG1 | 1.94 | 0.68 |
| 3:N:812:ALA:CB | 3:N:816:HIS:HB2 | 2.24 | 0.68 |
| 3:N:819:GLY:HA2 | 3:N:822:ALA:HB3 | 1.76 | 0.68 |
| 5:F:173:TYR:HA | 5:F:176:ILE:HD12 | 1.76 | 0.68 |
| 2:M:12:VAL:HG23 | 2:M:13:ILE:HG23 | 1.76 | 0.68 |
| 5:F:107:GLU:OE1 | 5:F:230:LYS:HE3 | 1.94 | 0.68 |
| 2:M:203:ASP:HB2 | 2:M:228:ALA:O | 1.94 | 0.67 |
| 3:N:219:GLU:HB3 | 3:N:337:LEU:HD12 | 1.76 | 0.67 |
| 3:D:1080:GLY:O | 3:D:1084:THR:HG22 | 1.93 | 0.67 |
| 3:D:237:LYS:CB | 3:D:238:PRO:HD2 | 2.16 | 0.67 |
| 3:D:154:THR:O | 3:D:157:GLU:HB2 | 1.94 | 0.67 |
| 3:D:186:VAL:HG12 | 3:D:187:LYS:N | 2.08 | 0.67 |
| 2:C:374:ASN:ND2 | 2:C:377:PRO:HD3 | 2.09 | 0.67 |
| 3:N:1353:GLN:OE1 | 3:N:1353:GLN:HA | 1.92 | 0.67 |
| 3:N:693:GLU:HA | 4:O:48:MET:CE | 2.23 | 0.67 |
| 1:K:138:LEU:HD12 | 1:K:139:ASN:H | 1.59 | 0.67 |
| 3:N:1498:ALA:HB3 | 4:O:84:ARG:NE | 2.09 | 0.67 |
| 2:M:1007:ALA:HA | 3:N:627:GLY:HA2 | 1.75 | 0.67 |
| 3:N:983:LEU:HD22 | 3:N:987:GLU:HB3 | 1.76 | 0.67 |
| 3:D:470:LEU:HB2 | 3:D:503:LEU:HD21 | 1.75 | 0.67 |
| 2:M:254:VAL:HB | 2:M:258:TYR:CZ | 2.29 | 0.67 |
| 3:N:287:GLY:HA3 | 3:N:311:LEU:HA | 1.76 | 0.67 |
| 2:C:313:LEU:C | 2:C:315:ALA:H | 1.98 | 0.67 |
| 3:N:130:SER:N | 3:N:568:ARG:NH2 | 2.43 | 0.67 |
| 3:N:82:LYS:H | 3:N:82:LYS:HD2 | 1.59 | 0.67 |
| 3:N:85:VAL:HG22 | 3:N:89:ARG:HG3 | 1.75 | 0.67 |
| 2:M:66:LEU:HA | 2:M:99:GLN:O | 1.94 | 0.67 |
| 3:N:1496:GLU:HA | 3:N:1499:ARG:CB | 2.23 | 0.67 |
| 2:M:690:ILE:O | 2:M:853:LEU:N | 2.21 | 0.67 |
| 3:N:623:VAL:CG1 | 3:N:624:ASP:N | 2.57 | 0.67 |
| 2:C:700:TYR:CB | 2:C:833:LEU:HD22 | 2.25 | 0.67 |
| 3:D:629:SER:C | 3:D:744:GLN:HG2 | 2.15 | 0.67 |
| 2:M:205:GLU:O | 2:M:209:ARG:HB2 | 1.95 | 0.67 |
| 3:N:223:LEU:O | 3:N:332:TYR:HA | 1.94 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:194:VAL:HG22 | 2:C:221:LEU:HG | 1.75 | 0.67 |
| 3:D:238:PRO:HB3 | 3:D:317:VAL:C | 2.14 | 0.67 |
| 3:D:135:LEU:HD23 | 3:D:135:LEU:H | 1.57 | 0.67 |
| 5:F:126:LEU:O | 5:F:129:GLU:HB3 | 1.93 | 0.67 |
| 5:P:407:LYS:O | 5:P:411:HIS:HB3 | 1.94 | 0.67 |
| 3:D:1016:PRO:HA | 3:D:1021:TYR:CD1 | 2.29 | 0.67 |
| 3:D:906:GLN:HB3 | 3:D:911:LEU:HD21 | 1.77 | 0.67 |
| 3:D:947:ILE:HG23 | 3:D:947:ILE:O | 1.93 | 0.67 |
| 2:C:694:LEU:HD21 | 2:C:868:ASP:CB | 2.21 | 0.67 |
| 3:N:230:TRP:CZ2 | 3:N:233:LYS:HE3 | 2.28 | 0.67 |
| 2:C:1104:GLU:H | 2:C:1104:GLU:CD | 1.98 | 0.67 |
| 3:D:534:ARG:HH21 | 5:F:313:GLU:CB | 2.00 | 0.67 |
| 3:N:401:TYR:O | 3:N:444:VAL:HG22 | 1.95 | 0.67 |
| 3:N:352:ASN:O | 3:N:368:VAL:HG13 | 1.93 | 0.67 |
| 5:P:419:ARG:O | 5:P:421:PHE:N | 2.27 | 0.67 |
| 3:D:806:PHE:CA | 3:D:809:PRO:HD2 | 2.24 | 0.67 |
| 3:D:1015:TYR:N | 3:D:1016:PRO:HD3 | 2.09 | 0.67 |
| 3:D:96:ALA:HB3 | 3:D:554:LEU:HD23 | 1.77 | 0.67 |
| 2:C:710:ILE:HG22 | 2:C:823:VAL:HB | 1.75 | 0.67 |
| 1:L:213:GLN:O | 1:L:217:ILE:HG13 | 1.95 | 0.67 |
| 3:N:371:ILE:HG13 | 3:N:372:ASP:H | 1.57 | 0.67 |
| 2:M:958:THR:CG2 | 2:M:961:GLU:HB2 | 2.22 | 0.67 |
| 3:N:931:LEU:CA | 3:N:934:LEU:HD12 | 2.23 | 0.67 |
| 1:L:226:SER:O | 1:L:228:PRO:HD3 | 1.93 | 0.67 |
| 2:C:1038:TRP:CH2 | 3:D:1096:ARG:HA | 2.29 | 0.67 |
| 3:D:133:ILE:HG22 | 3:D:455:ARG:O | 1.95 | 0.67 |
| 3:D:440:VAL:CG2 | 3:D:441:ARG:H | 2.05 | 0.67 |
| 2:M:94:LEU:O | 2:M:114:PHE:HA | 1.94 | 0.67 |
| 2:M:95:TYR:CG | 2:M:114:PHE:HB3 | 2.29 | 0.67 |
| 2:M:773:LEU:CD2 | 5:P:354:LEU:HD22 | 2.24 | 0.67 |
| 5:F:413:SER:CB | 5:F:414:ARG:HH21 | 2.07 | 0.67 |
| 2:C:37:GLU:HG2 | 2:C:71:TYR:CE2 | 2.29 | 0.67 |
| 3:D:631:ILE:HG12 | 3:D:743:ASP:O | 1.95 | 0.67 |
| 3:N:1397:LYS:HZ3 | 3:N:1432:LYS:HD2 | 1.58 | 0.67 |
| 5:P:159:ILE:O | 5:P:162:LYS:HB2 | 1.95 | 0.67 |
| 3:N:1029:ARG:HH11 | 3:N:1029:ARG:HG3 | 1.58 | 0.67 |
| 3:D:1337:GLU:N | 3:D:1337:GLU:OE1 | 2.26 | 0.67 |
| 2:C:175:GLU:C | 2:C:183:SER:HB2 | 2.15 | 0.67 |
| 3:N:438:ASP:HA | 3:N:445:ARG:NH2 | 2.09 | 0.67 |
| 5:P:77:THR:C | 5:P:79:ASP:H | 1.97 | 0.67 |
| 3:N:572:ARG:HH12 | 5:P:84:TYR:N | 1.93 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:105:VAL:HA | 3:D:110:SER:OG | 1.94 | 0.67 |
| 3:D:563:PRO:O | 3:D:566:ILE:HG12 | 1.95 | 0.67 |
| 3:D:1498:ALA:HB2 | 4:E:87:LYS:NZ | 2.10 | 0.67 |
| 5:F:314:PRO:HG2 | 5:F:315:VAL:H | 1.60 | 0.67 |
| 3:D:260:GLU:H | 3:D:270:LEU:HD12 | 1.58 | 0.67 |
| 3:D:258:VAL:CB | 3:D:273:ARG:HB2 | 2.09 | 0.67 |
| 4:E:7:ASP:HA | 4:E:10:PHE:CD1 | 2.30 | 0.67 |
| 3:D:654:LYS:HE2 | 3:D:658:LEU:HD11 | 1.75 | 0.67 |
| 2:C:876:VAL:HA | 2:C:881:ASN:HD21 | 1.60 | 0.67 |
| 2:M:1102:LEU:O | 3:N:5:VAL:HA | 1.93 | 0.67 |
| 1:K:188:GLN:HG3 | 1:K:189:ARG:N | 2.05 | 0.67 |
| 1:L:32:PHE:HA | 1:L:35:THR:HB | 1.76 | 0.67 |
| 2:M:918:LEU:HD12 | 2:M:968:LEU:HA | 1.76 | 0.67 |
| 2:M:37:GLU:HG2 | 2:M:71:TYR:HE2 | 1.58 | 0.67 |
| 3:N:957:PRO:HG2 | 3:N:1007:VAL:HA | 1.77 | 0.67 |
| 3:N:1046:GLN:HA | 3:N:1052:THR:HA | 1.77 | 0.67 |
| 1:L:68:ILE:HD12 | 1:L:71:VAL:CG1 | 2.24 | 0.67 |
| 2:M:254:VAL:HB | 2:M:258:TYR:CE1 | 2.29 | 0.67 |
| 2:M:397:GLU:N | 2:M:633:GLN:NE2 | 2.39 | 0.67 |
| 3:D:109:PRO:HB2 | 3:D:114:THR:OG1 | 1.93 | 0.67 |
| 3:D:563:PRO:HD2 | 3:D:566:ILE:HD11 | 1.77 | 0.67 |
| 3:N:421:LEU:CG | 3:N:428:LYS:HA | 2.13 | 0.67 |
| 3:D:1033:GLN:O | 3:D:1037:GLN:HG3 | 1.93 | 0.67 |
| 5:P:333:ILE:CD1 | 5:P:333:ILE:H | 2.08 | 0.67 |
| 3:D:60:CYS:SG | 3:D:76:CYS:HB3 | 2.34 | 0.67 |
| 2:C:395:LYS:HE2 | 2:C:403:SER:HB2 | 1.77 | 0.67 |
| 4:E:70:THR:C | 4:E:72:ARG:H | 1.98 | 0.67 |
| 3:N:249:TYR:CE1 | 3:N:330:THR:HG21 | 2.29 | 0.67 |
| 3:D:1106:VAL:HG12 | 3:D:1107:VAL:N | 2.10 | 0.67 |
| 3:N:1106:VAL:HG13 | 3:N:1219:GLU:O | 1.95 | 0.67 |
| 3:D:1383:ASP:HB3 | 3:D:1416:ALA:N | 2.05 | 0.67 |
| 1:K:41:ARG:HG2 | 1:K:45:LEU:HD11 | 1.77 | 0.67 |
| 3:N:79:GLU:HG2 | 3:N:80:VAL:N | 2.09 | 0.67 |
| 3:N:1069:GLU:HA | 3:N:1072:ILE:CD1 | 2.25 | 0.67 |
| 3:N:593:ASN:HB3 | 3:N:594:PRO:HD3 | 1.77 | 0.67 |
| 3:N:1337:GLU:N | 3:N:1337:GLU:OE1 | 2.27 | 0.67 |
| 1:A:118:ALA:O | 1:A:120:VAL:HG23 | 1.95 | 0.67 |
| 3:D:234:GLU:C | 3:D:236:TYR:H | 1.98 | 0.67 |
| 3:D:217:LYS:HB2 | 3:D:339:TRP:NE1 | 2.09 | 0.67 |
| 3:D:297:ILE:HD13 | 3:D:298:VAL:CG2 | 2.16 | 0.67 |
| 3:D:334:THR:C | 3:D:335:LEU:HD12 | 2.15 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:E:8:LYS:O | 4:E:12:MET:HG3 | 1.95 | 0.67 |
| 4:E:6:ILE:HG23 | 4:E:7:ASP:H | 1.60 | 0.67 |
| 1:B:208:LEU:HG | 1:B:209:GLU:N | 2.09 | 0.67 |
| 3:D:1398:TRP:N | 3:D:1398:TRP:CE3 | 2.61 | 0.67 |
| 3:N:1033:GLN:N | 3:N:1033:GLN:CD | 2.41 | 0.67 |
| 2:M:670:GLN:O | 2:M:672:VAL:HG12 | 1.95 | 0.67 |
| 2:C:857:ASP:CB | 2:C:978:ARG:HG2 | 2.25 | 0.67 |
| 2:C:762:LYS:HB2 | 2:C:786:LYS:HD2 | 1.77 | 0.67 |
| 2:C:79:PRO:HG2 | 2:C:82:GLU:CB | 2.25 | 0.67 |
| 2:C:474:VAL:HG12 | 2:C:530:GLU:O | 1.94 | 0.67 |
| 3:D:408:GLU:HA | 3:D:421:LEU:O | 1.94 | 0.67 |
| 2:M:605:LYS:HB3 | 2:M:610:ARG:NH2 | 2.10 | 0.67 |
| 1:K:41:ARG:O | 1:K:45:LEU:HG | 1.95 | 0.67 |
| 3:N:1105:ILE:HD11 | 3:N:1374:GLN:NE2 | 2.10 | 0.67 |
| 3:N:141:ILE:HD12 | 3:N:450:TYR:H | 1.59 | 0.66 |
| 2:C:1089:VAL:HA | 2:C:1092:LEU:HD12 | 1.77 | 0.66 |
| 3:D:127:LEU:CD2 | 3:D:128:TYR:N | 2.57 | 0.66 |
| 3:D:520:LEU:HD23 | 3:D:525:ARG:HB3 | 1.77 | 0.66 |
| 3:D:819:GLY:CA | 3:D:824:ASN:HD22 | 2.08 | 0.66 |
| 5:F:385:GLU:HA | 5:F:388:ALA:CB | 2.23 | 0.66 |
| 3:D:787:LEU:HD21 | 3:D:947:ILE:HD13 | 1.76 | 0.66 |
| 3:N:711:LEU:HD22 | 3:N:778:LEU:CD2 | 2.25 | 0.66 |
| 3:D:430:ASP:OD1 | 3:D:430:ASP:N | 2.28 | 0.66 |
| 3:N:1273:VAL:HG22 | 3:N:1326:THR:OG1 | 1.94 | 0.66 |
| 3:N:264:LEU:HD22 | 3:N:316:GLN:HE21 | 1.60 | 0.66 |
| 3:N:262:LYS:O | 3:N:268:ALA:HA | 1.95 | 0.66 |
| 3:D:317:VAL:HG23 | 3:D:338:GLU:C | 2.16 | 0.66 |
| 3:D:592:THR:HG21 | 3:D:598:ARG:HH12 | 1.59 | 0.66 |
| 2:C:93:PRO:HA | 2:C:117:HIS:HB3 | 1.77 | 0.66 |
| 5:F:340:SER:OG | 5:F:342:VAL:HB | 1.95 | 0.66 |
| 3:N:1424:VAL:HG23 | 3:N:1425:THR:N | 2.09 | 0.66 |
| 3:N:1269:LYS:C | 3:N:1271:LYS:H | 1.97 | 0.66 |
| 3:N:1031:ASN:CG | 3:N:1034:GLN:HG3 | 2.14 | 0.66 |
| 3:N:1098:LEU:N | 3:N:1098:LEU:HD12 | 2.04 | 0.66 |
| 1:K:199:ILE:HB | 1:K:207:PRO:HB3 | 1.76 | 0.66 |
| 3:D:644:LEU:C | 3:D:721:VAL:HG22 | 2.16 | 0.66 |
| 3:D:14:SER:HB2 | 3:D:17:LYS:HB2 | 1.77 | 0.66 |
| 2:M:577:PRO:HA | 2:M:671:ASN:OD1 | 1.96 | 0.66 |
| 3:N:323:GLU:CD | 3:N:334:THR:HB | 2.15 | 0.66 |
| 2:C:219:GLN:C | 2:C:221:LEU:H | 1.98 | 0.66 |
| 2:C:200:LEU:HD22 | 2:C:300:ASP:HB3 | 1.78 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1083:ASP:HB2 | 3:D:1239:ARG:CZ | 2.25 | 0.66 |
| 3:N:128:TYR:HD2 | 3:N:128:TYR:H | 1.42 | 0.66 |
| 5:P:83:GLN:O | 5:P:86:HIS:ND1 | 2.26 | 0.66 |
| 3:D:245:LEU:N | 3:D:246:PRO:HD3 | 2.09 | 0.66 |
| 5:F:347:GLN:O | 5:F:350:LEU:HB3 | 1.96 | 0.66 |
| 2:C:367:LEU:CG | 2:C:372:LEU:HD21 | 2.26 | 0.66 |
| 3:N:1489:GLN:HA | 3:N:1492:LEU:HD12 | 1.76 | 0.66 |
| 3:N:1112:CYS:H | 3:N:1201:CYS:CB | 2.07 | 0.66 |
| 5:F:164:LYS:HA | 5:F:171:LYS:HE3 | 1.76 | 0.66 |
| 5:F:321:ILE:HG22 | 5:F:322:GLY:N | 2.09 | 0.66 |
| 3:N:1237:THR:O | 3:N:1255:GLY:HA3 | 1.96 | 0.66 |
| 1:A:42:ARG:NH1 | 1:B:34:VAL:HB | 2.10 | 0.66 |
| 1:A:10:VAL:N | 1:A:26:GLU:O | 2.28 | 0.66 |
| 2:C:415:PRO:HB2 | 2:C:418:LEU:CB | 2.23 | 0.66 |
| 5:F:104:ARG:HG3 | 5:F:105:LYS:N | 2.09 | 0.66 |
| 3:N:253:ALA:H | 3:N:301:GLY:CA | 2.05 | 0.66 |
| 3:N:828:LYS:HD3 | 3:N:828:LYS:H | 1.60 | 0.66 |
| 2:M:511:GLU:O | 2:M:525:SER:HA | 1.96 | 0.66 |
| 3:D:736:PHE:O | 3:D:738:ALA:N | 2.29 | 0.66 |
| 3:N:206:ARG:HG3 | 3:N:207:PHE:N | 2.11 | 0.66 |
| 2:M:498:GLN:HB2 | 2:M:514:VAL:HG23 | 1.76 | 0.66 |
| 3:D:264:LEU:HD12 | 3:D:267:GLY:HA3 | 1.76 | 0.66 |
| 2:C:402:SER:HA | 2:C:566:THR:HG23 | 1.77 | 0.66 |
| 2:M:349:ALA:O | 2:M:353:ARG:HG3 | 1.95 | 0.66 |
| 3:N:1384:PRO:HB3 | 3:N:1387:SER:O | 1.95 | 0.66 |
| 2:C:230:ARG:O | 2:C:233:GLU:HG3 | 1.95 | 0.66 |
| 3:N:455:ARG:HB2 | 3:N:460:ALA:HB2 | 1.76 | 0.66 |
| 3:D:1094:LEU:HD21 | 3:D:1229:ILE:HG22 | 1.78 | 0.66 |
| 3:D:367:ILE:HG22 | 3:D:368:VAL:HG23 | 1.78 | 0.66 |
| 5:F:396:ARG:HA | 5:F:399:GLN:NE2 | 2.09 | 0.66 |
| 3:N:252:ARG:CZ | 3:N:300:LYS:HG2 | 2.26 | 0.66 |
| 3:N:1103:HIS:CD2 | 3:N:1462:LEU:H | 2.13 | 0.66 |
| 3:D:629:SER:HA | 3:D:744:GLN:HE21 | 1.59 | 0.66 |
| 2:C:20:GLU:O | 2:C:23:VAL:HG22 | 1.96 | 0.66 |
| 5:F:279:GLN:HA | 5:F:284:ARG:O | 1.96 | 0.66 |
| 3:N:1277:ILE:HG22 | 3:N:1278:ASP:N | 2.10 | 0.66 |
| 3:D:175:VAL:CG1 | 3:D:192:ALA:HB1 | 2.25 | 0.66 |
| 3:D:342:PRO:O | 3:D:343:LYS:HG3 | 1.95 | 0.66 |
| 3:N:98:PRO:HA | 3:N:514:LEU:O | 1.96 | 0.66 |
| 1:B:30:ARG:HA | 1:B:193:ASP:OD1 | 1.95 | 0.66 |
| 2:M:290:LEU:CD2 | 2:M:302:VAL:HG21 | 2.26 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:186:VAL:CG2 | 2:C:187:ASN:N | 2.50 | 0.66 |
| 2:C:195:LEU:CB | 2:C:238:LEU:HD21 | 2.23 | 0.66 |
| 3:D:1107:VAL:HG21 | 3:D:1219:GLU:HB3 | 1.77 | 0.66 |
| 3:D:661:MET:SD | 3:D:673:ALA:HB1 | 2.35 | 0.66 |
| 2:C:110:GLU:CD | 2:C:369:PRO:HB3 | 2.16 | 0.66 |
| 3:D:1171:VAL:HG12 | 3:D:1175:ILE:HD11 | 1.75 | 0.66 |
| 3:N:1406:ARG:HD3 | 3:N:1412:LYS:HZ3 | 1.57 | 0.66 |
| 2:C:988:VAL:CG1 | 3:D:948:THR:HB | 2.23 | 0.66 |
| 3:N:876:SER:OG | 3:N:879:ARG:HG2 | 1.95 | 0.66 |
| 3:N:939:PHE:O | 3:N:942:SER:N | 2.29 | 0.66 |
| 2:M:909:ALA:HB1 | 2:M:914:ILE:CD1 | 2.24 | 0.66 |
| 3:D:1121:PRO:HD3 | 3:D:1346:ARG:HH21 | 1.61 | 0.66 |
| 4:O:46:PRO:O | 4:O:56:ASP:HA | 1.96 | 0.66 |
| 2:C:292:ARG:HE | 2:C:295:ASP:HB3 | 1.60 | 0.66 |
| 3:N:244:GLU:O | 3:N:246:PRO:CD | 2.38 | 0.66 |
| 3:N:154:THR:HG22 | 3:N:157:GLU:HG3 | 1.76 | 0.66 |
| 3:N:568:ARG:HA | 3:N:571:LYS:HD2 | 1.78 | 0.66 |
| 3:D:522:PRO:HA | 3:D:525:ARG:NH1 | 2.11 | 0.66 |
| 3:D:250:LEU:HD11 | 3:D:304:LEU:CD2 | 2.25 | 0.66 |
| 2:M:87:ASP:HA | 2:M:131:GLY:HA3 | 1.76 | 0.66 |
| 2:C:867:VAL:HG23 | 2:C:868:ASP:N | 2.09 | 0.66 |
| 3:N:812:ALA:CA | 3:N:816:HIS:HB2 | 2.26 | 0.66 |
| 5:F:365:GLU:O | 5:F:368:VAL:HG22 | 1.94 | 0.66 |
| 1:L:124:ASN:ND2 | 1:L:127:LEU:HD22 | 2.11 | 0.66 |
| 3:N:989:TYR:HA | 3:N:992:ILE:HD12 | 1.77 | 0.66 |
| 3:N:99:ALA:O | 3:N:514:LEU:N | 2.28 | 0.66 |
| 2:M:194:VAL:HG21 | 2:M:221:LEU:O | 1.94 | 0.66 |
| 2:C:162:ILE:HD12 | 2:C:172:ILE:CD1 | 2.26 | 0.66 |
| 3:N:137:PRO:CG | 3:N:138:LYS:H | 2.09 | 0.66 |
| 3:N:149:LYS:HG2 | 3:N:150:ARG:N | 2.10 | 0.66 |
| 3:N:154:THR:O | 3:N:157:GLU:HB2 | 1.95 | 0.66 |
| 3:D:327:GLU:HG3 | 3:D:327:GLU:O | 1.95 | 0.66 |
| 2:M:595:LEU:HD21 | 2:M:639:GLN:NE2 | 2.10 | 0.66 |
| 5:P:288:TYR:CE1 | 5:P:305:GLU:HB2 | 2.31 | 0.66 |
| 1:L:104:GLU:CB | 1:L:137:ARG:HG3 | 2.22 | 0.66 |
| 3:D:82:LYS:HD2 | 3:D:82:LYS:H | 1.61 | 0.66 |
| 3:D:83:SER:OG | 5:F:337:HIS:NE2 | 2.29 | 0.66 |
| 3:D:414:ARG:HD3 | 3:D:451:ASP:OD1 | 1.95 | 0.66 |
| 1:K:186:LEU:HD23 | 1:K:188:GLN:NE2 | 2.10 | 0.66 |
| 2:M:988:VAL:HG12 | 3:N:948:THR:OG1 | 1.95 | 0.66 |
| 3:N:623:VAL:HG12 | 3:N:624:ASP:N | 2.10 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:K:42:ARG:HH12 | 1:L:34:VAL:HB | 1.60 | 0.66 |
| 2:C:136:ILE:HD13 | 2:C:392:SER:HA | 1.76 | 0.66 |
| 5:P:111:GLU:HA | 5:P:114:LYS:HD2 | 1.77 | 0.66 |
| 3:D:175:VAL:HG13 | 3:D:193:PRO:HD2 | 1.76 | 0.66 |
| 3:N:264:LEU:HB2 | 3:N:267:GLY:N | 2.11 | 0.66 |
| 3:D:711:LEU:HD22 | 3:D:778:LEU:HD23 | 1.78 | 0.66 |
| 3:N:643:GLY:HA3 | 3:N:727:GLN:HB2 | 1.76 | 0.66 |
| 3:N:179:VAL:C | 3:N:181:ASP:H | 1.99 | 0.66 |
| 3:D:219:GLU:HG2 | 3:D:220:ARG:H | 1.59 | 0.66 |
| 2:M:397:GLU:HG2 | 2:M:632:ASN:HB2 | 1.77 | 0.66 |
| 2:M:403:SER:O | 2:M:406:HIS:HB3 | 1.96 | 0.66 |
| 3:D:1103:HIS:HD2 | 3:D:1463:LYS:H | 1.43 | 0.66 |
| 3:D:133:ILE:HG23 | 3:D:456:MET:CG | 2.25 | 0.66 |
| 3:D:258:VAL:H | 3:D:273:ARG:N | 1.93 | 0.66 |
| 3:N:674:ARG:NH2 | 5:P:342:VAL:HG22 | 2.11 | 0.66 |
| 2:M:720:GLU:HB3 | 2:M:760:SER:HB3 | 1.78 | 0.66 |
| 5:F:371:LEU:HD23 | 5:F:375:LEU:HD11 | 1.75 | 0.66 |
| 3:D:397:LYS:HE3 | 3:D:448:GLU:OE2 | 1.96 | 0.66 |
| 3:N:1464:GLU:O | 3:N:1467:ILE:HG22 | 1.95 | 0.66 |
| 2:C:672:VAL:HG23 | 2:C:868:ASP:OD2 | 1.95 | 0.66 |
| 3:D:172:PRO:HB2 | 3:D:175:VAL:CG2 | 2.26 | 0.66 |
| 3:N:887:ALA:HA | 3:N:890:VAL:HG22 | 1.77 | 0.66 |
| 3:N:1124:GLN:N | 3:N:1133:ARG:O | 2.27 | 0.66 |
| 2:M:232:GLU:O | 2:M:235:LEU:HB3 | 1.96 | 0.66 |
| 1:B:239:ALA:O | 1:B:241:GLU:N | 2.28 | 0.66 |
| 2:C:191:PHE:CE2 | 2:C:196:LEU:HD21 | 2.30 | 0.66 |
| 2:C:436:GLY:HA2 | 2:C:539:VAL:HA | 1.76 | 0.66 |
| 3:D:109:PRO:HB2 | 3:D:114:THR:HG21 | 1.76 | 0.66 |
| 3:D:259:VAL:HG23 | 3:D:270:LEU:HD13 | 1.78 | 0.66 |
| 3:D:248:PRO:HA | 3:D:308:LYS:NZ | 2.10 | 0.66 |
| 2:C:38:LYS:CG | 2:C:39:ARG:H | 2.07 | 0.66 |
| 3:D:1399:ASP:O | 3:D:1403:LEU:HB3 | 1.96 | 0.66 |
| 3:N:1267:ARG:NH1 | 3:N:1267:ARG:CB | 2.54 | 0.66 |
| 2:C:676:ILE:CG2 | 2:C:988:VAL:HG13 | 2.25 | 0.66 |
| 3:N:614:PHE:HA | 3:N:617:ASN:HD22 | 1.60 | 0.66 |
| 2:M:419:THR:HG22 | 2:M:420:ARG:N | 2.11 | 0.66 |
| 2:M:876:VAL:H | 2:M:877:PRO:HD2 | 1.60 | 0.66 |
| 2:C:754:ILE:HG12 | 2:C:791:ARG:CD | 2.26 | 0.66 |
| 3:N:592:THR:HG21 | 3:N:598:ARG:HH12 | 1.60 | 0.66 |
| 2:C:243:ARG:CG | 2:C:244:PRO:HA | 2.26 | 0.66 |
| 2:M:428:ARG:CZ | 2:M:451:LEU:HD21 | 2.25 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:474:GLU:HG2 | 3:D:475:LYS:N | 2.10 | 0.66 |
| 3:D:1144:LEU:HA | 3:D:1147:ARG:HG3 | 1.77 | 0.66 |
| 1:A:143:ARG:NH1 | 1:A:158:ILE:HG23 | 2.11 | 0.66 |
| 1:L:156:HIS:CG | 1:L:156:HIS:O | 2.49 | 0.66 |
| 3:N:325:GLU:O | 3:N:325:GLU:HG3 | 1.96 | 0.65 |
| 3:N:153:LEU:HD21 | 3:N:158:TYR:HA | 1.78 | 0.65 |
| 3:N:133:ILE:HD13 | 3:N:456:MET:HE1 | 1.78 | 0.65 |
| 3:N:565:ILE:HG12 | 3:N:566:ILE:N | 2.11 | 0.65 |
| 3:N:553:ARG:HH11 | 5:P:214:GLN:CB | 2.08 | 0.65 |
| 3:D:455:ARG:HD3 | 3:D:459:GLU:CD | 2.16 | 0.65 |
| 3:D:545:ARG:HH11 | 3:D:545:ARG:HB3 | 1.61 | 0.65 |
| 3:D:365:ASP:O | 3:D:379:ALA:HB2 | 1.96 | 0.65 |
| 2:M:649:VAL:HG13 | 2:M:650:ARG:NH2 | 2.10 | 0.65 |
| 5:P:274:THR:HG22 | 5:P:278:LEU:HD11 | 1.77 | 0.65 |
| 3:D:1397:LYS:HB2 | 3:D:1398:TRP:CE3 | 2.31 | 0.65 |
| 1:L:161:ARG:H | 1:L:164:ALA:HB2 | 1.60 | 0.65 |
| 2:C:889:HIS:CD2 | 2:C:970:GLY:HA3 | 2.31 | 0.65 |
| 2:C:674:VAL:HA | 2:C:869:VAL:HG13 | 1.78 | 0.65 |
| 2:C:987:ILE:HA | 3:D:948:THR:CG2 | 2.25 | 0.65 |
| 3:N:207:PHE:CE1 | 5:P:98:GLU:HG3 | 2.31 | 0.65 |
| 2:C:402:SER:HA | 2:C:566:THR:CG2 | 2.26 | 0.65 |
| 2:C:724:ARG:HH21 | 2:C:734:LEU:CB | 2.09 | 0.65 |
| 2:C:197:LEU:CD1 | 2:C:221:LEU:HD11 | 2.25 | 0.65 |
| 2:C:170:PRO:HD3 | 2:C:263:ASP:HB3 | 1.77 | 0.65 |
| 2:C:274:ARG:O | 2:C:278:GLU:HB3 | 1.96 | 0.65 |
| 3:N:115:LEU:O | 3:N:116:LEU:HD23 | 1.96 | 0.65 |
| 3:N:22:SER:CB | 3:N:92:HIS:ND1 | 2.59 | 0.65 |
| 3:D:1102:THR:O | 3:D:1222:GLY:HA3 | 1.96 | 0.65 |
| 3:D:615:ARG:HG3 | 3:D:616:GLN:N | 2.11 | 0.65 |
| 4:O:41:GLU:HB2 | 4:O:42:PRO:CD | 2.20 | 0.65 |
| 2:C:988:VAL:H | 3:D:948:THR:HG21 | 1.61 | 0.65 |
| 3:N:257:GLY:CA | 3:N:274:ARG:HA | 2.26 | 0.65 |
| 3:N:1459:LEU:HD12 | 3:N:1470:ARG:NH1 | 2.10 | 0.65 |
| 1:K:154:GLU:H | 1:K:154:GLU:CD | 1.98 | 0.65 |
| 3:N:1085:ALA:CA | 3:N:1088:THR:HG22 | 2.26 | 0.65 |
| 3:D:1311:LEU:CD1 | 3:D:1312:LEU:H | 2.09 | 0.65 |
| 2:C:712:ALA:HB3 | 2:C:821:GLU:H | 1.61 | 0.65 |
| 5:P:392:VAL:CG1 | 5:P:396:ARG:HB3 | 2.26 | 0.65 |
| 5:F:173:TYR:O | 5:F:176:ILE:HB | 1.96 | 0.65 |
| 2:M:216:GLU:OE2 | 2:M:217:LEU:HG | 1.95 | 0.65 |
| 3:N:630:VAL:HA | 3:N:744:GLN:HG2 | 1.78 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:198:ARG:HA | 2:M:202:TYR:O | 1.97 | 0.65 |
| 2:M:204:GLN:C | 2:M:209:ARG:HD3 | 2.17 | 0.65 |
| 2:C:456:ALA:HB1 | 2:C:538:GLN:O | 1.97 | 0.65 |
| 3:D:539:ASP:HB3 | 3:D:600:LEU:HB3 | 1.78 | 0.65 |
| 3:D:356:PRO:HG2 | 3:D:359:ALA:HB2 | 1.78 | 0.65 |
| 3:D:403:PHE:CZ | 3:D:442:ASN:HB3 | 2.29 | 0.65 |
| 1:B:69:PRO:O | 1:B:71:VAL:HG23 | 1.95 | 0.65 |
| 1:B:18:ARG:O | 1:B:207:PRO:HD3 | 1.97 | 0.65 |
| 1:B:216:GLU:OE2 | 1:B:220:GLU:HB2 | 1.97 | 0.65 |
| 3:N:315:ARG:HD2 | 3:N:315:ARG:H | 1.60 | 0.65 |
| 1:L:137:ARG:HG2 | 1:L:137:ARG:HH11 | 1.60 | 0.65 |
| 3:D:168:THR:HB | 3:D:206:ARG:NH2 | 2.12 | 0.65 |
| 3:N:1468:LEU:CD2 | 3:N:1469:GLY:N | 2.60 | 0.65 |
| 5:P:330:GLY:O | 5:P:332:PHE:N | 2.30 | 0.65 |
| 3:N:1400:VAL:HB | 3:N:1401:GLU:OE1 | 1.96 | 0.65 |
| 5:P:153:PRO:HG2 | 5:P:154:LYS:HG3 | 1.77 | 0.65 |
| 3:N:403:PHE:HB2 | 3:N:423:ASP:OD2 | 1.96 | 0.65 |
| 2:M:305:PRO:O | 2:M:308:ARG:HG2 | 1.95 | 0.65 |
| 2:M:542:VAL:HG23 | 2:M:543:ASN:N | 2.06 | 0.65 |
| 3:N:212:ARG:HD3 | 3:N:342:PRO:CB | 2.26 | 0.65 |
| 3:D:526:PRO:O | 3:D:537:THR:HG22 | 1.95 | 0.65 |
| 3:D:352:ASN:O | 3:D:368:VAL:HG13 | 1.97 | 0.65 |
| 3:D:441:ARG:HD3 | 3:D:443:VAL:HG21 | 1.78 | 0.65 |
| 2:C:70:GLU:OE1 | 2:C:97:ARG:HD3 | 1.96 | 0.65 |
| 5:P:263:HIS:HA | 5:P:266:GLU:OE2 | 1.97 | 0.65 |
| 3:D:166:GLN:O | 3:D:167:GLU:HG2 | 1.96 | 0.65 |
| 2:M:186:VAL:HG13 | 2:M:187:ASN:N | 2.08 | 0.65 |
| 2:C:742:VAL:HG12 | 2:C:743:VAL:N | 2.11 | 0.65 |
| 2:M:1086:ARG:HB3 | 2:M:1112:PHE:CE2 | 2.30 | 0.65 |
| 2:M:930:LYS:C | 2:M:932:GLU:H | 2.00 | 0.65 |
| 1:A:108:GLU:HG2 | 1:A:109:VAL:H | 1.59 | 0.65 |
| 3:N:207:PHE:CE1 | 5:P:97:GLU:HB2 | 2.31 | 0.65 |
| 5:F:353:GLU:HA | 5:F:356:LYS:HD2 | 1.79 | 0.65 |
| 5:P:234:LYS:HE2 | 5:P:236:SER:CB | 2.26 | 0.65 |
| 2:M:293:PHE:CD1 | 2:M:294:GLU:HG3 | 2.31 | 0.65 |
| 2:M:203:ASP:O | 2:M:207:LEU:HD12 | 1.96 | 0.65 |
| 2:C:257:VAL:HG12 | 2:C:263:ASP:OD1 | 1.96 | 0.65 |
| 3:D:1083:ASP:HB2 | 3:D:1239:ARG:NH1 | 2.12 | 0.65 |
| 3:N:524:LEU:C | 3:N:526:PRO:HD3 | 2.17 | 0.65 |
| 5:F:217:ASN:O | 5:F:220:LEU:HB3 | 1.96 | 0.65 |
| 2:M:367:LEU:HD23 | 2:M:367:LEU:O | 1.96 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:D:414:ARG:HD3 | 3:D:451:ASP:CG | 2.17 | 0.65 |
| 5:F:76:SER:O | 5:F:78:SER:N | 2.28 | 0.65 |
| 1:B:74:ASP:HB3 | 1:B:77:GLU:CB | 2.27 | 0.65 |
| 3:D:851:LEU:O | 3:D:854:ALA:HB3 | 1.96 | 0.65 |
| 3:N:1342:GLU:HA | 3:N:1345:GLU:OE1 | 1.97 | 0.65 |
| 1:A:86:VAL:HG13 | 1:A:123:MET:HB2 | 1.77 | 0.65 |
| 3:D:1341:PRO:O | 3:D:1344:VAL:HG12 | 1.97 | 0.65 |
| 3:D:1376:MET:HE1 | 3:D:1421:LEU:HD13 | 1.78 | 0.65 |
| 3:D:881:LEU:HG | 3:D:885:ILE:HD11 | 1.79 | 0.65 |
| 2:C:1:MET:HB3 | 2:C:898:GLY:O | 1.97 | 0.65 |
| 4:E:42:PRO:HA | 4:E:45:ARG:HD2 | 1.77 | 0.65 |
| 2:C:405:ARG:HD2 | 2:C:442:GLU:OE2 | 1.96 | 0.65 |
| 3:D:354:VAL:HB | 3:D:367:ILE:O | 1.97 | 0.65 |
| 3:D:288:MET:CE | 3:D:307:ALA:HB2 | 2.26 | 0.65 |
| 1:B:137:ARG:HH11 | 1:B:137:ARG:HG2 | 1.61 | 0.65 |
| 5:F:373:LYS:HB3 | 5:F:379:ARG:N | 2.11 | 0.65 |
| 2:C:370:ALA:HA | 2:C:373:VAL:CG2 | 2.25 | 0.65 |
| 2:C:672:VAL:HG23 | 2:C:673:LEU:N | 2.11 | 0.65 |
| 1:A:5:LYS:HZ2 | 1:A:28:LEU:C | 2.00 | 0.65 |
| 1:K:41:ARG:NH2 | 2:M:860:HIS:CD2 | 2.64 | 0.65 |
| 3:N:207:PHE:HZ | 5:P:98:GLU:HG3 | 1.62 | 0.65 |
| 2:M:498:GLN:OE1 | 3:N:1067:VAL:HG13 | 1.95 | 0.65 |
| 2:M:435:TYR:HA | 3:N:1071:PHE:CE2 | 2.32 | 0.65 |
| 3:D:965:GLU:O | 3:D:968:ASP:N | 2.30 | 0.65 |
| 1:A:186:LEU:HD23 | 1:A:188:GLN:HE21 | 1.60 | 0.65 |
| 2:C:205:GLU:O | 2:C:209:ARG:HB2 | 1.96 | 0.65 |
| 3:N:148:GLU:O | 3:N:150:ARG:N | 2.29 | 0.65 |
| 3:D:1098:LEU:CD1 | 3:D:1098:LEU:H | 2.10 | 0.65 |
| 3:D:610:LYS:HZ3 | 3:D:1442:ASN:H | 1.44 | 0.65 |
| 5:F:207:LEU:O | 5:F:212:LEU:HD21 | 1.96 | 0.65 |
| 3:D:252:ARG:HG3 | 3:D:300:LYS:C | 2.17 | 0.65 |
| 3:D:225:LEU:HD12 | 3:D:333:LEU:CD1 | 2.26 | 0.65 |
| 2:M:151:ASP:HB3 | 2:M:157:ARG:O | 1.97 | 0.65 |
| 2:C:45:GLN:O | 2:C:49:ARG:HG3 | 1.97 | 0.65 |
| 2:C:56:GLU:HB3 | 2:C:359:MET:SD | 2.36 | 0.65 |
| 5:P:302:LYS:HD2 | 5:P:302:LYS:C | 2.17 | 0.65 |
| 5:F:280:GLN:CG | 5:F:281:GLU:H | 1.95 | 0.65 |
| 3:N:274:ARG:HE | 3:N:279:VAL:CG1 | 2.08 | 0.65 |
| 3:N:1108:ARG:CD | 3:N:1199:GLY:HA3 | 2.26 | 0.65 |
| 2:M:153:ALA:O | 2:M:155:PRO:HD3 | 1.96 | 0.65 |
| 4:O:37:ASN:HD22 | 4:O:37:ASN:N | 1.93 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:238:PRO:HD3 | 3:D:318:ARG:HA | 1.77 | 0.65 |
| 3:N:441:ARG:O | 3:N:443:VAL:N | 2.30 | 0.65 |
| 3:D:811:GLU:HB2 | 3:D:816:HIS:ND1 | 2.11 | 0.65 |
| 3:D:1406:ARG:HA | 3:D:1412:LYS:HG2 | 1.78 | 0.65 |
| 2:C:508:ILE:HD12 | 2:C:526:PRO:HB3 | 1.79 | 0.65 |
| 2:C:643:VAL:HG23 | 2:C:647:GLN:CD | 2.17 | 0.65 |
| 3:N:1313:VAL:HG22 | 3:N:1314:LYS:N | 2.12 | 0.65 |
| 1:L:86:VAL:HG13 | 1:L:123:MET:HB2 | 1.78 | 0.65 |
| 1:L:5:LYS:HZ1 | 1:L:189:ARG:HD2 | 1.61 | 0.65 |
| 2:C:1030:GLN:O | 3:D:622:ARG:HA | 1.97 | 0.65 |
| 3:D:1042:ARG:HG2 | 3:D:1042:ARG:HH11 | 1.62 | 0.65 |
| 3:N:131:LYS:HB3 | 3:N:568:ARG:HG2 | 1.77 | 0.65 |
| 3:D:259:VAL:CA | 3:D:270:LEU:HD11 | 2.27 | 0.65 |
| 3:D:245:LEU:HA | 3:D:309:GLY:H | 1.62 | 0.65 |
| 3:D:249:TYR:CD1 | 3:D:330:THR:HG21 | 2.32 | 0.65 |
| 1:B:101:LEU:HB3 | 1:B:140:MET:SD | 2.37 | 0.65 |
| 3:D:673:ALA:HA | 3:D:676:MET:HB3 | 1.78 | 0.65 |
| 5:P:367:MET:CB | 5:P:371:LEU:HG | 2.27 | 0.65 |
| 5:F:421:PHE:CD2 | 5:F:422:LEU:N | 2.65 | 0.65 |
| 3:D:56:TYR:OH | 3:D:82:LYS:HE3 | 1.97 | 0.65 |
| 3:N:959:GLU:H | 3:N:959:GLU:CD | 2.00 | 0.65 |
| 3:N:962:GLN:HB3 | 3:N:966:GLU:OE2 | 1.96 | 0.65 |
| 3:N:625:TYR:HB3 | 3:N:749:VAL:HB | 1.79 | 0.65 |
| 5:P:94:LEU:CG | 5:P:190:ALA:HB1 | 2.26 | 0.65 |
| 3:D:647:ARG:O | 3:D:650:LEU:HB3 | 1.97 | 0.65 |
| 3:N:166:GLN:HA | 3:N:395:VAL:O | 1.96 | 0.65 |
| 3:D:315:ARG:H | 3:D:315:ARG:HD2 | 1.62 | 0.65 |
| 3:N:544:TYR:O | 3:N:547:LEU:HB3 | 1.97 | 0.65 |
| 3:D:128:TYR:HD1 | 3:D:457:GLY:CA | 2.08 | 0.65 |
| 3:D:12:LEU:HD21 | 3:D:1452:ILE:HD13 | 1.78 | 0.65 |
| 3:D:400:VAL:HG23 | 3:D:443:VAL:CG1 | 2.27 | 0.65 |
| 5:P:413:SER:HB2 | 5:P:414:ARG:HH21 | 1.61 | 0.65 |
| 3:N:1406:ARG:HG2 | 3:N:1412:LYS:HD3 | 1.79 | 0.65 |
| 2:C:1115:LEU:HB3 | 3:D:85:VAL:CG2 | 2.21 | 0.65 |
| 3:N:972:LEU:HD23 | 3:N:972:LEU:N | 2.12 | 0.65 |
| 2:M:914:ILE:HD12 | 2:M:914:ILE:N | 2.11 | 0.65 |
| 3:N:1175:ILE:O | 3:N:1179:GLU:HG3 | 1.97 | 0.65 |
| 3:N:1122:LEU:C | 3:N:1135:ARG:HG3 | 2.17 | 0.65 |
| 1:A:83:LYS:HE3 | 1:A:168:ASP:O | 1.96 | 0.65 |
| 3:N:931:LEU:HA | 3:N:934:LEU:CD1 | 2.27 | 0.65 |
| 2:M:41:ASN:ND2 | 2:M:41:ASN:C | 2.49 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:45:GLN:O | 2:M:49:ARG:HG3 | 1.96 | 0.65 |
| 3:D:887:ALA:HA | 3:D:890:VAL:CG2 | 2.27 | 0.65 |
| 3:N:174:GLY:HA2 | 3:N:389:GLU:CG | 2.27 | 0.65 |
| 4:E:70:THR:O | 4:E:72:ARG:N | 2.30 | 0.64 |
| 3:N:261:LEU:HD22 | 3:N:268:ALA:O | 1.97 | 0.64 |
| 2:C:425:PHE:HZ | 3:D:1239:ARG:NH2 | 1.94 | 0.64 |
| 2:C:328:LEU:HD12 | 2:C:433:THR:O | 1.97 | 0.64 |
| 3:D:546:ARG:O | 3:D:550:ARG:HG3 | 1.97 | 0.64 |
| 5:F:213:ILE:HG22 | 5:F:217:ASN:HD21 | 1.62 | 0.64 |
| 2:M:313:LEU:C | 2:M:315:ALA:H | 2.00 | 0.64 |
| 2:M:600:ASP:HA | 2:M:649:VAL:O | 1.97 | 0.64 |
| 5:F:271:LEU:HD11 | 5:F:307:THR:HG21 | 1.78 | 0.64 |
| 3:D:1403:LEU:C | 3:D:1405:GLU:H | 2.01 | 0.64 |
| 3:N:1403:LEU:HB3 | 3:N:1408:ILE:CD1 | 2.27 | 0.64 |
| 3:D:58:CYS:HB2 | 3:D:76:CYS:SG | 2.37 | 0.64 |
| 1:B:176:ARG:HG2 | 1:B:177:VAL:N | 2.12 | 0.64 |
| 3:N:1120:VAL:HB | 3:N:1144:LEU:HD21 | 1.79 | 0.64 |
| 2:C:685:GLU:O | 2:C:686:ASP:HB2 | 1.95 | 0.64 |
| 3:N:149:LYS:HG2 | 3:N:150:ARG:H | 1.63 | 0.64 |
| 3:N:537:THR:C | 5:P:317:LEU:HG | 2.17 | 0.64 |
| 2:C:1037:VAL:HG21 | 9:D:1529:NE6:H9 | 1.79 | 0.64 |
| 3:D:1472:ILE:HG23 | 3:D:1474:ALA:H | 1.61 | 0.64 |
| 3:D:280:ALA:HB1 | 3:D:282:TYR:CE1 | 2.32 | 0.64 |
| 3:D:421:LEU:HB3 | 3:D:427:VAL:O | 1.97 | 0.64 |
| 3:N:352:ASN:N | 3:N:369:ALA:O | 2.31 | 0.64 |
| 3:D:659:LYS:HG3 | 3:D:663:GLU:OE2 | 1.96 | 0.64 |
| 3:N:965:GLU:OE2 | 3:N:969:ARG:HB3 | 1.96 | 0.64 |
| 2:M:1009:SER:HB3 | 3:N:651:GLU:CD | 2.17 | 0.64 |
| 2:C:836:GLY:O | 2:C:848:VAL:HG13 | 1.97 | 0.64 |
| 2:M:613:VAL:O | 2:M:620:LEU:HA | 1.97 | 0.64 |
| 2:M:172:ILE:HG22 | 2:M:173:ASP:N | 2.12 | 0.64 |
| 1:K:89:PHE:HB2 | 1:K:146:ARG:HH21 | 1.63 | 0.64 |
| 3:N:225:LEU:HB3 | 3:N:226:PRO:HD2 | 1.78 | 0.64 |
| 2:C:139:GLN:HB3 | 2:C:411:SER:HB3 | 1.80 | 0.64 |
| 3:N:113:GLY:C | 3:N:115:LEU:H | 2.01 | 0.64 |
| 3:N:96:ALA:HB3 | 3:N:554:LEU:HD23 | 1.79 | 0.64 |
| 3:N:25:GLU:HB2 | 3:N:92:HIS:CE1 | 2.33 | 0.64 |
| 3:D:10:ILE:O | 3:D:1454:GLY:HA2 | 1.97 | 0.64 |
| 3:D:524:LEU:C | 3:D:526:PRO:HD3 | 2.18 | 0.64 |
| 1:A:208:LEU:HG | 1:A:209:GLU:N | 2.11 | 0.64 |
| 5:P:299:TRP:CE3 | 5:P:303:ARG:HD3 | 2.32 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:793:THR:O | 3:D:905:PRO:HA | 1.96 | 0.64 |
| 3:N:852:ALA:HB1 | 3:N:857:ILE:HD11 | 1.78 | 0.64 |
| 3:N:1114:THR:HB | 3:N:1195:GLN:CG | 2.27 | 0.64 |
| 3:N:1147:ARG:HB3 | 3:N:1188:VAL:CG2 | 2.27 | 0.64 |
| 3:D:417:PRO:HB3 | 3:D:429:SER:C | 2.18 | 0.64 |
| 3:N:699:VAL:HG12 | 3:N:717:GLN:CG | 2.26 | 0.64 |
| 3:D:1121:PRO:CD | 3:D:1346:ARG:HH21 | 2.10 | 0.64 |
| 3:N:1324:PRO:O | 3:N:1325:LEU:HD23 | 1.98 | 0.64 |
| 5:F:145:PRO:O | 5:F:149:GLU:HB2 | 1.97 | 0.64 |
| 2:C:809:GLY:C | 2:C:811:PRO:HD2 | 2.18 | 0.64 |
| 5:P:219:GLY:HA3 | 5:P:246:ALA:CB | 2.27 | 0.64 |
| 2:M:896:PHE:C | 2:M:898:GLY:N | 2.50 | 0.64 |
| 2:M:1009:SER:HB3 | 3:N:651:GLU:OE2 | 1.97 | 0.64 |
| 1:K:33:GLY:HA3 | 1:K:181:VAL:HG22 | 1.79 | 0.64 |
| 1:L:170:VAL:O | 1:L:170:VAL:HG23 | 1.96 | 0.64 |
| 4:E:73:LEU:HD12 | 4:E:74:VAL:H | 1.61 | 0.64 |
| 3:N:1293:PHE:CZ | 3:N:1300:SER:HB3 | 2.32 | 0.64 |
| 2:C:140:ILE:HG23 | 2:C:410:ILE:CG2 | 2.27 | 0.64 |
| 3:N:112:ILE:HG23 | 3:N:512:MET:SD | 2.38 | 0.64 |
| 3:D:298:VAL:O | 3:D:298:VAL:HG12 | 1.97 | 0.64 |
| 2:M:93:PRO:HA | 2:M:117:HIS:CB | 2.24 | 0.64 |
| 3:D:785:ILE:HD13 | 3:D:935:LYS:HA | 1.79 | 0.64 |
| 1:B:68:ILE:HD12 | 1:B:71:VAL:HB | 1.79 | 0.64 |
| 3:D:806:PHE:CD1 | 3:D:809:PRO:HB2 | 2.31 | 0.64 |
| 3:D:815:ALA:HA | 3:D:818:ARG:CD | 2.27 | 0.64 |
| 5:F:339:PRO:HB3 | 5:F:343:ASP:HB2 | 1.78 | 0.64 |
| 5:F:346:THR:O | 5:F:350:LEU:N | 2.31 | 0.64 |
| 3:N:1106:VAL:HG12 | 3:N:1107:VAL:N | 2.13 | 0.64 |
| 2:M:672:VAL:CG2 | 2:M:673:LEU:N | 2.61 | 0.64 |
| 3:N:844:ALA:HB1 | 3:N:867:ARG:HH11 | 1.61 | 0.64 |
| 1:B:72:LYS:HD3 | 1:B:72:LYS:C | 2.17 | 0.64 |
| 1:B:82:LEU:O | 1:B:85:LEU:HB3 | 1.97 | 0.64 |
| 2:M:495:THR:HB | 2:M:530:GLU:HG3 | 1.80 | 0.64 |
| 1:A:167:VAL:HG12 | 1:A:168:ASP:N | 2.11 | 0.64 |
| 3:N:818:ARG:O | 3:N:822:ALA:N | 2.27 | 0.64 |
| 2:M:71:TYR:HD2 | 2:M:71:TYR:N | 1.95 | 0.64 |
| 3:D:142:LEU:HD23 | 3:D:146:PRO:CA | 2.27 | 0.64 |
| 3:N:1130:ARG:HH22 | 3:N:1323:GLN:NE2 | 1.94 | 0.64 |
| 2:C:815:LEU:HD11 | 2:C:821:GLU:HA | 1.79 | 0.64 |
| 2:C:705:ILE:HD12 | 2:C:705:ILE:N | 2.13 | 0.64 |
| 2:C:939:ARG:HD2 | 2:C:982:PRO:CD | 2.28 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:D:212:ARG:HG3 | 3:D:343:LYS:O | 1.98 | 0.64 |
| 1:A:56:VAL:HG22 | 1:A:142:VAL:HA | 1.78 | 0.64 |
| 3:D:1333:HIS:O | 3:D:1336:LEU:HB3 | 1.98 | 0.64 |
| 2:C:469:THR:HG23 | 2:C:470:PRO:HD2 | 1.80 | 0.64 |
| 2:C:470:PRO:HG3 | 2:C:485:TYR:CZ | 2.32 | 0.64 |
| 3:N:119:SER:HB3 | 3:N:123:LEU:CG | 2.27 | 0.64 |
| 3:D:125:GLN:HE22 | 3:D:587:ARG:HE | 1.45 | 0.64 |
| 3:D:355:VAL:HG11 | 3:D:385:VAL:CG2 | 2.24 | 0.64 |
| 3:D:227:LEU:HD22 | 3:D:328:GLY:C | 2.18 | 0.64 |
| 1:A:206:THR:HB | 1:A:209:GLU:CG | 2.18 | 0.64 |
| 3:D:1031:ASN:N | 3:D:1034:GLN:HE21 | 1.96 | 0.64 |
| 2:C:878:SER:HA | 3:D:1034:GLN:OE1 | 1.98 | 0.64 |
| 3:N:302:GLN:N | 3:N:303:PRO:HD2 | 2.12 | 0.64 |
| 2:C:693:GLU:HG3 | 2:C:697:ARG:HH11 | 1.63 | 0.64 |
| 3:N:1258:ARG:NE | 3:N:1262:LEU:HD11 | 2.13 | 0.64 |
| 1:K:55:SER:HB3 | 1:K:166:PRO:HA | 1.78 | 0.64 |
| 2:M:41:ASN:O | 2:M:46:ALA:HB2 | 1.97 | 0.64 |
| 3:N:403:PHE:CD1 | 3:N:404:GLU:N | 2.65 | 0.64 |
| 3:N:163:TYR:OH | 5:P:186:HIS:HE1 | 1.81 | 0.64 |
| 3:N:433:GLY:CA | 3:N:449:SER:N | 2.60 | 0.64 |
| 3:D:815:ALA:HA | 3:D:818:ARG:HD2 | 1.79 | 0.64 |
| 5:F:381:HIS:C | 5:F:385:GLU:HG3 | 2.17 | 0.64 |
| 2:C:95:TYR:CD2 | 2:C:114:PHE:HB3 | 2.32 | 0.64 |
| 2:C:37:GLU:OE2 | 2:C:70:GLU:HB3 | 1.98 | 0.64 |
| 2:M:760:SER:O | 2:M:785:VAL:HA | 1.98 | 0.64 |
| 3:D:1396:GLU:O | 3:D:1397:LYS:HD3 | 1.98 | 0.64 |
| 3:D:1406:ARG:HB3 | 3:D:1412:LYS:HE2 | 1.79 | 0.64 |
| 2:M:1015:LEU:HA | 5:P:335:ASP:HB2 | 1.78 | 0.64 |
| 3:D:851:LEU:N | 3:D:851:LEU:HD23 | 2.12 | 0.64 |
| 2:C:363:SER:CB | 2:C:366:SER:HB3 | 2.21 | 0.64 |
| 5:F:278:LEU:HB3 | 5:F:286:PRO:HG3 | 1.80 | 0.64 |
| 3:N:807:ALA:N | 3:N:809:PRO:HD2 | 2.12 | 0.64 |
| 1:A:11:PHE:HD2 | 1:B:227:ASN:O | 1.80 | 0.64 |
| 2:M:191:PHE:CE2 | 2:M:196:LEU:HD21 | 2.32 | 0.64 |
| 2:C:230:ARG:NH1 | 2:C:230:ARG:HG3 | 2.12 | 0.64 |
| 2:M:649:VAL:CA | 2:M:650:ARG:HH21 | 2.08 | 0.64 |
| 3:D:658:LEU:HA | 3:D:661:MET:CE | 2.17 | 0.64 |
| 2:M:100:LEU:HD23 | 2:M:368:THR:HA | 1.80 | 0.64 |
| 5:P:302:LYS:HD2 | 5:P:303:ARG:H | 1.55 | 0.64 |
| 2:C:971:LYS:NZ | 3:D:950:GLY:HA3 | 2.13 | 0.64 |
| 3:N:1434:TRP:O | 3:N:1437:ALA:HB3 | 1.97 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:N:1114:THR:HB | 3:N:1195:GLN:HG3 | 1.80 | 0.64 |
| 1:K:34:VAL:HG21 | 2:M:939:ARG:HH21 | 1.62 | 0.64 |
| 2:M:1007:ALA:HB2 | 3:N:648:MET:HG3 | 1.78 | 0.64 |
| 5:F:300:ASP:O | 5:F:304:VAL:HG23 | 1.98 | 0.64 |
| 3:N:157:GLU:O | 3:N:161:LEU:HG | 1.97 | 0.64 |
| 3:D:437:VAL:HG11 | 5:F:175:HIS:CB | 2.21 | 0.64 |
| 3:D:574:LEU:O | 3:D:578:VAL:HG23 | 1.98 | 0.64 |
| 5:F:115:LYS:HD2 | 5:F:119:ILE:HD11 | 1.79 | 0.64 |
| 5:F:209:PHE:O | 5:F:213:ILE:HG13 | 1.98 | 0.64 |
| 3:D:260:GLU:H | 3:D:270:LEU:CD1 | 2.10 | 0.64 |
| 2:M:63:GLY:H | 2:M:103:LYS:CA | 2.10 | 0.64 |
| 3:D:800:LYS:O | 3:D:830:ALA:HB3 | 1.98 | 0.64 |
| 2:C:904:PRO:HD2 | 2:C:908:GLY:HA2 | 1.78 | 0.64 |
| 2:C:549:PHE:CD2 | 2:C:886:LEU:HB2 | 2.32 | 0.64 |
| 3:N:793:THR:HG21 | 3:N:906:GLN:HG2 | 1.79 | 0.64 |
| 2:M:698:ASP:HA | 2:M:832:LYS:CE | 2.28 | 0.64 |
| 2:M:317:VAL:O | 2:M:317:VAL:HG12 | 1.98 | 0.64 |
| 2:M:317:VAL:N | 2:M:318:PRO:CD | 2.61 | 0.64 |
| 2:C:897:LEU:O | 2:C:899:GLN:HG2 | 1.98 | 0.64 |
| 3:N:680:GLN:HA | 3:N:683:ILE:CD1 | 2.27 | 0.64 |
| 3:N:507:ASN:ND2 | 3:N:1452:ILE:O | 2.31 | 0.64 |
| 2:C:194:VAL:HA | 2:C:197:LEU:CG | 2.28 | 0.64 |
| 3:D:1464:GLU:CG | 3:D:1465:ASN:H | 2.10 | 0.64 |
| 3:D:87:ARG:HB3 | 3:D:523:ASP:HB2 | 1.79 | 0.64 |
| 5:P:370:LYS:O | 5:P:375:LEU:N | 2.30 | 0.64 |
| 3:D:826:PRO:O | 3:D:829:VAL:HG22 | 1.97 | 0.64 |
| 3:D:1031:ASN:N | 3:D:1034:GLN:NE2 | 2.44 | 0.64 |
| 3:N:1464:GLU:CG | 3:N:1465:ASN:H | 2.10 | 0.64 |
| 2:M:1008:ARG:NH1 | 2:M:1020:PRO:HB3 | 2.13 | 0.64 |
| 1:K:34:VAL:HB | 1:L:42:ARG:NH1 | 2.12 | 0.64 |
| 3:N:1372:VAL:HA | 3:N:1375:MET:HE2 | 1.79 | 0.64 |
| 5:P:152:ASP:N | 5:P:153:PRO:HD2 | 2.13 | 0.64 |
| 2:C:380:ALA:C | 2:C:384:GLU:HG2 | 2.18 | 0.64 |
| 3:D:1364:HIS:ND1 | 3:D:1366:LYS:HG3 | 2.12 | 0.64 |
| 4:O:25:LYS:HA | 4:O:28:GLN:CD | 2.17 | 0.64 |
| 2:M:439:CYS:SG | 2:M:441:VAL:HG13 | 2.38 | 0.64 |
| 4:E:39:VAL:HG11 | 4:E:72:ARG:O | 1.97 | 0.64 |
| 2:C:584:GLU:H | 2:C:584:GLU:CD | 2.00 | 0.64 |
| 3:D:569:ASN:O | 3:D:573:MET:HG3 | 1.97 | 0.64 |
| 5:P:383:LEU:HD21 | 5:P:394:ARG:HD3 | 1.80 | 0.64 |
| 1:L:76:VAL:HA | 1:L:79:ILE:CD1 | 2.21 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:52:PHE:HE1 | 2:C:66:LEU:HG | 1.63 | 0.64 |
| 5:P:261:PRO:O | 5:P:264:MET:HB2 | 1.97 | 0.64 |
| 3:N:796:ARG:HE | 3:N:861:GLN:CB | 2.11 | 0.64 |
| 3:D:168:THR:HB | 3:D:206:ARG:HH22 | 1.62 | 0.64 |
| 3:N:761:ILE:HD12 | 4:O:20:THR:HA | 1.80 | 0.64 |
| 3:N:479:GLU:C | 3:N:481:MET:H | 2.01 | 0.64 |
| 3:N:656:PHE:HZ | 3:N:751:LEU:HD23 | 1.62 | 0.64 |
| 3:N:209:ARG:O | 3:N:346:ARG:HA | 1.98 | 0.64 |
| 5:F:300:ASP:O | 5:F:303:ARG:HB3 | 1.97 | 0.64 |
| 3:D:1310:ARG:HD3 | 3:D:1327:ARG:HD3 | 1.78 | 0.64 |
| 2:M:1000:MET:HB2 | 2:M:1003:ASP:HB2 | 1.79 | 0.64 |
| 4:E:47:LYS:O | 4:E:48:MET:HG3 | 1.96 | 0.63 |
| 5:P:209:PHE:O | 5:P:213:ILE:HG13 | 1.97 | 0.63 |
| 1:B:208:LEU:O | 1:B:211:LEU:HB3 | 1.98 | 0.63 |
| 3:D:676:MET:HG3 | 3:D:677:LEU:CD2 | 2.28 | 0.63 |
| 2:M:56:GLU:O | 2:M:64:LEU:HD23 | 1.98 | 0.63 |
| 1:B:197:LEU:HD12 | 1:B:198:ARG:H | 1.63 | 0.63 |
| 2:C:605:LYS:CB | 2:C:610:ARG:HH21 | 2.09 | 0.63 |
| 5:F:305:GLU:O | 5:F:308:LEU:HG | 1.97 | 0.63 |
| 3:N:989:TYR:CE1 | 3:N:993:LEU:HD21 | 2.33 | 0.63 |
| 1:L:47:SER:C | 1:L:48:ILE:HD12 | 2.18 | 0.63 |
| 5:F:251:ILE:O | 5:F:255:ALA:HB2 | 1.98 | 0.63 |
| 2:M:1113:GLU:O | 2:M:1113:GLU:HG3 | 1.97 | 0.63 |
| 3:D:109:PRO:HB2 | 3:D:114:THR:CG2 | 2.28 | 0.63 |
| 3:D:241:ILE:HG22 | 3:D:242:LEU:N | 2.11 | 0.63 |
| 1:A:36:LEU:O | 1:A:40:LEU:HD12 | 1.98 | 0.63 |
| 5:P:265:VAL:CA | 5:P:268:ILE:HD12 | 2.25 | 0.63 |
| 5:F:292:ALA:HB1 | 5:F:299:TRP:O | 1.98 | 0.63 |
| 2:M:243:ARG:CG | 2:M:244:PRO:HA | 2.24 | 0.63 |
| 2:M:1058:ASP:OD2 | 2:M:1084:SER:CB | 2.45 | 0.63 |
| 2:M:48:PHE:CE1 | 2:M:71:TYR:HB3 | 2.32 | 0.63 |
| 1:L:70:GLY:O | 1:L:133:GLU:HG2 | 1.98 | 0.63 |
| 3:N:1083:ASP:OD2 | 3:N:1238:MET:HB3 | 1.97 | 0.63 |
| 3:N:1367:HIS:O | 3:N:1371:VAL:HG23 | 1.97 | 0.63 |
| 2:M:710:ILE:HD13 | 2:M:790:LEU:HB2 | 1.79 | 0.63 |
| 1:K:228:PRO:O | 1:K:229:GLN:HG3 | 1.97 | 0.63 |
| 2:M:212:GLY:HA3 | 2:M:218:VAL:HG11 | 1.80 | 0.63 |
| 2:C:144:PRO:HB2 | 2:C:266:ARG:HB3 | 1.80 | 0.63 |
| 3:D:1108:ARG:HE | 3:D:1199:GLY:HA3 | 1.62 | 0.63 |
| 3:D:154:THR:HG22 | 3:D:157:GLU:HG3 | 1.80 | 0.63 |
| 3:N:402:PRO:CG | 3:N:443:VAL:HG22 | 2.29 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:402:PRO:HA | 3:N:443:VAL:HA | 1.80 | 0.63 |
| 2:C:38:LYS:HG3 | 2:C:39:ARG:N | 2.07 | 0.63 |
| 2:M:588:VAL:HG23 | 2:M:589:ARG:N | 2.12 | 0.63 |
| 2:C:101:ILE:CG2 | 2:C:102:HIS:N | 2.61 | 0.63 |
| 3:D:1381:VAL:HG13 | 3:D:1389:LEU:HA | 1.80 | 0.63 |
| 2:C:1115:LEU:HD13 | 3:D:85:VAL:CB | 2.24 | 0.63 |
| 2:C:676:ILE:HG13 | 2:C:873:PRO:HG3 | 1.81 | 0.63 |
| 2:C:855:VAL:O | 2:C:858:MET:HB3 | 1.98 | 0.63 |
| 2:M:1035:MET:O | 2:M:1038:TRP:HB2 | 1.97 | 0.63 |
| 2:M:1040:LEU:HD23 | 3:N:763:MET:CE | 2.28 | 0.63 |
| 5:F:322:GLY:O | 5:F:324:GLU:HG3 | 1.97 | 0.63 |
| 3:N:186:VAL:HA | 3:N:200:ASP:OD2 | 1.98 | 0.63 |
| 3:D:1120:VAL:HB | 3:D:1144:LEU:HD21 | 1.81 | 0.63 |
| 3:D:1206:GLY:O | 3:D:1215:VAL:HG12 | 1.97 | 0.63 |
| 2:M:211:LEU:C | 2:M:213:ALA:H | 1.99 | 0.63 |
| 2:C:260:LEU:HD13 | 2:C:291:ALA:CB | 2.28 | 0.63 |
| 3:N:397:LYS:HE3 | 3:N:448:GLU:OE2 | 1.98 | 0.63 |
| 3:N:566:ILE:HA | 3:N:569:ASN:HB3 | 1.81 | 0.63 |
| 5:P:76:SER:O | 5:P:78:SER:N | 2.26 | 0.63 |
| 2:C:1100:GLN:HB3 | 3:D:9:ARG:HB3 | 1.80 | 0.63 |
| 3:D:1486:VAL:HG22 | 4:E:75:PHE:HB3 | 1.80 | 0.63 |
| 3:N:358:GLY:HA2 | 3:N:385:VAL:CB | 2.28 | 0.63 |
| 5:F:413:SER:HA | 5:F:416:ARG:NH1 | 2.14 | 0.63 |
| 3:N:1486:VAL:HA | 4:O:75:PHE:HA | 1.80 | 0.63 |
| 1:L:58:ILE:O | 1:L:61:VAL:HG13 | 1.98 | 0.63 |
| 2:M:694:LEU:HD21 | 2:M:868:ASP:CB | 2.28 | 0.63 |
| 1:A:109:VAL:HB | 1:A:130:ALA:H | 1.63 | 0.63 |
| 3:D:968:ASP:O | 3:D:972:LEU:HD23 | 1.98 | 0.63 |
| 2:M:480:THR:HG22 | 2:M:482:GLU:N | 2.12 | 0.63 |
| 2:C:292:ARG:HH21 | 2:C:295:ASP:CG | 2.01 | 0.63 |
| 2:M:394:PHE:HB3 | 2:M:632:ASN:ND2 | 2.14 | 0.63 |
| 2:C:176:VAL:HG12 | 2:C:181:VAL:O | 1.99 | 0.63 |
| 3:D:119:SER:O | 3:D:121:THR:N | 2.31 | 0.63 |
| 3:D:528:VAL:O | 3:D:535:PHE:HB3 | 1.98 | 0.63 |
| 3:N:441:ARG:O | 3:N:443:VAL:HG23 | 1.99 | 0.63 |
| 3:D:210:ARG:N | 3:D:389:GLU:HB2 | 2.14 | 0.63 |
| 3:D:187:LYS:HG3 | 3:D:198:ARG:CG | 2.27 | 0.63 |
| 2:C:367:LEU:HG | 2:C:372:LEU:HD11 | 1.81 | 0.63 |
| 3:N:671:LYS:CA | 3:N:674:ARG:HB2 | 2.28 | 0.63 |
| 1:B:197:LEU:HD12 | 1:B:198:ARG:N | 2.14 | 0.63 |
| 3:N:1151:ARG:C | 3:N:1162:GLU:HB3 | 2.18 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:101:LEU:HD12 | 1:K:102:LYS:N | 2.12 | 0.63 |
| 1:K:5:LYS:HZ2 | 1:K:28:LEU:C | 2.02 | 0.63 |
| 1:B:70:GLY:O | 1:B:133:GLU:HG2 | 1.99 | 0.63 |
| 2:M:328:LEU:HG | 2:M:433:THR:HB | 1.79 | 0.63 |
| 3:N:1254:GLN:HG2 | 3:N:1255:GLY:N | 2.13 | 0.63 |
| 3:D:960:LYS:HG2 | 3:D:964:LEU:CD1 | 2.28 | 0.63 |
| 3:N:1256:LEU:HB3 | 3:N:1257:PRO:HD3 | 1.80 | 0.63 |
| 2:M:198:ARG:HE | 2:M:231:PRO:HD3 | 1.64 | 0.63 |
| 3:N:227:LEU:HD12 | 3:N:331:VAL:CG2 | 2.29 | 0.63 |
| 2:C:174:LEU:HD21 | 2:C:184:MET:HG2 | 1.80 | 0.63 |
| 2:C:232:GLU:O | 2:C:236:ILE:HG13 | 1.98 | 0.63 |
| 2:C:542:VAL:CG2 | 2:C:543:ASN:H | 2.07 | 0.63 |
| 3:D:22:SER:HA | 3:D:90:MET:O | 1.98 | 0.63 |
| 3:D:442:ASN:HD22 | 3:D:442:ASN:N | 1.96 | 0.63 |
| 2:M:63:GLY:H | 2:M:103:LYS:HA | 1.61 | 0.63 |
| 2:M:776:SER:CB | 5:P:379:ARG:HH22 | 2.11 | 0.63 |
| 2:M:941:VAL:HG12 | 2:M:945:ARG:HH21 | 1.62 | 0.63 |
| 3:N:172:PRO:O | 3:N:175:VAL:HG23 | 1.98 | 0.63 |
| 2:C:135:VAL:HG23 | 2:C:395:LYS:HA | 1.79 | 0.63 |
| 2:M:217:LEU:C | 2:M:219:GLN:H | 2.02 | 0.63 |
| 1:B:117:VAL:HG12 | 1:B:118:ALA:N | 2.12 | 0.63 |
| 3:N:501:ALA:O | 3:N:505:SER:CB | 2.46 | 0.63 |
| 2:M:148:PHE:N | 2:M:323:ASP:OD2 | 2.31 | 0.63 |
| 3:N:92:HIS:HA | 3:N:519:VAL:HG23 | 1.81 | 0.63 |
| 3:D:113:GLY:C | 3:D:115:LEU:N | 2.50 | 0.63 |
| 3:D:550:ARG:NH1 | 3:D:573:MET:HB3 | 2.14 | 0.63 |
| 3:D:259:VAL:HG23 | 3:D:270:LEU:CD1 | 2.28 | 0.63 |
| 1:B:206:THR:HG22 | 1:B:208:LEU:HB3 | 1.81 | 0.63 |
| 2:M:853:LEU:HB2 | 2:M:858:MET:HE3 | 1.81 | 0.63 |
| 2:C:649:VAL:HG13 | 2:C:653:ASP:CB | 2.29 | 0.63 |
| 3:N:811:GLU:HB2 | 3:N:816:HIS:ND1 | 2.14 | 0.63 |
| 3:N:819:GLY:HA2 | 3:N:824:ASN:ND2 | 2.14 | 0.63 |
| 3:N:772:PRO:HG3 | 3:N:1210:SER:CB | 2.27 | 0.63 |
| 2:M:468:ARG:HA | 2:M:486:MET:O | 1.99 | 0.63 |
| 2:C:343:GLN:O | 2:C:346:VAL:HG22 | 1.99 | 0.63 |
| 2:C:578:VAL:HG23 | 2:C:579:VAL:HG12 | 1.80 | 0.63 |
| 3:N:531:ASP:O | 3:N:533:GLY:N | 2.32 | 0.63 |
| 2:C:211:LEU:O | 2:C:213:ALA:N | 2.31 | 0.63 |
| 2:C:176:VAL:CG1 | 2:C:182:VAL:HA | 2.29 | 0.63 |
| 2:C:178:PRO:O | 2:C:179:ASN:C | 2.36 | 0.63 |
| 2:C:193:LEU:CD1 | 2:C:196:LEU:HD12 | 2.29 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:520:GLU:O | 2:C:522:VAL:HG23 | 1.98 | 0.63 |
| 3:D:592:THR:HG21 | 3:D:598:ARG:NH1 | 2.14 | 0.63 |
| 3:D:274:ARG:NH2 | 3:D:279:VAL:HG13 | 2.13 | 0.63 |
| 4:O:73:LEU:HD12 | 4:O:74:VAL:H | 1.64 | 0.63 |
| 3:D:1403:LEU:HG | 3:D:1408:ILE:HG13 | 1.80 | 0.63 |
| 2:C:987:ILE:HG23 | 3:D:948:THR:CG2 | 2.28 | 0.63 |
| 3:D:434:ARG:HD3 | 3:D:449:SER:HB3 | 1.80 | 0.63 |
| 3:N:849:ALA:O | 3:N:852:ALA:HB3 | 1.98 | 0.63 |
| 2:M:34:VAL:N | 2:M:35:PRO:CD | 2.61 | 0.63 |
| 2:M:504:GLU:O | 2:M:506:ASN:N | 2.32 | 0.63 |
| 1:K:78:ILE:O | 1:K:81:ASN:HB2 | 1.98 | 0.63 |
| 5:P:138:SER:HA | 5:P:141:VAL:HG13 | 1.81 | 0.63 |
| 2:C:380:ALA:O | 2:C:384:GLU:HG2 | 1.99 | 0.63 |
| 1:B:152:PRO:HG2 | 1:B:155:LYS:HB3 | 1.80 | 0.63 |
| 1:L:5:LYS:HE2 | 1:L:189:ARG:NH1 | 2.13 | 0.63 |
| 2:M:380:ALA:C | 2:M:384:GLU:HG2 | 2.19 | 0.63 |
| 2:M:726:ILE:C | 2:M:728:HIS:H | 2.01 | 0.63 |
| 4:E:42:PRO:HA | 4:E:45:ARG:CD | 2.28 | 0.63 |
| 2:C:184:MET:HG3 | 2:C:193:LEU:CD1 | 2.28 | 0.63 |
| 2:C:199:VAL:HG21 | 2:C:238:LEU:CD1 | 2.29 | 0.63 |
| 3:N:125:GLN:HG2 | 5:P:75:ILE:O | 1.98 | 0.63 |
| 3:D:1107:VAL:CG2 | 3:D:1219:GLU:HB3 | 2.29 | 0.63 |
| 3:D:119:SER:CB | 3:D:122:GLU:HB2 | 2.28 | 0.63 |
| 3:D:127:LEU:CD2 | 3:D:461:ILE:HD11 | 2.28 | 0.63 |
| 3:D:182:GLY:HA2 | 3:D:203:ALA:CB | 2.19 | 0.63 |
| 3:D:55:ASP:OD1 | 3:D:83:SER:N | 2.32 | 0.63 |
| 3:N:814:ALA:O | 3:N:818:ARG:HG3 | 1.99 | 0.63 |
| 3:N:1397:LYS:C | 3:N:1398:TRP:CD1 | 2.72 | 0.63 |
| 3:D:1372:VAL:HA | 3:D:1375:MET:HE2 | 1.80 | 0.63 |
| 2:M:328:LEU:CD1 | 2:M:437:ARG:HD2 | 2.29 | 0.63 |
| 1:L:110:LYS:HD2 | 1:L:126:ASP:HA | 1.80 | 0.63 |
| 3:D:178:LEU:HG | 3:D:181:ASP:HB2 | 1.81 | 0.63 |
| 2:M:726:ILE:CD1 | 2:M:728:HIS:HB2 | 2.29 | 0.63 |
| 1:A:106:PRO:HD3 | 1:A:134:GLU:OE1 | 1.99 | 0.63 |
| 4:E:85:LEU:HD23 | 4:E:85:LEU:H | 1.63 | 0.63 |
| 5:P:164:LYS:HA | 5:P:171:LYS:HE3 | 1.81 | 0.63 |
| 3:N:212:ARG:HA | 3:N:343:LYS:O | 1.99 | 0.62 |
| 2:C:322:VAL:HG12 | 2:C:323:ASP:H | 1.63 | 0.62 |
| 3:N:131:LYS:HB3 | 3:N:131:LYS:HZ3 | 1.62 | 0.62 |
| 3:N:85:VAL:HG22 | 3:N:89:ARG:CG | 2.29 | 0.62 |
| 1:B:215:VAL:CG2 | 1:B:216:GLU:N | 2.62 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:M:158:TYR:CE1 | 2:M:313:LEU:HG | 2.33 | 0.62 |
| 2:C:56:GLU:HB2 | 2:C:64:LEU:CD2 | 2.29 | 0.62 |
| 2:M:89:THR:HG23 | 2:M:129:ILE:HA | 1.81 | 0.62 |
| 3:D:907:GLU:OE2 | 3:D:910:SER:HB3 | 1.99 | 0.62 |
| 1:K:186:LEU:O | 1:K:188:GLN:HG2 | 1.99 | 0.62 |
| 3:N:1091:SER:C | 3:N:1093:TYR:N | 2.46 | 0.62 |
| 3:D:875:THR:HG22 | 3:D:879:ARG:HG3 | 1.81 | 0.62 |
| 2:M:939:ARG:O | 2:M:943:VAL:HG23 | 1.99 | 0.62 |
| 1:L:91:ASN:HB3 | 1:L:94:LEU:CG | 2.26 | 0.62 |
| 3:D:644:LEU:HD12 | 3:D:645:PRO:CD | 2.28 | 0.62 |
| 2:C:894:GLY:HA2 | 2:C:897:LEU:HB2 | 1.81 | 0.62 |
| 3:D:962:GLN:HB3 | 3:D:966:GLU:OE2 | 1.99 | 0.62 |
| 2:C:1100:GLN:HA | 2:C:1100:GLN:NE2 | 2.14 | 0.62 |
| 5:P:339:PRO:HB3 | 5:P:343:ASP:HB2 | 1.80 | 0.62 |
| 5:F:382:THR:HG22 | 5:F:394:ARG:HB2 | 1.82 | 0.62 |
| 2:C:649:VAL:HG22 | 2:C:650:ARG:NH2 | 2.14 | 0.62 |
| 2:C:695:LEU:O | 2:C:698:ASP:N | 2.29 | 0.62 |
| 3:N:690:ALA:O | 3:N:693:GLU:HB3 | 1.98 | 0.62 |
| 1:K:208:LEU:HG | 1:K:212:ASN:HD21 | 1.64 | 0.62 |
| 2:M:979:THR:C | 2:M:981:GLU:H | 2.02 | 0.62 |
| 3:N:1498:ALA:HB3 | 4:O:84:ARG:NH2 | 2.13 | 0.62 |
| 3:N:1400:VAL:HG12 | 3:N:1404:ASN:ND2 | 2.13 | 0.62 |
| 2:C:1010:THR:HA | 3:D:624:ASP:OD1 | 1.97 | 0.62 |
| 3:N:921:ARG:HB3 | 3:N:921:ARG:HH11 | 1.63 | 0.62 |
| 2:M:353:ARG:O | 2:M:357:GLU:HG3 | 1.99 | 0.62 |
| 1:L:156:HIS:O | 1:L:158:ILE:N | 2.32 | 0.62 |
| 4:O:37:ASN:N | 4:O:37:ASN:ND2 | 2.46 | 0.62 |
| 2:M:265:ARG:HG3 | 2:M:265:ARG:O | 1.98 | 0.62 |
| 2:C:218:VAL:O | 2:C:218:VAL:HG22 | 1.98 | 0.62 |
| 2:C:221:LEU:HD23 | 2:C:222:MET:HG3 | 1.81 | 0.62 |
| 2:C:260:LEU:HB2 | 2:C:291:ALA:HB2 | 1.81 | 0.62 |
| 3:N:452:ILE:HD12 | 3:N:452:ILE:O | 1.99 | 0.62 |
| 3:N:45:PHE:HB3 | 3:N:86:ARG:HH22 | 1.64 | 0.62 |
| 3:N:552:ASN:HA | 3:N:555:LYS:HD2 | 1.81 | 0.62 |
| 3:N:576:GLU:HA | 3:N:579:ASP:OD2 | 1.99 | 0.62 |
| 3:N:410:SER:CB | 5:P:178:ARG:HG3 | 2.29 | 0.62 |
| 3:D:318:ARG:HG2 | 3:D:319:ALA:N | 2.14 | 0.62 |
| 1:L:66:SER:HB2 | 1:L:75:VAL:HG21 | 1.80 | 0.62 |
| 3:D:798:GLU:HG3 | 3:D:799:LYS:N | 2.14 | 0.62 |
| 3:N:1342:GLU:CD | 3:N:1342:GLU:H | 2.01 | 0.62 |
| 3:N:1341:PRO:O | 3:N:1342:GLU:C | 2.35 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:417:PRO:HG2 | 3:D:428:LYS:HE2 | 1.81 | 0.62 |
| 3:N:1396:GLU:C | 3:N:1398:TRP:H | 2.02 | 0.62 |
| 3:D:1330:ILE:HD12 | 3:D:1347:TYR:CE1 | 2.34 | 0.62 |
| 1:A:57:TYR:HE1 | 1:A:163:ASN:HB2 | 1.65 | 0.62 |
| 3:N:173:PRO:HG3 | 3:N:209:ARG:NH1 | 2.15 | 0.62 |
| 5:P:92:PRO:O | 5:P:94:LEU:N | 2.31 | 0.62 |
| 3:D:1324:PRO:O | 3:D:1325:LEU:HD23 | 1.98 | 0.62 |
| 1:K:31:GLY:N | 1:K:193:ASP:OD2 | 2.32 | 0.62 |
| 2:M:204:GLN:O | 2:M:209:ARG:HD3 | 1.98 | 0.62 |
| 3:N:244:GLU:CG | 3:N:245:LEU:H | 2.12 | 0.62 |
| 5:P:80:PRO:HA | 5:P:83:GLN:OE1 | 2.00 | 0.62 |
| 2:C:1100:GLN:CG | 2:C:1102:LEU:HD21 | 2.28 | 0.62 |
| 4:E:6:ILE:O | 4:E:9:LEU:HB2 | 1.99 | 0.62 |
| 5:P:353:GLU:HA | 5:P:356:LYS:CG | 2.30 | 0.62 |
| 2:M:101:ILE:HD13 | 2:M:107:LEU:HD22 | 1.79 | 0.62 |
| 3:D:849:ALA:O | 3:D:852:ALA:HB3 | 1.98 | 0.62 |
| 3:D:629:SER:CA | 3:D:744:GLN:HE21 | 2.13 | 0.62 |
| 1:K:209:GLU:HA | 1:K:212:ASN:HD22 | 1.63 | 0.62 |
| 3:N:1213:ARG:HH11 | 3:N:1213:ARG:CG | 2.11 | 0.62 |
| 5:P:93:LEU:O | 5:P:93:LEU:HG | 1.99 | 0.62 |
| 3:D:1211:MET:HB2 | 3:D:1213:ARG:NH1 | 2.15 | 0.62 |
| 2:C:810:ASP:N | 2:C:811:PRO:CD | 2.62 | 0.62 |
| 2:M:660:ALA:HB1 | 2:M:667:ALA:O | 2.00 | 0.62 |
| 2:C:267:TYR:CE1 | 2:C:464:LEU:HD12 | 2.34 | 0.62 |
| 3:D:157:GLU:O | 3:D:161:LEU:HG | 1.97 | 0.62 |
| 3:D:510:GLU:CD | 3:D:510:GLU:H | 2.02 | 0.62 |
| 2:M:806:LEU:O | 2:M:821:GLU:HB2 | 2.00 | 0.62 |
| 3:D:794:GLN:HE22 | 3:D:905:PRO:HG2 | 1.64 | 0.62 |
| 3:N:1031:ASN:ND2 | 3:N:1034:GLN:HG3 | 2.15 | 0.62 |
| 3:N:1118:ILE:HD13 | 3:N:1190:SER:HB2 | 1.81 | 0.62 |
| 1:B:76:VAL:O | 1:B:80:LEU:HG | 1.99 | 0.62 |
| 3:D:841:TYR:HB2 | 3:D:864:VAL:CG1 | 2.29 | 0.62 |
| 3:N:1342:GLU:N | 3:N:1342:GLU:CD | 2.52 | 0.62 |
| 2:M:1059:ASP:OD2 | 2:M:1062:GLY:HA3 | 1.98 | 0.62 |
| 2:M:1085:PHE:CD2 | 3:N:1468:LEU:HA | 2.34 | 0.62 |
| 2:M:1098:ASP:HB2 | 3:N:17:LYS:HE2 | 1.81 | 0.62 |
| 1:K:208:LEU:HG | 1:K:209:GLU:N | 2.14 | 0.62 |
| 2:M:984:GLU:O | 3:N:946:GLY:HA3 | 2.00 | 0.62 |
| 1:K:64:GLU:OE2 | 1:K:76:VAL:HG13 | 2.00 | 0.62 |
| 2:M:781:LYS:HA | 2:M:781:LYS:CE | 2.28 | 0.62 |
| 3:N:1206:GLY:O | 3:N:1215:VAL:HG12 | 1.99 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:607:ASP:HB3 | 2:C:610:ARG:NH1 | 2.14 | 0.62 |
| 2:C:1051:GLU:HG3 | 2:C:1052:MET:H | 1.62 | 0.62 |
| 3:D:1269:LYS:HE2 | 3:D:1269:LYS:H | 1.63 | 0.62 |
| 3:N:999:THR:O | 3:N:1003:VAL:HG23 | 1.99 | 0.62 |
| 1:L:48:ILE:C | 1:L:148:VAL:HG12 | 2.20 | 0.62 |
| 1:K:226:SER:O | 1:K:228:PRO:HD3 | 1.99 | 0.62 |
| 2:M:549:PHE:CE2 | 2:M:886:LEU:HB2 | 2.33 | 0.62 |
| 2:M:170:PRO:CD | 2:M:263:ASP:HB3 | 2.29 | 0.62 |
| 2:C:191:PHE:HD2 | 2:C:195:LEU:HD11 | 1.64 | 0.62 |
| 3:N:139:GLY:HA3 | 3:N:147:VAL:HG23 | 1.79 | 0.62 |
| 2:C:1100:GLN:HG3 | 2:C:1102:LEU:CD2 | 2.28 | 0.62 |
| 3:D:1217:ILE:HD12 | 3:D:1217:ILE:N | 2.01 | 0.62 |
| 3:D:1498:ALA:HB2 | 4:E:87:LYS:HZ3 | 1.63 | 0.62 |
| 3:D:269:PHE:CD1 | 3:D:283:PHE:HB2 | 2.33 | 0.62 |
| 2:M:773:LEU:CD1 | 2:M:777:ILE:HD11 | 2.28 | 0.62 |
| 5:P:349:LEU:HA | 5:P:352:GLU:OE2 | 1.99 | 0.62 |
| 3:N:613:ARG:O | 3:N:1441:GLN:HG3 | 2.00 | 0.62 |
| 3:N:1121:PRO:HD2 | 3:N:1346:ARG:HH21 | 1.65 | 0.62 |
| 2:C:479:VAL:H | 2:C:506:ASN:HB3 | 1.64 | 0.62 |
| 1:L:219:ARG:HG2 | 1:L:219:ARG:NH1 | 2.12 | 0.62 |
| 3:D:701:LEU:CD2 | 3:D:715:ALA:HB2 | 2.29 | 0.62 |
| 1:A:1:MET:H1 | 1:A:6:LEU:HD13 | 1.63 | 0.62 |
| 3:D:1147:ARG:HB2 | 3:D:1166:LEU:HD12 | 1.81 | 0.62 |
| 3:D:272:LEU:HD12 | 3:D:282:TYR:CE1 | 2.33 | 0.62 |
| 3:D:366:LYS:HE2 | 3:D:369:ALA:HB2 | 1.82 | 0.62 |
| 5:F:417:LYS:HB2 | 5:F:418:LEU:HD12 | 1.82 | 0.62 |
| 1:L:57:TYR:CD1 | 1:L:163:ASN:HB2 | 2.34 | 0.62 |
| 3:N:1379:VAL:C | 3:N:1420:LEU:HD22 | 2.20 | 0.62 |
| 3:N:658:LEU:O | 3:N:661:MET:HB2 | 2.00 | 0.62 |
| 3:D:1286:THR:HG22 | 3:D:1288:GLU:OE1 | 1.99 | 0.62 |
| 3:D:984:THR:HG22 | 3:D:987:GLU:CG | 2.30 | 0.62 |
| 5:P:152:ASP:N | 5:P:153:PRO:CD | 2.62 | 0.62 |
| 1:L:26:GLU:HB2 | 1:L:27:PRO:HA | 1.81 | 0.62 |
| 3:N:954:ALA:HB3 | 3:N:1062:ARG:HD2 | 1.81 | 0.62 |
| 3:D:1246:VAL:HG11 | 3:D:1249:ALA:O | 2.00 | 0.62 |
| 2:M:343:GLN:HG2 | 2:M:385:PHE:HB2 | 1.82 | 0.62 |
| 3:D:1048:PRO:O | 3:D:1079:LYS:NZ | 2.32 | 0.62 |
| 3:N:27:GLU:HB2 | 3:N:28:LYS:HE2 | 1.81 | 0.62 |
| 2:C:1104:GLU:HA | 3:D:7:LYS:HZ3 | 1.62 | 0.62 |
| 3:D:654:LYS:O | 3:D:657:LEU:HB3 | 2.00 | 0.62 |
| 5:P:305:GLU:O | 5:P:308:LEU:HG | 1.99 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:551:ASN:O | 3:D:554:LEU:HB3 | 1.99 | 0.62 |
| 2:M:672:VAL:HG23 | 2:M:673:LEU:N | 2.13 | 0.62 |
| 1:B:64:GLU:HA | 1:B:75:VAL:HG11 | 1.80 | 0.62 |
| 1:B:47:SER:C | 1:B:48:ILE:HD12 | 2.20 | 0.62 |
| 3:N:673:ALA:O | 3:N:676:MET:HB3 | 2.00 | 0.62 |
| 3:N:634:GLY:HA3 | 3:N:637:LEU:HG | 1.82 | 0.62 |
| 3:N:207:PHE:HB3 | 5:P:97:GLU:OE1 | 1.99 | 0.62 |
| 3:D:264:LEU:HB3 | 3:D:316:GLN:NE2 | 2.15 | 0.62 |
| 4:E:61:GLU:CD | 4:E:61:GLU:N | 2.52 | 0.62 |
| 3:N:985:ASP:O | 3:N:988:ARG:HB3 | 1.98 | 0.62 |
| 3:N:989:TYR:O | 3:N:992:ILE:HB | 2.00 | 0.62 |
| 1:L:68:ILE:HG13 | 1:L:71:VAL:O | 2.00 | 0.62 |
| 2:M:726:ILE:HG13 | 2:M:728:HIS:CB | 2.29 | 0.62 |
| 2:M:218:VAL:O | 2:M:218:VAL:HG22 | 2.00 | 0.62 |
| 3:N:156:GLU:H | 3:N:156:GLU:CD | 2.04 | 0.62 |
| 3:D:1465:ASN:OD1 | 3:D:1470:ARG:HD3 | 2.00 | 0.62 |
| 5:P:385:GLU:HA | 5:P:388:ALA:HB3 | 1.80 | 0.62 |
| 3:D:657:LEU:HG | 3:D:661:MET:HE2 | 1.80 | 0.62 |
| 2:C:56:GLU:O | 2:C:64:LEU:HD23 | 1.99 | 0.62 |
| 3:D:1381:VAL:HG12 | 3:D:1391:GLU:O | 2.00 | 0.62 |
| 3:D:79:GLU:CG | 3:D:80:VAL:H | 2.11 | 0.62 |
| 3:N:865:THR:HA | 3:N:873:LEU:O | 2.00 | 0.62 |
| 2:C:672:VAL:CG2 | 2:C:673:LEU:N | 2.63 | 0.62 |
| 2:M:1037:VAL:HG12 | 2:M:1041:GLU:CD | 2.19 | 0.62 |
| 2:M:958:THR:HG23 | 2:M:961:GLU:HB3 | 1.80 | 0.62 |
| 5:F:321:ILE:HG13 | 5:F:332:PHE:HE1 | 1.63 | 0.62 |
| 2:M:522:VAL:HG12 | 2:M:523:ILE:N | 2.15 | 0.62 |
| 1:L:153:ALA:HB2 | 1:L:168:ASP:N | 2.14 | 0.62 |
| 3:N:470:LEU:HB2 | 3:N:503:LEU:CD2 | 2.30 | 0.62 |
| 2:C:555:ALA:O | 2:C:558:ALA:HB3 | 1.99 | 0.62 |
| 3:D:349:PRO:HB3 | 5:F:97:GLU:HG2 | 1.81 | 0.62 |
| 2:M:205:GLU:CA | 2:M:209:ARG:HH11 | 2.11 | 0.62 |
| 3:N:249:TYR:HB3 | 3:N:307:ALA:CB | 2.27 | 0.62 |
| 3:D:561:GLY:HA3 | 5:F:132:ARG:HD3 | 1.82 | 0.62 |
| 5:F:132:ARG:NH2 | 5:F:184:ARG:HH12 | 1.96 | 0.62 |
| 5:F:409:LYS:HD2 | 5:F:410:TYR:H | 1.64 | 0.62 |
| 3:N:1462:LEU:HD23 | 3:N:1473:PRO:HD2 | 1.81 | 0.62 |
| 1:L:201:THR:HG21 | 1:L:207:PRO:HA | 1.80 | 0.62 |
| 3:N:479:GLU:O | 3:N:481:MET:N | 2.32 | 0.62 |
| 3:N:801:GLY:CA | 3:N:830:ALA:HB3 | 2.30 | 0.62 |
| 3:N:1368:ILE:O | 3:N:1372:VAL:HG23 | 1.99 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:K:178:ALA:HB2 | 2:M:864:GLY:N | 2.15 | 0.62 |
| 3:D:1086:LEU:HD12 | 3:D:1238:MET:SD | 2.40 | 0.61 |
| 3:D:136:ASP:CB | 3:D:137:PRO:CD | 2.78 | 0.61 |
| 3:D:1486:VAL:HG22 | 4:E:75:PHE:CB | 2.30 | 0.61 |
| 5:F:101:GLU:HG3 | 5:F:105:LYS:HE3 | 1.82 | 0.61 |
| 5:F:223:ALA:HB2 | 5:F:242:TRP:HB2 | 1.82 | 0.61 |
| 3:D:937:TYR:H | 3:D:937:TYR:HD1 | 1.46 | 0.61 |
| 5:P:382:THR:CG2 | 5:P:394:ARG:HB2 | 2.30 | 0.61 |
| 1:B:209:GLU:HA | 1:B:212:ASN:ND2 | 2.14 | 0.61 |
| 1:B:213:GLN:O | 1:B:216:GLU:HB3 | 2.00 | 0.61 |
| 2:M:606:VAL:HG22 | 2:M:645:VAL:HG13 | 1.81 | 0.61 |
| 1:B:185:ARG:HB3 | 1:B:190:THR:HG23 | 1.80 | 0.61 |
| 2:M:759:THR:HB | 2:M:785:VAL:CG1 | 2.29 | 0.61 |
| 4:O:71:GLY:C | 4:O:73:LEU:H | 2.03 | 0.61 |
| 1:L:20:TYR:C | 1:L:207:PRO:HG2 | 2.20 | 0.61 |
| 2:C:672:VAL:HG23 | 2:C:868:ASP:HB2 | 1.81 | 0.61 |
| 2:M:328:LEU:HG | 2:M:433:THR:CB | 2.30 | 0.61 |
| 5:P:102:LEU:HG | 5:P:187:LEU:HD22 | 1.81 | 0.61 |
| 3:N:1333:HIS:O | 3:N:1336:LEU:HB3 | 2.00 | 0.61 |
| 2:C:728:HIS:NE2 | 2:C:730:SER:HB3 | 2.15 | 0.61 |
| 2:M:230:ARG:HH21 | 2:M:237:ARG:HH22 | 0.77 | 0.61 |
| 3:N:553:ARG:NH1 | 5:P:211:ASP:HA | 2.12 | 0.61 |
| 3:D:45:PHE:O | 3:D:47:GLU:N | 2.33 | 0.61 |
| 5:P:353:GLU:HA | 5:P:356:LYS:CD | 2.29 | 0.61 |
| 1:B:215:VAL:HG23 | 1:B:216:GLU:N | 2.15 | 0.61 |
| 5:F:367:MET:HB3 | 5:F:371:LEU:HG | 1.83 | 0.61 |
| 3:D:915:VAL:O | 3:D:918:ALA:HB3 | 2.00 | 0.61 |
| 3:N:1468:LEU:HD23 | 3:N:1469:GLY:N | 2.15 | 0.61 |
| 1:L:90:LEU:HD12 | 1:L:119:ASP:HA | 1.81 | 0.61 |
| 2:M:18:LEU:HG | 2:M:590:ASP:OD1 | 2.01 | 0.61 |
| 2:M:182:VAL:HG22 | 2:M:220:GLY:O | 1.99 | 0.61 |
| 3:N:223:LEU:O | 3:N:224:ARG:HD2 | 2.00 | 0.61 |
| 4:E:87:LYS:HE3 | 4:E:91:ARG:NH2 | 2.16 | 0.61 |
| 3:N:417:PRO:HB3 | 3:N:430:ASP:CA | 2.25 | 0.61 |
| 3:D:367:ILE:HD11 | 3:D:379:ALA:HA | 1.82 | 0.61 |
| 5:F:417:LYS:C | 5:F:419:ARG:H | 2.03 | 0.61 |
| 1:A:206:THR:HG22 | 1:A:208:LEU:N | 2.15 | 0.61 |
| 2:C:373:VAL:HG12 | 2:C:374:ASN:N | 2.15 | 0.61 |
| 3:D:1424:VAL:HG23 | 3:D:1425:THR:N | 2.14 | 0.61 |
| 3:D:858:VAL:HG12 | 3:D:859:ASP:N | 2.15 | 0.61 |
| 2:C:571:LEU:HD22 | 2:C:701:THR:N | 2.15 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:N:479:GLU:C | 3:N:481:MET:N | 2.51 | 0.61 |
| 3:N:350:HIS:HB3 | 5:P:232:ARG:NH1 | 2.14 | 0.61 |
| 1:K:110:LYS:CB | 1:K:112:ARG:HG2 | 2.26 | 0.61 |
| 1:A:111:ALA:C | 1:A:113:ASP:H | 2.01 | 0.61 |
| 3:D:1183:ILE:HG13 | 3:D:1184:GLN:H | 1.64 | 0.61 |
| 2:M:1030:GLN:CG | 3:N:626:SER:HB2 | 2.30 | 0.61 |
| 3:D:1314:LYS:HB2 | 3:D:1317:ASP:OD2 | 1.99 | 0.61 |
| 5:P:223:ALA:HB2 | 5:P:242:TRP:HB2 | 1.83 | 0.61 |
| 2:M:436:GLY:HA2 | 2:M:539:VAL:HA | 1.81 | 0.61 |
| 5:F:361:LEU:HG | 5:F:362:SER:N | 2.15 | 0.61 |
| 2:C:162:ILE:CD1 | 2:C:172:ILE:HD12 | 2.30 | 0.61 |
| 3:D:252:ARG:HG3 | 3:D:300:LYS:CA | 2.29 | 0.61 |
| 2:C:101:ILE:CG2 | 2:C:107:LEU:HD23 | 2.30 | 0.61 |
| 5:F:288:TYR:HB3 | 5:F:301:ALA:CA | 2.30 | 0.61 |
| 2:C:6:PHE:HB3 | 2:C:908:GLY:HA2 | 1.81 | 0.61 |
| 5:F:74:LYS:O | 5:F:77:THR:HB | 2.00 | 0.61 |
| 5:F:79:ASP:O | 5:F:79:ASP:OD1 | 2.17 | 0.61 |
| 3:N:18:ILE:CG2 | 3:N:518:PRO:HG3 | 2.30 | 0.61 |
| 1:K:101:LEU:HD13 | 1:K:113:ASP:O | 2.01 | 0.61 |
| 2:M:926:PHE:CD1 | 2:M:929:ARG:HG3 | 2.35 | 0.61 |
| 1:L:143:ARG:C | 1:L:143:ARG:HD3 | 2.20 | 0.61 |
| 3:N:206:ARG:NE | 3:N:392:SER:HB2 | 2.15 | 0.61 |
| 2:C:631:SER:HB2 | 2:C:637:LEU:HD21 | 1.83 | 0.61 |
| 3:D:972:LEU:CD2 | 3:D:972:LEU:N | 2.63 | 0.61 |
| 3:N:633:VAL:O | 3:N:635:PRO:HD3 | 1.99 | 0.61 |
| 2:M:687:ALA:HB1 | 2:M:850:ALA:HB2 | 1.81 | 0.61 |
| 3:D:642:CYS:SG | 3:D:716:PHE:HB2 | 2.40 | 0.61 |
| 2:C:138:SER:HB2 | 2:C:333:ILE:HD11 | 1.81 | 0.61 |
| 2:C:431:HIS:CE1 | 2:C:433:THR:H | 2.18 | 0.61 |
| 3:N:567:ILE:HG22 | 3:N:571:LYS:CE | 2.23 | 0.61 |
| 5:P:84:TYR:C | 5:P:86:HIS:H | 2.02 | 0.61 |
| 3:D:133:ILE:O | 3:D:152:LEU:HD12 | 2.00 | 0.61 |
| 3:D:544:TYR:O | 3:D:547:LEU:HB3 | 2.00 | 0.61 |
| 2:M:112:GLU:O | 2:M:113:VAL:HG13 | 2.01 | 0.61 |
| 3:D:288:MET:HE2 | 3:D:307:ALA:HB2 | 1.81 | 0.61 |
| 5:F:267:THR:O | 5:F:271:LEU:HG | 1.99 | 0.61 |
| 3:N:1032:PRO:HB2 | 3:N:1033:GLN:NE2 | 2.15 | 0.61 |
| 1:K:185:ARG:HA | 1:K:190:THR:HA | 1.82 | 0.61 |
| 2:M:676:ILE:CG2 | 2:M:988:VAL:HG13 | 2.31 | 0.61 |
| 2:M:1056:LYS:NZ | 3:N:749:VAL:H | 1.97 | 0.61 |
| 1:B:85:LEU:HD12 | 1:B:86:VAL:H | 1.65 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:1092:LEU:O | 2:M:1095:LEU:HB2 | 2.00 | 0.61 |
| 3:N:811:GLU:HB2 | 3:N:816:HIS:CE1 | 2.35 | 0.61 |
| 2:C:317:VAL:N | 2:C:318:PRO:CD | 2.62 | 0.61 |
| 1:K:25:LEU:HD11 | 1:L:224:TYR:HB3 | 1.83 | 0.61 |
| 2:M:493:ARG:HB2 | 2:M:494:TYR:CE1 | 2.35 | 0.61 |
| 1:K:195:LEU:HD12 | 1:K:196:THR:N | 2.14 | 0.61 |
| 2:M:200:LEU:HB2 | 2:M:202:TYR:CD2 | 2.35 | 0.61 |
| 3:N:525:ARG:O | 3:N:525:ARG:HG3 | 1.99 | 0.61 |
| 3:D:119:SER:C | 3:D:121:THR:H | 2.04 | 0.61 |
| 3:D:358:GLY:HA2 | 3:D:385:VAL:CB | 2.29 | 0.61 |
| 1:B:101:LEU:HD22 | 1:B:114:PHE:CD1 | 2.35 | 0.61 |
| 5:F:382:THR:HG22 | 5:F:394:ARG:CB | 2.30 | 0.61 |
| 3:D:661:MET:CE | 3:D:677:LEU:HD11 | 2.30 | 0.61 |
| 3:N:142:LEU:HD13 | 3:N:144:GLY:H | 1.65 | 0.61 |
| 2:C:676:ILE:O | 2:C:676:ILE:HG12 | 1.99 | 0.61 |
| 3:N:820:GLU:HG3 | 3:N:836:VAL:CG1 | 2.31 | 0.61 |
| 3:D:204:LEU:HD12 | 3:D:205:TYR:N | 2.15 | 0.61 |
| 3:D:167:GLU:O | 3:D:394:LEU:HD12 | 2.01 | 0.61 |
| 3:D:1277:ILE:HG22 | 3:D:1278:ASP:N | 2.08 | 0.61 |
| 1:B:48:ILE:HG22 | 1:B:173:PRO:HD2 | 1.83 | 0.61 |
| 3:N:1468:LEU:C | 3:N:1468:LEU:HD23 | 2.19 | 0.61 |
| 3:D:1368:ILE:O | 3:D:1372:VAL:HG23 | 2.00 | 0.61 |
| 3:N:225:LEU:HB3 | 3:N:226:PRO:CD | 2.31 | 0.61 |
| 2:C:263:ASP:HB2 | 2:C:264:PRO:CD | 2.31 | 0.61 |
| 3:N:89:ARG:NH1 | 3:N:89:ARG:HG2 | 2.14 | 0.61 |
| 2:C:1058:ASP:HB3 | 2:C:1082:PRO:HB3 | 1.83 | 0.61 |
| 3:D:257:GLY:HA2 | 3:D:274:ARG:CA | 2.22 | 0.61 |
| 3:D:406:ASP:CB | 3:D:424:GLY:N | 2.63 | 0.61 |
| 3:D:806:PHE:CD2 | 3:D:809:PRO:HB2 | 2.34 | 0.61 |
| 2:C:352:ALA:O | 2:C:355:VAL:HG12 | 2.00 | 0.61 |
| 5:P:372:ARG:HG3 | 5:P:378:GLY:O | 2.00 | 0.61 |
| 2:M:89:THR:OG1 | 2:M:130:ASN:N | 2.34 | 0.61 |
| 2:C:776:SER:HB3 | 2:C:780:GLU:CD | 2.21 | 0.61 |
| 3:D:953:ASP:OD2 | 3:D:1019:PRO:HG2 | 1.99 | 0.61 |
| 3:N:483:HIS:HD1 | 3:N:483:HIS:H | 1.47 | 0.61 |
| 1:L:179:PHE:CD1 | 1:L:195:LEU:HD11 | 2.36 | 0.61 |
| 2:M:944:LEU:HD21 | 2:M:963:LEU:CD2 | 2.30 | 0.61 |
| 5:F:153:PRO:HG2 | 5:F:154:LYS:HG3 | 1.81 | 0.61 |
| 1:L:89:PHE:CD2 | 1:L:94:LEU:HB2 | 2.35 | 0.61 |
| 3:N:1015:TYR:N | 3:N:1016:PRO:HD3 | 2.15 | 0.61 |
| 4:E:48:MET:O | 4:E:54:LEU:HA | 2.00 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:284:LEU:HB3 | 3:N:288:MET:HB3 | 1.81 | 0.61 |
| 2:C:334:ARG:NH1 | 2:C:418:LEU:HD11 | 2.15 | 0.61 |
| 3:N:93:ILE:HB | 3:N:517:VAL:HB | 1.82 | 0.61 |
| 3:D:154:THR:HG22 | 3:D:157:GLU:OE2 | 2.01 | 0.61 |
| 1:A:35:THR:O | 1:A:39:PRO:HG2 | 2.00 | 0.61 |
| 2:M:649:VAL:HA | 2:M:650:ARG:NH2 | 2.14 | 0.61 |
| 5:P:367:MET:HB2 | 5:P:371:LEU:CD1 | 2.30 | 0.61 |
| 2:M:239:PHE:CZ | 2:M:246:ASP:HB3 | 2.36 | 0.61 |
| 2:C:676:ILE:HD11 | 3:D:949:ILE:HB | 1.83 | 0.61 |
| 2:C:549:PHE:CE2 | 2:C:886:LEU:HB2 | 2.36 | 0.61 |
| 3:N:1033:GLN:HA | 3:N:1036:ARG:NH1 | 2.15 | 0.61 |
| 3:N:1112:CYS:SG | 3:N:1114:THR:HG22 | 2.41 | 0.61 |
| 2:M:1049:LEU:HD11 | 2:M:1053:LEU:HD11 | 1.83 | 0.61 |
| 2:C:575:GLN:H | 2:C:667:ALA:HB1 | 1.64 | 0.61 |
| 2:C:926:PHE:CD1 | 2:C:929:ARG:HG3 | 2.36 | 0.61 |
| 2:M:1085:PHE:CE2 | 3:N:1468:LEU:HA | 2.34 | 0.61 |
| 3:N:349:PRO:CB | 5:P:232:ARG:HH22 | 2.12 | 0.61 |
| 2:C:504:GLU:HG3 | 2:C:507:ARG:CD | 2.30 | 0.61 |
| 1:B:23:PHE:CD1 | 1:B:23:PHE:N | 2.68 | 0.61 |
| 1:B:143:ARG:HD3 | 1:B:143:ARG:C | 2.21 | 0.61 |
| 5:P:113:ILE:HD13 | 5:P:128:ARG:HB3 | 1.83 | 0.61 |
| 3:D:1305:LEU:HD23 | 3:D:1305:LEU:N | 2.15 | 0.61 |
| 3:N:322:VAL:HB | 3:N:335:LEU:HD21 | 1.83 | 0.61 |
| 2:C:187:ASN:O | 2:C:188:LYS:HG2 | 2.00 | 0.61 |
| 2:C:230:ARG:CG | 2:C:233:GLU:HG3 | 2.22 | 0.61 |
| 3:N:112:ILE:O | 3:N:115:LEU:HB3 | 2.00 | 0.61 |
| 1:B:114:PHE:O | 1:B:116:PRO:HD3 | 2.01 | 0.61 |
| 3:N:1305:LEU:N | 3:N:1305:LEU:HD23 | 2.15 | 0.61 |
| 2:C:946:ARG:HH11 | 2:C:984:GLU:HB2 | 1.66 | 0.61 |
| 3:D:1033:GLN:H | 3:D:1033:GLN:CD | 2.04 | 0.61 |
| 3:N:1094:LEU:CD1 | 3:N:1098:LEU:HD11 | 2.29 | 0.61 |
| 3:N:881:LEU:HD21 | 3:N:941:PHE:CZ | 2.35 | 0.61 |
| 2:M:910:LYS:N | 2:M:913:GLU:OE1 | 2.34 | 0.61 |
| 1:L:241:GLU:H | 1:L:242:PRO:CD | 2.10 | 0.61 |
| 2:M:1067:TYR:CE1 | 2:M:1071:ILE:HD11 | 2.35 | 0.61 |
| 3:N:809:PRO:HA | 3:N:810:GLU:OE2 | 2.01 | 0.61 |
| 3:D:1122:LEU:HG | 3:D:1184:GLN:O | 2.01 | 0.61 |
| 3:D:881:LEU:HD21 | 3:D:941:PHE:HZ | 1.65 | 0.61 |
| 3:N:1126:ASP:OD1 | 3:N:1129:THR:HA | 2.01 | 0.61 |
| 3:N:1367:HIS:HA | 3:N:1370:ILE:HD12 | 1.83 | 0.61 |
| 2:M:685:GLU:HB3 | 3:N:740:PHE:CD1 | 2.36 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:937:ASP:HB3 | 2:C:940:GLU:HG3 | 1.81 | 0.61 |
| 2:M:261:ILE:CG2 | 2:M:262:ALA:N | 2.64 | 0.61 |
| 2:C:178:PRO:O | 2:C:220:GLY:CA | 2.32 | 0.61 |
| 2:C:303:PHE:N | 2:C:303:PHE:CD1 | 2.69 | 0.61 |
| 3:N:121:THR:CG2 | 3:N:122:GLU:H | 2.01 | 0.61 |
| 2:C:1015:LEU:O | 2:C:1018:GLN:NE2 | 2.34 | 0.61 |
| 3:D:100:ALA:HA | 3:D:513:ILE:HD12 | 1.83 | 0.61 |
| 3:D:833:GLU:N | 3:D:833:GLU:CD | 2.54 | 0.61 |
| 5:F:380:GLU:N | 5:F:385:GLU:OE2 | 2.34 | 0.61 |
| 5:P:271:LEU:N | 5:P:271:LEU:HD23 | 2.16 | 0.61 |
| 1:L:101:LEU:HD22 | 1:L:114:PHE:CD1 | 2.35 | 0.61 |
| 5:F:144:ILE:HG13 | 5:F:144:ILE:O | 2.01 | 0.61 |
| 2:M:689:VAL:O | 2:M:690:ILE:HD13 | 2.00 | 0.61 |
| 3:D:852:ALA:HB1 | 3:D:857:ILE:HD11 | 1.83 | 0.61 |
| 2:C:666:LEU:HD12 | 2:C:667:ALA:N | 2.16 | 0.61 |
| 1:L:233:VAL:HG12 | 1:L:235:ALA:H | 1.66 | 0.61 |
| 1:K:73:GLU:CD | 1:K:131:THR:H | 2.04 | 0.61 |
| 3:N:1400:VAL:HA | 3:N:1408:ILE:CD1 | 2.30 | 0.61 |
| 2:C:813:VAL:CG1 | 2:C:815:LEU:HG | 2.31 | 0.61 |
| 1:B:219:ARG:HG2 | 1:B:219:ARG:HH11 | 1.65 | 0.61 |
| 3:D:1137:ARG:O | 3:D:1141:GLU:HG3 | 2.01 | 0.61 |
| 2:M:224:GLU:HB3 | 2:M:227:PHE:CG | 2.36 | 0.60 |
| 2:M:285:LEU:HD11 | 2:M:288:ARG:C | 2.21 | 0.60 |
| 2:M:400:PRO:HB3 | 2:M:591:SER:HB2 | 1.82 | 0.60 |
| 3:N:280:ALA:HB1 | 3:N:282:TYR:OH | 2.01 | 0.60 |
| 3:N:287:GLY:O | 3:N:311:LEU:HD22 | 2.01 | 0.60 |
| 3:N:141:ILE:CB | 3:N:450:TYR:HD2 | 2.13 | 0.60 |
| 5:P:86:HIS:C | 5:P:88:ILE:H | 2.03 | 0.60 |
| 3:N:401:TYR:CE2 | 3:N:429:SER:HB2 | 2.36 | 0.60 |
| 3:N:408:GLU:CB | 3:N:422:ALA:HB2 | 2.28 | 0.60 |
| 5:F:370:LYS:HG3 | 5:F:371:LEU:N | 2.14 | 0.60 |
| 3:N:1008:PHE:HZ | 3:N:1032:PRO:HA | 1.64 | 0.60 |
| 3:N:828:LYS:N | 3:N:828:LYS:CD | 2.64 | 0.60 |
| 3:N:660:LYS:HG3 | 3:N:694:VAL:HG22 | 1.83 | 0.60 |
| 2:M:923:GLU:O | 2:M:927:GLY:N | 2.34 | 0.60 |
| 3:N:807:ALA:HA | 3:N:833:GLU:HB2 | 1.83 | 0.60 |
| 2:M:486:MET:SD | 2:M:491:GLU:N | 2.74 | 0.60 |
| 3:N:230:TRP:NE1 | 3:N:233:LYS:HG3 | 2.16 | 0.60 |
| 3:N:501:ALA:O | 3:N:505:SER:HB2 | 2.01 | 0.60 |
| 2:C:683:ASN:H | 2:C:683:ASN:ND2 | 1.98 | 0.60 |
| 2:C:233:GLU:HB2 | 2:C:237:ARG:NH2 | 2.15 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:483:VAL:HG22 | 2:C:484:VAL:N | 2.16 | 0.60 |
| 2:C:496:ILE:HA | 2:C:531:PHE:O | 2.01 | 0.60 |
| 3:N:131:LYS:HE3 | 3:N:565:ILE:HA | 1.83 | 0.60 |
| 3:N:44:LEU:O | 3:N:525:ARG:NH2 | 2.33 | 0.60 |
| 3:N:139:GLY:HA2 | 3:N:452:ILE:HG22 | 1.81 | 0.60 |
| 3:N:356:PRO:HB3 | 3:N:440:VAL:CB | 2.28 | 0.60 |
| 3:D:355:VAL:HG21 | 3:D:367:ILE:HG23 | 1.81 | 0.60 |
| 3:D:401:TYR:O | 3:D:444:VAL:HG22 | 2.02 | 0.60 |
| 3:D:241:ILE:HG12 | 3:D:312:ARG:HG3 | 1.82 | 0.60 |
| 2:M:157:ARG:NH1 | 2:M:314:THR:HA | 2.16 | 0.60 |
| 3:N:968:ASP:HA | 3:N:971:LEU:HD12 | 1.82 | 0.60 |
| 3:D:433:GLY:CA | 3:D:449:SER:H | 2.04 | 0.60 |
| 2:M:1035:MET:HA | 2:M:1038:TRP:CE3 | 2.35 | 0.60 |
| 3:N:1122:LEU:O | 3:N:1134:LEU:HD12 | 2.00 | 0.60 |
| 2:M:1060:ILE:O | 2:M:1063:ARG:HG2 | 2.00 | 0.60 |
| 3:N:348:GLN:HB2 | 3:N:351:MET:SD | 2.41 | 0.60 |
| 2:M:36:PRO:HG2 | 2:M:38:LYS:HB3 | 1.84 | 0.60 |
| 3:N:924:MET:O | 3:N:927:THR:HB | 2.01 | 0.60 |
| 3:D:15:PRO:O | 3:D:19:ARG:HG3 | 2.01 | 0.60 |
| 2:C:896:PHE:C | 2:C:898:GLY:H | 2.04 | 0.60 |
| 3:N:1321:ALA:O | 3:N:1339:LYS:HG3 | 2.01 | 0.60 |
| 2:C:250:ARG:CB | 2:C:253:ALA:HB2 | 2.31 | 0.60 |
| 2:M:326:ASP:HA | 2:M:331:ARG:HD2 | 1.82 | 0.60 |
| 3:N:104:PHE:CD1 | 3:N:104:PHE:N | 2.68 | 0.60 |
| 3:N:126:VAL:O | 3:N:132:TYR:CD1 | 2.53 | 0.60 |
| 3:N:566:ILE:HG21 | 5:P:192:LEU:HD22 | 1.83 | 0.60 |
| 3:D:593:ASN:HB3 | 3:D:594:PRO:HD3 | 1.84 | 0.60 |
| 3:D:408:GLU:CG | 3:D:422:ALA:HB2 | 2.31 | 0.60 |
| 1:B:218:LEU:O | 1:B:221:HIS:HB2 | 2.01 | 0.60 |
| 5:F:340:SER:N | 5:F:343:ASP:OD2 | 2.34 | 0.60 |
| 2:M:355:VAL:CA | 2:M:358:ARG:HG3 | 2.30 | 0.60 |
| 3:N:1406:ARG:HD3 | 3:N:1412:LYS:HZ1 | 1.66 | 0.60 |
| 3:D:951:ILE:HD11 | 3:D:1062:ARG:CG | 2.26 | 0.60 |
| 5:F:367:MET:HA | 5:F:370:LYS:HG2 | 1.83 | 0.60 |
| 2:C:654:LEU:HD12 | 2:C:655:LEU:N | 2.13 | 0.60 |
| 3:N:1450:ALA:O | 3:N:1454:GLY:N | 2.34 | 0.60 |
| 1:L:38:ASN:ND2 | 2:M:979:THR:HA | 2.17 | 0.60 |
| 3:N:729:HIS:HE1 | 3:N:935:LYS:NZ | 1.99 | 0.60 |
| 2:C:1021:LEU:HD21 | 5:F:332:PHE:O | 2.01 | 0.60 |
| 2:C:1049:LEU:O | 2:C:1052:MET:HB3 | 2.01 | 0.60 |
| 5:P:245:GLN:HA | 5:P:245:GLN:HE21 | 1.66 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:13:ILE:HD13 | 2:C:13:ILE:H | 1.66 | 0.60 |
| 3:N:1302:GLU:HG2 | 3:N:1303:TYR:H | 1.67 | 0.60 |
| 3:N:243:ALA:HB3 | 3:N:311:LEU:CD1 | 2.30 | 0.60 |
| 3:D:1498:ALA:HA | 3:D:1501:GLU:HB2 | 1.82 | 0.60 |
| 3:D:274:ARG:HH21 | 3:D:279:VAL:HG13 | 1.65 | 0.60 |
| 3:N:355:VAL:HG13 | 3:N:356:PRO:HD2 | 1.83 | 0.60 |
| 3:N:367:ILE:HB | 3:N:377:VAL:HG11 | 1.82 | 0.60 |
| 3:D:248:PRO:CA | 3:D:308:LYS:HZ3 | 2.09 | 0.60 |
| 3:D:323:GLU:HB2 | 3:D:334:THR:OG1 | 2.00 | 0.60 |
| 3:D:729:HIS:O | 3:D:732:VAL:HG22 | 2.01 | 0.60 |
| 2:C:36:PRO:HG2 | 2:C:38:LYS:HG2 | 1.83 | 0.60 |
| 1:A:35:THR:N | 1:B:42:ARG:NH1 | 2.48 | 0.60 |
| 2:C:352:ALA:CA | 2:C:355:VAL:HG12 | 2.27 | 0.60 |
| 3:D:82:LYS:O | 3:D:85:VAL:HG12 | 2.01 | 0.60 |
| 3:N:59:ALA:HB3 | 3:N:76:CYS:CB | 2.31 | 0.60 |
| 3:N:1097:LYS:HB2 | 3:N:1098:LEU:HD12 | 1.84 | 0.60 |
| 3:N:1099:VAL:CG1 | 9:N:1528:NE6:H14 | 2.29 | 0.60 |
| 3:N:274:ARG:NE | 3:N:279:VAL:HG11 | 2.17 | 0.60 |
| 1:L:211:LEU:O | 1:L:215:VAL:HG13 | 2.01 | 0.60 |
| 3:N:1341:PRO:HA | 3:N:1344:VAL:HG12 | 1.83 | 0.60 |
| 3:N:1466:VAL:O | 3:N:1468:LEU:N | 2.34 | 0.60 |
| 3:N:351:MET:HA | 3:N:370:ALA:HB2 | 1.84 | 0.60 |
| 1:B:13:VAL:CG2 | 1:B:14:ARG:H | 2.15 | 0.60 |
| 3:N:106:LYS:CE | 3:N:106:LYS:HA | 2.25 | 0.60 |
| 2:C:1021:LEU:HD23 | 5:F:334:PRO:HB3 | 1.83 | 0.60 |
| 1:L:48:ILE:HG22 | 1:L:173:PRO:HD2 | 1.82 | 0.60 |
| 3:D:713:ILE:O | 3:D:714:GLN:HG3 | 2.02 | 0.60 |
| 2:M:722:ILE:HG13 | 2:M:722:ILE:O | 2.01 | 0.60 |
| 3:D:634:GLY:HA3 | 3:D:637:LEU:HG | 1.83 | 0.60 |
| 2:M:305:PRO:HA | 2:M:308:ARG:HG2 | 1.83 | 0.60 |
| 3:N:212:ARG:HD3 | 3:N:342:PRO:HB3 | 1.83 | 0.60 |
| 2:C:202:TYR:HB2 | 2:C:207:LEU:HD11 | 1.84 | 0.60 |
| 5:P:200:LYS:HA | 5:P:209:PHE:HE1 | 1.66 | 0.60 |
| 3:D:210:ARG:HB2 | 3:D:389:GLU:HB2 | 1.82 | 0.60 |
| 3:N:362:GLU:H | 3:N:365:ASP:CB | 2.15 | 0.60 |
| 3:D:241:ILE:CD1 | 3:D:310:LEU:HD22 | 2.30 | 0.60 |
| 3:D:322:VAL:CG2 | 3:D:333:LEU:HD22 | 2.31 | 0.60 |
| 1:A:34:VAL:O | 1:A:36:LEU:N | 2.34 | 0.60 |
| 3:N:671:LYS:HE2 | 3:N:675:ARG:HD3 | 1.82 | 0.60 |
| 3:D:1152:GLU:HG2 | 3:D:1153:VAL:H | 1.66 | 0.60 |
| 3:N:1107:VAL:HG11 | 3:N:1217:ILE:HA | 1.84 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:873:PRO:O | 2:C:876:VAL:HG23 | 2.01 | 0.60 |
| 2:M:42:VAL:HG13 | 2:M:43:GLY:N | 2.17 | 0.60 |
| 3:D:341:GLU:OE1 | 3:D:343:LYS:HE3 | 2.02 | 0.60 |
| 3:D:1117:TYR:CD1 | 3:D:1118:ILE:N | 2.69 | 0.60 |
| 3:N:227:LEU:HD12 | 3:N:331:VAL:HG22 | 1.82 | 0.60 |
| 3:D:1442:ASN:HD21 | 3:D:1445:HIS:HB2 | 1.66 | 0.60 |
| 1:L:75:VAL:O | 1:L:79:ILE:HG13 | 2.02 | 0.60 |
| 1:B:63:HIS:CD2 | 1:B:65:PHE:HB2 | 2.36 | 0.60 |
| 2:C:34:VAL:N | 2:C:35:PRO:CD | 2.64 | 0.60 |
| 2:C:71:TYR:HD2 | 2:C:71:TYR:N | 1.97 | 0.60 |
| 2:M:61:LYS:O | 2:M:103:LYS:HB2 | 2.01 | 0.60 |
| 5:P:367:MET:O | 5:P:370:LYS:HG2 | 2.02 | 0.60 |
| 3:N:1019:PRO:O | 3:N:1023:MET:HG3 | 2.00 | 0.60 |
| 1:K:100:LEU:HB3 | 1:K:115:LEU:CD1 | 2.28 | 0.60 |
| 1:A:108:GLU:HG2 | 1:A:109:VAL:N | 2.15 | 0.60 |
| 2:M:41:ASN:HB2 | 2:M:46:ALA:HA | 1.82 | 0.60 |
| 1:L:87:VAL:HG12 | 1:L:122:ILE:HA | 1.84 | 0.60 |
| 1:A:55:SER:HB2 | 1:A:165:ILE:O | 2.02 | 0.60 |
| 5:F:86:HIS:C | 5:F:88:ILE:H | 2.05 | 0.60 |
| 2:M:276:LYS:HB3 | 2:M:280:LYS:HZ2 | 1.65 | 0.60 |
| 2:C:415:PRO:O | 2:C:419:THR:N | 2.32 | 0.60 |
| 3:N:462:GLN:HG2 | 3:N:466:LYS:HE3 | 1.83 | 0.60 |
| 2:C:1112:PHE:O | 2:C:1113:GLU:HG2 | 2.01 | 0.60 |
| 3:D:136:ASP:HB3 | 3:D:137:PRO:CD | 2.28 | 0.60 |
| 3:D:1485:GLN:O | 4:E:75:PHE:HA | 2.02 | 0.60 |
| 5:F:101:GLU:CG | 5:F:105:LYS:HE3 | 2.32 | 0.60 |
| 3:D:658:LEU:O | 3:D:661:MET:HB2 | 2.02 | 0.60 |
| 3:D:673:ALA:CA | 3:D:676:MET:HB3 | 2.32 | 0.60 |
| 5:P:282:LEU:C | 5:P:284:ARG:H | 2.05 | 0.60 |
| 3:N:675:ARG:O | 3:N:678:GLU:HG2 | 2.02 | 0.60 |
| 3:D:1405:GLU:CD | 3:D:1406:ARG:H | 2.04 | 0.60 |
| 3:D:828:LYS:H | 3:D:828:LYS:HD3 | 1.67 | 0.60 |
| 3:N:769:LEU:O | 3:N:778:LEU:N | 2.27 | 0.60 |
| 2:C:790:LEU:HD12 | 2:C:791:ARG:N | 2.15 | 0.60 |
| 1:K:110:LYS:HB3 | 1:K:125:PRO:O | 2.02 | 0.60 |
| 2:M:974:LEU:HB2 | 2:M:983:ILE:HD12 | 1.83 | 0.60 |
| 3:N:1165:TYR:CE2 | 3:N:1206:GLY:HA2 | 2.36 | 0.60 |
| 3:D:1341:PRO:O | 3:D:1343:ALA:N | 2.35 | 0.60 |
| 1:A:138:LEU:HD12 | 1:A:139:ASN:N | 2.14 | 0.60 |
| 5:P:151:LEU:C | 5:P:153:PRO:HD2 | 2.22 | 0.60 |
| 5:P:253:ASP:CB | 5:P:259:ARG:HH12 | 2.15 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:L:123:MET:HE2 | 1:L:204:SER:HA | 1.83 | 0.60 |
| 5:F:308:LEU:HD23 | 5:F:308:LEU:H | 1.66 | 0.60 |
| 3:D:172:PRO:HB2 | 3:D:175:VAL:HG21 | 1.83 | 0.60 |
| 2:M:542:VAL:CG2 | 2:M:543:ASN:H | 2.07 | 0.60 |
| 3:D:376:GLU:O | 3:D:378:ILE:HG13 | 2.01 | 0.60 |
| 2:M:774:LEU:HD23 | 5:P:418:LEU:CD2 | 2.31 | 0.60 |
| 3:D:834:THR:HA | 3:D:838:ARG:HD2 | 1.84 | 0.60 |
| 2:C:100:LEU:CD2 | 2:C:367:LEU:HD23 | 2.30 | 0.60 |
| 2:C:56:GLU:HB2 | 2:C:64:LEU:HD23 | 1.84 | 0.60 |
| 5:F:263:HIS:HA | 5:F:266:GLU:CD | 2.21 | 0.60 |
| 3:D:1264:GLU:OE2 | 3:D:1424:VAL:HG22 | 2.02 | 0.60 |
| 1:L:58:ILE:HB | 1:L:61:VAL:CG1 | 2.31 | 0.60 |
| 5:F:367:MET:O | 5:F:370:LYS:HG2 | 2.02 | 0.60 |
| 3:D:1038:LEU:HD23 | 3:D:1061:PHE:HB2 | 1.84 | 0.60 |
| 3:N:1162:GLU:O | 3:N:1162:GLU:HG3 | 2.02 | 0.60 |
| 1:B:80:LEU:HB3 | 3:D:844:ALA:HB2 | 1.83 | 0.60 |
| 2:C:649:VAL:HG22 | 2:C:650:ARG:HH21 | 1.67 | 0.60 |
| 2:C:573:ARG:HB2 | 2:C:670:GLN:NE2 | 2.16 | 0.60 |
| 2:C:760:SER:O | 2:C:786:LYS:N | 2.34 | 0.60 |
| 3:N:170:PRO:C | 3:N:171:LEU:HD23 | 2.21 | 0.60 |
| 3:D:142:LEU:HD13 | 3:D:144:GLY:H | 1.66 | 0.60 |
| 1:A:20:TYR:HD1 | 1:A:199:ILE:O | 1.85 | 0.60 |
| 1:A:224:TYR:HD2 | 1:A:224:TYR:N | 2.00 | 0.60 |
| 1:K:1:MET:H1 | 1:K:6:LEU:HD22 | 1.67 | 0.60 |
| 2:C:353:ARG:O | 2:C:357:GLU:HG3 | 2.02 | 0.60 |
| 2:M:550:LEU:HD12 | 2:M:550:LEU:O | 2.01 | 0.60 |
| 3:D:1066:THR:N | 3:D:1069:GLU:HB2 | 2.16 | 0.60 |
| 5:F:175:HIS:O | 5:F:178:ARG:HB2 | 2.02 | 0.60 |
| 3:D:302:GLN:N | 3:D:303:PRO:HD2 | 2.16 | 0.60 |
| 3:D:400:VAL:HG23 | 3:D:443:VAL:HG11 | 1.81 | 0.60 |
| 2:C:66:LEU:HA | 2:C:99:GLN:O | 2.02 | 0.60 |
| 2:M:369:PRO:O | 2:M:372:LEU:HD21 | 2.01 | 0.60 |
| 3:N:1268:PRO:O | 3:N:1271:LYS:HB2 | 2.02 | 0.60 |
| 3:D:65:ARG:HB3 | 5:F:375:LEU:O | 2.02 | 0.60 |
| 3:N:617:ASN:HB3 | 3:N:619:LEU:HG | 1.84 | 0.60 |
| 3:N:867:ARG:HA | 3:N:871:LYS:O | 2.01 | 0.60 |
| 3:D:167:GLU:O | 3:D:394:LEU:HA | 2.02 | 0.60 |
| 1:A:231:ALA:N | 1:B:13:VAL:O | 2.30 | 0.60 |
| 3:N:1208:ASP:CG | 3:N:1211:MET:HG2 | 2.22 | 0.60 |
| 3:D:1286:THR:CG2 | 3:D:1289:LYS:H | 2.15 | 0.60 |
| 3:D:1000:THR:HG23 | 3:D:1041:LEU:HD23 | 1.83 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:D:1041:LEU:CD1 | 3:D:1058:ARG:HA | 2.32 | 0.60 |
| 3:D:699:VAL:HG12 | 3:D:717:GLN:CG | 2.31 | 0.60 |
| 2:C:939:ARG:NH1 | 2:C:942:GLU:OE2 | 2.34 | 0.60 |
| 5:P:169:GLU:H | 5:P:169:GLU:CD | 2.04 | 0.60 |
| 2:M:228:ALA:O | 2:M:229:MET:HG3 | 2.02 | 0.60 |
| 3:D:463:GLN:HB3 | 3:D:467:GLU:OE2 | 2.01 | 0.60 |
| 3:D:295:GLY:C | 3:D:302:GLN:HB3 | 2.21 | 0.60 |
| 3:D:297:ILE:HG23 | 3:D:298:VAL:N | 2.17 | 0.60 |
| 5:P:298:GLY:O | 5:P:303:ARG:NH1 | 2.35 | 0.60 |
| 5:P:367:MET:CE | 5:P:371:LEU:HD21 | 2.32 | 0.60 |
| 3:N:1107:VAL:CG1 | 3:N:1217:ILE:HA | 2.32 | 0.60 |
| 3:D:911:LEU:O | 3:D:914:LEU:HB3 | 2.02 | 0.60 |
| 3:N:252:ARG:HG3 | 3:N:300:LYS:CA | 2.32 | 0.60 |
| 3:N:860:LEU:O | 3:N:876:SER:HB2 | 2.01 | 0.60 |
| 3:N:939:PHE:O | 3:N:940:THR:C | 2.40 | 0.60 |
| 2:C:710:ILE:HD13 | 2:C:790:LEU:HB2 | 1.83 | 0.60 |
| 2:C:504:GLU:HG3 | 2:C:507:ARG:HD2 | 1.84 | 0.60 |
| 1:K:152:PRO:CG | 1:K:155:LYS:HB2 | 2.29 | 0.60 |
| 2:M:71:TYR:CD2 | 2:M:71:TYR:N | 2.68 | 0.60 |
| 2:C:185:LYS:HE2 | 2:C:190:LYS:NZ | 2.17 | 0.60 |
| 3:N:1403:LEU:HB3 | 3:N:1408:ILE:HD12 | 1.83 | 0.60 |
| 2:C:1048:THR:O | 2:C:1051:GLU:HG3 | 2.02 | 0.60 |
| 5:F:234:LYS:CE | 5:F:236:SER:HB3 | 2.32 | 0.60 |
| 2:C:474:VAL:HG12 | 2:C:530:GLU:C | 2.22 | 0.60 |
| 2:C:683:ASN:H | 2:C:683:ASN:HD22 | 1.50 | 0.60 |
| 3:D:1045:MET:HG3 | 3:D:1073:SER:HA | 1.83 | 0.60 |
| 2:C:233:GLU:CD | 2:C:234:ALA:N | 2.53 | 0.59 |
| 3:N:32:ILE:HG12 | 3:N:39:PRO:HA | 1.84 | 0.59 |
| 3:N:433:GLY:HA3 | 3:N:448:GLU:HA | 1.84 | 0.59 |
| 3:D:259:VAL:HG21 | 3:D:292:VAL:O | 2.02 | 0.59 |
| 3:D:408:GLU:OE2 | 3:D:422:ALA:HB2 | 2.01 | 0.59 |
| 3:D:811:GLU:HB3 | 3:D:815:ALA:HB3 | 1.84 | 0.59 |
| 2:C:93:PRO:HA | 2:C:117:HIS:CB | 2.31 | 0.59 |
| 1:L:99:LEU:HB3 | 1:L:114:PHE:CE2 | 2.37 | 0.59 |
| 3:D:799:LYS:HB3 | 3:D:800:LYS:HE2 | 1.83 | 0.59 |
| 3:D:483:HIS:HB2 | 3:D:484:PRO:CD | 2.27 | 0.59 |
| 2:C:691:SER:CB | 2:C:868:ASP:HA | 2.31 | 0.59 |
| 3:N:1173:LEU:O | 3:N:1176:LYS:HB3 | 2.02 | 0.59 |
| 3:N:1478:SER:O | 3:N:1482:ARG:HG3 | 2.01 | 0.59 |
| 1:L:209:GLU:O | 1:L:213:GLN:HG3 | 2.02 | 0.59 |
| 2:M:1090:LYS:HE2 | 2:M:1112:PHE:CZ | 2.37 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:K:100:LEU:CD2 | 1:K:101:LEU:H | 2.12 | 0.59 |
| 1:K:211:LEU:O | 1:K:214:ALA:HB3 | 2.02 | 0.59 |
| 1:K:36:LEU:O | 1:K:39:PRO:HD2 | 2.02 | 0.59 |
| 1:K:86:VAL:CG1 | 1:K:123:MET:HB2 | 2.32 | 0.59 |
| 2:C:18:LEU:C | 2:C:20:GLU:H | 2.04 | 0.59 |
| 3:D:1286:THR:HB | 3:D:1289:LYS:H | 1.66 | 0.59 |
| 3:N:167:GLU:O | 3:N:394:LEU:HA | 2.02 | 0.59 |
| 1:L:5:LYS:C | 1:L:7:LYS:N | 2.55 | 0.59 |
| 2:C:12:VAL:HG23 | 2:C:13:ILE:HD12 | 1.84 | 0.59 |
| 3:D:1117:TYR:C | 3:D:1193:THR:HG21 | 2.22 | 0.59 |
| 3:D:901:GLN:HB3 | 3:D:904:VAL:CG2 | 2.32 | 0.59 |
| 3:N:774:SER:HB3 | 3:N:1362:LYS:O | 2.02 | 0.59 |
| 2:M:401:LEU:O | 2:M:405:ARG:N | 2.34 | 0.59 |
| 2:C:182:VAL:HG21 | 2:C:194:VAL:CG2 | 2.32 | 0.59 |
| 2:C:492:ASP:CA | 2:C:518:LYS:HB3 | 2.31 | 0.59 |
| 3:N:84:ILE:O | 3:N:87:ARG:HG2 | 2.02 | 0.59 |
| 3:D:527:MET:HA | 3:D:537:THR:HG23 | 1.83 | 0.59 |
| 2:M:595:LEU:O | 2:M:654:LEU:HD12 | 2.01 | 0.59 |
| 2:C:966:LEU:HD21 | 2:C:986:PRO:CG | 2.32 | 0.59 |
| 2:C:700:TYR:HB2 | 2:C:833:LEU:HD22 | 1.83 | 0.59 |
| 3:D:41:ARG:HH21 | 3:D:48:ARG:CZ | 2.14 | 0.59 |
| 3:N:658:LEU:CA | 3:N:661:MET:HE3 | 2.31 | 0.59 |
| 3:N:661:MET:O | 3:N:664:LYS:O | 2.21 | 0.59 |
| 1:A:76:VAL:HA | 1:A:79:ILE:CD1 | 2.27 | 0.59 |
| 2:M:504:GLU:O | 2:M:507:ARG:HD2 | 2.02 | 0.59 |
| 1:K:11:PHE:HB2 | 1:L:224:TYR:O | 2.02 | 0.59 |
| 2:M:498:GLN:HA | 2:M:533:ASP:OD2 | 2.01 | 0.59 |
| 5:F:353:GLU:HA | 5:F:356:LYS:CG | 2.31 | 0.59 |
| 2:C:154:ARG:HG2 | 2:C:156:GLY:H | 1.67 | 0.59 |
| 2:M:333:ILE:HG22 | 2:M:465:GLY:O | 2.02 | 0.59 |
| 2:C:166:PRO:HG2 | 2:C:169:GLY:N | 2.17 | 0.59 |
| 2:C:321:GLU:CD | 2:C:321:GLU:H | 2.06 | 0.59 |
| 3:N:135:LEU:HD12 | 3:N:148:GLU:CB | 2.33 | 0.59 |
| 3:D:103:TRP:CZ2 | 3:D:604:THR:HG23 | 2.37 | 0.59 |
| 3:N:408:GLU:HB2 | 3:N:421:LEU:O | 2.02 | 0.59 |
| 3:D:400:VAL:HG22 | 3:D:402:PRO:HD3 | 1.84 | 0.59 |
| 3:D:639:LEU:O | 3:D:639:LEU:HD12 | 2.01 | 0.59 |
| 1:A:35:THR:C | 1:A:36:LEU:HD12 | 2.22 | 0.59 |
| 1:B:38:ASN:O | 1:B:42:ARG:HG3 | 2.02 | 0.59 |
| 3:D:654:LYS:CB | 3:D:655:PRO:HD3 | 2.32 | 0.59 |
| 5:P:300:ASP:HB3 | 5:P:302:LYS:HZ2 | 1.67 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:713:ARG:HD2 | 2:M:720:GLU:OE2 | 2.01 | 0.59 |
| 3:D:1170:ASP:O | 3:D:1173:LEU:HB3 | 2.02 | 0.59 |
| 3:D:1405:GLU:CG | 3:D:1406:ARG:H | 2.14 | 0.59 |
| 3:N:966:GLU:HA | 3:N:969:ARG:NE | 2.17 | 0.59 |
| 3:N:968:ASP:O | 3:N:971:LEU:HB2 | 2.03 | 0.59 |
| 3:D:1031:ASN:OD1 | 3:D:1034:GLN:HG3 | 2.01 | 0.59 |
| 3:N:1341:PRO:O | 3:N:1344:VAL:N | 2.35 | 0.59 |
| 2:M:474:VAL:HG12 | 2:M:530:GLU:C | 2.22 | 0.59 |
| 1:K:218:LEU:O | 1:K:221:HIS:HB2 | 2.02 | 0.59 |
| 2:M:504:GLU:HG3 | 2:M:507:ARG:HB2 | 1.84 | 0.59 |
| 3:D:1121:PRO:HG2 | 3:D:1135:ARG:HH11 | 1.66 | 0.59 |
| 3:N:1273:VAL:HG23 | 3:N:1325:LEU:HB2 | 1.84 | 0.59 |
| 2:C:1030:GLN:HG2 | 3:D:626:SER:HB2 | 1.83 | 0.59 |
| 3:N:960:LYS:HG2 | 3:N:964:LEU:CD1 | 2.32 | 0.59 |
| 2:C:585:GLU:HB2 | 2:C:665:PHE:CE2 | 2.36 | 0.59 |
| 2:M:497:ALA:HA | 2:M:515:ALA:HA | 1.84 | 0.59 |
| 2:M:164:PRO:HG3 | 2:M:170:PRO:HB2 | 1.83 | 0.59 |
| 2:M:198:ARG:NH2 | 2:M:231:PRO:HD3 | 2.16 | 0.59 |
| 2:M:226:VAL:HA | 2:M:229:MET:SD | 2.42 | 0.59 |
| 2:C:166:PRO:HG3 | 2:C:263:ASP:HA | 1.84 | 0.59 |
| 2:C:430:VAL:O | 2:C:430:VAL:HG13 | 2.02 | 0.59 |
| 3:D:1048:PRO:HA | 3:D:1079:LYS:HE3 | 1.83 | 0.59 |
| 3:D:1066:THR:HG22 | 3:D:1068:LEU:H | 1.67 | 0.59 |
| 3:N:140:ALA:N | 3:N:450:TYR:CE2 | 2.70 | 0.59 |
| 3:N:149:LYS:HE2 | 3:N:151:GLN:HG3 | 1.83 | 0.59 |
| 3:N:361:VAL:CG1 | 3:N:379:ALA:HB1 | 2.32 | 0.59 |
| 3:N:362:GLU:H | 3:N:365:ASP:HB2 | 1.66 | 0.59 |
| 1:B:59:GLU:HB2 | 1:B:139:ASN:HD22 | 1.67 | 0.59 |
| 3:D:658:LEU:HD23 | 3:D:661:MET:CE | 2.32 | 0.59 |
| 3:D:921:ARG:HB3 | 3:D:921:ARG:NH1 | 2.17 | 0.59 |
| 3:D:433:GLY:C | 3:D:434:ARG:HD2 | 2.23 | 0.59 |
| 1:L:201:THR:CG2 | 1:L:207:PRO:HA | 2.32 | 0.59 |
| 1:A:181:VAL:HG13 | 1:A:193:ASP:HB3 | 1.85 | 0.59 |
| 1:A:78:ILE:O | 1:A:82:LEU:HG | 2.02 | 0.59 |
| 2:C:17:PRO:HD2 | 2:C:20:GLU:OE1 | 2.01 | 0.59 |
| 3:D:1288:GLU:O | 3:D:1307:LYS:HD3 | 2.03 | 0.59 |
| 3:D:1335:LEU:CD2 | 3:D:1344:VAL:HA | 2.32 | 0.59 |
| 1:B:176:ARG:HB3 | 1:B:200:TRP:CD1 | 2.37 | 0.59 |
| 2:C:807:ARG:C | 2:C:809:GLY:N | 2.52 | 0.59 |
| 3:N:984:THR:HG22 | 3:N:987:GLU:CB | 2.33 | 0.59 |
| 3:N:605:ASP:O | 3:N:609:GLY:HA2 | 2.02 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:617:ASP:OD2 | 2:M:619:ARG:HG3 | 2.03 | 0.59 |
| 2:C:930:LYS:C | 2:C:932:GLU:H | 2.04 | 0.59 |
| 2:C:682:TYR:CE1 | 2:C:851:LYS:HD2 | 2.37 | 0.59 |
| 2:M:261:ILE:C | 2:M:288:ARG:HH21 | 2.06 | 0.59 |
| 3:N:387:LEU:CD1 | 3:N:387:LEU:H | 2.16 | 0.59 |
| 2:C:283:ILE:CG2 | 2:C:284:ARG:H | 2.03 | 0.59 |
| 3:N:527:MET:SD | 3:N:537:THR:HG21 | 2.42 | 0.59 |
| 3:N:551:ASN:O | 3:N:555:LYS:HG3 | 2.01 | 0.59 |
| 3:D:820:GLU:CG | 3:D:836:VAL:HG11 | 2.26 | 0.59 |
| 3:D:163:TYR:O | 3:D:447:VAL:HG11 | 2.02 | 0.59 |
| 2:M:187:ASN:O | 2:M:188:LYS:HG3 | 2.02 | 0.59 |
| 3:N:1161:GLU:HG3 | 3:N:1164:ARG:CB | 2.32 | 0.59 |
| 2:C:571:LEU:HD13 | 2:C:699:PHE:O | 2.02 | 0.59 |
| 2:C:929:ARG:O | 2:C:934:PHE:HB2 | 2.03 | 0.59 |
| 2:M:31:GLN:NE2 | 2:M:40:GLU:O | 2.35 | 0.59 |
| 2:M:881:ASN:ND2 | 2:M:881:ASN:N | 2.50 | 0.59 |
| 3:D:1047:LYS:HD2 | 3:D:1051:GLU:CG | 2.32 | 0.59 |
| 2:M:688:ILE:HD11 | 2:M:847:GLY:HA3 | 1.84 | 0.59 |
| 2:M:385:PHE:HD1 | 2:M:389:SER:HB2 | 1.68 | 0.59 |
| 2:C:205:GLU:CA | 2:C:209:ARG:HH11 | 2.16 | 0.59 |
| 2:C:140:ILE:HG23 | 2:C:410:ILE:HG21 | 1.84 | 0.59 |
| 4:E:87:LYS:HG2 | 4:E:88:GLU:N | 2.17 | 0.59 |
| 5:F:204:GLY:O | 5:F:206:GLY:N | 2.36 | 0.59 |
| 5:F:330:GLY:HA2 | 5:F:333:ILE:HD12 | 1.82 | 0.59 |
| 2:M:776:SER:HB3 | 5:P:379:ARG:NH2 | 2.14 | 0.59 |
| 1:L:98:THR:HA | 1:L:142:VAL:O | 2.02 | 0.59 |
| 3:D:826:PRO:HB2 | 3:D:829:VAL:HG13 | 1.82 | 0.59 |
| 3:N:297:ILE:CG2 | 3:N:298:VAL:H | 2.13 | 0.59 |
| 3:N:1147:ARG:O | 3:N:1166:LEU:HG | 2.03 | 0.59 |
| 5:F:77:THR:O | 5:F:77:THR:HG23 | 2.03 | 0.59 |
| 1:K:14:ARG:CD | 1:L:233:VAL:HA | 2.32 | 0.59 |
| 1:K:206:THR:HB | 1:K:209:GLU:CD | 2.22 | 0.59 |
| 3:N:1398:TRP:O | 3:N:1402:ALA:N | 2.35 | 0.59 |
| 3:N:204:LEU:O | 3:N:393:ILE:HG23 | 2.03 | 0.59 |
| 3:D:995:LEU:HG | 3:D:996:TRP:N | 2.17 | 0.59 |
| 1:K:176:ARG:CZ | 2:M:865:THR:CG2 | 2.81 | 0.59 |
| 5:F:167:PRO:HD2 | 5:F:170:HIS:HD2 | 1.66 | 0.59 |
| 2:M:841:ASN:ND2 | 2:M:845:ASN:HB3 | 2.18 | 0.59 |
| 2:C:816:LYS:H | 2:C:816:LYS:HD2 | 1.68 | 0.59 |
| 2:M:405:ARG:NH2 | 2:M:409:ARG:CZ | 2.65 | 0.59 |
| 3:N:334:THR:C | 3:N:335:LEU:HD12 | 2.23 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:P:184:ARG:O | 5:P:188:ILE:HG13 | 2.02 | 0.59 |
| 3:D:1107:VAL:CG1 | 3:D:1217:ILE:HA | 2.32 | 0.59 |
| 3:D:1495:ILE:HG13 | 4:E:84:ARG:HH12 | 1.68 | 0.59 |
| 5:P:370:LYS:HA | 5:P:374:GLY:HA3 | 1.83 | 0.59 |
| 1:L:56:VAL:HG12 | 1:L:57:TYR:N | 2.17 | 0.59 |
| 2:M:1068:GLU:O | 2:M:1072:LYS:HG2 | 2.03 | 0.59 |
| 1:K:122:ILE:CG2 | 1:K:124:ASN:H | 2.08 | 0.59 |
| 2:M:195:LEU:HB3 | 2:M:238:LEU:HD21 | 1.84 | 0.59 |
| 3:D:165:LYS:O | 3:D:396:VAL:HA | 2.02 | 0.59 |
| 3:D:565:ILE:HG23 | 3:D:566:ILE:H | 1.67 | 0.59 |
| 3:D:355:VAL:HG13 | 3:D:356:PRO:HD2 | 1.85 | 0.59 |
| 2:M:69:LEU:HB3 | 2:M:97:ARG:HB2 | 1.85 | 0.59 |
| 2:M:310:LEU:O | 2:M:314:THR:HG23 | 2.02 | 0.59 |
| 3:D:807:ALA:HA | 3:D:833:GLU:CG | 2.32 | 0.59 |
| 2:M:101:ILE:CG2 | 2:M:102:HIS:H | 2.14 | 0.59 |
| 2:M:355:VAL:HA | 2:M:358:ARG:HE | 1.67 | 0.59 |
| 3:N:1434:TRP:CE3 | 3:N:1457:ASP:HB2 | 2.38 | 0.59 |
| 3:N:475:LYS:O | 3:N:478:LEU:HB3 | 2.03 | 0.59 |
| 2:M:42:VAL:CG1 | 2:M:43:GLY:N | 2.66 | 0.59 |
| 2:M:463:GLU:H | 2:M:463:GLU:CD | 2.06 | 0.59 |
| 2:C:560:MET:HB3 | 2:C:564:MET:CE | 2.33 | 0.59 |
| 2:M:198:ARG:HE | 2:M:231:PRO:CD | 2.15 | 0.59 |
| 3:D:1489:GLN:NE2 | 4:E:72:ARG:HA | 2.17 | 0.59 |
| 2:C:269:LEU:HD12 | 2:C:288:ARG:CB | 2.31 | 0.59 |
| 5:P:77:THR:O | 5:P:79:ASP:N | 2.36 | 0.59 |
| 5:P:386:VAL:HG23 | 5:P:387:GLY:H | 1.67 | 0.59 |
| 1:B:112:ARG:CB | 1:B:112:ARG:HH11 | 2.16 | 0.59 |
| 1:L:76:VAL:O | 1:L:79:ILE:HB | 2.02 | 0.59 |
| 1:B:41:ARG:HG3 | 1:B:41:ARG:HH11 | 1.68 | 0.59 |
| 3:N:1217:ILE:N | 3:N:1217:ILE:HD12 | 2.05 | 0.59 |
| 3:N:58:CYS:HB2 | 3:N:76:CYS:SG | 2.42 | 0.59 |
| 3:N:252:ARG:HG3 | 3:N:300:LYS:HA | 1.84 | 0.59 |
| 2:M:243:ARG:HG3 | 2:M:244:PRO:CA | 2.24 | 0.59 |
| 5:F:79:ASP:OD1 | 5:F:82:ARG:HB2 | 2.03 | 0.59 |
| 3:N:10:ILE:HG23 | 3:N:10:ILE:O | 2.03 | 0.59 |
| 3:D:881:LEU:O | 3:D:885:ILE:HG13 | 2.02 | 0.59 |
| 2:C:632:ASN:HB3 | 2:C:633:GLN:HE22 | 1.67 | 0.59 |
| 5:P:111:GLU:HG3 | 5:P:114:LYS:NZ | 2.15 | 0.59 |
| 5:P:111:GLU:O | 5:P:114:LYS:HB2 | 2.03 | 0.59 |
| 5:P:222:ARG:HG2 | 5:P:242:TRP:CZ3 | 2.37 | 0.59 |
| 3:N:1108:ARG:NE | 3:N:1199:GLY:HA3 | 2.18 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:709:HIS:CD2 | 3:D:711:LEU:HB2 | 2.38 | 0.59 |
| 2:C:1050:GLN:HG2 | 2:C:1079:PRO:HG2 | 1.83 | 0.59 |
| 3:D:1085:ALA:HA | 3:D:1088:THR:CG2 | 2.32 | 0.59 |
| 3:N:121:THR:O | 3:N:122:GLU:C | 2.40 | 0.59 |
| 3:N:554:LEU:O | 3:N:555:LYS:C | 2.41 | 0.59 |
| 3:D:1474:ALA:O | 3:D:1477:GLY:N | 2.36 | 0.59 |
| 5:F:392:VAL:CG1 | 5:F:396:ARG:HD3 | 2.30 | 0.59 |
| 2:M:588:VAL:CG2 | 2:M:589:ARG:N | 2.64 | 0.59 |
| 2:M:712:ALA:O | 2:M:820:ARG:HG3 | 2.03 | 0.59 |
| 3:D:1422:MET:SD | 3:D:1427:SER:HA | 2.43 | 0.59 |
| 1:K:188:GLN:CG | 1:K:189:ARG:H | 2.03 | 0.59 |
| 1:L:42:ARG:HH22 | 2:M:939:ARG:NH2 | 2.00 | 0.59 |
| 5:P:329:TYR:O | 5:P:332:PHE:HD1 | 1.84 | 0.59 |
| 2:M:1005:MET:HG2 | 3:N:629:SER:CB | 2.31 | 0.59 |
| 2:C:917:LEU:HD23 | 2:C:920:GLN:OE1 | 2.03 | 0.59 |
| 3:D:966:GLU:HA | 3:D:969:ARG:CZ | 2.33 | 0.59 |
| 1:B:238:GLU:HB3 | 1:B:240:LYS:HZ2 | 1.68 | 0.59 |
| 2:M:185:LYS:CG | 2:M:190:LYS:HD3 | 2.29 | 0.58 |
| 2:M:582:GLY:O | 2:M:584:GLU:HG2 | 2.03 | 0.58 |
| 3:N:225:LEU:HD12 | 3:N:333:LEU:CD1 | 2.32 | 0.58 |
| 1:B:235:ALA:CB | 1:B:236:PRO:HD3 | 2.30 | 0.58 |
| 3:N:127:LEU:HD23 | 3:N:128:TYR:CA | 2.32 | 0.58 |
| 3:D:274:ARG:NE | 3:D:279:VAL:HG11 | 2.17 | 0.58 |
| 3:D:248:PRO:CB | 3:D:308:LYS:HZ1 | 2.16 | 0.58 |
| 3:N:1491:THR:C | 3:N:1493:LYS:H | 2.06 | 0.58 |
| 3:N:1376:MET:HA | 3:N:1376:MET:HE2 | 1.84 | 0.58 |
| 2:M:352:ALA:CA | 2:M:355:VAL:HG12 | 2.31 | 0.58 |
| 2:M:813:VAL:CG1 | 2:M:815:LEU:HG | 2.33 | 0.58 |
| 3:D:1403:LEU:HD23 | 3:D:1408:ILE:HD11 | 1.82 | 0.58 |
| 3:D:800:LYS:HZ1 | 3:D:826:PRO:HD3 | 1.68 | 0.58 |
| 1:K:111:ALA:CA | 1:K:129:ILE:HD11 | 2.31 | 0.58 |
| 1:K:88:ARG:HD2 | 1:K:90:LEU:HD23 | 1.84 | 0.58 |
| 4:O:33:HIS:HB2 | 4:O:37:ASN:OD1 | 2.02 | 0.58 |
| 2:C:421:GLU:O | 2:C:421:GLU:HG2 | 2.02 | 0.58 |
| 2:M:301:GLU:HA | 2:M:304:LEU:CD2 | 2.26 | 0.58 |
| 2:M:545:ASN:HB3 | 2:M:583:LEU:HD11 | 1.85 | 0.58 |
| 2:C:399:ASN:HB2 | 2:C:400:PRO:CD | 2.33 | 0.58 |
| 3:D:525:ARG:N | 3:D:526:PRO:CD | 2.63 | 0.58 |
| 4:E:28:GLN:O | 4:E:32:ARG:HG3 | 2.03 | 0.58 |
| 2:M:595:LEU:HD21 | 2:M:639:GLN:HE22 | 1.67 | 0.58 |
| 2:M:815:LEU:HD11 | 2:M:821:GLU:HA | 1.85 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:K:184:THR:HG23 | 1:K:192:LEU:HB2 | 1.85 | 0.58 |
| 3:N:1068:LEU:O | 3:N:1072:ILE:HG13 | 2.04 | 0.58 |
| 3:D:211:VAL:HG13 | 3:D:386:HIS:O | 2.03 | 0.58 |
| 2:M:232:GLU:O | 2:M:236:ILE:HG13 | 2.03 | 0.58 |
| 2:C:267:TYR:CB | 2:C:272:ALA:HB2 | 2.16 | 0.58 |
| 3:D:1498:ALA:HB3 | 4:E:84:ARG:NE | 2.19 | 0.58 |
| 3:D:564:GLU:O | 3:D:567:ILE:HB | 2.03 | 0.58 |
| 3:D:274:ARG:CB | 3:D:279:VAL:HG21 | 2.17 | 0.58 |
| 2:M:774:LEU:HD23 | 5:P:418:LEU:HD23 | 1.84 | 0.58 |
| 1:B:44:LEU:O | 1:B:174:VAL:HG21 | 2.03 | 0.58 |
| 5:F:269:ASN:O | 5:F:273:ARG:HG3 | 2.03 | 0.58 |
| 3:D:1384:PRO:HB3 | 3:D:1387:SER:O | 2.04 | 0.58 |
| 3:N:1035:ILE:O | 3:N:1038:LEU:N | 2.36 | 0.58 |
| 2:M:689:VAL:CG2 | 2:M:870:ILE:HB | 2.32 | 0.58 |
| 1:A:169:ALA:HB1 | 1:A:171:PHE:CE1 | 2.38 | 0.58 |
| 3:N:699:VAL:CG1 | 3:N:717:GLN:HG2 | 2.28 | 0.58 |
| 3:N:167:GLU:HB3 | 3:N:169:TYR:OH | 2.02 | 0.58 |
| 3:N:167:GLU:HB3 | 3:N:169:TYR:CZ | 2.38 | 0.58 |
| 2:C:1:MET:CB | 2:C:899:GLN:HA | 2.33 | 0.58 |
| 3:N:917:GLN:O | 3:N:921:ARG:HG2 | 2.03 | 0.58 |
| 5:F:303:ARG:O | 5:F:304:VAL:C | 2.40 | 0.58 |
| 3:D:972:LEU:N | 3:D:972:LEU:HD22 | 2.18 | 0.58 |
| 5:F:172:ARG:HG3 | 5:F:173:TYR:N | 2.17 | 0.58 |
| 1:B:154:GLU:HG2 | 3:D:840:LYS:HE3 | 1.85 | 0.58 |
| 4:O:49:GLN:HA | 4:O:53:GLY:O | 2.03 | 0.58 |
| 2:M:385:PHE:O | 2:M:389:SER:N | 2.37 | 0.58 |
| 3:N:280:ALA:HB1 | 3:N:282:TYR:CE1 | 2.38 | 0.58 |
| 2:C:176:VAL:C | 2:C:178:PRO:HD3 | 2.22 | 0.58 |
| 2:C:198:ARG:HA | 2:C:202:TYR:O | 2.03 | 0.58 |
| 2:C:1054:THR:HG22 | 2:C:1082:PRO:HG3 | 1.86 | 0.58 |
| 3:D:408:GLU:OE1 | 3:D:444:VAL:HG11 | 2.03 | 0.58 |
| 3:D:241:ILE:HG13 | 3:D:312:ARG:CZ | 2.33 | 0.58 |
| 2:C:874:LEU:HD13 | 3:D:783:ARG:HB3 | 1.86 | 0.58 |
| 3:N:826:PRO:HD2 | 3:N:829:VAL:CG1 | 2.30 | 0.58 |
| 3:N:799:LYS:H | 3:N:829:VAL:CG1 | 2.16 | 0.58 |
| 3:N:1117:TYR:CA | 3:N:1193:THR:HG21 | 2.32 | 0.58 |
| 2:M:1033:GLY:O | 2:M:1037:VAL:HG23 | 2.03 | 0.58 |
| 2:C:615:TYR:O | 2:C:618:GLY:N | 2.37 | 0.58 |
| 2:M:1072:LYS:HB2 | 2:M:1074:GLU:HG3 | 1.84 | 0.58 |
| 1:K:74:ASP:O | 1:K:75:VAL:C | 2.42 | 0.58 |
| 1:K:75:VAL:O | 1:K:79:ILE:HG13 | 2.04 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:K:9:PRO:HG2 | 1:K:28:LEU:CD2 | 2.33 | 0.58 |
| 3:N:1398:TRP:HA | 3:N:1401:GLU:HB2 | 1.84 | 0.58 |
| 3:N:1086:LEU:HD12 | 3:N:1238:MET:SD | 2.44 | 0.58 |
| 3:D:792:ILE:HG21 | 3:D:941:PHE:CD1 | 2.37 | 0.58 |
| 3:D:887:ALA:CB | 3:D:893:GLU:HA | 2.33 | 0.58 |
| 5:F:147:LEU:O | 5:F:148:LYS:HB2 | 2.02 | 0.58 |
| 2:M:835:VAL:HA | 2:M:849:VAL:CG1 | 2.34 | 0.58 |
| 3:D:1364:HIS:CE1 | 3:D:1366:LYS:HG3 | 2.38 | 0.58 |
| 1:L:52:ALA:HB1 | 1:L:170:VAL:H | 1.67 | 0.58 |
| 4:O:61:GLU:H | 4:O:61:GLU:CD | 2.07 | 0.58 |
| 3:D:894:LYS:O | 3:D:898:GLU:HG3 | 2.02 | 0.58 |
| 2:M:79:PRO:HG2 | 2:M:82:GLU:HB2 | 1.84 | 0.58 |
| 2:C:204:GLN:NE2 | 2:C:225:SER:HB3 | 2.18 | 0.58 |
| 5:F:113:ILE:HA | 5:F:116:LEU:CD1 | 2.23 | 0.58 |
| 5:F:223:ALA:HB2 | 5:F:242:TRP:CB | 2.33 | 0.58 |
| 3:D:252:ARG:HA | 3:D:301:GLY:HA3 | 1.85 | 0.58 |
| 3:D:241:ILE:HG12 | 3:D:312:ARG:CG | 2.33 | 0.58 |
| 2:M:712:ALA:HB3 | 2:M:821:GLU:H | 1.68 | 0.58 |
| 5:F:371:LEU:HA | 5:F:375:LEU:CG | 2.31 | 0.58 |
| 3:N:796:ARG:NE | 3:N:861:GLN:HB2 | 2.18 | 0.58 |
| 2:C:710:ILE:CG2 | 2:C:823:VAL:HB | 2.32 | 0.58 |
| 2:C:614:ARG:HE | 2:C:618:GLY:HA2 | 1.68 | 0.58 |
| 2:C:18:LEU:C | 2:C:20:GLU:N | 2.54 | 0.58 |
| 1:K:107:LYS:HE2 | 1:K:108:GLU:O | 2.04 | 0.58 |
| 2:M:44:ILE:HG23 | 2:M:344:PHE:CE1 | 2.28 | 0.58 |
| 1:L:128:HIS:HE1 | 1:L:131:THR:HG23 | 1.69 | 0.58 |
| 2:M:327:HIS:HB3 | 2:M:330:ASN:ND2 | 2.18 | 0.58 |
| 2:M:906:PHE:HZ | 3:N:1070:TYR:CD2 | 2.21 | 0.58 |
| 5:F:321:ILE:HD11 | 5:F:329:TYR:N | 2.18 | 0.58 |
| 2:C:937:ASP:O | 2:C:940:GLU:HB2 | 2.04 | 0.58 |
| 5:P:167:PRO:HD2 | 5:P:170:HIS:HD2 | 1.67 | 0.58 |
| 2:C:122:THR:HG22 | 2:C:123:GLU:H | 1.68 | 0.58 |
| 3:N:221:ALA:O | 3:N:334:THR:HG23 | 2.04 | 0.58 |
| 2:C:195:LEU:CD2 | 2:C:195:LEU:H | 1.93 | 0.58 |
| 2:C:467:ILE:HG22 | 2:C:468:ARG:N | 2.18 | 0.58 |
| 3:N:27:GLU:C | 3:N:28:LYS:HD3 | 2.24 | 0.58 |
| 3:N:100:ALA:HA | 3:N:513:ILE:HD12 | 1.85 | 0.58 |
| 3:N:536:ALA:C | 5:P:317:LEU:HD21 | 2.24 | 0.58 |
| 5:P:214:GLN:O | 5:P:217:ASN:HB2 | 2.04 | 0.58 |
| 3:D:160:GLU:C | 3:D:161:LEU:HD23 | 2.24 | 0.58 |
| 3:D:540:LEU:O | 3:D:544:TYR:N | 2.33 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:542:ASP:HA | 3:D:545:ARG:HG3 | 1.84 | 0.58 |
| 3:D:591:VAL:HG12 | 3:D:599:PRO:HA | 1.84 | 0.58 |
| 4:E:84:ARG:O | 4:E:87:LYS:HB3 | 2.04 | 0.58 |
| 3:D:563:PRO:HG3 | 5:F:185:GLN:OE1 | 2.04 | 0.58 |
| 3:D:298:VAL:HB | 3:D:300:LYS:HE3 | 1.86 | 0.58 |
| 5:P:382:THR:HG23 | 5:P:397:ILE:HG21 | 1.85 | 0.58 |
| 5:P:270:LYS:HE3 | 5:P:295:MET:SD | 2.43 | 0.58 |
| 3:D:490:ALA:O | 3:D:493:ARG:HG2 | 2.03 | 0.58 |
| 3:D:800:LYS:CD | 3:D:800:LYS:H | 2.17 | 0.58 |
| 3:N:1472:ILE:HG22 | 3:N:1474:ALA:H | 1.68 | 0.58 |
| 5:F:189:GLU:CA | 5:F:192:LEU:HG | 2.26 | 0.58 |
| 5:F:85:LEU:C | 5:F:87:GLU:H | 2.07 | 0.58 |
| 3:D:843:PHE:CD1 | 3:D:849:ALA:HA | 2.39 | 0.58 |
| 2:M:1098:ASP:HB2 | 3:N:17:LYS:CE | 2.33 | 0.58 |
| 3:N:661:MET:HB3 | 3:N:667:ALA:HB2 | 1.85 | 0.58 |
| 1:K:122:ILE:HG22 | 1:K:123:MET:N | 2.17 | 0.58 |
| 2:M:857:ASP:CB | 2:M:978:ARG:HG2 | 2.34 | 0.58 |
| 3:D:990:ASP:C | 3:D:994:GLN:HE21 | 2.07 | 0.58 |
| 5:P:157:GLU:CD | 5:P:157:GLU:H | 2.06 | 0.58 |
| 1:L:23:PHE:N | 1:L:23:PHE:CD1 | 2.71 | 0.58 |
| 1:L:151:VAL:HB | 1:L:169:ALA:HB3 | 1.84 | 0.58 |
| 3:N:149:LYS:HG2 | 3:N:150:ARG:HG2 | 1.84 | 0.58 |
| 3:D:152:LEU:HG | 3:D:153:LEU:N | 2.18 | 0.58 |
| 3:D:99:ALA:O | 3:D:514:LEU:HB2 | 2.03 | 0.58 |
| 4:E:84:ARG:O | 4:E:88:GLU:HG2 | 2.04 | 0.58 |
| 3:D:438:ASP:O | 3:D:439:LEU:HD23 | 2.03 | 0.58 |
| 2:M:310:LEU:HD12 | 2:M:314:THR:HG23 | 1.86 | 0.58 |
| 2:C:73:LEU:HB3 | 2:C:93:PRO:O | 2.03 | 0.58 |
| 2:C:572:ILE:CD1 | 2:C:701:THR:HB | 2.33 | 0.58 |
| 1:K:138:LEU:HD21 | 1:K:140:MET:HE3 | 1.86 | 0.58 |
| 3:N:469:ASP:OD1 | 3:N:471:GLU:HB2 | 2.03 | 0.58 |
| 3:N:187:LYS:HG3 | 3:N:198:ARG:HA | 1.86 | 0.58 |
| 2:C:122:THR:HG22 | 2:C:123:GLU:N | 2.17 | 0.58 |
| 2:C:511:GLU:O | 2:C:525:SER:HA | 2.04 | 0.58 |
| 3:N:245:LEU:CA | 3:N:309:GLY:H | 2.07 | 0.58 |
| 2:C:232:GLU:O | 2:C:235:LEU:HB3 | 2.04 | 0.58 |
| 3:N:131:LYS:HB2 | 3:N:456:MET:HE2 | 1.85 | 0.58 |
| 3:D:1463:LYS:O | 3:D:1467:ILE:HG22 | 2.04 | 0.58 |
| 3:D:1478:SER:C | 3:D:1482:ARG:HG3 | 2.24 | 0.58 |
| 3:D:528:VAL:HG12 | 3:D:529:GLN:O | 2.04 | 0.58 |
| 3:D:653:PHE:CD1 | 3:D:653:PHE:N | 2.71 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:100:LEU:HD21 | 2:C:367:LEU:CD2 | 2.33 | 0.58 |
| 2:C:988:VAL:N | 3:D:948:THR:HG21 | 2.18 | 0.58 |
| 2:C:676:ILE:CD1 | 3:D:949:ILE:HB | 2.34 | 0.58 |
| 3:N:653:PHE:CD1 | 3:N:653:PHE:N | 2.70 | 0.58 |
| 1:L:33:GLY:O | 1:L:195:LEU:HD22 | 2.03 | 0.58 |
| 1:A:128:HIS:CE1 | 1:A:131:THR:HG23 | 2.39 | 0.58 |
| 3:D:1256:LEU:HB3 | 3:D:1257:PRO:HD3 | 1.86 | 0.58 |
| 3:N:167:GLU:C | 3:N:394:LEU:HD12 | 2.24 | 0.58 |
| 3:D:142:LEU:HD23 | 3:D:146:PRO:HA | 1.85 | 0.58 |
| 2:C:636:ALA:O | 2:C:637:LEU:HD23 | 2.04 | 0.58 |
| 3:N:230:TRP:HE1 | 3:N:233:LYS:CG | 2.16 | 0.58 |
| 3:N:1159:ARG:O | 3:N:1160:LEU:HD23 | 2.04 | 0.58 |
| 3:D:1147:ARG:O | 3:D:1166:LEU:HG | 2.04 | 0.58 |
| 2:M:884:GLN:O | 2:M:887:GLU:HB3 | 2.04 | 0.58 |
| 2:C:764:GLU:HB3 | 2:C:766:GLU:OE2 | 2.04 | 0.58 |
| 3:N:1182:GLU:O | 3:N:1182:GLU:HG2 | 2.02 | 0.58 |
| 2:C:293:PHE:CD1 | 2:C:294:GLU:HG3 | 2.39 | 0.58 |
| 4:E:39:VAL:CG1 | 4:E:72:ARG:HB3 | 2.33 | 0.58 |
| 3:N:456:MET:N | 3:N:456:MET:SD | 2.77 | 0.58 |
| 3:D:153:LEU:HG | 3:D:154:THR:N | 2.19 | 0.58 |
| 3:D:465:LEU:HD22 | 3:D:509:PRO:HB2 | 1.84 | 0.58 |
| 3:D:563:PRO:O | 3:D:565:ILE:N | 2.36 | 0.58 |
| 3:D:325:GLU:CG | 3:D:332:TYR:HB3 | 2.34 | 0.58 |
| 5:P:355:GLU:OE1 | 5:P:356:LYS:N | 2.36 | 0.58 |
| 2:C:73:LEU:HB3 | 2:C:94:LEU:HA | 1.85 | 0.58 |
| 3:D:1153:VAL:HG12 | 3:D:1155:VAL:HG23 | 1.86 | 0.58 |
| 3:N:1446:VAL:O | 3:N:1449:GLU:HG2 | 2.03 | 0.58 |
| 3:N:858:VAL:CG1 | 3:N:859:ASP:N | 2.67 | 0.58 |
| 5:F:94:LEU:HD11 | 5:F:190:ALA:HB3 | 1.86 | 0.58 |
| 2:M:939:ARG:HD2 | 2:M:982:PRO:CD | 2.33 | 0.58 |
| 1:A:109:VAL:HG12 | 1:A:129:ILE:HB | 1.86 | 0.58 |
| 3:N:172:PRO:HB2 | 3:N:175:VAL:HG21 | 1.86 | 0.58 |
| 3:N:1067:VAL:HG13 | 3:N:1068:LEU:H | 1.68 | 0.58 |
| 2:M:1031:ARG:HB2 | 3:N:622:ARG:NH1 | 2.18 | 0.58 |
| 3:N:135:LEU:CD1 | 3:N:148:GLU:HB2 | 2.32 | 0.58 |
| 3:N:153:LEU:HD21 | 3:N:158:TYR:CA | 2.34 | 0.58 |
| 3:D:1104:GLU:O | 3:D:1108:ARG:NH2 | 2.37 | 0.58 |
| 3:D:165:LYS:O | 3:D:396:VAL:HG23 | 2.02 | 0.58 |
| 3:D:288:MET:SD | 3:D:305:ALA:HB1 | 2.43 | 0.58 |
| 2:M:596:TYR:HA | 2:M:653:ASP:O | 2.04 | 0.58 |
| 2:M:807:ARG:C | 2:M:809:GLY:N | 2.51 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:266:GLU:HB3 | 3:N:286:VAL:HG22 | 1.84 | 0.58 |
| 3:D:953:ASP:O | 3:D:955:VAL:HG23 | 2.04 | 0.58 |
| 3:D:801:GLY:CA | 3:D:830:ALA:HB3 | 2.34 | 0.58 |
| 2:C:949:LYS:HZ3 | 3:D:796:ARG:NH1 | 2.02 | 0.58 |
| 2:M:1037:VAL:HG13 | 2:M:1049:LEU:HD21 | 1.86 | 0.58 |
| 2:C:639:GLN:HA | 2:C:657:ASP:O | 2.03 | 0.58 |
| 3:N:656:PHE:CZ | 3:N:751:LEU:HD23 | 2.39 | 0.58 |
| 1:A:80:LEU:O | 1:A:83:LYS:HB2 | 2.04 | 0.58 |
| 3:N:587:ARG:NH1 | 3:N:587:ARG:HB3 | 2.19 | 0.58 |
| 2:M:432:ARG:HG3 | 2:M:433:THR:N | 2.19 | 0.58 |
| 5:P:95:THR:O | 5:P:98:GLU:N | 2.37 | 0.58 |
| 3:N:1066:THR:O | 3:N:1067:VAL:C | 2.42 | 0.58 |
| 2:C:994:ILE:HG22 | 2:C:995:MET:N | 2.18 | 0.58 |
| 2:M:261:ILE:CG2 | 2:M:262:ALA:H | 2.17 | 0.57 |
| 2:C:523:ILE:O | 2:C:524:VAL:HG13 | 2.03 | 0.57 |
| 3:D:406:ASP:HB2 | 3:D:423:ASP:C | 2.24 | 0.57 |
| 3:D:222:GLY:HA2 | 3:D:333:LEU:O | 2.03 | 0.57 |
| 5:P:382:THR:HG22 | 5:P:394:ARG:HA | 1.85 | 0.57 |
| 5:P:262:VAL:C | 5:P:264:MET:N | 2.54 | 0.57 |
| 5:P:379:ARG:HB2 | 5:P:379:ARG:HH11 | 1.68 | 0.57 |
| 3:N:1489:GLN:NE2 | 4:O:73:LEU:N | 2.52 | 0.57 |
| 3:N:266:GLU:HB3 | 3:N:286:VAL:HG21 | 1.83 | 0.57 |
| 3:D:418:GLY:O | 3:D:428:LYS:HE2 | 2.04 | 0.57 |
| 1:L:28:LEU:HD22 | 1:L:32:PHE:HB2 | 1.86 | 0.57 |
| 1:K:45:LEU:HB2 | 2:M:856:GLU:HG3 | 1.86 | 0.57 |
| 3:N:930:LEU:HG | 3:N:934:LEU:HD11 | 1.86 | 0.57 |
| 1:K:76:VAL:HA | 1:K:79:ILE:CD1 | 2.30 | 0.57 |
| 2:M:327:HIS:CE1 | 2:M:488:ALA:HB1 | 2.39 | 0.57 |
| 2:M:23:VAL:HG12 | 2:M:121:MET:HE1 | 1.85 | 0.57 |
| 2:M:23:VAL:HG23 | 2:M:24:GLU:N | 2.19 | 0.57 |
| 2:M:833:LEU:HD11 | 2:M:837:ASP:HB2 | 1.86 | 0.57 |
| 3:N:502:PHE:CE2 | 3:N:1452:ILE:HG23 | 2.39 | 0.57 |
| 5:P:171:LYS:O | 5:P:174:LEU:HB3 | 2.03 | 0.57 |
| 1:K:143:ARG:HH11 | 1:K:158:ILE:HG23 | 1.68 | 0.57 |
| 3:N:269:PHE:HE2 | 3:N:271:VAL:HG22 | 1.68 | 0.57 |
| 4:E:25:LYS:HA | 4:E:28:GLN:CD | 2.23 | 0.57 |
| 4:E:37:ASN:HA | 4:E:93:TYR:CE2 | 2.38 | 0.57 |
| 3:D:284:LEU:HD12 | 3:D:290:PRO:CB | 2.28 | 0.57 |
| 5:F:413:SER:HA | 5:F:416:ARG:NH2 | 2.19 | 0.57 |
| 2:C:987:ILE:CA | 3:D:948:THR:HG21 | 2.34 | 0.57 |
| 3:N:1445:HIS:O | 3:N:1449:GLU:HG2 | 2.04 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:N:788:GLY:HA3 | 3:N:938:GLY:O | 2.04 | 0.57 |
| 3:D:875:THR:CG2 | 3:D:879:ARG:HG3 | 2.34 | 0.57 |
| 3:N:661:MET:SD | 3:N:673:ALA:HB1 | 2.44 | 0.57 |
| 1:L:36:LEU:O | 1:L:40:LEU:HD12 | 2.04 | 0.57 |
| 3:D:499:VAL:HG12 | 3:D:503:LEU:HD12 | 1.84 | 0.57 |
| 3:N:1028:ALA:O | 3:N:1029:ARG:HB2 | 2.03 | 0.57 |
| 3:D:474:GLU:OE2 | 3:D:475:LYS:HG3 | 2.04 | 0.57 |
| 2:M:289:THR:O | 2:M:290:LEU:HD23 | 2.03 | 0.57 |
| 4:E:40:LEU:HD21 | 4:E:44:GLU:CB | 2.34 | 0.57 |
| 2:C:182:VAL:HG22 | 2:C:221:LEU:HA | 1.86 | 0.57 |
| 2:C:517:ARG:H | 2:C:520:GLU:HB2 | 1.68 | 0.57 |
| 3:D:1085:ALA:HA | 3:D:1088:THR:HG22 | 1.85 | 0.57 |
| 3:D:1445:HIS:O | 3:D:1449:GLU:HG2 | 2.04 | 0.57 |
| 3:D:450:TYR:CE2 | 3:D:452:ILE:HG22 | 2.39 | 0.57 |
| 3:D:608:SER:HB2 | 3:D:614:PHE:CD1 | 2.39 | 0.57 |
| 3:N:399:ARG:HB3 | 3:N:401:TYR:CE1 | 2.36 | 0.57 |
| 5:P:412:GLU:HA | 5:P:412:GLU:OE2 | 2.03 | 0.57 |
| 5:P:356:LYS:HD3 | 5:P:417:LYS:NZ | 2.19 | 0.57 |
| 2:C:39:ARG:O | 2:C:40:GLU:HB2 | 2.04 | 0.57 |
| 5:F:393:THR:HG22 | 5:F:394:ARG:N | 2.19 | 0.57 |
| 3:D:800:LYS:NZ | 3:D:826:PRO:HD3 | 2.19 | 0.57 |
| 3:D:433:GLY:O | 3:D:434:ARG:HD2 | 2.04 | 0.57 |
| 3:N:1382:THR:O | 3:N:1389:LEU:HD21 | 2.05 | 0.57 |
| 3:N:1149:LEU:HG | 3:N:1162:GLU:HA | 1.86 | 0.57 |
| 2:M:31:GLN:HA | 2:M:35:PRO:HG2 | 1.87 | 0.57 |
| 1:L:144:VAL:HG12 | 1:L:145:ASP:N | 2.19 | 0.57 |
| 2:M:38:LYS:HG3 | 2:M:39:ARG:N | 2.16 | 0.57 |
| 3:N:106:LYS:HB3 | 3:N:586:ARG:NH1 | 2.18 | 0.57 |
| 1:L:90:LEU:HG | 1:L:119:ASP:O | 2.05 | 0.57 |
| 4:E:57:ASP:O | 4:E:63:TRP:NE1 | 2.37 | 0.57 |
| 3:N:1333:HIS:HA | 3:N:1421:LEU:HD23 | 1.84 | 0.57 |
| 2:M:1069:ALA:HB1 | 2:M:1075:ASP:O | 2.04 | 0.57 |
| 2:M:203:ASP:CB | 2:M:228:ALA:O | 2.51 | 0.57 |
| 2:M:198:ARG:HH11 | 2:M:203:ASP:N | 2.02 | 0.57 |
| 2:C:203:ASP:OD1 | 2:C:205:GLU:HB3 | 2.03 | 0.57 |
| 3:N:537:THR:HA | 5:P:317:LEU:HD11 | 1.87 | 0.57 |
| 2:C:1083:GLU:CD | 3:D:88:TYR:HH | 2.07 | 0.57 |
| 3:D:458:ALA:O | 3:D:459:GLU:C | 2.41 | 0.57 |
| 3:D:86:ARG:O | 3:D:522:PRO:HD2 | 2.04 | 0.57 |
| 3:D:811:GLU:O | 3:D:815:ALA:CB | 2.50 | 0.57 |
| 1:B:41:ARG:O | 1:B:44:LEU:HB2 | 2.05 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:375:SER:C | 2:C:377:PRO:HD2 | 2.25 | 0.57 |
| 5:P:278:LEU:O | 5:P:279:GLN:C | 2.43 | 0.57 |
| 2:M:128:ILE:HA | 2:M:132:ALA:O | 2.04 | 0.57 |
| 2:C:773:LEU:O | 2:C:777:ILE:HG13 | 2.04 | 0.57 |
| 1:L:137:ARG:HG2 | 1:L:137:ARG:NH1 | 2.17 | 0.57 |
| 2:C:914:ILE:HD12 | 2:C:914:ILE:H | 1.68 | 0.57 |
| 3:N:793:THR:HG21 | 3:N:906:GLN:CG | 2.34 | 0.57 |
| 3:N:854:ALA:C | 3:N:856:GLY:H | 2.08 | 0.57 |
| 3:N:1167:SER:O | 3:N:1170:ASP:HB2 | 2.03 | 0.57 |
| 2:M:41:ASN:HA | 2:M:45:GLN:CB | 2.32 | 0.57 |
| 3:D:1344:VAL:O | 3:D:1347:TYR:HB3 | 2.04 | 0.57 |
| 1:L:85:LEU:HD12 | 1:L:86:VAL:N | 2.19 | 0.57 |
| 3:N:1120:VAL:CB | 3:N:1144:LEU:HD21 | 2.34 | 0.57 |
| 3:N:986:ARG:O | 3:N:987:GLU:C | 2.42 | 0.57 |
| 1:A:10:VAL:HG12 | 1:A:12:THR:HG23 | 1.87 | 0.57 |
| 3:D:903:ASP:O | 3:D:904:VAL:HG13 | 2.03 | 0.57 |
| 2:M:708:TYR:O | 2:M:824:ARG:HA | 2.05 | 0.57 |
| 2:M:601:GLY:O | 2:M:648:ARG:HA | 2.04 | 0.57 |
| 2:M:205:GLU:HA | 2:M:209:ARG:HH11 | 1.70 | 0.57 |
| 3:N:339:TRP:CH2 | 3:N:341:GLU:HG3 | 2.40 | 0.57 |
| 3:N:126:VAL:O | 3:N:132:TYR:HD1 | 1.88 | 0.57 |
| 3:D:1468:LEU:HD23 | 3:D:1470:ARG:HB2 | 1.85 | 0.57 |
| 3:D:540:LEU:O | 3:D:541:ASN:C | 2.43 | 0.57 |
| 4:E:26:ARG:HH21 | 4:E:38:THR:HA | 1.70 | 0.57 |
| 3:D:227:LEU:HD11 | 3:D:327:GLU:N | 2.19 | 0.57 |
| 3:D:247:GLU:HA | 3:D:308:LYS:HZ3 | 1.68 | 0.57 |
| 3:D:674:ARG:NH2 | 5:F:342:VAL:HG13 | 2.19 | 0.57 |
| 3:D:800:LYS:CE | 3:D:800:LYS:H | 2.16 | 0.57 |
| 2:C:878:SER:C | 2:C:879:ARG:HD2 | 2.25 | 0.57 |
| 2:C:910:LYS:HE3 | 2:C:912:PRO:HB2 | 1.86 | 0.57 |
| 1:K:184:THR:O | 1:K:192:LEU:HB2 | 2.05 | 0.57 |
| 2:M:971:LYS:HA | 2:M:988:VAL:HA | 1.86 | 0.57 |
| 3:N:881:LEU:HD21 | 3:N:941:PHE:HZ | 1.69 | 0.57 |
| 3:D:1278:ASP:HA | 3:D:1319:VAL:O | 2.05 | 0.57 |
| 2:C:479:VAL:HG23 | 2:C:506:ASN:O | 2.04 | 0.57 |
| 2:C:713:ARG:HA | 2:C:818:GLY:O | 2.04 | 0.57 |
| 3:N:704:ARG:HB2 | 3:N:745:MET:SD | 2.44 | 0.57 |
| 5:P:180:GLY:O | 5:P:183:ALA:HB3 | 2.05 | 0.57 |
| 2:C:630:ARG:HG3 | 2:C:634:GLY:HA2 | 1.85 | 0.57 |
| 3:D:966:GLU:HA | 3:D:969:ARG:NE | 2.20 | 0.57 |
| 2:M:173:ASP:O | 2:M:174:LEU:HD23 | 2.03 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:576:ALA:O | 2:M:900:ARG:NH1 | 2.37 | 0.57 |
| 3:N:217:LYS:HB2 | 3:N:339:TRP:CD1 | 2.39 | 0.57 |
| 2:C:198:ARG:NE | 2:C:231:PRO:HG3 | 2.19 | 0.57 |
| 2:C:444:PRO:HG3 | 2:C:452:ILE:HB | 1.85 | 0.57 |
| 3:N:133:ILE:HG23 | 3:N:456:MET:SD | 2.45 | 0.57 |
| 3:N:522:PRO:CA | 3:N:525:ARG:NH1 | 2.68 | 0.57 |
| 3:D:1104:GLU:N | 3:D:1104:GLU:OE1 | 2.37 | 0.57 |
| 2:C:1046:ALA:HA | 3:D:1472:ILE:HB | 1.85 | 0.57 |
| 3:D:160:GLU:CD | 3:D:165:LYS:HE2 | 2.25 | 0.57 |
| 3:D:546:ARG:O | 3:D:549:ASN:HB2 | 2.05 | 0.57 |
| 4:E:19:LEU:O | 4:E:22:VAL:HB | 2.04 | 0.57 |
| 5:P:401:GLU:O | 5:P:405:LEU:HG | 2.05 | 0.57 |
| 5:P:295:MET:HG3 | 5:P:299:TRP:CD2 | 2.39 | 0.57 |
| 3:D:80:VAL:O | 3:D:81:THR:HG23 | 2.05 | 0.57 |
| 2:C:882:LEU:O | 2:C:885:ILE:N | 2.38 | 0.57 |
| 5:F:192:LEU:HB3 | 11:F:424:HOH:O | 2.05 | 0.57 |
| 3:N:654:LYS:HB3 | 3:N:655:PRO:CD | 2.28 | 0.57 |
| 1:A:111:ALA:O | 1:A:113:ASP:N | 2.38 | 0.57 |
| 3:D:1311:LEU:HG | 3:D:1312:LEU:N | 2.20 | 0.57 |
| 2:C:799:ILE:O | 2:C:799:ILE:HG13 | 2.04 | 0.57 |
| 2:C:706:GLU:HG3 | 2:C:708:TYR:CE1 | 2.39 | 0.57 |
| 3:D:965:GLU:O | 3:D:967:ALA:N | 2.37 | 0.57 |
| 3:N:1046:GLN:CB | 3:N:1052:THR:HA | 2.34 | 0.57 |
| 4:E:86:GLN:O | 4:E:90:GLU:N | 2.37 | 0.57 |
| 2:C:715:THR:HG22 | 2:C:717:LEU:H | 1.68 | 0.57 |
| 3:D:1434:TRP:CE3 | 3:D:1457:ASP:HB2 | 2.40 | 0.57 |
| 3:N:1383:ASP:HB3 | 3:N:1416:ALA:H | 1.69 | 0.57 |
| 3:N:219:GLU:HG2 | 3:N:220:ARG:N | 2.15 | 0.57 |
| 3:N:241:ILE:HG12 | 3:N:312:ARG:CG | 2.32 | 0.57 |
| 3:D:1048:PRO:HG3 | 3:D:1075:HIS:CD2 | 2.34 | 0.57 |
| 3:N:125:GLN:HG3 | 3:N:126:VAL:N | 2.19 | 0.57 |
| 5:P:213:ILE:HG22 | 5:P:217:ASN:ND2 | 2.19 | 0.57 |
| 3:D:1107:VAL:HB | 3:D:1219:GLU:H | 1.69 | 0.57 |
| 3:D:119:SER:N | 3:D:123:LEU:HB2 | 2.20 | 0.57 |
| 3:D:223:LEU:HG | 3:D:224:ARG:N | 2.14 | 0.57 |
| 5:P:352:GLU:O | 5:P:354:LEU:N | 2.37 | 0.57 |
| 1:B:61:VAL:HG22 | 1:B:62:LEU:N | 2.20 | 0.57 |
| 2:M:604:ALA:HB3 | 2:M:612:VAL:O | 2.05 | 0.57 |
| 3:D:671:LYS:HE2 | 3:D:675:ARG:HD3 | 1.87 | 0.57 |
| 2:C:101:ILE:HD13 | 2:C:107:LEU:HD22 | 1.86 | 0.57 |
| 3:D:1156:LEU:HD12 | 3:D:1173:LEU:HD11 | 1.87 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:N:252:ARG:NE | 3:N:300:LYS:HA | 2.16 | 0.57 |
| 3:N:257:GLY:HA2 | 3:N:274:ARG:CA | 2.32 | 0.57 |
| 3:D:844:ALA:O | 3:D:867:ARG:HD2 | 2.04 | 0.57 |
| 1:K:124:ASN:HB3 | 1:K:127:LEU:HB2 | 1.87 | 0.57 |
| 1:K:25:LEU:HD21 | 1:L:224:TYR:HB2 | 1.86 | 0.57 |
| 2:C:603:VAL:HG21 | 2:C:647:GLN:HB3 | 1.85 | 0.57 |
| 1:A:57:TYR:O | 1:A:140:MET:HB2 | 2.05 | 0.57 |
| 5:F:163:LEU:HA | 5:F:166:LEU:CD1 | 2.35 | 0.57 |
| 2:C:805:ARG:NE | 2:C:807:ARG:HH21 | 2.02 | 0.57 |
| 3:N:284:LEU:HD12 | 3:N:290:PRO:HB3 | 1.85 | 0.57 |
| 2:C:194:VAL:CA | 2:C:197:LEU:HG | 2.35 | 0.57 |
| 2:C:148:PHE:N | 2:C:323:ASP:OD2 | 2.31 | 0.57 |
| 2:C:415:PRO:CB | 2:C:418:LEU:HB2 | 2.29 | 0.57 |
| 2:C:488:ALA:O | 2:C:491:GLU:HB3 | 2.05 | 0.57 |
| 3:D:108:VAL:CG1 | 3:D:109:PRO:HA | 2.34 | 0.57 |
| 3:D:537:THR:C | 5:F:317:LEU:HG | 2.24 | 0.57 |
| 3:D:591:VAL:HB | 3:D:598:ARG:O | 2.05 | 0.57 |
| 3:D:5:VAL:HG22 | 3:D:6:ARG:N | 2.19 | 0.57 |
| 3:D:924:MET:O | 3:D:927:THR:HB | 2.05 | 0.57 |
| 3:D:924:MET:HG2 | 4:E:7:ASP:OD2 | 2.05 | 0.57 |
| 5:F:386:VAL:CG2 | 5:F:387:GLY:H | 2.16 | 0.57 |
| 2:M:369:PRO:HD2 | 2:M:371:LYS:HD2 | 1.87 | 0.57 |
| 5:F:277:GLN:HA | 5:F:280:GLN:CD | 2.25 | 0.57 |
| 3:D:800:LYS:HD2 | 3:D:800:LYS:H | 1.69 | 0.57 |
| 3:N:771:SER:CB | 3:N:778:LEU:HD22 | 2.34 | 0.57 |
| 3:N:858:VAL:CG1 | 3:N:859:ASP:H | 2.17 | 0.57 |
| 3:N:584:ASN:ND2 | 3:N:590:PRO:HG2 | 2.18 | 0.57 |
| 2:C:596:TYR:HA | 2:C:653:ASP:O | 2.05 | 0.57 |
| 2:C:597:ALA:N | 2:C:653:ASP:O | 2.38 | 0.57 |
| 1:K:100:LEU:HD22 | 1:K:102:LYS:HE3 | 1.87 | 0.57 |
| 2:M:53:PRO:HB3 | 2:M:67:ASP:CG | 2.25 | 0.57 |
| 2:C:841:ASN:HD21 | 2:C:845:ASN:CB | 2.18 | 0.57 |
| 4:O:25:LYS:HA | 4:O:28:GLN:NE2 | 2.20 | 0.57 |
| 3:D:1293:PHE:CZ | 3:D:1300:SER:HB3 | 2.40 | 0.57 |
| 4:O:82:GLU:O | 4:O:85:LEU:HG | 2.04 | 0.57 |
| 2:C:224:GLU:HB3 | 2:C:227:PHE:CD1 | 2.40 | 0.57 |
| 3:N:457:GLY:O | 3:N:461:ILE:HG12 | 2.05 | 0.57 |
| 3:N:45:PHE:O | 3:N:47:GLU:N | 2.37 | 0.57 |
| 3:D:1464:GLU:O | 3:D:1467:ILE:HG22 | 2.04 | 0.57 |
| 2:M:69:LEU:HD23 | 2:M:70:GLU:HG3 | 1.87 | 0.57 |
| 1:A:39:PRO:HG3 | 1:B:39:PRO:CG | 2.30 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:M:605:LYS:CB | 2:M:610:ARG:HH21 | 2.16 | 0.57 |
| 2:C:345:ARG:O | 2:C:348:LEU:HB3 | 2.05 | 0.57 |
| 2:C:41:ASN:O | 2:C:43:GLY:N | 2.38 | 0.57 |
| 2:C:882:LEU:O | 2:C:883:GLY:C | 2.43 | 0.57 |
| 3:N:788:GLY:H | 3:N:942:SER:HB3 | 1.68 | 0.57 |
| 5:F:189:GLU:HA | 5:F:192:LEU:CD1 | 2.33 | 0.57 |
| 1:L:206:THR:HG22 | 1:L:208:LEU:H | 1.70 | 0.57 |
| 3:N:653:PHE:O | 3:N:654:LYS:C | 2.42 | 0.57 |
| 3:N:732:VAL:C | 3:N:734:GLU:N | 2.57 | 0.57 |
| 1:A:107:LYS:NZ | 1:A:108:GLU:O | 2.37 | 0.57 |
| 1:K:9:PRO:HD2 | 1:L:224:TYR:CE1 | 2.40 | 0.57 |
| 2:M:50:GLU:C | 2:M:52:PHE:N | 2.58 | 0.57 |
| 2:M:430:VAL:O | 2:M:430:VAL:HG13 | 2.04 | 0.57 |
| 2:M:488:ALA:O | 2:M:491:GLU:HB3 | 2.05 | 0.57 |
| 2:C:1052:MET:O | 2:C:1056:LYS:HB2 | 2.05 | 0.57 |
| 2:C:343:GLN:HG2 | 2:C:385:PHE:HB2 | 1.87 | 0.57 |
| 1:K:1:MET:O | 1:K:1:MET:SD | 2.62 | 0.57 |
| 1:L:5:LYS:C | 1:L:7:LYS:H | 2.07 | 0.57 |
| 2:M:380:ALA:O | 2:M:381:ALA:C | 2.43 | 0.57 |
| 2:C:122:THR:HB | 2:C:124:ASP:OD1 | 2.05 | 0.57 |
| 1:B:84:GLU:HB2 | 1:B:127:LEU:HD21 | 1.87 | 0.57 |
| 3:N:1042:ARG:HG2 | 3:N:1042:ARG:HH11 | 1.69 | 0.57 |
| 1:K:98:THR:CG2 | 1:K:141:GLU:HB3 | 2.35 | 0.57 |
| 2:M:193:LEU:CD2 | 2:M:307:LEU:HD22 | 2.34 | 0.57 |
| 2:C:513:VAL:O | 2:C:523:ILE:HA | 2.05 | 0.57 |
| 3:D:156:GLU:OE2 | 3:D:156:GLU:N | 2.38 | 0.57 |
| 3:D:99:ALA:O | 3:D:514:LEU:N | 2.38 | 0.57 |
| 3:D:530:VAL:HG22 | 3:D:534:ARG:O | 2.04 | 0.57 |
| 3:D:223:LEU:CG | 3:D:224:ARG:H | 2.13 | 0.57 |
| 5:F:383:LEU:CD2 | 5:F:394:ARG:HD3 | 2.34 | 0.57 |
| 1:A:209:GLU:HA | 1:A:212:ASN:ND2 | 2.20 | 0.57 |
| 2:C:69:LEU:CD2 | 2:C:70:GLU:HG3 | 2.34 | 0.57 |
| 2:M:352:ALA:HA | 2:M:355:VAL:CG1 | 2.33 | 0.57 |
| 1:L:163:ASN:O | 1:L:165:ILE:HG13 | 2.05 | 0.57 |
| 3:N:673:ALA:CA | 3:N:676:MET:HB3 | 2.34 | 0.57 |
| 1:K:41:ARG:HA | 1:K:44:LEU:HD12 | 1.87 | 0.57 |
| 1:K:86:VAL:HG21 | 1:K:202:ASP:HB2 | 1.86 | 0.57 |
| 1:L:38:ASN:O | 1:L:41:ARG:HB3 | 2.04 | 0.57 |
| 3:N:1402:ALA:HA | 3:N:1415:VAL:HG21 | 1.86 | 0.57 |
| 3:N:984:THR:HG22 | 3:N:987:GLU:HB2 | 1.87 | 0.57 |
| 5:F:245:GLN:CA | 5:F:245:GLN:HE21 | 2.13 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:726:ILE:C | 2:C:728:HIS:H | 2.08 | 0.57 |
| 3:D:821:VAL:C | 3:D:823:LEU:H | 2.07 | 0.57 |
| 1:A:14:ARG:HG3 | 1:A:14:ARG:O | 2.05 | 0.56 |
| 3:N:119:SER:N | 3:N:123:LEU:HB2 | 2.20 | 0.56 |
| 3:D:50:PHE:CD2 | 3:D:522:PRO:HD3 | 2.40 | 0.56 |
| 3:D:224:ARG:NH1 | 3:D:332:TYR:CD1 | 2.73 | 0.56 |
| 5:F:261:PRO:HB2 | 5:F:264:MET:HG2 | 1.87 | 0.56 |
| 2:M:128:ILE:C | 2:M:129:ILE:HD13 | 2.25 | 0.56 |
| 3:D:827:ILE:HG23 | 3:D:837:GLY:CA | 2.34 | 0.56 |
| 2:C:914:ILE:HD12 | 2:C:914:ILE:N | 2.20 | 0.56 |
| 1:A:49:PRO:CA | 1:A:148:VAL:HG12 | 2.35 | 0.56 |
| 2:C:654:LEU:CD1 | 2:C:655:LEU:H | 2.12 | 0.56 |
| 3:N:662:GLU:HA | 3:N:667:ALA:O | 2.03 | 0.56 |
| 1:K:110:LYS:HB2 | 1:K:112:ARG:CG | 2.28 | 0.56 |
| 1:K:39:PRO:O | 1:K:42:ARG:HB2 | 2.05 | 0.56 |
| 2:M:926:PHE:O | 2:M:929:ARG:N | 2.31 | 0.56 |
| 2:C:504:GLU:O | 2:C:506:ASN:N | 2.38 | 0.56 |
| 1:A:124:ASN:HB2 | 1:A:127:LEU:HB2 | 1.87 | 0.56 |
| 3:N:30:GLU:HG3 | 5:P:259:ARG:HB2 | 1.86 | 0.56 |
| 5:P:253:ASP:HA | 5:P:259:ARG:HH12 | 1.69 | 0.56 |
| 5:P:245:GLN:NE2 | 5:P:245:GLN:CA | 2.68 | 0.56 |
| 2:M:122:THR:HG22 | 2:M:123:GLU:N | 2.19 | 0.56 |
| 2:C:1039:ALA:HA | 3:D:1227:GLN:HE22 | 1.70 | 0.56 |
| 3:N:1292:VAL:HG12 | 3:N:1293:PHE:N | 2.19 | 0.56 |
| 3:N:250:LEU:HD13 | 3:N:306:GLU:HG2 | 1.86 | 0.56 |
| 3:N:1479:ASP:HA | 3:N:1483:PHE:HE1 | 1.70 | 0.56 |
| 2:M:265:ARG:HD2 | 2:M:268:ASP:HA | 1.85 | 0.56 |
| 2:M:582:GLY:N | 2:M:584:GLU:OE2 | 2.29 | 0.56 |
| 3:N:22:SER:C | 3:N:24:GLY:H | 2.08 | 0.56 |
| 3:D:1445:HIS:O | 3:D:1446:VAL:C | 2.44 | 0.56 |
| 3:D:257:GLY:N | 3:D:272:LEU:HD22 | 2.20 | 0.56 |
| 3:D:225:LEU:HD22 | 3:D:243:ALA:HB2 | 1.87 | 0.56 |
| 3:D:186:VAL:HG12 | 3:D:187:LYS:H | 1.68 | 0.56 |
| 5:F:381:HIS:H | 5:F:385:GLU:CD | 2.09 | 0.56 |
| 5:P:308:LEU:H | 5:P:308:LEU:HD23 | 1.69 | 0.56 |
| 3:N:1093:TYR:O | 3:N:1097:LYS:HG2 | 2.04 | 0.56 |
| 2:C:577:PRO:HG3 | 2:C:993:PHE:CG | 2.40 | 0.56 |
| 3:N:685:ASP:O | 3:N:687:VAL:N | 2.37 | 0.56 |
| 1:K:64:GLU:HG3 | 1:K:64:GLU:O | 2.04 | 0.56 |
| 2:M:91:GLN:HB2 | 2:M:118:ILE:C | 2.26 | 0.56 |
| 3:D:970:LYS:HA | 3:D:973:GLN:NE2 | 2.20 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:N:188:GLY:H | 3:N:198:ARG:CA | 2.17 | 0.56 |
| 2:C:293:PHE:HD1 | 2:C:294:GLU:HG3 | 1.68 | 0.56 |
| 4:E:50:THR:O | 4:E:55:PHE:CE1 | 2.58 | 0.56 |
| 4:E:40:LEU:HD13 | 4:E:72:ARG:NH1 | 2.20 | 0.56 |
| 2:C:285:LEU:HD12 | 2:C:289:THR:O | 2.04 | 0.56 |
| 2:C:413:LEU:CA | 2:C:419:THR:HG21 | 2.35 | 0.56 |
| 2:C:498:GLN:HA | 2:C:533:ASP:OD2 | 2.05 | 0.56 |
| 3:D:1066:THR:HB | 3:D:1069:GLU:HG3 | 1.86 | 0.56 |
| 3:D:556:LYS:O | 3:D:560:GLN:N | 2.38 | 0.56 |
| 5:F:132:ARG:HB3 | 5:F:136:LEU:HD11 | 1.87 | 0.56 |
| 5:F:210:LEU:HA | 5:F:213:ILE:CD1 | 2.16 | 0.56 |
| 3:D:1479:ASP:HA | 3:D:1482:ARG:NE | 2.19 | 0.56 |
| 3:D:249:TYR:HD2 | 3:D:288:MET:HE1 | 1.71 | 0.56 |
| 3:D:225:LEU:O | 3:D:330:THR:HA | 2.05 | 0.56 |
| 2:M:641:PRO:O | 2:M:642:ARG:HD3 | 2.06 | 0.56 |
| 1:A:206:THR:HG23 | 1:A:207:PRO:HD2 | 1.86 | 0.56 |
| 2:C:54:ILE:HD12 | 2:C:352:ALA:HB1 | 1.87 | 0.56 |
| 2:C:55:GLU:CD | 2:C:57:GLU:HB3 | 2.26 | 0.56 |
| 2:C:352:ALA:HA | 2:C:355:VAL:CG1 | 2.33 | 0.56 |
| 2:M:101:ILE:HG23 | 2:M:107:LEU:HD23 | 1.88 | 0.56 |
| 5:P:300:ASP:CG | 5:P:302:LYS:HE3 | 2.26 | 0.56 |
| 2:M:772:ARG:NH2 | 5:P:379:ARG:HG3 | 2.20 | 0.56 |
| 5:P:370:LYS:HG3 | 5:P:371:LEU:H | 1.68 | 0.56 |
| 3:D:1412:LYS:O | 3:D:1414:PRO:HD3 | 2.05 | 0.56 |
| 3:D:1263:PHE:CE1 | 3:D:1352:ILE:HD13 | 2.40 | 0.56 |
| 3:D:1397:LYS:HB2 | 3:D:1398:TRP:HZ3 | 1.68 | 0.56 |
| 3:D:800:LYS:HE3 | 3:D:826:PRO:HD3 | 1.86 | 0.56 |
| 3:D:1038:LEU:O | 3:D:1060:SER:HB2 | 2.05 | 0.56 |
| 3:N:1094:LEU:HG | 3:N:1095:THR:N | 2.19 | 0.56 |
| 2:M:1039:ALA:HB3 | 3:N:713:ILE:HD12 | 1.87 | 0.56 |
| 2:M:853:LEU:HB2 | 2:M:858:MET:CE | 2.35 | 0.56 |
| 3:N:939:PHE:O | 3:N:941:PHE:N | 2.38 | 0.56 |
| 3:N:792:ILE:HG21 | 3:N:941:PHE:CD1 | 2.41 | 0.56 |
| 3:D:428:LYS:HG2 | 3:D:429:SER:H | 1.69 | 0.56 |
| 3:N:657:LEU:HG | 3:N:661:MET:CE | 2.34 | 0.56 |
| 3:N:350:HIS:ND1 | 5:P:232:ARG:NH2 | 2.52 | 0.56 |
| 2:M:959:PRO:HA | 2:M:962:GLN:OE1 | 2.04 | 0.56 |
| 2:M:508:ILE:HG22 | 2:M:509:ALA:N | 2.20 | 0.56 |
| 1:B:13:VAL:CG2 | 1:B:14:ARG:N | 2.67 | 0.56 |
| 3:N:1401:GLU:H | 3:N:1401:GLU:CD | 2.09 | 0.56 |
| 3:N:1403:LEU:O | 3:N:1408:ILE:HG13 | 2.05 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:206:ARG:HG3 | 3:N:207:PHE:H | 1.70 | 0.56 |
| 3:N:173:PRO:HG3 | 3:N:209:ARG:HH12 | 1.71 | 0.56 |
| 5:F:156:VAL:HG23 | 5:F:157:GLU:CD | 2.26 | 0.56 |
| 2:C:1014:SER:CA | 2:C:1021:LEU:HD22 | 2.35 | 0.56 |
| 5:P:172:ARG:HG3 | 5:P:173:TYR:N | 2.19 | 0.56 |
| 4:E:62:THR:O | 4:E:66:LYS:HG2 | 2.05 | 0.56 |
| 1:K:176:ARG:NE | 2:M:865:THR:HG22 | 2.20 | 0.56 |
| 1:A:9:PRO:HB2 | 1:A:25:LEU:HD11 | 1.87 | 0.56 |
| 3:N:95:LEU:HB3 | 3:N:97:THR:O | 2.04 | 0.56 |
| 2:C:715:THR:HB | 2:C:718:GLY:O | 2.04 | 0.56 |
| 1:B:95:GLN:HE22 | 1:B:146:ARG:NH1 | 2.02 | 0.56 |
| 2:M:745:ILE:HG22 | 2:M:746:GLY:N | 2.20 | 0.56 |
| 2:M:551:GLU:N | 2:M:551:GLU:OE1 | 2.39 | 0.56 |
| 5:P:361:LEU:HD12 | 5:P:362:SER:H | 1.70 | 0.56 |
| 2:C:198:ARG:HH21 | 2:C:231:PRO:HD3 | 1.70 | 0.56 |
| 2:C:258:TYR:O | 2:C:290:LEU:HD12 | 2.05 | 0.56 |
| 3:N:122:GLU:O | 3:N:126:VAL:CB | 2.53 | 0.56 |
| 3:N:138:LYS:O | 3:N:452:ILE:HG22 | 2.06 | 0.56 |
| 3:N:571:LYS:O | 3:N:574:LEU:HB3 | 2.06 | 0.56 |
| 5:P:76:SER:C | 5:P:78:SER:H | 2.06 | 0.56 |
| 3:D:135:LEU:HD11 | 3:D:148:GLU:CG | 2.36 | 0.56 |
| 3:D:9:ARG:HG2 | 3:D:10:ILE:N | 2.20 | 0.56 |
| 5:F:117:SER:O | 5:F:121:GLY:N | 2.38 | 0.56 |
| 3:D:256:GLU:O | 3:D:274:ARG:HB2 | 2.04 | 0.56 |
| 3:D:210:ARG:H | 3:D:389:GLU:HB2 | 1.70 | 0.56 |
| 2:M:649:VAL:HG13 | 2:M:650:ARG:HH21 | 1.69 | 0.56 |
| 2:C:51:THR:HG21 | 2:C:348:LEU:HG | 1.87 | 0.56 |
| 1:K:12:THR:HA | 1:L:229:GLN:CB | 2.20 | 0.56 |
| 3:D:1149:LEU:HD23 | 3:D:1161:GLU:O | 2.05 | 0.56 |
| 2:M:7:GLY:HA3 | 2:M:907:ASP:OD2 | 2.05 | 0.56 |
| 3:N:880:ILE:O | 3:N:883:ALA:HB3 | 2.05 | 0.56 |
| 2:C:672:VAL:HG21 | 2:C:868:ASP:HB2 | 1.87 | 0.56 |
| 1:B:73:GLU:HG3 | 1:B:130:ALA:HB1 | 1.87 | 0.56 |
| 2:C:614:ARG:HA | 2:C:619:ARG:O | 2.06 | 0.56 |
| 2:C:594:ALA:HB1 | 2:C:654:LEU:CD1 | 2.35 | 0.56 |
| 1:B:47:SER:O | 1:B:48:ILE:HD12 | 2.05 | 0.56 |
| 1:K:13:VAL:HG22 | 1:K:14:ARG:N | 2.21 | 0.56 |
| 3:N:1165:TYR:CE2 | 3:N:1214:PRO:HB3 | 2.41 | 0.56 |
| 3:N:169:TYR:HB3 | 3:N:195:VAL:HG11 | 1.88 | 0.56 |
| 3:N:1041:LEU:HG | 3:N:1043:GLY:H | 1.71 | 0.56 |
| 2:C:167:LYS:HB3 | 2:C:167:LYS:NZ | 2.20 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:F:302:LYS:O | 5:F:305:GLU:HB3 | 2.05 | 0.56 |
| 2:M:1055:LEU:HD21 | 2:M:1079:PRO:HG3 | 1.87 | 0.56 |
| 2:M:548:PRO:HG3 | 2:M:842:ARG:NH2 | 2.20 | 0.56 |
| 3:N:227:LEU:HD11 | 3:N:327:GLU:N | 2.20 | 0.56 |
| 2:C:194:VAL:HA | 2:C:197:LEU:CD1 | 2.36 | 0.56 |
| 2:C:405:ARG:NH2 | 2:C:409:ARG:HD2 | 2.21 | 0.56 |
| 3:N:135:LEU:HG | 3:N:151:GLN:O | 2.04 | 0.56 |
| 3:D:118:LEU:HA | 3:D:123:LEU:CD1 | 2.32 | 0.56 |
| 3:D:100:ALA:HB3 | 3:D:128:TYR:HE2 | 1.68 | 0.56 |
| 3:D:134:VAL:HG12 | 3:D:152:LEU:HA | 1.86 | 0.56 |
| 3:D:545:ARG:HB3 | 3:D:545:ARG:NH1 | 2.19 | 0.56 |
| 2:C:1015:LEU:N | 5:F:333:ILE:O | 2.31 | 0.56 |
| 2:C:93:PRO:HA | 2:C:117:HIS:CA | 2.35 | 0.56 |
| 1:K:71:VAL:HG22 | 1:K:132:LEU:HD22 | 1.87 | 0.56 |
| 2:C:41:ASN:HB3 | 2:C:49:ARG:CZ | 2.35 | 0.56 |
| 5:P:305:GLU:HA | 5:P:308:LEU:HD11 | 1.87 | 0.56 |
| 5:F:267:THR:HA | 5:F:270:LYS:HB3 | 1.88 | 0.56 |
| 5:F:291:ILE:HD12 | 5:F:291:ILE:O | 2.05 | 0.56 |
| 1:L:99:LEU:HB3 | 1:L:114:PHE:CD2 | 2.41 | 0.56 |
| 1:L:57:TYR:HB2 | 1:L:164:ALA:HA | 1.88 | 0.56 |
| 2:C:911:GLU:HB2 | 2:C:912:PRO:HD3 | 1.87 | 0.56 |
| 3:N:295:GLY:CA | 3:N:302:GLN:HB3 | 2.33 | 0.56 |
| 1:B:85:LEU:HD12 | 1:B:86:VAL:N | 2.20 | 0.56 |
| 3:D:417:PRO:HB2 | 3:D:428:LYS:CG | 2.30 | 0.56 |
| 2:C:1007:ALA:HB2 | 3:D:648:MET:HG3 | 1.88 | 0.56 |
| 3:N:598:ARG:HH11 | 3:N:598:ARG:HG2 | 1.71 | 0.56 |
| 3:N:1394:VAL:O | 3:N:1398:TRP:CD1 | 2.58 | 0.56 |
| 3:N:1409:ALA:C | 3:N:1411:GLY:H | 2.08 | 0.56 |
| 5:P:157:GLU:O | 5:P:158:GLU:C | 2.42 | 0.56 |
| 3:D:710:ARG:HG3 | 3:D:711:LEU:HD12 | 1.88 | 0.56 |
| 3:D:1365:ASP:O | 3:D:1366:LYS:C | 2.44 | 0.56 |
| 1:B:88:ARG:O | 1:B:120:VAL:HA | 2.06 | 0.56 |
| 3:N:1216:SER:HB2 | 4:O:15:SER:HA | 1.86 | 0.56 |
| 2:M:769:PRO:HG2 | 3:N:65:ARG:HH12 | 1.69 | 0.56 |
| 3:N:511:TRP:N | 3:N:511:TRP:CE3 | 2.73 | 0.56 |
| 2:C:658:GLY:N | 2:C:661:SER:OG | 2.39 | 0.56 |
| 2:M:203:ASP:HA | 2:M:228:ALA:HB1 | 1.87 | 0.56 |
| 2:M:269:LEU:HA | 2:M:288:ARG:HB2 | 1.88 | 0.56 |
| 1:B:233:VAL:HG12 | 1:B:235:ALA:H | 1.70 | 0.56 |
| 2:C:492:ASP:HA | 2:C:518:LYS:CB | 2.35 | 0.56 |
| 3:N:553:ARG:O | 3:N:556:LYS:HB2 | 2.05 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:45:PHE:HB3 | 3:D:86:ARG:HH22 | 1.71 | 0.56 |
| 3:D:403:PHE:CD2 | 3:D:442:ASN:O | 2.59 | 0.56 |
| 5:P:411:HIS:O | 5:P:414:ARG:HB2 | 2.05 | 0.56 |
| 1:A:38:ASN:HB3 | 1:A:39:PRO:CD | 2.32 | 0.56 |
| 3:D:661:MET:C | 3:D:667:ALA:HB3 | 2.25 | 0.56 |
| 5:F:343:ASP:N | 5:F:343:ASP:OD1 | 2.37 | 0.56 |
| 5:P:278:LEU:CB | 5:P:286:PRO:HG3 | 2.24 | 0.56 |
| 3:N:1032:PRO:HB2 | 3:N:1033:GLN:HE22 | 1.71 | 0.56 |
| 2:M:690:ILE:CG2 | 2:M:852:ILE:HG23 | 2.30 | 0.56 |
| 3:N:785:ILE:HG12 | 3:N:939:PHE:CE2 | 2.41 | 0.56 |
| 2:C:691:SER:HA | 2:C:858:MET:CE | 2.36 | 0.56 |
| 3:D:417:PRO:CB | 3:D:430:ASP:HA | 2.32 | 0.56 |
| 5:F:321:ILE:HG22 | 5:F:322:GLY:H | 1.70 | 0.56 |
| 3:N:996:TRP:CD2 | 3:N:1056:PRO:HG2 | 2.41 | 0.56 |
| 3:N:907:GLU:O | 3:N:908:LYS:C | 2.44 | 0.56 |
| 2:M:400:PRO:O | 2:M:401:LEU:C | 2.42 | 0.56 |
| 3:N:284:LEU:HD13 | 3:N:288:MET:CG | 2.34 | 0.56 |
| 3:N:219:GLU:C | 3:N:337:LEU:HG | 2.26 | 0.56 |
| 2:C:198:ARG:HG3 | 2:C:231:PRO:HA | 1.86 | 0.56 |
| 3:N:23:TYR:O | 3:N:49:ILE:HG23 | 2.06 | 0.56 |
| 3:N:536:ALA:O | 3:N:537:THR:HG23 | 2.06 | 0.56 |
| 3:D:596:SER:C | 3:D:598:ARG:H | 2.09 | 0.56 |
| 4:E:28:GLN:O | 4:E:31:LEU:HB2 | 2.05 | 0.56 |
| 5:F:131:VAL:O | 5:F:135:ILE:HG13 | 2.05 | 0.56 |
| 3:D:280:ALA:HB1 | 3:D:282:TYR:CZ | 2.40 | 0.56 |
| 3:D:210:ARG:HB2 | 3:D:389:GLU:CB | 2.35 | 0.56 |
| 3:D:403:PHE:CE1 | 3:D:442:ASN:HB3 | 2.41 | 0.56 |
| 1:B:38:ASN:CB | 1:B:39:PRO:HD3 | 2.32 | 0.56 |
| 5:F:418:LEU:H | 5:F:418:LEU:CD1 | 2.02 | 0.56 |
| 2:C:44:ILE:O | 2:C:47:ALA:HB3 | 2.06 | 0.56 |
| 5:F:264:MET:HE2 | 5:F:264:MET:HA | 1.88 | 0.56 |
| 1:L:97:VAL:HG12 | 1:L:98:THR:N | 2.21 | 0.56 |
| 1:K:13:VAL:CG2 | 1:K:14:ARG:N | 2.68 | 0.56 |
| 5:F:368:VAL:HG23 | 5:F:369:LEU:HG | 1.88 | 0.56 |
| 2:M:1030:GLN:HE22 | 3:N:628:ARG:HH21 | 1.53 | 0.56 |
| 3:N:207:PHE:HB2 | 3:N:391:ALA:HB3 | 1.87 | 0.56 |
| 1:B:176:ARG:HD3 | 3:D:884:ARG:HH22 | 1.70 | 0.56 |
| 4:O:6:ILE:HA | 4:O:9:LEU:HD12 | 1.88 | 0.56 |
| 3:N:602:SER:O | 3:N:606:ILE:HG13 | 2.06 | 0.56 |
| 1:L:68:ILE:HD12 | 1:L:71:VAL:HG11 | 1.86 | 0.56 |
| 2:M:710:ILE:CG2 | 2:M:823:VAL:HB | 2.36 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:408:ARG:NH2 | 2:C:457:ALA:O | 2.38 | 0.56 |
| 2:M:204:GLN:HB2 | 2:M:209:ARG:CZ | 2.36 | 0.56 |
| 2:C:164:PRO:HB3 | 2:C:264:PRO:O | 2.05 | 0.56 |
| 2:C:198:ARG:HE | 2:C:231:PRO:CD | 2.19 | 0.56 |
| 5:P:84:TYR:O | 5:P:86:HIS:N | 2.39 | 0.56 |
| 3:D:540:LEU:HD21 | 3:D:606:ILE:CD1 | 2.36 | 0.56 |
| 2:M:72:ARG:O | 2:M:95:TYR:N | 2.38 | 0.56 |
| 5:F:402:ASN:H | 5:F:402:ASN:ND2 | 2.03 | 0.56 |
| 5:F:402:ASN:HD22 | 5:F:402:ASN:N | 2.04 | 0.56 |
| 1:A:209:GLU:HA | 1:A:212:ASN:HD22 | 1.71 | 0.56 |
| 5:P:270:LYS:HA | 5:P:273:ARG:HD2 | 1.87 | 0.56 |
| 3:D:1161:GLU:HG3 | 3:D:1164:ARG:CB | 2.29 | 0.56 |
| 3:N:965:GLU:O | 3:N:966:GLU:C | 2.44 | 0.56 |
| 3:D:794:GLN:NE2 | 3:D:905:PRO:HG2 | 2.19 | 0.56 |
| 3:N:1094:LEU:HD12 | 3:N:1098:LEU:HD11 | 1.87 | 0.56 |
| 3:N:1365:ASP:O | 3:N:1366:LYS:C | 2.44 | 0.56 |
| 2:C:649:VAL:HA | 2:C:650:ARG:NH2 | 2.17 | 0.56 |
| 1:A:5:LYS:NZ | 1:A:28:LEU:C | 2.59 | 0.56 |
| 2:M:31:GLN:HG2 | 2:M:35:PRO:CB | 2.31 | 0.56 |
| 3:N:592:THR:CG2 | 3:N:600:LEU:HD21 | 2.31 | 0.56 |
| 1:B:19:GLU:HG2 | 1:B:203:GLY:CA | 2.35 | 0.56 |
| 5:F:159:ILE:O | 5:F:163:LEU:HG | 2.06 | 0.56 |
| 2:C:807:ARG:CZ | 2:C:807:ARG:HB2 | 2.35 | 0.56 |
| 1:L:112:ARG:HH11 | 1:L:112:ARG:HB3 | 1.70 | 0.56 |
| 1:L:86:VAL:CG1 | 1:L:123:MET:HB2 | 2.36 | 0.56 |
| 5:P:231:ARG:HB2 | 5:P:233:PHE:CZ | 2.41 | 0.56 |
| 3:N:69:GLU:HG3 | 3:N:71:LYS:HZ3 | 1.70 | 0.56 |
| 2:M:545:ASN:CB | 2:M:583:LEU:HD11 | 2.35 | 0.56 |
| 2:C:230:ARG:HH11 | 2:C:230:ARG:HG3 | 1.71 | 0.56 |
| 2:C:439:CYS:SG | 2:C:441:VAL:HG13 | 2.46 | 0.56 |
| 2:C:460:ARG:HH21 | 2:C:462:ASP:HB3 | 1.70 | 0.56 |
| 3:N:152:LEU:HG | 3:N:153:LEU:N | 2.19 | 0.56 |
| 3:D:1440:PHE:HE2 | 3:D:1463:LYS:NZ | 2.03 | 0.56 |
| 3:D:520:LEU:O | 3:D:525:ARG:NH1 | 2.39 | 0.56 |
| 5:F:223:ALA:HB2 | 5:F:242:TRP:CG | 2.41 | 0.56 |
| 2:M:600:ASP:HB3 | 2:M:650:ARG:CA | 2.29 | 0.56 |
| 2:M:358:ARG:HD2 | 2:M:372:LEU:HA | 1.86 | 0.56 |
| 5:F:271:LEU:O | 5:F:272:SER:C | 2.44 | 0.56 |
| 3:D:1156:LEU:HD12 | 3:D:1173:LEU:CD1 | 2.35 | 0.56 |
| 3:D:71:LYS:H | 3:D:80:VAL:CG2 | 2.19 | 0.56 |
| 1:K:111:ALA:HB3 | 1:K:124:ASN:O | 2.05 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:D:1344:VAL:CG1 | 3:D:1345:GLU:N | 2.69 | 0.56 |
| 2:M:486:MET:SD | 2:M:491:GLU:HA | 2.46 | 0.56 |
| 2:C:380:ALA:O | 2:C:381:ALA:C | 2.42 | 0.56 |
| 3:D:959:GLU:H | 3:D:959:GLU:CD | 2.09 | 0.56 |
| 3:N:470:LEU:N | 3:N:470:LEU:HD23 | 2.20 | 0.56 |
| 3:N:188:GLY:N | 3:N:197:SER:O | 2.39 | 0.56 |
| 3:D:1310:ARG:HB3 | 3:D:1327:ARG:HG3 | 1.88 | 0.56 |
| 3:N:1216:SER:OG | 4:O:16:LYS:HB2 | 2.05 | 0.56 |
| 5:F:244:ARG:O | 5:F:247:ILE:HB | 2.06 | 0.56 |
| 3:D:685:ASP:O | 3:D:687:VAL:N | 2.39 | 0.56 |
| 4:E:45:ARG:O | 4:E:47:LYS:HG2 | 2.06 | 0.56 |
| 3:N:225:LEU:HD11 | 3:N:242:LEU:HD21 | 1.88 | 0.56 |
| 3:N:566:ILE:O | 3:N:569:ASN:HB3 | 2.05 | 0.56 |
| 3:N:574:LEU:HG | 3:N:575:GLN:N | 2.20 | 0.56 |
| 3:D:583:ASP:HB2 | 3:D:604:THR:OG1 | 2.05 | 0.56 |
| 3:N:420:VAL:C | 3:N:421:LEU:HD23 | 2.26 | 0.56 |
| 3:D:442:ASN:ND2 | 3:D:442:ASN:N | 2.54 | 0.56 |
| 3:D:937:TYR:HA | 3:D:940:THR:OG1 | 2.06 | 0.56 |
| 1:B:188:GLN:HG2 | 1:B:189:ARG:HG3 | 1.88 | 0.56 |
| 2:C:876:VAL:O | 2:C:880:MET:N | 2.39 | 0.56 |
| 2:C:691:SER:HA | 2:C:858:MET:HE3 | 1.88 | 0.56 |
| 1:A:44:LEU:O | 1:A:48:ILE:HG12 | 2.06 | 0.56 |
| 1:B:76:VAL:HA | 1:B:79:ILE:CG1 | 2.36 | 0.56 |
| 2:M:1083:GLU:O | 2:M:1087:VAL:HG23 | 2.05 | 0.56 |
| 1:K:208:LEU:O | 1:K:211:LEU:HB3 | 2.05 | 0.56 |
| 1:L:179:PHE:CB | 1:L:197:LEU:HD13 | 2.34 | 0.56 |
| 2:M:328:LEU:HD11 | 2:M:434:HIS:HA | 1.87 | 0.56 |
| 3:N:1048:PRO:HA | 3:N:1079:LYS:NZ | 2.20 | 0.56 |
| 5:F:142:ARG:CD | 5:F:145:PRO:HA | 2.35 | 0.56 |
| 2:C:1008:ARG:HG2 | 2:C:1009:SER:N | 2.21 | 0.56 |
| 3:N:925:GLU:HG2 | 4:O:7:ASP:OD2 | 2.05 | 0.56 |
| 2:C:1031:ARG:HB2 | 3:D:622:ARG:HH12 | 1.71 | 0.56 |
| 3:D:821:VAL:HG22 | 3:D:840:LYS:NZ | 2.21 | 0.56 |
| 3:D:758:GLU:HG2 | 3:D:1476:THR:HG21 | 1.88 | 0.56 |
| 2:C:950:LEU:HB2 | 2:C:952:LEU:HG | 1.87 | 0.56 |
| 2:M:115:LEU:HB3 | 2:M:375:SER:HB3 | 1.88 | 0.56 |
| 2:M:191:PHE:CD2 | 2:M:195:LEU:HD12 | 2.42 | 0.55 |
| 3:N:246:PRO:HD2 | 3:N:308:LYS:HA | 1.88 | 0.55 |
| 2:C:305:PRO:HG3 | 2:C:308:ARG:NH2 | 2.20 | 0.55 |
| 2:C:522:VAL:HG12 | 2:C:523:ILE:N | 2.20 | 0.55 |
| 3:D:102:ILE:O | 3:D:104:PHE:N | 2.39 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:102:ILE:C | 3:D:104:PHE:H | 2.10 | 0.55 |
| 3:D:119:SER:CB | 3:D:123:LEU:H | 2.02 | 0.55 |
| 3:D:1465:ASN:HD22 | 3:D:1473:PRO:HD3 | 1.69 | 0.55 |
| 3:D:5:VAL:HG22 | 3:D:6:ARG:H | 1.71 | 0.55 |
| 3:D:406:ASP:CB | 3:D:424:GLY:H | 2.18 | 0.55 |
| 3:D:248:PRO:CB | 3:D:308:LYS:NZ | 2.69 | 0.55 |
| 4:E:6:ILE:CG2 | 4:E:7:ASP:N | 2.69 | 0.55 |
| 5:F:386:VAL:CG2 | 5:F:387:GLY:N | 2.69 | 0.55 |
| 5:P:365:GLU:HA | 5:P:368:VAL:HG13 | 1.88 | 0.55 |
| 3:D:957:PRO:HG3 | 3:D:1010:ASN:ND2 | 2.04 | 0.55 |
| 3:D:398:ALA:HB2 | 3:D:447:VAL:HG22 | 1.88 | 0.55 |
| 3:N:1194:CYS:HB2 | 3:N:1204:CYS:CB | 2.36 | 0.55 |
| 3:D:864:VAL:CG1 | 3:D:865:THR:N | 2.69 | 0.55 |
| 2:C:1005:MET:HG2 | 3:D:629:SER:CB | 2.35 | 0.55 |
| 2:M:974:LEU:HD11 | 2:M:989:VAL:HG11 | 1.87 | 0.55 |
| 1:A:85:LEU:HD12 | 1:A:124:ASN:OD1 | 2.05 | 0.55 |
| 3:D:1280:VAL:HG12 | 3:D:1281:VAL:N | 2.21 | 0.55 |
| 3:D:72:VAL:HG12 | 3:D:73:CYS:N | 2.21 | 0.55 |
| 2:M:879:ARG:N | 2:M:879:ARG:HD2 | 2.21 | 0.55 |
| 2:M:224:GLU:HB3 | 2:M:227:PHE:CB | 2.36 | 0.55 |
| 2:M:277:ALA:O | 2:M:281:LEU:N | 2.39 | 0.55 |
| 2:C:415:PRO:HG2 | 2:C:418:LEU:HD12 | 1.88 | 0.55 |
| 3:N:413:ASP:O | 3:N:434:ARG:HA | 2.06 | 0.55 |
| 5:P:86:HIS:C | 5:P:88:ILE:N | 2.60 | 0.55 |
| 3:D:1094:LEU:HG | 3:D:1095:THR:N | 2.21 | 0.55 |
| 3:D:136:ASP:HB2 | 3:D:453:ASP:O | 2.05 | 0.55 |
| 5:F:221:ILE:O | 5:F:224:VAL:HB | 2.06 | 0.55 |
| 2:M:98:LEU:H | 2:M:111:ASP:HA | 1.71 | 0.55 |
| 5:P:399:GLN:O | 5:P:402:ASN:HB2 | 2.06 | 0.55 |
| 2:C:768:THR:HB | 2:C:771:GLU:HB3 | 1.88 | 0.55 |
| 5:F:401:GLU:O | 5:F:404:ALA:HB3 | 2.06 | 0.55 |
| 2:C:355:VAL:HA | 2:C:358:ARG:HG3 | 1.89 | 0.55 |
| 2:C:56:GLU:OE1 | 2:C:359:MET:HB2 | 2.05 | 0.55 |
| 5:P:262:VAL:HA | 5:P:265:VAL:HG23 | 1.88 | 0.55 |
| 2:M:89:THR:HG23 | 2:M:128:ILE:O | 2.06 | 0.55 |
| 3:N:5:VAL:HG12 | 3:N:6:ARG:N | 2.22 | 0.55 |
| 2:M:573:ARG:O | 2:M:670:GLN:NE2 | 2.39 | 0.55 |
| 3:N:857:ILE:O | 3:N:858:VAL:HG23 | 2.05 | 0.55 |
| 1:A:30:ARG:HG3 | 2:C:938:LYS:NZ | 2.22 | 0.55 |
| 3:N:350:HIS:HB3 | 5:P:232:ARG:CZ | 2.36 | 0.55 |
| 3:D:884:ARG:HG2 | 3:D:885:ILE:N | 2.21 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:F:162:LYS:O | 5:F:166:LEU:HG | 2.07 | 0.55 |
| 2:M:498:GLN:HB2 | 2:M:514:VAL:CG2 | 2.36 | 0.55 |
| 3:N:1253:THR:HG22 | 3:N:1254:GLN:N | 2.18 | 0.55 |
| 1:A:1:MET:HA | 1:A:6:LEU:HD22 | 1.88 | 0.55 |
| 2:C:939:ARG:O | 2:C:942:GLU:HB3 | 2.05 | 0.55 |
| 3:D:1293:PHE:CE2 | 3:D:1300:SER:HB3 | 2.41 | 0.55 |
| 2:C:1015:LEU:HA | 5:F:335:ASP:HB2 | 1.88 | 0.55 |
| 3:D:10:ILE:O | 3:D:10:ILE:HG23 | 2.06 | 0.55 |
| 3:D:1481:VAL:HG22 | 4:E:18:ARG:CZ | 2.36 | 0.55 |
| 2:C:1015:LEU:HB2 | 5:F:333:ILE:HG22 | 1.88 | 0.55 |
| 3:D:245:LEU:HG | 3:D:309:GLY:HA2 | 1.88 | 0.55 |
| 1:B:58:ILE:CD1 | 1:B:60:ASP:H | 2.19 | 0.55 |
| 3:D:810:GLU:O | 3:D:812:ALA:N | 2.40 | 0.55 |
| 3:N:1377:LYS:HD3 | 3:N:1378:TYR:CE1 | 2.41 | 0.55 |
| 5:P:305:GLU:OE2 | 5:P:309:LYS:NZ | 2.37 | 0.55 |
| 3:D:828:LYS:HD3 | 3:D:828:LYS:N | 2.21 | 0.55 |
| 2:C:948:GLU:HB3 | 2:C:953:VAL:HG23 | 1.88 | 0.55 |
| 3:N:1363:LEU:C | 3:N:1363:LEU:HD23 | 2.27 | 0.55 |
| 3:N:875:THR:HG21 | 3:N:902:LEU:HD11 | 1.87 | 0.55 |
| 5:F:94:LEU:HD11 | 5:F:190:ALA:CB | 2.36 | 0.55 |
| 1:L:210:ALA:O | 1:L:211:LEU:C | 2.45 | 0.55 |
| 3:D:41:ARG:HH21 | 3:D:48:ARG:NH1 | 2.03 | 0.55 |
| 1:K:42:ARG:HD3 | 1:L:35:THR:HA | 1.89 | 0.55 |
| 5:P:321:ILE:O | 5:P:323:ASP:N | 2.40 | 0.55 |
| 3:N:591:VAL:HG12 | 3:N:599:PRO:CA | 2.36 | 0.55 |
| 3:N:1311:LEU:CD1 | 3:N:1312:LEU:H | 2.17 | 0.55 |
| 3:N:167:GLU:OE1 | 3:N:169:TYR:CE2 | 2.60 | 0.55 |
| 3:D:984:THR:HG23 | 3:D:987:GLU:H | 1.72 | 0.55 |
| 2:M:560:MET:HB3 | 2:M:564:MET:CE | 2.37 | 0.55 |
| 3:D:1246:VAL:CG1 | 3:D:1249:ALA:O | 2.54 | 0.55 |
| 3:N:1302:GLU:HG2 | 3:N:1303:TYR:N | 2.20 | 0.55 |
| 3:D:1504:GLU:O | 3:D:1505:ALA:HB3 | 2.05 | 0.55 |
| 3:N:41:ARG:HH21 | 3:N:48:ARG:NH1 | 2.04 | 0.55 |
| 3:N:522:PRO:HG3 | 3:N:525:ARG:HH22 | 1.70 | 0.55 |
| 3:N:544:TYR:O | 3:N:545:ARG:C | 2.42 | 0.55 |
| 5:F:175:HIS:HA | 5:F:178:ARG:HB2 | 1.87 | 0.55 |
| 3:D:274:ARG:HE | 3:D:279:VAL:HG11 | 1.71 | 0.55 |
| 3:D:296:GLU:N | 3:D:302:GLN:OE1 | 2.39 | 0.55 |
| 1:L:79:ILE:HA | 1:L:82:LEU:HG | 1.88 | 0.55 |
| 5:F:373:LYS:HB3 | 5:F:379:ARG:H | 1.70 | 0.55 |
| 2:C:373:VAL:CG1 | 2:C:374:ASN:N | 2.69 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:166:GLN:HB3 | 3:D:394:LEU:HD11 | 1.89 | 0.55 |
| 3:D:41:ARG:HG3 | 3:D:41:ARG:HH11 | 1.70 | 0.55 |
| 1:A:83:LYS:HZ1 | 1:A:170:VAL:HG22 | 1.71 | 0.55 |
| 3:D:629:SER:HB3 | 3:D:726:ILE:HD11 | 1.89 | 0.55 |
| 3:D:1353:GLN:O | 3:D:1355:VAL:N | 2.39 | 0.55 |
| 2:M:953:VAL:HG13 | 2:M:966:LEU:HD13 | 1.88 | 0.55 |
| 3:N:191:LEU:HD23 | 3:N:195:VAL:HG11 | 1.88 | 0.55 |
| 3:D:16:GLU:N | 3:D:16:GLU:CD | 2.57 | 0.55 |
| 3:N:1337:GLU:CD | 3:N:1337:GLU:H | 2.09 | 0.55 |
| 5:P:147:LEU:O | 5:P:148:LYS:HB2 | 2.05 | 0.55 |
| 2:C:266:ARG:CD | 2:C:273:GLY:HA3 | 2.37 | 0.55 |
| 3:N:36:THR:CG2 | 3:N:38:LYS:HE2 | 2.37 | 0.55 |
| 5:P:209:PHE:HA | 5:P:212:LEU:CD1 | 2.36 | 0.55 |
| 2:C:1114:GLY:C | 2:C:1116:ALA:H | 2.09 | 0.55 |
| 3:D:128:TYR:CD1 | 3:D:457:GLY:HA2 | 2.27 | 0.55 |
| 3:D:529:GLN:HA | 3:D:535:PHE:CD2 | 2.40 | 0.55 |
| 5:P:406:ARG:O | 5:P:409:LYS:HG3 | 2.06 | 0.55 |
| 1:B:68:ILE:HD12 | 1:B:71:VAL:CG1 | 2.37 | 0.55 |
| 1:L:74:ASP:OD2 | 1:L:75:VAL:N | 2.40 | 0.55 |
| 1:B:63:HIS:HD2 | 1:B:65:PHE:HB2 | 1.71 | 0.55 |
| 2:M:641:PRO:HA | 2:M:655:LEU:O | 2.06 | 0.55 |
| 2:C:1066:ALA:O | 2:C:1070:ILE:HG13 | 2.06 | 0.55 |
| 3:D:654:LYS:O | 3:D:658:LEU:HG | 2.07 | 0.55 |
| 3:N:1304:LYS:O | 3:N:1305:LEU:HB3 | 2.05 | 0.55 |
| 3:D:1028:ALA:O | 3:D:1029:ARG:HB2 | 2.06 | 0.55 |
| 3:N:835:SER:HB3 | 3:N:838:ARG:HG3 | 1.89 | 0.55 |
| 3:D:28:LYS:HG2 | 3:D:42:ASP:CB | 2.36 | 0.55 |
| 2:M:1059:ASP:HA | 2:M:1083:GLU:OE2 | 2.07 | 0.55 |
| 2:M:1111:ILE:HD11 | 2:M:1112:PHE:CE1 | 2.41 | 0.55 |
| 2:C:23:VAL:HG23 | 2:C:24:GLU:N | 2.21 | 0.55 |
| 1:K:55:SER:HA | 1:K:167:VAL:HG23 | 1.88 | 0.55 |
| 1:K:74:ASP:OD1 | 1:K:76:VAL:N | 2.39 | 0.55 |
| 3:D:1376:MET:HE1 | 3:D:1421:LEU:CD1 | 2.37 | 0.55 |
| 1:B:176:ARG:HG2 | 1:B:177:VAL:H | 1.71 | 0.55 |
| 3:D:409:VAL:HB | 5:F:164:LYS:NZ | 2.22 | 0.55 |
| 3:N:1126:ASP:OD2 | 3:N:1129:THR:HG23 | 2.06 | 0.55 |
| 3:N:622:ARG:HG2 | 3:N:622:ARG:HH11 | 1.72 | 0.55 |
| 2:C:493:ARG:HB2 | 2:C:494:TYR:CE1 | 2.42 | 0.55 |
| 3:N:891:GLU:HB2 | 3:N:926:LYS:NZ | 2.21 | 0.55 |
| 2:M:200:LEU:HD13 | 2:M:300:ASP:HB3 | 1.88 | 0.55 |
| 2:M:389:SER:HB3 | 2:M:392:SER:HB3 | 1.89 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:323:GLU:HB2 | 3:N:334:THR:CB | 2.36 | 0.55 |
| 3:N:525:ARG:NH1 | 3:N:525:ARG:HG2 | 2.20 | 0.55 |
| 3:D:1103:HIS:CD2 | 3:D:1462:LEU:H | 2.24 | 0.55 |
| 3:D:119:SER:OG | 3:D:122:GLU:HB2 | 2.07 | 0.55 |
| 3:D:508:ARG:CB | 3:D:510:GLU:OE1 | 2.54 | 0.55 |
| 5:F:127:ILE:O | 5:F:130:VAL:N | 2.39 | 0.55 |
| 5:F:314:PRO:HG2 | 5:F:315:VAL:N | 2.21 | 0.55 |
| 3:N:430:ASP:N | 3:N:430:ASP:OD1 | 2.38 | 0.55 |
| 3:D:365:ASP:O | 3:D:379:ALA:CB | 2.54 | 0.55 |
| 3:D:288:MET:O | 3:D:290:PRO:HD3 | 2.05 | 0.55 |
| 4:E:5:GLY:O | 4:E:9:LEU:HG | 2.05 | 0.55 |
| 1:B:112:ARG:O | 1:B:114:PHE:N | 2.40 | 0.55 |
| 2:C:32:ALA:C | 2:C:35:PRO:HD2 | 2.27 | 0.55 |
| 2:C:95:TYR:CG | 2:C:114:PHE:HB3 | 2.41 | 0.55 |
| 1:A:34:VAL:CB | 1:B:42:ARG:HH12 | 1.96 | 0.55 |
| 3:D:673:ALA:O | 3:D:677:LEU:HG | 2.07 | 0.55 |
| 1:A:206:THR:HG22 | 1:A:208:LEU:H | 1.70 | 0.55 |
| 5:F:288:TYR:O | 5:F:291:ILE:HG23 | 2.06 | 0.55 |
| 3:N:1492:LEU:O | 3:N:1495:ILE:HG22 | 2.07 | 0.55 |
| 3:D:494:LYS:HA | 3:D:1388:ARG:HH12 | 1.72 | 0.55 |
| 3:D:1398:TRP:HB3 | 3:D:1402:ALA:HB3 | 1.89 | 0.55 |
| 3:D:1409:ALA:C | 3:D:1410:GLU:HG3 | 2.26 | 0.55 |
| 3:D:826:PRO:HD2 | 3:D:829:VAL:HG11 | 1.89 | 0.55 |
| 3:D:914:LEU:O | 3:D:914:LEU:HD12 | 2.07 | 0.55 |
| 2:M:892:LEU:O | 2:M:895:TYR:HB3 | 2.07 | 0.55 |
| 5:F:75:ILE:HG22 | 5:F:76:SER:N | 2.21 | 0.55 |
| 5:F:80:PRO:HA | 5:F:83:GLN:NE2 | 2.16 | 0.55 |
| 2:M:1056:LYS:HZ3 | 3:N:749:VAL:H | 1.54 | 0.55 |
| 1:K:203:GLY:C | 1:K:205:VAL:N | 2.59 | 0.55 |
| 1:L:32:PHE:O | 1:L:36:LEU:HD12 | 2.06 | 0.55 |
| 1:L:28:LEU:HD13 | 1:L:33:GLY:N | 2.22 | 0.55 |
| 3:N:1394:VAL:HG21 | 3:N:1397:LYS:NZ | 2.22 | 0.55 |
| 3:D:986:ARG:HG3 | 3:D:990:ASP:OD2 | 2.05 | 0.55 |
| 2:C:806:LEU:HD22 | 2:C:813:VAL:CG2 | 2.36 | 0.55 |
| 3:D:14:SER:O | 3:D:18:ILE:HG13 | 2.05 | 0.55 |
| 5:F:245:GLN:CA | 5:F:245:GLN:NE2 | 2.70 | 0.55 |
| 3:D:178:LEU:HG | 3:D:181:ASP:CB | 2.35 | 0.55 |
| 2:M:790:LEU:HD12 | 2:M:790:LEU:C | 2.27 | 0.55 |
| 3:N:317:VAL:HB | 3:N:339:TRP:HB3 | 1.89 | 0.55 |
| 2:C:139:GLN:HG2 | 2:C:391:LEU:HD21 | 1.87 | 0.55 |
| 2:C:176:VAL:HG12 | 2:C:183:SER:N | 2.21 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:410:ILE:HD12 | 2:C:410:ILE:N | 2.22 | 0.55 |
| 3:D:108:VAL:HG12 | 3:D:109:PRO:HA | 1.86 | 0.55 |
| 3:D:1481:VAL:O | 3:D:1482:ARG:C | 2.45 | 0.55 |
| 3:D:573:MET:O | 3:D:576:GLU:HB3 | 2.06 | 0.55 |
| 5:F:117:SER:HB2 | 5:F:122:LEU:O | 2.06 | 0.55 |
| 5:F:401:GLU:O | 5:F:405:LEU:HG | 2.07 | 0.55 |
| 3:D:655:PRO:O | 3:D:656:PHE:C | 2.45 | 0.55 |
| 2:M:87:ASP:O | 2:M:130:ASN:HA | 2.07 | 0.55 |
| 3:D:954:ALA:CB | 3:D:1062:ARG:HD2 | 2.33 | 0.55 |
| 3:N:970:LYS:HG3 | 3:N:974:ILE:HD11 | 1.89 | 0.55 |
| 2:C:879:ARG:N | 2:C:879:ARG:HD2 | 2.22 | 0.55 |
| 3:D:864:VAL:CG1 | 3:D:865:THR:H | 2.20 | 0.55 |
| 2:C:600:ASP:HA | 2:C:649:VAL:O | 2.06 | 0.55 |
| 2:M:474:VAL:HG11 | 2:M:529:VAL:HG12 | 1.89 | 0.55 |
| 1:K:198:ARG:NH2 | 2:M:932:GLU:OE2 | 2.40 | 0.55 |
| 1:K:86:VAL:HG12 | 1:K:124:ASN:OD1 | 2.06 | 0.55 |
| 1:L:28:LEU:HD11 | 1:L:36:LEU:CD1 | 2.37 | 0.55 |
| 3:N:1404:ASN:CA | 3:N:1408:ILE:HB | 2.35 | 0.55 |
| 3:N:1211:MET:HB2 | 3:N:1213:ARG:NH1 | 2.21 | 0.55 |
| 2:M:1030:GLN:OE1 | 3:N:628:ARG:HB2 | 2.06 | 0.55 |
| 3:N:1012:GLU:HB2 | 3:N:1021:TYR:OH | 2.07 | 0.55 |
| 2:C:396:ASP:O | 2:C:403:SER:CA | 2.54 | 0.55 |
| 1:L:10:VAL:HG22 | 1:L:26:GLU:O | 2.07 | 0.55 |
| 3:N:264:LEU:HD22 | 3:N:316:GLN:NE2 | 2.21 | 0.55 |
| 3:N:607:LEU:HG | 3:N:608:SER:N | 2.21 | 0.55 |
| 4:E:80:VAL:HB | 4:E:81:PRO:HD2 | 1.89 | 0.55 |
| 3:N:760:ARG:NH1 | 4:O:61:GLU:HB2 | 2.22 | 0.55 |
| 3:D:1220:ALA:O | 3:D:1224:VAL:HG23 | 2.07 | 0.55 |
| 2:C:989:VAL:HG23 | 2:C:990:GLY:N | 2.21 | 0.55 |
| 2:M:235:LEU:HD22 | 2:M:236:ILE:HG13 | 1.89 | 0.55 |
| 3:N:261:LEU:HD23 | 3:N:270:LEU:HA | 1.88 | 0.55 |
| 3:N:218:LYS:HA | 3:N:337:LEU:O | 2.07 | 0.55 |
| 2:C:437:ARG:O | 2:C:455:LEU:HD12 | 2.07 | 0.55 |
| 3:N:139:GLY:O | 3:N:147:VAL:HB | 2.06 | 0.55 |
| 3:D:1448:THR:O | 3:D:1452:ILE:HG12 | 2.07 | 0.55 |
| 3:D:209:ARG:N | 3:D:389:GLU:O | 2.40 | 0.55 |
| 4:E:6:ILE:CG2 | 4:E:7:ASP:H | 2.19 | 0.55 |
| 5:P:382:THR:HG23 | 5:P:397:ILE:CG2 | 2.37 | 0.55 |
| 1:L:66:SER:O | 1:L:75:VAL:HG23 | 2.07 | 0.55 |
| 2:M:151:ASP:H | 2:M:158:TYR:HA | 1.71 | 0.55 |
| 3:D:1377:LYS:HD3 | 3:D:1378:TYR:CE1 | 2.42 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:N:1030:GLY:HA2 | 3:N:1034:GLN:NE2 | 2.22 | 0.55 |
| 3:N:610:LYS:NZ | 3:N:1442:ASN:N | 2.52 | 0.55 |
| 3:N:18:ILE:HG23 | 3:N:518:PRO:HG3 | 1.89 | 0.55 |
| 3:N:637:LEU:HD12 | 3:N:729:HIS:N | 2.21 | 0.55 |
| 1:L:108:GLU:HG3 | 1:L:131:THR:CG2 | 2.33 | 0.55 |
| 2:C:815:LEU:CD1 | 2:C:821:GLU:HA | 2.37 | 0.55 |
| 5:P:245:GLN:CA | 5:P:245:GLN:HE21 | 2.20 | 0.55 |
| 3:N:921:ARG:HH11 | 3:N:921:ARG:CB | 2.19 | 0.55 |
| 3:N:1221:VAL:CG1 | 3:N:1370:ILE:HD13 | 2.37 | 0.55 |
| 5:P:128:ARG:HA | 5:P:131:VAL:CG2 | 2.36 | 0.55 |
| 2:M:841:ASN:ND2 | 2:M:884:GLN:OE1 | 2.40 | 0.55 |
| 2:C:560:MET:HB3 | 2:C:564:MET:HE3 | 1.87 | 0.55 |
| 3:D:1294:VAL:O | 3:D:1295:GLU:HG3 | 2.07 | 0.55 |
| 2:M:1006:HIS:HA | 2:M:1027:PHE:CZ | 2.41 | 0.55 |
| 5:F:138:SER:O | 5:F:141:VAL:HG22 | 2.07 | 0.55 |
| 2:M:237:ARG:O | 2:M:240:THR:CB | 2.55 | 0.55 |
| 3:N:280:ALA:HB1 | 3:N:282:TYR:CZ | 2.42 | 0.55 |
| 3:D:1078:ARG:HG3 | 3:D:1078:ARG:HH11 | 1.72 | 0.55 |
| 3:N:27:GLU:HB2 | 3:N:28:LYS:CE | 2.37 | 0.55 |
| 3:N:416:ALA:CB | 3:N:432:TYR:CG | 2.90 | 0.55 |
| 3:N:41:ARG:NH2 | 3:N:48:ARG:NH1 | 2.54 | 0.55 |
| 3:D:1104:GLU:O | 3:D:1106:VAL:HG23 | 2.07 | 0.55 |
| 3:D:133:ILE:HG22 | 3:D:455:ARG:C | 2.27 | 0.55 |
| 3:D:99:ALA:N | 3:D:514:LEU:O | 2.39 | 0.55 |
| 3:N:356:PRO:CB | 3:N:440:VAL:HB | 2.34 | 0.55 |
| 3:D:930:LEU:O | 3:D:933:ALA:HB3 | 2.07 | 0.55 |
| 5:P:413:SER:CB | 5:P:414:ARG:HH21 | 2.20 | 0.55 |
| 3:D:812:ALA:C | 3:D:814:ALA:N | 2.59 | 0.55 |
| 5:F:405:LEU:O | 5:F:408:LEU:HB3 | 2.07 | 0.55 |
| 2:M:589:ARG:HG2 | 2:M:596:TYR:CZ | 2.41 | 0.55 |
| 2:M:780:GLU:HG2 | 5:P:379:ARG:HH21 | 1.69 | 0.55 |
| 2:M:719:PRO:HB3 | 2:M:820:ARG:NH1 | 2.21 | 0.55 |
| 3:D:909:ASN:O | 3:D:910:SER:C | 2.45 | 0.55 |
| 3:D:413:ASP:O | 3:D:434:ARG:HA | 2.07 | 0.55 |
| 3:N:759:ALA:O | 3:N:763:MET:HB2 | 2.06 | 0.55 |
| 2:C:599:GLU:HA | 2:C:599:GLU:OE1 | 2.07 | 0.55 |
| 2:C:695:LEU:HD21 | 2:C:833:LEU:HB3 | 1.89 | 0.55 |
| 3:D:1354:LYS:O | 3:D:1358:ALA:HB2 | 2.07 | 0.55 |
| 1:A:86:VAL:HG22 | 1:A:123:MET:HG3 | 1.89 | 0.55 |
| 5:F:368:VAL:CG2 | 5:F:369:LEU:H | 2.14 | 0.55 |
| 3:D:869:MET:HE1 | 3:D:893:GLU:HG2 | 1.89 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:D:178:LEU:HG | 3:D:181:ASP:OD2 | 2.07 | 0.55 |
| 2:C:728:HIS:ND1 | 2:C:729:LEU:N | 2.55 | 0.55 |
| 4:E:85:LEU:O | 4:E:86:GLN:C | 2.45 | 0.55 |
| 2:M:549:PHE:CD2 | 2:M:886:LEU:HB2 | 2.42 | 0.55 |
| 3:N:715:ALA:O | 3:N:764:LEU:HD12 | 2.07 | 0.55 |
| 2:C:293:PHE:HD1 | 2:C:294:GLU:N | 2.04 | 0.55 |
| 2:M:226:VAL:O | 2:M:230:ARG:CZ | 2.55 | 0.55 |
| 3:N:238:PRO:HB3 | 3:N:317:VAL:C | 2.28 | 0.55 |
| 2:C:267:TYR:HE1 | 2:C:464:LEU:HD12 | 1.71 | 0.55 |
| 2:C:439:CYS:HB2 | 2:C:541:SER:CB | 2.35 | 0.55 |
| 3:N:139:GLY:HA2 | 3:N:452:ILE:CG2 | 2.37 | 0.55 |
| 3:N:574:LEU:O | 3:N:577:ALA:HB3 | 2.07 | 0.55 |
| 5:P:192:LEU:O | 5:P:196:VAL:HG23 | 2.06 | 0.55 |
| 3:D:1095:THR:C | 3:D:1099:VAL:HG23 | 2.27 | 0.55 |
| 3:N:368:VAL:H | 3:N:377:VAL:HB | 1.71 | 0.55 |
| 4:E:6:ILE:CA | 4:E:9:LEU:HD12 | 2.24 | 0.55 |
| 5:P:350:LEU:O | 5:P:352:GLU:N | 2.39 | 0.55 |
| 5:P:400:ILE:O | 5:P:401:GLU:C | 2.45 | 0.55 |
| 1:B:112:ARG:NH2 | 1:B:125:PRO:C | 2.60 | 0.55 |
| 3:D:660:LYS:HD2 | 3:D:693:GLU:OE2 | 2.06 | 0.55 |
| 5:F:260:ILE:HG13 | 5:F:261:PRO:HD2 | 1.88 | 0.55 |
| 3:D:1380:GLU:O | 3:D:1418:LYS:N | 2.30 | 0.55 |
| 3:N:1379:VAL:O | 3:N:1393:GLN:N | 2.40 | 0.55 |
| 3:N:795:VAL:HG13 | 3:N:879:ARG:HH12 | 1.71 | 0.55 |
| 3:N:808:THR:N | 3:N:809:PRO:CD | 2.63 | 0.55 |
| 3:N:812:ALA:HB2 | 3:N:816:HIS:HB2 | 1.89 | 0.55 |
| 1:K:5:LYS:HZ2 | 1:K:29:GLU:N | 2.05 | 0.55 |
| 3:N:628:ARG:N | 3:N:648:MET:HE1 | 2.21 | 0.55 |
| 1:A:70:GLY:H | 2:C:607:ASP:CB | 2.20 | 0.55 |
| 2:M:486:MET:HG3 | 2:M:490:GLU:OE1 | 2.07 | 0.55 |
| 3:N:207:PHE:CZ | 5:P:97:GLU:HB2 | 2.42 | 0.55 |
| 2:M:23:VAL:HA | 2:M:121:MET:CE | 2.33 | 0.55 |
| 3:N:921:ARG:O | 3:N:922:LEU:HD23 | 2.07 | 0.55 |
| 2:C:167:LYS:HB3 | 2:C:167:LYS:HZ3 | 1.72 | 0.55 |
| 3:N:988:ARG:HG2 | 3:N:992:ILE:HD11 | 1.87 | 0.55 |
| 3:N:186:VAL:HG12 | 3:N:187:LYS:N | 2.22 | 0.55 |
| 5:P:167:PRO:HB2 | 5:P:169:GLU:OE1 | 2.07 | 0.55 |
| 3:D:1179:GLU:C | 3:D:1181:GLY:H | 2.10 | 0.55 |
| 3:N:259:VAL:O | 3:N:260:GLU:HG3 | 2.07 | 0.54 |
| 2:C:266:ARG:HB2 | 2:C:272:ALA:CB | 2.36 | 0.54 |
| 2:C:399:ASN:HB2 | 2:C:400:PRO:HD3 | 1.89 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:512:ARG:HG3 | 2:C:523:ILE:HD11 | 1.88 | 0.54 |
| 3:D:1083:ASP:HB2 | 3:D:1239:ARG:HH12 | 1.71 | 0.54 |
| 3:N:39:PRO:HG2 | 3:N:53:ILE:HD11 | 1.89 | 0.54 |
| 3:D:1108:ARG:NE | 3:D:1199:GLY:HA3 | 2.21 | 0.54 |
| 5:F:224:VAL:O | 5:F:225:GLU:C | 2.46 | 0.54 |
| 2:C:41:ASN:HB2 | 2:C:45:GLN:C | 2.28 | 0.54 |
| 5:P:367:MET:SD | 5:P:371:LEU:HD11 | 2.46 | 0.54 |
| 2:M:807:ARG:HB3 | 2:M:807:ARG:HH11 | 1.72 | 0.54 |
| 3:D:489:ARG:HH21 | 3:D:1389:LEU:CD1 | 2.20 | 0.54 |
| 3:N:1267:ARG:CZ | 3:N:1267:ARG:HB2 | 2.36 | 0.54 |
| 3:N:966:GLU:HA | 3:N:969:ARG:CZ | 2.37 | 0.54 |
| 1:L:19:GLU:O | 1:L:200:TRP:HA | 2.07 | 0.54 |
| 1:B:66:SER:O | 1:B:75:VAL:HG23 | 2.07 | 0.54 |
| 1:L:215:VAL:CG2 | 1:L:216:GLU:N | 2.70 | 0.54 |
| 1:K:34:VAL:HG11 | 1:L:42:ARG:HH12 | 1.71 | 0.54 |
| 3:N:812:ALA:C | 3:N:814:ALA:N | 2.56 | 0.54 |
| 3:D:984:THR:HG22 | 3:D:987:GLU:HB2 | 1.88 | 0.54 |
| 3:D:1499:ARG:HG3 | 3:D:1499:ARG:NH1 | 2.22 | 0.54 |
| 3:N:1197:ARG:HG2 | 3:N:1198:TYR:CD2 | 2.41 | 0.54 |
| 3:N:582:LEU:O | 3:N:603:LEU:HB2 | 2.07 | 0.54 |
| 3:D:622:ARG:HG2 | 3:D:622:ARG:NH1 | 2.22 | 0.54 |
| 3:D:1087:ARG:HD2 | 3:D:1234:THR:HA | 1.89 | 0.54 |
| 2:M:224:GLU:HB3 | 2:M:227:PHE:CD1 | 2.42 | 0.54 |
| 2:C:517:ARG:CB | 2:C:520:GLU:HB2 | 2.35 | 0.54 |
| 3:N:432:TYR:CD2 | 3:N:450:TYR:HB2 | 2.42 | 0.54 |
| 3:N:527:MET:HA | 3:N:537:THR:CG2 | 2.37 | 0.54 |
| 2:C:1089:VAL:O | 2:C:1093:GLN:HG3 | 2.08 | 0.54 |
| 3:D:539:ASP:O | 3:D:542:ASP:HB2 | 2.07 | 0.54 |
| 5:P:386:VAL:CG2 | 5:P:387:GLY:N | 2.71 | 0.54 |
| 3:N:1101:VAL:HG21 | 3:N:1424:VAL:HB | 1.87 | 0.54 |
| 5:P:265:VAL:O | 5:P:266:GLU:C | 2.46 | 0.54 |
| 5:P:306:GLU:O | 5:P:307:THR:C | 2.45 | 0.54 |
| 3:D:800:LYS:N | 3:D:800:LYS:HE2 | 2.22 | 0.54 |
| 3:D:851:LEU:H | 3:D:851:LEU:HD23 | 1.70 | 0.54 |
| 2:C:572:ILE:HG13 | 2:C:573:ARG:N | 2.21 | 0.54 |
| 2:M:1058:ASP:HB3 | 2:M:1082:PRO:HB3 | 1.89 | 0.54 |
| 3:N:659:LYS:HG3 | 3:N:663:GLU:OE2 | 2.08 | 0.54 |
| 1:L:28:LEU:CD2 | 1:L:29:GLU:H | 2.20 | 0.54 |
| 3:N:807:ALA:HA | 3:N:833:GLU:CB | 2.36 | 0.54 |
| 3:N:736:PHE:O | 3:N:738:ALA:N | 2.39 | 0.54 |
| 5:P:155:THR:HA | 5:P:158:GLU:OE2 | 2.07 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:20:TYR:CD1 | 1:A:21:GLY:N | 2.75 | 0.54 |
| 1:L:153:ALA:HB2 | 1:L:167:VAL:C | 2.27 | 0.54 |
| 3:N:500:ARG:O | 3:N:504:ASP:N | 2.33 | 0.54 |
| 2:C:1031:ARG:N | 3:D:622:ARG:HH12 | 2.05 | 0.54 |
| 3:N:1310:ARG:HB3 | 3:N:1327:ARG:HB2 | 1.88 | 0.54 |
| 3:N:1137:ARG:O | 3:N:1141:GLU:HG3 | 2.07 | 0.54 |
| 2:M:281:LEU:HB3 | 2:M:305:PRO:CB | 2.37 | 0.54 |
| 3:D:1489:GLN:HA | 3:D:1492:LEU:CD1 | 2.37 | 0.54 |
| 3:N:241:ILE:HG13 | 3:N:312:ARG:CZ | 2.37 | 0.54 |
| 3:N:288:MET:HE1 | 3:N:307:ALA:CB | 2.35 | 0.54 |
| 2:C:174:LEU:CD2 | 2:C:184:MET:HG2 | 2.37 | 0.54 |
| 2:C:263:ASP:N | 2:C:263:ASP:OD2 | 2.40 | 0.54 |
| 3:N:90:MET:HE2 | 3:N:519:VAL:C | 2.27 | 0.54 |
| 3:D:238:PRO:HB3 | 3:D:318:ARG:HA | 1.87 | 0.54 |
| 3:D:1483:PHE:N | 3:D:1483:PHE:CD1 | 2.75 | 0.54 |
| 3:D:1486:VAL:HG22 | 4:E:75:PHE:HA | 1.89 | 0.54 |
| 3:D:253:ALA:N | 3:D:301:GLY:CA | 2.62 | 0.54 |
| 3:D:209:ARG:HA | 3:D:347:VAL:HB | 1.88 | 0.54 |
| 3:D:185:VAL:HG23 | 3:D:203:ALA:H | 1.73 | 0.54 |
| 2:M:650:ARG:HE | 2:M:650:ARG:H | 0.72 | 0.54 |
| 3:D:827:ILE:CG2 | 3:D:837:GLY:HA3 | 2.36 | 0.54 |
| 2:M:1048:THR:O | 2:M:1052:MET:HB2 | 2.06 | 0.54 |
| 2:C:640:ARG:HB2 | 2:C:642:ARG:NH2 | 2.23 | 0.54 |
| 2:C:695:LEU:HD22 | 2:C:832:LYS:HE2 | 1.89 | 0.54 |
| 2:M:1061:GLU:HA | 2:M:1064:ASN:ND2 | 2.22 | 0.54 |
| 2:C:808:ARG:H | 2:C:815:LEU:HD11 | 1.72 | 0.54 |
| 5:P:253:ASP:CA | 5:P:259:ARG:NH1 | 2.67 | 0.54 |
| 3:D:710:ARG:N | 3:D:1227:GLN:OE1 | 2.31 | 0.54 |
| 1:L:188:GLN:HG3 | 1:L:189:ARG:H | 1.72 | 0.54 |
| 3:D:1087:ARG:HD2 | 3:D:1234:THR:C | 2.27 | 0.54 |
| 3:N:1281:VAL:HG23 | 3:N:1317:ASP:O | 2.06 | 0.54 |
| 1:K:103:ALA:O | 1:K:104:GLU:HG3 | 2.07 | 0.54 |
| 1:B:224:TYR:HD2 | 1:B:224:TYR:N | 2.06 | 0.54 |
| 2:M:166:PRO:HB2 | 2:M:169:GLY:CA | 2.37 | 0.54 |
| 2:M:332:ARG:HG2 | 2:M:333:ILE:N | 2.23 | 0.54 |
| 2:C:148:PHE:CZ | 2:C:309:TYR:HD2 | 2.25 | 0.54 |
| 2:C:277:ALA:HB1 | 2:C:281:LEU:HD12 | 1.89 | 0.54 |
| 2:C:305:PRO:O | 2:C:308:ARG:HG2 | 2.07 | 0.54 |
| 2:C:512:ARG:CG | 2:C:523:ILE:HD11 | 2.37 | 0.54 |
| 2:C:556:ASN:O | 2:C:559:LEU:HB3 | 2.07 | 0.54 |
| 3:D:1107:VAL:HG11 | 3:D:1217:ILE:HA | 1.89 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:128:TYR:HE2 | 3:D:575:GLN:NE2 | 2.04 | 0.54 |
| 1:B:112:ARG:CZ | 1:B:112:ARG:HB3 | 2.38 | 0.54 |
| 3:D:803:GLY:C | 3:D:805:GLU:N | 2.61 | 0.54 |
| 2:C:768:THR:HG22 | 2:C:770:GLU:N | 2.23 | 0.54 |
| 2:C:1071:ILE:C | 2:C:1073:GLY:H | 2.11 | 0.54 |
| 5:F:290:GLU:HA | 5:F:293:GLU:OE1 | 2.07 | 0.54 |
| 5:P:370:LYS:HA | 5:P:374:GLY:H | 1.73 | 0.54 |
| 3:D:1374:GLN:O | 3:D:1377:LYS:HB3 | 2.05 | 0.54 |
| 2:M:1100:GLN:CG | 2:M:1102:LEU:HD21 | 2.36 | 0.54 |
| 3:N:1032:PRO:O | 3:N:1033:GLN:C | 2.46 | 0.54 |
| 2:C:577:PRO:HA | 2:C:671:ASN:OD1 | 2.08 | 0.54 |
| 2:C:976:ASP:OD1 | 2:C:978:ARG:HG3 | 2.07 | 0.54 |
| 1:B:76:VAL:CA | 1:B:79:ILE:HD12 | 2.29 | 0.54 |
| 1:A:75:VAL:O | 1:A:78:ILE:HB | 2.07 | 0.54 |
| 1:A:79:ILE:O | 1:A:80:LEU:C | 2.45 | 0.54 |
| 1:A:123:MET:CE | 1:A:123:MET:HA | 2.37 | 0.54 |
| 5:P:98:GLU:O | 5:P:99:GLU:C | 2.46 | 0.54 |
| 3:N:996:TRP:CE3 | 3:N:1056:PRO:HG2 | 2.42 | 0.54 |
| 3:N:1029:ARG:NH1 | 3:N:1029:ARG:HG3 | 2.22 | 0.54 |
| 2:C:1030:GLN:CG | 3:D:626:SER:HB2 | 2.36 | 0.54 |
| 1:B:224:TYR:N | 1:B:224:TYR:CD2 | 2.74 | 0.54 |
| 2:M:799:ILE:HD12 | 2:M:800:VAL:O | 2.07 | 0.54 |
| 2:M:630:ARG:HH11 | 2:M:630:ARG:HG2 | 1.72 | 0.54 |
| 3:N:217:LYS:CD | 3:N:262:LYS:HZ1 | 2.21 | 0.54 |
| 2:C:212:GLY:HA3 | 2:C:218:VAL:HG11 | 1.89 | 0.54 |
| 3:D:114:THR:HG22 | 3:D:114:THR:O | 2.07 | 0.54 |
| 3:D:1462:LEU:HD22 | 3:D:1472:ILE:HD12 | 1.88 | 0.54 |
| 3:D:582:LEU:CA | 3:D:603:LEU:HD12 | 2.16 | 0.54 |
| 2:C:1015:LEU:HD12 | 5:F:335:ASP:HB2 | 1.90 | 0.54 |
| 3:N:441:ARG:C | 3:N:443:VAL:N | 2.59 | 0.54 |
| 3:D:210:ARG:CB | 3:D:389:GLU:HG3 | 2.35 | 0.54 |
| 3:D:268:ALA:HB3 | 3:D:290:PRO:HG3 | 1.90 | 0.54 |
| 3:D:925:GLU:CD | 4:E:6:ILE:HG22 | 2.28 | 0.54 |
| 3:D:653:PHE:HD1 | 3:D:653:PHE:N | 2.04 | 0.54 |
| 5:F:289:GLU:O | 5:F:293:GLU:HG3 | 2.08 | 0.54 |
| 3:N:1500:LYS:O | 3:N:1503:VAL:HG23 | 2.08 | 0.54 |
| 4:O:71:GLY:O | 4:O:73:LEU:N | 2.41 | 0.54 |
| 1:L:161:ARG:CB | 1:L:164:ALA:HB2 | 2.28 | 0.54 |
| 2:M:554:ASP:HB2 | 2:M:880:MET:HB2 | 1.90 | 0.54 |
| 3:N:614:PHE:HZ | 9:N:1528:NE6:H21 | 1.72 | 0.54 |
| 1:L:176:ARG:HD2 | 1:L:200:TRP:NE1 | 2.21 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:73:GLU:HB2 | 1:B:78:ILE:HD11 | 1.90 | 0.54 |
| 3:D:860:LEU:HA | 3:D:877:PRO:CB | 2.36 | 0.54 |
| 3:D:706:PRO:HB2 | 3:D:708:LEU:CD2 | 2.36 | 0.54 |
| 3:D:984:THR:HG22 | 3:D:987:GLU:CB | 2.38 | 0.54 |
| 5:P:142:ARG:HD3 | 5:P:145:PRO:HA | 1.90 | 0.54 |
| 5:P:107:GLU:O | 5:P:110:MET:HB3 | 2.07 | 0.54 |
| 5:P:242:TRP:CA | 5:P:245:GLN:HG2 | 2.35 | 0.54 |
| 2:M:520:GLU:OE1 | 2:M:520:GLU:HA | 2.06 | 0.54 |
| 3:N:1001:GLU:CA | 3:N:1001:GLU:OE2 | 2.53 | 0.54 |
| 3:D:1366:LYS:O | 3:D:1369:GLU:N | 2.41 | 0.54 |
| 3:N:1046:GLN:CA | 3:N:1052:THR:HA | 2.38 | 0.54 |
| 2:M:136:ILE:HG21 | 2:M:336:VAL:HG13 | 1.90 | 0.54 |
| 2:C:327:HIS:HA | 2:C:431:HIS:NE2 | 2.22 | 0.54 |
| 3:N:154:THR:HG22 | 3:N:157:GLU:CD | 2.27 | 0.54 |
| 3:D:118:LEU:HD23 | 3:D:123:LEU:HD13 | 1.89 | 0.54 |
| 4:E:27:ALA:O | 4:E:31:LEU:HG | 2.07 | 0.54 |
| 3:D:560:GLN:HA | 5:F:132:ARG:HH12 | 1.73 | 0.54 |
| 1:B:104:GLU:HB3 | 1:B:137:ARG:CB | 2.37 | 0.54 |
| 2:M:605:LYS:CB | 2:M:610:ARG:NH2 | 2.70 | 0.54 |
| 5:P:365:GLU:HA | 5:P:368:VAL:CG1 | 2.38 | 0.54 |
| 2:M:809:GLY:C | 2:M:811:PRO:CD | 2.74 | 0.54 |
| 4:O:70:THR:O | 4:O:72:ARG:N | 2.40 | 0.54 |
| 3:N:959:GLU:O | 3:N:962:GLN:HB2 | 2.07 | 0.54 |
| 3:N:796:ARG:C | 3:N:797:LYS:HG3 | 2.27 | 0.54 |
| 2:M:913:GLU:O | 2:M:917:LEU:HG | 2.08 | 0.54 |
| 2:M:953:VAL:HG13 | 2:M:966:LEU:CD1 | 2.38 | 0.54 |
| 2:M:486:MET:SD | 2:M:491:GLU:CA | 2.96 | 0.54 |
| 5:P:102:LEU:O | 5:P:106:VAL:HG23 | 2.08 | 0.54 |
| 3:D:1283:ILE:HD12 | 3:D:1315:ASP:OD2 | 2.07 | 0.54 |
| 3:D:1315:ASP:O | 3:D:1317:ASP:N | 2.40 | 0.54 |
| 3:D:985:ASP:O | 3:D:988:ARG:HB3 | 2.08 | 0.54 |
| 3:N:1120:VAL:N | 3:N:1186:VAL:O | 2.37 | 0.54 |
| 3:N:500:ARG:O | 3:N:504:ASP:CB | 2.56 | 0.54 |
| 3:N:1124:GLN:HG3 | 3:N:1133:ARG:HB3 | 1.88 | 0.54 |
| 3:D:730:PRO:HA | 3:D:733:CYS:SG | 2.48 | 0.54 |
| 2:C:1032:PHE:N | 3:D:621:LYS:O | 2.33 | 0.54 |
| 2:M:389:SER:HB3 | 2:M:392:SER:CB | 2.38 | 0.54 |
| 2:M:396:ASP:HB2 | 2:M:406:HIS:CD2 | 2.43 | 0.54 |
| 3:N:147:VAL:CG2 | 3:N:148:GLU:N | 2.56 | 0.54 |
| 3:N:154:THR:HG23 | 3:N:156:GLU:OE2 | 2.08 | 0.54 |
| 3:D:109:PRO:HG2 | 3:D:111:LYS:CE | 2.38 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:154:THR:HG23 | 3:D:156:GLU:OE2 | 2.08 | 0.54 |
| 1:B:58:ILE:HD13 | 1:B:59:GLU:N | 2.23 | 0.54 |
| 2:M:151:ASP:HB2 | 2:M:158:TYR:HA | 1.89 | 0.54 |
| 2:C:73:LEU:CB | 2:C:93:PRO:O | 2.56 | 0.54 |
| 2:C:889:HIS:HD2 | 2:C:970:GLY:HA3 | 1.71 | 0.54 |
| 2:C:953:VAL:HG12 | 2:C:965:GLU:HB3 | 1.88 | 0.54 |
| 3:N:59:ALA:HB3 | 3:N:76:CYS:HB2 | 1.89 | 0.54 |
| 2:M:672:VAL:HG23 | 2:M:868:ASP:OD2 | 2.08 | 0.54 |
| 3:N:792:ILE:HD13 | 3:N:941:PHE:CE1 | 2.42 | 0.54 |
| 2:C:694:LEU:CD2 | 2:C:868:ASP:HB3 | 2.30 | 0.54 |
| 2:M:1086:ARG:HD3 | 2:M:1112:PHE:CD2 | 2.42 | 0.54 |
| 3:D:1354:LYS:HA | 3:D:1357:ARG:HD2 | 1.90 | 0.54 |
| 1:K:57:TYR:HE1 | 1:K:163:ASN:HB2 | 1.73 | 0.54 |
| 2:C:1013:TYR:O | 2:C:1014:SER:C | 2.46 | 0.54 |
| 2:C:133:ASP:HB2 | 2:C:632:ASN:OD1 | 2.06 | 0.54 |
| 2:C:346:VAL:HB | 2:C:350:ARG:NH2 | 2.23 | 0.54 |
| 3:D:177:ALA:HB3 | 3:D:191:LEU:O | 2.07 | 0.54 |
| 2:C:915:LYS:HD3 | 2:C:968:LEU:O | 2.07 | 0.54 |
| 2:M:896:PHE:O | 2:M:898:GLY:N | 2.40 | 0.54 |
| 3:D:349:PRO:CG | 5:F:97:GLU:HG2 | 2.37 | 0.54 |
| 2:M:252:LYS:HD3 | 2:M:298:PHE:CE1 | 2.43 | 0.54 |
| 2:C:498:GLN:OE1 | 3:D:1067:VAL:HG13 | 2.07 | 0.54 |
| 3:N:564:GLU:CD | 3:N:565:ILE:N | 2.61 | 0.54 |
| 3:N:84:ILE:HG23 | 3:N:85:VAL:N | 2.22 | 0.54 |
| 3:N:570:GLU:OE2 | 5:P:214:GLN:HG3 | 2.07 | 0.54 |
| 3:D:604:THR:O | 3:D:607:LEU:HB3 | 2.07 | 0.54 |
| 2:M:603:VAL:CG1 | 2:M:645:VAL:HA | 2.37 | 0.54 |
| 2:C:30:LEU:HD23 | 2:C:44:ILE:CD1 | 2.38 | 0.54 |
| 2:M:808:ARG:NH2 | 2:M:819:VAL:O | 2.40 | 0.54 |
| 3:N:1486:VAL:HG13 | 4:O:74:VAL:O | 2.08 | 0.54 |
| 3:D:794:GLN:OE1 | 3:D:905:PRO:HG3 | 2.06 | 0.54 |
| 3:D:167:GLU:HB3 | 3:D:169:TYR:CE1 | 2.43 | 0.54 |
| 3:N:1476:THR:HG21 | 4:O:20:THR:HB | 1.89 | 0.54 |
| 2:M:1088:LEU:CA | 2:M:1091:GLU:OE1 | 2.52 | 0.54 |
| 1:A:83:LYS:NZ | 1:A:170:VAL:HG22 | 2.23 | 0.54 |
| 2:M:983:ILE:O | 2:M:984:GLU:C | 2.46 | 0.54 |
| 3:D:1311:LEU:CG | 3:D:1312:LEU:N | 2.71 | 0.54 |
| 2:C:133:ASP:HB3 | 2:C:395:LYS:HB3 | 1.90 | 0.54 |
| 2:C:895:TYR:CD2 | 2:C:895:TYR:C | 2.81 | 0.54 |
| 3:N:1216:SER:CB | 4:O:16:LYS:H | 2.20 | 0.54 |
| 2:C:159:ILE:HG22 | 2:C:174:LEU:O | 2.08 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:533:ASP:HB3 | 2:C:538:GLN:OE1 | 2.08 | 0.54 |
| 3:N:411:THR:CG2 | 5:P:179:GLU:HG3 | 2.26 | 0.54 |
| 3:D:153:LEU:CD1 | 3:D:157:GLU:HB3 | 2.38 | 0.54 |
| 3:D:564:GLU:HA | 3:D:567:ILE:HB | 1.88 | 0.54 |
| 3:D:592:THR:CG2 | 3:D:600:LEU:HD21 | 2.38 | 0.54 |
| 3:D:6:ARG:HH21 | 3:D:1482:ARG:HH22 | 1.56 | 0.54 |
| 4:E:88:GLU:OE1 | 4:E:91:ARG:NH1 | 2.41 | 0.54 |
| 3:D:287:GLY:C | 3:D:311:LEU:HD22 | 2.28 | 0.54 |
| 1:B:56:VAL:HG12 | 1:B:57:TYR:N | 2.21 | 0.54 |
| 3:D:819:GLY:HA2 | 3:D:824:ASN:ND2 | 2.23 | 0.54 |
| 3:D:1404:ASN:HA | 3:D:1409:ALA:H | 1.70 | 0.54 |
| 3:D:65:ARG:HG2 | 3:D:67:ARG:HG2 | 1.89 | 0.54 |
| 3:D:955:VAL:O | 3:D:957:PRO:HD3 | 2.08 | 0.54 |
| 3:N:1112:CYS:N | 3:N:1201:CYS:CB | 2.70 | 0.54 |
| 2:C:595:LEU:HD21 | 2:C:639:GLN:NE2 | 2.23 | 0.54 |
| 3:N:692:GLU:O | 3:N:693:GLU:C | 2.45 | 0.54 |
| 2:C:24:GLU:HA | 2:C:27:ARG:HB3 | 1.88 | 0.54 |
| 3:N:806:PHE:CD2 | 3:N:809:PRO:HB2 | 2.43 | 0.54 |
| 5:P:329:TYR:O | 5:P:332:PHE:CD1 | 2.61 | 0.54 |
| 3:N:1395:LEU:O | 3:N:1398:TRP:CD1 | 2.61 | 0.54 |
| 3:D:1121:PRO:O | 3:D:1122:LEU:HD23 | 2.07 | 0.54 |
| 1:A:72:LYS:O | 2:C:608:GLY:HA2 | 2.08 | 0.54 |
| 2:M:449:ILE:HD13 | 3:N:1082:ALA:HA | 1.90 | 0.54 |
| 3:D:996:TRP:O | 3:D:997:THR:C | 2.46 | 0.54 |
| 3:N:924:MET:CG | 3:N:925:GLU:N | 2.71 | 0.54 |
| 1:L:112:ARG:HH12 | 1:L:125:PRO:HB2 | 1.72 | 0.54 |
| 2:M:861:LEU:HB2 | 2:M:863:ASP:OD1 | 2.08 | 0.54 |
| 1:A:1:MET:N | 1:A:6:LEU:HB2 | 2.21 | 0.54 |
| 1:A:11:PHE:HB2 | 1:A:25:LEU:HD13 | 1.90 | 0.54 |
| 3:N:1123:PHE:HA | 3:N:1133:ARG:O | 2.08 | 0.54 |
| 2:C:685:GLU:CG | 3:D:739:ASP:HB3 | 2.37 | 0.54 |
| 1:B:117:VAL:CG1 | 1:B:118:ALA:N | 2.70 | 0.54 |
| 3:N:1216:SER:HB2 | 4:O:16:LYS:H | 1.71 | 0.54 |
| 2:M:185:LYS:NZ | 2:M:190:LYS:NZ | 2.56 | 0.54 |
| 2:C:289:THR:O | 2:C:290:LEU:HD23 | 2.08 | 0.54 |
| 3:N:127:LEU:HD23 | 3:N:128:TYR:HA | 1.89 | 0.54 |
| 3:N:87:ARG:HG3 | 3:N:88:TYR:CE2 | 2.43 | 0.54 |
| 5:P:221:ILE:O | 5:P:224:VAL:HB | 2.08 | 0.54 |
| 3:D:437:VAL:HG13 | 3:D:437:VAL:O | 2.06 | 0.54 |
| 3:D:136:ASP:OD2 | 3:D:455:ARG:HD2 | 2.08 | 0.54 |
| 3:D:541:ASN:O | 3:D:545:ARG:HG3 | 2.08 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:441:ARG:HB3 | 3:D:443:VAL:HG23 | 1.89 | 0.54 |
| 3:D:489:ARG:HH21 | 3:D:1389:LEU:HD12 | 1.73 | 0.54 |
| 2:C:943:VAL:O | 2:C:946:ARG:N | 2.41 | 0.54 |
| 3:D:414:ARG:HH11 | 3:D:451:ASP:CG | 2.11 | 0.54 |
| 1:L:20:TYR:HA | 1:L:199:ILE:O | 2.06 | 0.54 |
| 3:N:1478:SER:C | 3:N:1482:ARG:HG3 | 2.29 | 0.54 |
| 3:N:14:SER:HB3 | 3:N:16:GLU:OE2 | 2.08 | 0.54 |
| 1:A:152:PRO:O | 1:A:155:LYS:CB | 2.56 | 0.54 |
| 3:D:630:VAL:HA | 3:D:744:GLN:HA | 1.89 | 0.54 |
| 1:A:123:MET:HA | 1:A:123:MET:HE2 | 1.89 | 0.54 |
| 2:M:492:ASP:HA | 2:M:518:LYS:HB3 | 1.90 | 0.54 |
| 5:P:95:THR:O | 5:P:96:LEU:C | 2.46 | 0.54 |
| 3:D:887:ALA:HA | 3:D:890:VAL:HG22 | 1.90 | 0.54 |
| 3:D:1311:LEU:HG | 3:D:1313:VAL:H | 1.73 | 0.54 |
| 3:N:1102:THR:HG22 | 3:N:1374:GLN:HG3 | 1.89 | 0.54 |
| 3:N:499:VAL:HG12 | 3:N:503:LEU:HD12 | 1.90 | 0.54 |
| 2:C:10:ARG:NH1 | 2:C:481:ASP:OD1 | 2.41 | 0.54 |
| 3:D:1123:PHE:HA | 3:D:1133:ARG:O | 2.08 | 0.54 |
| 3:D:1360:GLY:HA2 | 3:D:1362:LYS:NZ | 2.23 | 0.54 |
| 2:M:166:PRO:HG2 | 2:M:262:ALA:O | 2.08 | 0.53 |
| 2:M:299:LYS:HG2 | 2:M:300:ASP:N | 2.23 | 0.53 |
| 3:N:133:ILE:HD12 | 3:N:456:MET:HE1 | 1.89 | 0.53 |
| 3:D:1092:GLY:O | 3:D:1093:TYR:C | 2.46 | 0.53 |
| 3:D:109:PRO:O | 3:D:111:LYS:HE3 | 2.08 | 0.53 |
| 3:D:1481:VAL:HG12 | 4:E:21:VAL:HG21 | 1.88 | 0.53 |
| 2:M:649:VAL:CG1 | 2:M:653:ASP:HB2 | 2.38 | 0.53 |
| 5:P:256:ARG:HB3 | 5:P:258:ILE:O | 2.07 | 0.53 |
| 5:P:301:ALA:O | 5:P:304:VAL:HB | 2.08 | 0.53 |
| 5:P:308:LEU:H | 5:P:308:LEU:CD2 | 2.21 | 0.53 |
| 1:B:181:VAL:HG22 | 1:B:195:LEU:HD13 | 1.90 | 0.53 |
| 2:C:674:VAL:HB | 2:C:869:VAL:HG13 | 1.89 | 0.53 |
| 2:C:984:GLU:HG3 | 3:D:944:THR:O | 2.08 | 0.53 |
| 3:D:169:TYR:O | 3:D:392:SER:HA | 2.08 | 0.53 |
| 2:C:599:GLU:HG3 | 2:C:600:ASP:H | 1.72 | 0.53 |
| 2:C:649:VAL:CG1 | 2:C:653:ASP:HB2 | 2.38 | 0.53 |
| 3:N:654:LYS:CB | 3:N:655:PRO:HD3 | 2.30 | 0.53 |
| 1:K:20:TYR:C | 1:K:207:PRO:HG2 | 2.28 | 0.53 |
| 1:A:127:LEU:HD12 | 1:A:128:HIS:N | 2.23 | 0.53 |
| 5:F:365:GLU:HA | 5:F:368:VAL:CG1 | 2.36 | 0.53 |
| 3:N:1205:TYR:HD2 | 3:N:1215:VAL:HG11 | 1.73 | 0.53 |
| 2:C:343:GLN:HG2 | 2:C:385:PHE:CG | 2.44 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:P:223:ALA:HB2 | 5:P:242:TRP:CB | 2.38 | 0.53 |
| 2:M:517:ARG:O | 2:M:520:GLU:HG2 | 2.07 | 0.53 |
| 1:L:150:TYR:CZ | 1:L:168:ASP:HB3 | 2.42 | 0.53 |
| 3:D:768:ASN:C | 3:D:769:LEU:HD12 | 2.28 | 0.53 |
| 2:C:994:ILE:CG2 | 2:C:995:MET:N | 2.70 | 0.53 |
| 2:C:685:GLU:HG2 | 3:D:739:ASP:HB3 | 1.90 | 0.53 |
| 4:O:85:LEU:H | 4:O:85:LEU:HD23 | 1.72 | 0.53 |
| 3:D:625:TYR:O | 3:D:749:VAL:HG23 | 2.08 | 0.53 |
| 1:A:200:TRP:N | 1:A:200:TRP:CD1 | 2.76 | 0.53 |
| 2:C:254:VAL:HB | 2:C:258:TYR:CE1 | 2.43 | 0.53 |
| 2:C:461:VAL:HA | 2:C:466:PHE:O | 2.08 | 0.53 |
| 2:C:5:ARG:HG2 | 2:C:902:ILE:HD12 | 1.90 | 0.53 |
| 3:N:411:THR:H | 3:N:437:VAL:CG2 | 2.21 | 0.53 |
| 2:C:1102:LEU:CD1 | 3:D:9:ARG:HB2 | 2.39 | 0.53 |
| 2:C:1104:GLU:C | 2:C:1106:ASP:H | 2.10 | 0.53 |
| 3:D:119:SER:C | 3:D:121:THR:N | 2.60 | 0.53 |
| 4:E:26:ARG:O | 4:E:30:LEU:HB2 | 2.08 | 0.53 |
| 3:D:215:TYR:CE1 | 3:D:380:GLU:HB2 | 2.43 | 0.53 |
| 3:D:351:MET:HA | 3:D:370:ALA:HB2 | 1.89 | 0.53 |
| 1:B:56:VAL:HG22 | 1:B:142:VAL:HG13 | 1.90 | 0.53 |
| 1:B:206:THR:CG2 | 1:B:208:LEU:HB3 | 2.38 | 0.53 |
| 2:M:622:GLU:O | 2:M:624:PRO:HD3 | 2.08 | 0.53 |
| 5:F:272:SER:O | 5:F:275:ALA:HB3 | 2.08 | 0.53 |
| 3:D:448:GLU:N | 3:D:448:GLU:OE1 | 2.42 | 0.53 |
| 3:N:1435:LEU:O | 3:N:1438:ALA:N | 2.41 | 0.53 |
| 2:M:672:VAL:CG2 | 2:M:868:ASP:HB2 | 2.38 | 0.53 |
| 3:N:799:LYS:HB2 | 3:N:826:PRO:HG2 | 1.89 | 0.53 |
| 3:N:841:TYR:HB2 | 3:N:864:VAL:CG1 | 2.34 | 0.53 |
| 3:N:915:VAL:O | 3:N:918:ALA:HB3 | 2.07 | 0.53 |
| 3:D:1277:ILE:HG21 | 3:D:1299:PHE:CE1 | 2.43 | 0.53 |
| 2:C:666:LEU:HD12 | 2:C:667:ALA:H | 1.72 | 0.53 |
| 3:N:10:ILE:O | 3:N:1451:ALA:HA | 2.08 | 0.53 |
| 1:A:75:VAL:O | 1:A:79:ILE:HG13 | 2.08 | 0.53 |
| 3:N:734:GLU:OE2 | 3:N:780:LYS:NZ | 2.38 | 0.53 |
| 1:A:228:PRO:C | 1:A:229:GLN:HG3 | 2.28 | 0.53 |
| 2:C:603:VAL:CG2 | 2:C:647:GLN:HB3 | 2.37 | 0.53 |
| 2:C:384:GLU:HA | 2:C:388:ARG:HH21 | 1.74 | 0.53 |
| 2:M:292:ARG:HE | 2:M:295:ASP:HB3 | 1.71 | 0.53 |
| 4:E:46:PRO:HG2 | 4:E:63:TRP:CD1 | 2.44 | 0.53 |
| 3:D:1216:SER:OG | 4:E:16:LYS:HB3 | 2.09 | 0.53 |
| 3:D:958:GLU:OE2 | 3:D:961:LYS:HG3 | 2.08 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:N:989:TYR:CZ | 3:N:993:LEU:HD11 | 2.43 | 0.53 |
| 2:M:738:ASP:OD2 | 2:M:739:GLU:OE2 | 2.26 | 0.53 |
| 2:C:728:HIS:CG | 2:C:729:LEU:N | 2.77 | 0.53 |
| 3:N:163:TYR:OH | 5:P:186:HIS:CE1 | 2.61 | 0.53 |
| 2:M:998:TYR:HE2 | 2:M:1000:MET:HA | 1.72 | 0.53 |
| 3:N:894:LYS:O | 3:N:898:GLU:HG3 | 2.08 | 0.53 |
| 1:A:189:ARG:HA | 11:A:317:HOH:O | 2.08 | 0.53 |
| 3:N:817:GLU:O | 3:N:821:VAL:HG23 | 2.07 | 0.53 |
| 2:M:140:ILE:HD12 | 2:M:331:ARG:NH2 | 2.23 | 0.53 |
| 3:N:238:PRO:CG | 3:N:318:ARG:HG2 | 2.38 | 0.53 |
| 2:C:141:HIS:CD2 | 2:C:334:ARG:HG2 | 2.43 | 0.53 |
| 3:N:124:GLU:HG3 | 3:N:128:TYR:CZ | 2.44 | 0.53 |
| 3:D:1447:LEU:O | 3:D:1448:THR:C | 2.47 | 0.53 |
| 2:M:69:LEU:HB3 | 2:M:97:ARG:CB | 2.39 | 0.53 |
| 3:D:325:GLU:HG2 | 3:D:332:TYR:HB3 | 1.91 | 0.53 |
| 3:D:937:TYR:CD1 | 3:D:937:TYR:N | 2.77 | 0.53 |
| 5:P:352:GLU:O | 5:P:353:GLU:C | 2.46 | 0.53 |
| 2:M:101:ILE:HA | 2:M:106:GLY:O | 2.08 | 0.53 |
| 2:M:355:VAL:HA | 2:M:358:ARG:NE | 2.23 | 0.53 |
| 5:F:287:THR:O | 5:F:288:TYR:C | 2.46 | 0.53 |
| 3:D:414:ARG:HA | 3:D:433:GLY:O | 2.09 | 0.53 |
| 3:N:1032:PRO:O | 3:N:1035:ILE:N | 2.41 | 0.53 |
| 3:N:1465:ASN:ND2 | 3:N:1472:ILE:HA | 2.23 | 0.53 |
| 3:N:1171:VAL:O | 3:N:1172:HIS:C | 2.46 | 0.53 |
| 2:C:571:LEU:CD1 | 2:C:700:TYR:HA | 2.39 | 0.53 |
| 1:A:30:ARG:HH21 | 1:A:191:ASP:CB | 2.22 | 0.53 |
| 3:D:703:ASN:HD22 | 3:D:704:ARG:H | 1.56 | 0.53 |
| 1:K:122:ILE:HG22 | 1:K:124:ASN:N | 2.11 | 0.53 |
| 2:M:923:GLU:O | 2:M:924:VAL:C | 2.47 | 0.53 |
| 2:M:926:PHE:HE2 | 2:M:960:GLU:HG3 | 1.74 | 0.53 |
| 1:L:144:VAL:HG12 | 1:L:145:ASP:H | 1.73 | 0.53 |
| 1:K:9:PRO:HB2 | 1:K:25:LEU:HD11 | 1.90 | 0.53 |
| 1:K:5:LYS:C | 1:K:7:LYS:H | 2.11 | 0.53 |
| 2:C:603:VAL:CG1 | 2:C:645:VAL:HA | 2.38 | 0.53 |
| 3:D:1286:THR:HG22 | 3:D:1288:GLU:N | 2.21 | 0.53 |
| 2:M:1005:MET:HE1 | 3:N:648:MET:HB2 | 1.89 | 0.53 |
| 3:N:626:SER:HA | 3:N:747:VAL:O | 2.09 | 0.53 |
| 1:A:70:GLY:N | 2:C:607:ASP:HB2 | 2.22 | 0.53 |
| 2:C:397:GLU:HA | 2:C:403:SER:HB3 | 1.89 | 0.53 |
| 2:C:634:GLY:HA3 | 2:C:704:HIS:CE1 | 2.42 | 0.53 |
| 5:P:81:VAL:CG2 | 5:P:82:ARG:H | 2.19 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:1045:MET:O | 3:D:1053:PHE:HD1 | 1.91 | 0.53 |
| 3:N:821:VAL:C | 3:N:823:LEU:H | 2.11 | 0.53 |
| 2:C:208:ALA:HB2 | 2:C:221:LEU:HD22 | 1.90 | 0.53 |
| 5:P:132:ARG:HG2 | 5:P:181:GLU:HG2 | 1.90 | 0.53 |
| 5:P:208:SER:HB3 | 5:P:211:ASP:CG | 2.29 | 0.53 |
| 3:D:250:LEU:CD1 | 3:D:304:LEU:HA | 2.39 | 0.53 |
| 3:N:363:ALA:HA | 3:N:380:GLU:HA | 1.90 | 0.53 |
| 3:D:639:LEU:N | 3:D:729:HIS:CE1 | 2.76 | 0.53 |
| 2:M:774:LEU:C | 2:M:774:LEU:HD13 | 2.29 | 0.53 |
| 3:D:812:ALA:CA | 3:D:816:HIS:HB2 | 2.26 | 0.53 |
| 1:A:36:LEU:C | 1:A:40:LEU:HD12 | 2.28 | 0.53 |
| 1:K:69:PRO:O | 1:K:71:VAL:HG23 | 2.06 | 0.53 |
| 2:M:603:VAL:CG2 | 2:M:647:GLN:HB3 | 2.38 | 0.53 |
| 3:D:397:LYS:O | 3:D:447:VAL:HG13 | 2.09 | 0.53 |
| 3:D:434:ARG:HH21 | 3:D:451:ASP:CG | 2.10 | 0.53 |
| 3:D:436:GLU:HB2 | 3:D:445:ARG:O | 2.09 | 0.53 |
| 5:F:82:ARG:O | 5:F:85:LEU:HB2 | 2.09 | 0.53 |
| 3:N:372:ASP:C | 3:N:374:GLU:N | 2.61 | 0.53 |
| 1:A:150:TYR:HD1 | 1:A:170:VAL:HG12 | 1.73 | 0.53 |
| 2:M:41:ASN:HD22 | 2:M:42:VAL:N | 2.05 | 0.53 |
| 2:M:572:ILE:HG13 | 2:M:701:THR:O | 2.09 | 0.53 |
| 2:M:437:ARG:HG3 | 2:M:437:ARG:HH11 | 1.73 | 0.53 |
| 5:P:95:THR:O | 5:P:98:GLU:HB2 | 2.08 | 0.53 |
| 1:B:19:GLU:HG2 | 1:B:203:GLY:N | 2.23 | 0.53 |
| 2:C:396:ASP:OD1 | 2:C:402:SER:HB2 | 2.09 | 0.53 |
| 5:P:110:MET:HG2 | 5:P:111:GLU:N | 2.23 | 0.53 |
| 2:C:91:GLN:HB3 | 2:C:119:PRO:HA | 1.90 | 0.53 |
| 5:F:353:GLU:HA | 5:F:356:LYS:CD | 2.38 | 0.53 |
| 3:D:972:LEU:HD23 | 3:D:972:LEU:H | 1.71 | 0.53 |
| 1:L:182:GLU:O | 1:L:194:LYS:HB3 | 2.08 | 0.53 |
| 5:F:231:ARG:HB2 | 5:F:233:PHE:CZ | 2.44 | 0.53 |
| 3:N:124:GLU:O | 3:N:125:GLN:C | 2.47 | 0.53 |
| 3:D:591:VAL:HG11 | 3:D:597:ASP:O | 2.09 | 0.53 |
| 2:M:94:LEU:N | 2:M:116:GLY:O | 2.40 | 0.53 |
| 5:P:403:LYS:NZ | 5:P:407:LYS:HE2 | 2.22 | 0.53 |
| 5:P:410:TYR:O | 5:P:413:SER:HB2 | 2.09 | 0.53 |
| 2:M:603:VAL:HG21 | 2:M:647:GLN:HB3 | 1.89 | 0.53 |
| 2:M:625:LEU:CD1 | 2:M:639:GLN:HB2 | 2.37 | 0.53 |
| 3:N:1287:GLU:HB3 | 3:N:1288:GLU:OE1 | 2.09 | 0.53 |
| 3:D:1400:VAL:O | 3:D:1404:ASN:ND2 | 2.42 | 0.53 |
| 3:D:56:TYR:H | 3:D:81:THR:C | 2.11 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:N:1031:ASN:OD1 | 3:N:1034:GLN:HG3 | 2.09 | 0.53 |
| 3:N:1396:GLU:C | 3:N:1398:TRP:N | 2.61 | 0.53 |
| 1:B:9:PRO:HA | 1:B:27:PRO:HD2 | 1.90 | 0.53 |
| 2:C:1048:THR:O | 2:C:1052:MET:HB2 | 2.08 | 0.53 |
| 2:C:841:ASN:CG | 2:C:845:ASN:HB3 | 2.29 | 0.53 |
| 3:D:984:THR:CG2 | 3:D:987:GLU:H | 2.21 | 0.53 |
| 3:N:530:VAL:O | 3:N:531:ASP:C | 2.47 | 0.53 |
| 3:N:99:ALA:O | 3:N:514:LEU:HB2 | 2.08 | 0.53 |
| 3:N:99:ALA:N | 3:N:514:LEU:O | 2.39 | 0.53 |
| 3:D:218:LYS:HA | 3:D:337:LEU:O | 2.09 | 0.53 |
| 3:D:956:ILE:HG12 | 3:D:1039:CYS:O | 2.08 | 0.53 |
| 3:N:259:VAL:HG23 | 3:N:270:LEU:HD11 | 1.89 | 0.53 |
| 2:C:204:GLN:C | 2:C:209:ARG:HD3 | 2.28 | 0.53 |
| 2:C:329:GLY:CA | 2:C:488:ALA:HB3 | 2.38 | 0.53 |
| 3:N:125:GLN:O | 3:N:126:VAL:C | 2.47 | 0.53 |
| 3:N:139:GLY:HA3 | 3:N:147:VAL:CG2 | 2.38 | 0.53 |
| 3:N:538:SER:OG | 3:N:540:LEU:HG | 2.09 | 0.53 |
| 3:D:1232:PRO:HB2 | 3:D:1356:TYR:HE2 | 1.74 | 0.53 |
| 3:D:1436:SER:O | 3:D:1439:SER:HB3 | 2.08 | 0.53 |
| 3:D:154:THR:H | 3:D:157:GLU:CD | 2.12 | 0.53 |
| 3:D:9:ARG:CG | 3:D:10:ILE:N | 2.71 | 0.53 |
| 3:D:244:GLU:OE2 | 3:D:310:LEU:HD23 | 2.08 | 0.53 |
| 1:B:210:ALA:O | 1:B:211:LEU:C | 2.46 | 0.53 |
| 3:D:812:ALA:O | 3:D:813:LEU:C | 2.46 | 0.53 |
| 2:C:772:ARG:HD3 | 5:F:373:LYS:HD2 | 1.89 | 0.53 |
| 3:N:1101:VAL:CG2 | 3:N:1428:ALA:HB2 | 2.21 | 0.53 |
| 2:C:983:ILE:HG23 | 3:D:944:THR:O | 2.08 | 0.53 |
| 3:N:1094:LEU:HD23 | 3:N:1230:GLY:HA2 | 1.91 | 0.53 |
| 1:L:176:ARG:HG2 | 1:L:177:VAL:H | 1.71 | 0.53 |
| 2:M:573:ARG:HB2 | 2:M:670:GLN:NE2 | 2.23 | 0.53 |
| 5:F:94:LEU:CG | 5:F:190:ALA:HB1 | 2.38 | 0.53 |
| 2:M:1010:THR:HA | 3:N:624:ASP:OD1 | 2.09 | 0.53 |
| 1:B:75:VAL:O | 1:B:79:ILE:HG13 | 2.08 | 0.53 |
| 2:C:571:LEU:HD11 | 2:C:700:TYR:HA | 1.90 | 0.53 |
| 3:D:1286:THR:HB | 3:D:1289:LYS:N | 2.23 | 0.53 |
| 2:M:1030:GLN:NE2 | 3:N:628:ARG:HH21 | 2.05 | 0.53 |
| 1:L:90:LEU:O | 1:L:92:PRO:HD3 | 2.08 | 0.53 |
| 2:C:806:LEU:HB2 | 2:C:822:VAL:CG2 | 2.38 | 0.53 |
| 5:P:110:MET:HG2 | 5:P:114:LYS:HE3 | 1.90 | 0.53 |
| 1:A:214:ALA:HA | 1:A:217:ILE:HD12 | 1.91 | 0.53 |
| 1:L:83:LYS:HE2 | 1:L:168:ASP:HB2 | 1.91 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:N:1371:VAL:O | 3:N:1374:GLN:HB2 | 2.09 | 0.53 |
| 3:D:1119:SER:HB3 | 3:D:1185:GLU:HB3 | 1.91 | 0.53 |
| 2:C:87:ASP:OD1 | 2:C:824:ARG:NH2 | 2.40 | 0.53 |
| 5:P:239:ALA:O | 5:P:240:THR:C | 2.46 | 0.53 |
| 1:L:186:LEU:C | 1:L:188:GLN:H | 2.11 | 0.53 |
| 2:C:293:PHE:CD1 | 2:C:294:GLU:N | 2.77 | 0.53 |
| 2:M:258:TYR:O | 2:M:290:LEU:HD12 | 2.09 | 0.53 |
| 3:D:432:TYR:N | 3:D:432:TYR:CD1 | 2.76 | 0.53 |
| 3:N:387:LEU:N | 3:N:387:LEU:CD1 | 2.70 | 0.53 |
| 2:C:193:LEU:HD12 | 2:C:196:LEU:CD1 | 2.36 | 0.53 |
| 2:C:263:ASP:HB2 | 2:C:264:PRO:HD3 | 1.89 | 0.53 |
| 2:C:545:ASN:CB | 2:C:583:LEU:HD11 | 2.38 | 0.53 |
| 3:N:458:ALA:O | 3:N:459:GLU:C | 2.46 | 0.53 |
| 3:D:546:ARG:HH21 | 3:D:577:ALA:CA | 2.22 | 0.53 |
| 4:E:84:ARG:HG2 | 4:E:88:GLU:HG3 | 1.91 | 0.53 |
| 1:B:138:LEU:HD11 | 1:B:140:MET:HE2 | 1.90 | 0.53 |
| 2:C:34:VAL:N | 2:C:35:PRO:HD3 | 2.23 | 0.53 |
| 5:F:289:GLU:CD | 5:F:289:GLU:N | 2.56 | 0.53 |
| 2:M:759:THR:HB | 2:M:785:VAL:HG12 | 1.91 | 0.53 |
| 4:O:70:THR:C | 4:O:72:ARG:H | 2.11 | 0.53 |
| 3:D:69:GLU:HG3 | 3:D:70:GLY:H | 1.73 | 0.53 |
| 3:D:800:LYS:HE3 | 3:D:826:PRO:HD2 | 1.90 | 0.53 |
| 3:D:828:LYS:CD | 3:D:828:LYS:H | 2.22 | 0.53 |
| 3:N:1094:LEU:O | 3:N:1095:THR:C | 2.47 | 0.53 |
| 3:N:909:ASN:O | 3:N:910:SER:C | 2.46 | 0.53 |
| 3:N:274:ARG:NE | 3:N:279:VAL:HG21 | 2.24 | 0.53 |
| 2:C:591:SER:O | 2:C:592:LEU:HB2 | 2.09 | 0.53 |
| 2:C:695:LEU:O | 2:C:832:LYS:NZ | 2.33 | 0.53 |
| 3:N:1121:PRO:CD | 3:N:1346:ARG:HH21 | 2.21 | 0.53 |
| 3:N:661:MET:HB3 | 3:N:667:ALA:CB | 2.39 | 0.53 |
| 1:K:11:PHE:HB3 | 1:L:227:ASN:O | 2.08 | 0.53 |
| 2:C:1048:THR:O | 2:C:1052:MET:N | 2.36 | 0.53 |
| 2:C:135:VAL:CG2 | 2:C:395:LYS:HA | 2.38 | 0.53 |
| 2:M:512:ARG:CG | 2:M:523:ILE:HD11 | 2.38 | 0.53 |
| 2:C:897:LEU:HD13 | 2:C:917:LEU:HD22 | 1.90 | 0.53 |
| 1:B:153:ALA:HB2 | 1:B:167:VAL:C | 2.29 | 0.53 |
| 3:N:630:VAL:CA | 3:N:744:GLN:HG2 | 2.37 | 0.53 |
| 1:L:52:ALA:HB2 | 1:L:170:VAL:C | 2.29 | 0.53 |
| 2:M:726:ILE:HG13 | 2:M:728:HIS:HB2 | 1.89 | 0.53 |
| 3:D:1302:GLU:HG2 | 3:D:1303:TYR:N | 2.23 | 0.53 |
| 5:F:243:ILE:O | 5:F:247:ILE:HG13 | 2.08 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:13:VAL:HG22 | 1:A:14:ARG:N | 2.23 | 0.53 |
| 2:C:231:PRO:O | 2:C:235:LEU:HB2 | 2.07 | 0.53 |
| 2:C:141:HIS:HD2 | 2:C:334:ARG:CG | 2.21 | 0.53 |
| 2:C:424:GLY:O | 2:C:427:VAL:N | 2.39 | 0.53 |
| 3:N:154:THR:HG22 | 3:N:157:GLU:CB | 2.39 | 0.53 |
| 3:N:153:LEU:HD12 | 3:N:157:GLU:OE1 | 2.08 | 0.53 |
| 3:D:1479:ASP:HA | 3:D:1482:ARG:HG3 | 1.89 | 0.53 |
| 5:F:115:LYS:HB3 | 5:F:119:ILE:HD11 | 1.91 | 0.53 |
| 3:D:297:ILE:CD1 | 3:D:298:VAL:HG23 | 2.18 | 0.53 |
| 3:D:401:TYR:HB2 | 3:D:444:VAL:CG2 | 2.38 | 0.53 |
| 2:M:311:PHE:HA | 2:M:314:THR:OG1 | 2.08 | 0.53 |
| 3:D:1162:GLU:HG3 | 3:D:1162:GLU:O | 2.08 | 0.53 |
| 3:D:481:MET:O | 3:D:489:ARG:HG3 | 2.07 | 0.53 |
| 3:N:959:GLU:HA | 3:N:962:GLN:NE2 | 2.23 | 0.53 |
| 3:N:965:GLU:O | 3:N:968:ASP:N | 2.42 | 0.53 |
| 3:N:953:ASP:OD2 | 3:N:1019:PRO:HG2 | 2.09 | 0.53 |
| 2:C:673:LEU:HB2 | 2:C:868:ASP:OD2 | 2.09 | 0.53 |
| 1:B:48:ILE:O | 1:B:148:VAL:HG12 | 2.09 | 0.53 |
| 3:N:657:LEU:HG | 3:N:661:MET:HE2 | 1.90 | 0.53 |
| 1:K:42:ARG:NH1 | 1:L:31:GLY:O | 2.42 | 0.53 |
| 5:F:274:THR:HG22 | 5:F:278:LEU:HD11 | 1.90 | 0.53 |
| 5:P:102:LEU:CD2 | 5:P:187:LEU:HB2 | 2.39 | 0.53 |
| 2:C:712:ALA:O | 2:C:820:ARG:N | 2.26 | 0.53 |
| 3:D:14:SER:O | 3:D:15:PRO:C | 2.47 | 0.53 |
| 3:D:1500:LYS:C | 3:D:1502:ALA:N | 2.61 | 0.53 |
| 2:C:728:HIS:CE1 | 2:C:730:SER:H | 2.27 | 0.53 |
| 2:C:730:SER:OG | 2:C:731:GLU:N | 2.42 | 0.53 |
| 3:N:1293:PHE:CE2 | 3:N:1300:SER:HB3 | 2.44 | 0.53 |
| 2:M:141:HIS:HB2 | 2:M:418:LEU:HD22 | 1.91 | 0.53 |
| 3:N:212:ARG:HB3 | 3:N:386:HIS:HB2 | 1.91 | 0.53 |
| 3:N:572:ARG:NH1 | 5:P:84:TYR:N | 2.57 | 0.53 |
| 3:D:135:LEU:HD11 | 3:D:148:GLU:HB2 | 1.90 | 0.53 |
| 3:N:353:VAL:HG23 | 3:N:353:VAL:O | 2.09 | 0.53 |
| 3:N:361:VAL:HA | 3:N:365:ASP:OD2 | 2.08 | 0.53 |
| 2:M:157:ARG:HD2 | 2:M:314:THR:HA | 1.90 | 0.53 |
| 2:C:30:LEU:HD23 | 2:C:44:ILE:HD12 | 1.91 | 0.53 |
| 2:M:56:GLU:OE2 | 2:M:356:ARG:HA | 2.08 | 0.53 |
| 4:O:42:PRO:HG2 | 4:O:43:GLU:H | 1.74 | 0.53 |
| 2:C:876:VAL:HG13 | 2:C:881:ASN:ND2 | 2.24 | 0.53 |
| 3:N:623:VAL:CG1 | 3:N:624:ASP:H | 2.21 | 0.53 |
| 3:N:625:TYR:N | 3:N:625:TYR:CD1 | 2.77 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:1347:TYR:CZ | 3:N:1351:GLU:HG2 | 2.42 | 0.53 |
| 5:P:323:ASP:OD1 | 5:P:325:LYS:HB2 | 2.09 | 0.53 |
| 3:N:168:THR:HG21 | 5:P:93:LEU:CD2 | 2.37 | 0.53 |
| 3:N:191:LEU:HD23 | 3:N:195:VAL:HG12 | 1.90 | 0.53 |
| 1:L:91:ASN:HB3 | 1:L:94:LEU:CD1 | 2.39 | 0.53 |
| 2:C:958:THR:HG23 | 2:C:961:GLU:HB2 | 1.91 | 0.53 |
| 3:N:1136:LYS:O | 3:N:1140:ILE:HG13 | 2.09 | 0.53 |
| 3:D:1046:GLN:NE2 | 3:D:1050:GLY:HA2 | 2.23 | 0.53 |
| 3:D:842:VAL:HG23 | 3:D:842:VAL:O | 2.09 | 0.53 |
| 2:M:164:PRO:HD3 | 2:M:266:ARG:CZ | 2.38 | 0.53 |
| 2:M:233:GLU:O | 2:M:237:ARG:HG3 | 2.09 | 0.53 |
| 3:N:287:GLY:C | 3:N:311:LEU:HD22 | 2.29 | 0.53 |
| 3:N:341:GLU:OE1 | 3:N:343:LYS:HE3 | 2.09 | 0.53 |
| 1:A:13:VAL:CG2 | 1:A:14:ARG:N | 2.71 | 0.53 |
| 2:C:431:HIS:ND1 | 2:C:432:ARG:N | 2.57 | 0.53 |
| 2:C:431:HIS:ND1 | 2:C:433:THR:N | 2.51 | 0.53 |
| 2:C:545:ASN:HB3 | 2:C:583:LEU:HD11 | 1.90 | 0.53 |
| 3:N:42:ASP:H | 3:N:46:ASP:CG | 2.11 | 0.53 |
| 3:N:140:ALA:N | 3:N:450:TYR:HE2 | 2.06 | 0.53 |
| 3:N:87:ARG:HB3 | 3:N:523:ASP:HB2 | 1.90 | 0.53 |
| 2:C:1058:ASP:OD2 | 2:C:1084:SER:N | 2.30 | 0.53 |
| 3:D:1464:GLU:CG | 3:D:1465:ASN:N | 2.71 | 0.53 |
| 5:F:110:MET:SD | 5:F:114:LYS:HE3 | 2.49 | 0.53 |
| 3:D:564:GLU:HB3 | 5:F:140:ARG:HD2 | 1.90 | 0.53 |
| 1:B:97:VAL:CG1 | 1:B:98:THR:H | 2.19 | 0.53 |
| 2:C:93:PRO:HA | 2:C:117:HIS:HA | 1.91 | 0.53 |
| 2:C:41:ASN:HB3 | 2:C:49:ARG:NE | 2.24 | 0.53 |
| 5:P:367:MET:O | 5:P:368:VAL:C | 2.47 | 0.53 |
| 3:N:1288:GLU:OE1 | 3:N:1288:GLU:N | 2.42 | 0.53 |
| 3:N:1106:VAL:CG1 | 3:N:1107:VAL:N | 2.72 | 0.53 |
| 3:D:1397:LYS:O | 3:D:1401:GLU:HB2 | 2.09 | 0.53 |
| 3:D:1405:GLU:O | 3:D:1412:LYS:CA | 2.50 | 0.53 |
| 5:F:355:GLU:CA | 5:F:358:LEU:HB3 | 2.36 | 0.53 |
| 1:B:5:LYS:O | 1:B:7:LYS:N | 2.42 | 0.53 |
| 3:N:1467:ILE:HD11 | 9:N:1528:NE6:C20 | 2.38 | 0.53 |
| 3:N:709:HIS:HA | 3:N:1227:GLN:HB3 | 1.90 | 0.53 |
| 3:N:711:LEU:C | 3:N:713:ILE:H | 2.12 | 0.53 |
| 3:D:204:LEU:HB3 | 3:D:394:LEU:O | 2.09 | 0.53 |
| 2:M:1040:LEU:HD23 | 3:N:763:MET:HE3 | 1.89 | 0.53 |
| 3:N:483:HIS:HB2 | 3:N:484:PRO:HD3 | 1.88 | 0.53 |
| 3:D:703:ASN:ND2 | 3:D:704:ARG:N | 2.57 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:L:30:ARG:HD3 | 2:M:854:PRO:CG | 2.38 | 0.53 |
| 2:M:961:GLU:O | 2:M:964:LYS:N | 2.41 | 0.53 |
| 4:O:84:ARG:O | 4:O:87:LYS:HB3 | 2.09 | 0.53 |
| 2:M:48:PHE:C | 2:M:50:GLU:H | 2.12 | 0.53 |
| 2:C:603:VAL:HG21 | 2:C:643:VAL:HG22 | 1.89 | 0.53 |
| 3:N:108:VAL:HA | 3:N:109:PRO:C | 2.29 | 0.53 |
| 1:L:94:LEU:O | 1:L:146:ARG:NH2 | 2.41 | 0.53 |
| 2:M:835:VAL:HG23 | 2:M:849:VAL:O | 2.09 | 0.53 |
| 1:A:219:ARG:O | 1:A:222:LEU:N | 2.42 | 0.53 |
| 2:M:463:GLU:OE2 | 2:M:464:LEU:HG | 2.09 | 0.53 |
| 2:C:939:ARG:CZ | 2:C:981:GLU:HG2 | 2.37 | 0.53 |
| 3:D:1488:ASP:HA | 4:E:73:LEU:CD1 | 2.39 | 0.53 |
| 3:N:511:TRP:N | 3:N:511:TRP:HE3 | 2.07 | 0.53 |
| 3:D:686:GLU:HA | 3:D:689:ASP:OD2 | 2.09 | 0.53 |
| 3:D:68:PHE:CZ | 5:F:376:ILE:HG12 | 2.44 | 0.53 |
| 2:M:26:TYR:O | 2:M:29:ALA:HB3 | 2.09 | 0.53 |
| 3:N:101:HIS:CE1 | 3:N:103:TRP:HB2 | 2.43 | 0.53 |
| 2:M:218:VAL:CG1 | 2:M:222:MET:HE2 | 2.38 | 0.52 |
| 2:M:232:GLU:HA | 2:M:235:LEU:CD1 | 2.37 | 0.52 |
| 3:N:148:GLU:O | 3:N:149:LYS:C | 2.46 | 0.52 |
| 3:N:466:LYS:HG2 | 3:N:510:GLU:HG2 | 1.91 | 0.52 |
| 3:D:12:LEU:HD12 | 3:D:511:TRP:HB2 | 1.91 | 0.52 |
| 5:F:120:THR:HG22 | 5:F:122:LEU:HG | 1.91 | 0.52 |
| 3:D:569:ASN:ND2 | 5:F:214:GLN:NE2 | 2.57 | 0.52 |
| 5:P:305:GLU:O | 5:P:309:LYS:HG3 | 2.09 | 0.52 |
| 3:N:1286:THR:CG2 | 3:N:1289:LYS:H | 2.22 | 0.52 |
| 3:D:1155:VAL:HG12 | 3:D:1156:LEU:N | 2.24 | 0.52 |
| 3:D:490:ALA:HA | 3:D:493:ARG:HE | 1.74 | 0.52 |
| 3:N:970:LYS:HE2 | 3:N:974:ILE:CG1 | 2.39 | 0.52 |
| 3:N:1381:VAL:CG1 | 3:N:1391:GLU:HB2 | 2.39 | 0.52 |
| 1:L:176:ARG:HB3 | 1:L:200:TRP:CD1 | 2.44 | 0.52 |
| 2:M:874:LEU:HD21 | 3:N:787:LEU:HD22 | 1.91 | 0.52 |
| 3:N:852:ALA:O | 3:N:855:HIS:N | 2.41 | 0.52 |
| 3:N:1112:CYS:HB3 | 3:N:1201:CYS:HB3 | 1.89 | 0.52 |
| 3:D:628:ARG:HG2 | 3:D:629:SER:N | 2.22 | 0.52 |
| 1:L:36:LEU:C | 1:L:39:PRO:HD2 | 2.29 | 0.52 |
| 3:N:535:PHE:CD1 | 3:N:535:PHE:N | 2.77 | 0.52 |
| 1:K:73:GLU:CD | 1:K:130:ALA:HA | 2.29 | 0.52 |
| 2:C:602:GLU:HG2 | 2:C:603:VAL:N | 2.23 | 0.52 |
| 5:P:154:LYS:O | 5:P:156:VAL:N | 2.42 | 0.52 |
| 2:M:18:LEU:O | 2:M:20:GLU:N | 2.41 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:16:GLU:O | 3:D:20:SER:N | 2.42 | 0.52 |
| 3:D:1114:THR:HB | 3:D:1195:GLN:CG | 2.37 | 0.52 |
| 2:C:353:ARG:HG2 | 2:C:353:ARG:NH1 | 2.21 | 0.52 |
| 1:A:24:VAL:HG12 | 1:A:25:LEU:N | 2.23 | 0.52 |
| 1:B:87:VAL:CG1 | 1:B:122:ILE:HG12 | 2.38 | 0.52 |
| 3:N:1336:LEU:O | 3:N:1340:GLY:N | 2.42 | 0.52 |
| 2:M:334:ARG:HH11 | 2:M:418:LEU:HD11 | 1.74 | 0.52 |
| 3:N:212:ARG:HD3 | 3:N:342:PRO:HB2 | 1.89 | 0.52 |
| 3:N:225:LEU:HD12 | 3:N:333:LEU:HD11 | 1.91 | 0.52 |
| 2:C:1101:THR:C | 2:C:1102:LEU:HD23 | 2.30 | 0.52 |
| 3:D:1091:SER:C | 3:D:1093:TYR:N | 2.58 | 0.52 |
| 3:D:520:LEU:HD21 | 3:D:524:LEU:CB | 2.39 | 0.52 |
| 3:D:556:LYS:O | 3:D:559:ALA:HB3 | 2.08 | 0.52 |
| 3:D:534:ARG:NH2 | 5:F:314:PRO:O | 2.43 | 0.52 |
| 3:D:302:GLN:O | 3:D:304:LEU:N | 2.41 | 0.52 |
| 3:D:351:MET:CG | 3:D:370:ALA:HB2 | 2.38 | 0.52 |
| 3:D:807:ALA:HB2 | 3:D:833:GLU:CD | 2.29 | 0.52 |
| 5:F:265:VAL:O | 5:F:266:GLU:C | 2.46 | 0.52 |
| 3:N:59:ALA:C | 3:N:61:GLY:H | 2.12 | 0.52 |
| 3:N:844:ALA:N | 3:N:848:GLU:OE1 | 2.42 | 0.52 |
| 3:D:207:PHE:O | 3:D:391:ALA:N | 2.42 | 0.52 |
| 3:N:1117:TYR:CD1 | 3:N:1118:ILE:N | 2.77 | 0.52 |
| 1:B:82:LEU:HD23 | 1:B:82:LEU:N | 2.23 | 0.52 |
| 2:C:649:VAL:CG1 | 2:C:653:ASP:CB | 2.87 | 0.52 |
| 1:A:30:ARG:HG3 | 2:C:938:LYS:HZ3 | 1.74 | 0.52 |
| 3:N:477:LEU:HD11 | 3:N:495:ARG:HD3 | 1.90 | 0.52 |
| 2:M:1095:LEU:O | 2:M:1096:ALA:HB3 | 2.09 | 0.52 |
| 1:K:112:ARG:HE | 1:K:125:PRO:HB2 | 1.74 | 0.52 |
| 2:M:918:LEU:HD13 | 2:M:967:PHE:O | 2.10 | 0.52 |
| 3:N:627:GLY:HA3 | 3:N:648:MET:HE2 | 1.91 | 0.52 |
| 2:C:1040:LEU:HD12 | 2:C:1049:LEU:HD13 | 1.90 | 0.52 |
| 3:D:989:TYR:CA | 3:D:992:ILE:HD12 | 2.37 | 0.52 |
| 5:F:308:LEU:CD2 | 5:F:308:LEU:H | 2.20 | 0.52 |
| 1:K:1:MET:N | 1:K:6:LEU:HD13 | 2.20 | 0.52 |
| 3:N:181:ASP:C | 3:N:183:GLU:N | 2.62 | 0.52 |
| 2:C:724:ARG:HH21 | 2:C:734:LEU:HB2 | 1.74 | 0.52 |
| 3:N:238:PRO:HD3 | 3:N:318:ARG:HA | 1.91 | 0.52 |
| 2:C:200:LEU:HD22 | 2:C:300:ASP:CB | 2.39 | 0.52 |
| 3:N:133:ILE:HB | 3:N:454:ALA:CB | 2.30 | 0.52 |
| 3:N:410:SER:O | 3:N:413:ASP:OD2 | 2.27 | 0.52 |
| 3:D:536:ALA:HB1 | 5:F:317:LEU:HD23 | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:D:252:ARG:NH2 | 3:D:300:LYS:HG2 | 2.24 | 0.52 |
| 3:N:1491:THR:C | 3:N:1493:LYS:N | 2.63 | 0.52 |
| 1:B:71:VAL:HG13 | 1:B:132:LEU:HD23 | 1.90 | 0.52 |
| 5:F:348:SER:O | 5:F:352:GLU:HG3 | 2.09 | 0.52 |
| 5:P:265:VAL:HG12 | 5:P:269:ASN:HD21 | 1.74 | 0.52 |
| 2:C:776:SER:CB | 2:C:780:GLU:HB2 | 2.39 | 0.52 |
| 3:D:1381:VAL:CG2 | 3:D:1382:THR:N | 2.72 | 0.52 |
| 3:D:1016:PRO:HA | 3:D:1021:TYR:HD1 | 1.70 | 0.52 |
| 3:D:30:GLU:HB3 | 3:D:40:GLU:CB | 2.39 | 0.52 |
| 2:M:918:LEU:HD12 | 2:M:968:LEU:O | 2.10 | 0.52 |
| 2:C:18:LEU:O | 2:C:20:GLU:N | 2.42 | 0.52 |
| 2:C:1000:MET:HB2 | 2:C:1003:ASP:HB2 | 1.91 | 0.52 |
| 1:A:109:VAL:CG1 | 1:A:129:ILE:HB | 2.39 | 0.52 |
| 5:P:93:LEU:O | 5:P:95:THR:N | 2.42 | 0.52 |
| 2:C:631:SER:O | 2:C:634:GLY:N | 2.36 | 0.52 |
| 3:D:760:ARG:HH12 | 4:E:61:GLU:HB2 | 1.74 | 0.52 |
| 4:E:70:THR:C | 4:E:72:ARG:N | 2.63 | 0.52 |
| 3:N:249:TYR:CE1 | 3:N:330:THR:CG2 | 2.92 | 0.52 |
| 2:C:288:ARG:HG3 | 2:C:289:THR:N | 2.24 | 0.52 |
| 2:C:517:ARG:O | 2:C:518:LYS:HG2 | 2.09 | 0.52 |
| 3:N:24:GLY:HA3 | 3:N:49:ILE:HG23 | 1.91 | 0.52 |
| 3:D:1103:HIS:HB2 | 3:D:1223:ILE:HD11 | 1.90 | 0.52 |
| 3:D:379:ALA:O | 3:D:380:GLU:HG3 | 2.10 | 0.52 |
| 1:B:137:ARG:HG2 | 1:B:137:ARG:NH1 | 2.24 | 0.52 |
| 2:M:310:LEU:CD1 | 2:M:314:THR:HG23 | 2.40 | 0.52 |
| 3:D:811:GLU:O | 3:D:816:HIS:N | 2.40 | 0.52 |
| 2:C:778:PHE:CE2 | 5:F:419:ARG:NH1 | 2.78 | 0.52 |
| 2:M:720:GLU:C | 2:M:721:ARG:HG3 | 2.29 | 0.52 |
| 3:D:826:PRO:HD2 | 3:D:829:VAL:CG2 | 2.40 | 0.52 |
| 2:M:970:GLY:O | 2:M:988:VAL:HA | 2.10 | 0.52 |
| 3:N:654:LYS:O | 3:N:657:LEU:HB3 | 2.09 | 0.52 |
| 2:M:68:PHE:CZ | 2:M:71:TYR:N | 2.77 | 0.52 |
| 2:M:1030:GLN:HG2 | 3:N:626:SER:HB2 | 1.92 | 0.52 |
| 2:M:499:ALA:HB2 | 2:M:533:ASP:HB2 | 1.90 | 0.52 |
| 2:C:806:LEU:HD22 | 2:C:813:VAL:HG22 | 1.91 | 0.52 |
| 5:P:110:MET:HE2 | 5:P:111:GLU:HG3 | 1.92 | 0.52 |
| 5:P:242:TRP:O | 5:P:245:GLN:HG2 | 2.10 | 0.52 |
| 3:D:14:SER:CB | 3:D:17:LYS:H | 2.20 | 0.52 |
| 3:N:181:ASP:O | 3:N:183:GLU:N | 2.35 | 0.52 |
| 4:O:37:ASN:HA | 4:O:93:TYR:CE2 | 2.43 | 0.52 |
| 3:N:1251:ASP:O | 3:N:1270:ALA:HB2 | 2.10 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:643:GLY:HA3 | 3:D:727:GLN:HB2 | 1.91 | 0.52 |
| 2:M:1114:GLY:C | 2:M:1116:ALA:H | 2.12 | 0.52 |
| 2:M:401:LEU:O | 2:M:404:LEU:HB3 | 2.10 | 0.52 |
| 3:N:322:VAL:CG2 | 3:N:333:LEU:HD22 | 2.40 | 0.52 |
| 1:A:16:GLN:NE2 | 1:B:235:ALA:HB1 | 2.25 | 0.52 |
| 2:C:240:THR:C | 2:C:242:LEU:H | 2.12 | 0.52 |
| 3:N:520:LEU:O | 3:N:525:ARG:NH1 | 2.43 | 0.52 |
| 2:C:1015:LEU:CD1 | 5:F:335:ASP:HA | 2.39 | 0.52 |
| 3:D:137:PRO:HG2 | 3:D:138:LYS:H | 1.74 | 0.52 |
| 3:D:152:LEU:HD12 | 3:D:153:LEU:H | 1.73 | 0.52 |
| 3:D:456:MET:SD | 3:D:568:ARG:HD3 | 2.49 | 0.52 |
| 3:D:226:PRO:CB | 3:D:231:VAL:HG21 | 2.40 | 0.52 |
| 5:P:355:GLU:C | 5:P:358:LEU:HB3 | 2.30 | 0.52 |
| 2:C:31:GLN:CA | 2:C:35:PRO:HG2 | 2.39 | 0.52 |
| 3:N:674:ARG:HG3 | 3:N:674:ARG:NH1 | 2.24 | 0.52 |
| 2:M:810:ASP:N | 2:M:811:PRO:CD | 2.73 | 0.52 |
| 4:O:40:LEU:HD12 | 4:O:41:GLU:H | 1.74 | 0.52 |
| 3:D:1403:LEU:C | 3:D:1405:GLU:N | 2.63 | 0.52 |
| 3:N:1435:LEU:O | 3:N:1436:SER:C | 2.47 | 0.52 |
| 2:M:419:THR:CG2 | 2:M:420:ARG:N | 2.72 | 0.52 |
| 3:D:207:PHE:HB2 | 3:D:391:ALA:CB | 2.37 | 0.52 |
| 1:A:178:ALA:CB | 2:C:864:GLY:HA3 | 2.39 | 0.52 |
| 2:M:1034:GLU:O | 2:M:1035:MET:C | 2.48 | 0.52 |
| 1:B:73:GLU:HG3 | 1:B:130:ALA:CB | 2.39 | 0.52 |
| 2:M:511:GLU:O | 2:M:526:PRO:HD3 | 2.10 | 0.52 |
| 2:M:1085:PHE:O | 2:M:1086:ARG:C | 2.48 | 0.52 |
| 3:D:703:ASN:HD22 | 3:D:704:ARG:N | 2.07 | 0.52 |
| 1:K:86:VAL:HG12 | 1:K:124:ASN:CG | 2.29 | 0.52 |
| 1:K:76:VAL:O | 1:K:80:LEU:HG | 2.10 | 0.52 |
| 3:N:587:ARG:HB3 | 3:N:587:ARG:CZ | 2.39 | 0.52 |
| 5:P:152:ASP:HA | 5:P:156:VAL:CG1 | 2.39 | 0.52 |
| 5:P:253:ASP:CA | 5:P:259:ARG:HH12 | 2.20 | 0.52 |
| 1:K:24:VAL:HG22 | 1:K:196:THR:HG23 | 1.91 | 0.52 |
| 3:N:985:ASP:OD2 | 3:N:985:ASP:N | 2.42 | 0.52 |
| 3:D:771:SER:O | 3:D:775:GLY:N | 2.42 | 0.52 |
| 2:C:211:LEU:C | 2:C:213:ALA:N | 2.59 | 0.52 |
| 3:N:602:SER:H | 3:N:605:ASP:CG | 2.11 | 0.52 |
| 2:C:1031:ARG:CA | 3:D:622:ARG:HH12 | 2.22 | 0.52 |
| 3:D:1117:TYR:HD1 | 3:D:1118:ILE:N | 2.08 | 0.52 |
| 1:K:98:THR:HG21 | 1:K:141:GLU:HB3 | 1.92 | 0.52 |
| 2:M:166:PRO:HB2 | 2:M:169:GLY:HA3 | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:E:39:VAL:HG11 | 4:E:72:ARG:HB3 | 1.91 | 0.52 |
| 3:N:219:GLU:CG | 3:N:220:ARG:H | 2.12 | 0.52 |
| 2:C:543:ASN:HB2 | 2:C:565:GLN:NE2 | 2.25 | 0.52 |
| 3:N:525:ARG:N | 3:N:526:PRO:CD | 2.69 | 0.52 |
| 3:N:552:ASN:O | 3:N:555:LYS:HB2 | 2.09 | 0.52 |
| 3:D:1098:LEU:H | 3:D:1098:LEU:HD12 | 1.75 | 0.52 |
| 3:D:1485:GLN:OE1 | 4:E:79:LEU:N | 2.41 | 0.52 |
| 3:D:411:THR:HA | 3:D:435:VAL:CG1 | 2.36 | 0.52 |
| 3:D:406:ASP:HB2 | 3:D:423:ASP:CA | 2.40 | 0.52 |
| 2:M:95:TYR:HA | 2:M:113:VAL:C | 2.29 | 0.52 |
| 3:D:227:LEU:HG | 3:D:326:GLU:CD | 2.30 | 0.52 |
| 2:M:157:ARG:CD | 2:M:314:THR:HG22 | 2.35 | 0.52 |
| 5:F:382:THR:CG2 | 5:F:394:ARG:HB2 | 2.39 | 0.52 |
| 1:A:34:VAL:C | 1:A:36:LEU:N | 2.63 | 0.52 |
| 1:B:38:ASN:HB2 | 11:B:702:HOH:O | 2.09 | 0.52 |
| 3:D:662:GLU:HA | 3:D:667:ALA:O | 2.09 | 0.52 |
| 5:F:417:LYS:C | 5:F:419:ARG:N | 2.63 | 0.52 |
| 2:M:102:HIS:CG | 2:M:365:ASP:OD1 | 2.63 | 0.52 |
| 5:F:291:ILE:O | 5:F:292:ALA:C | 2.47 | 0.52 |
| 3:N:674:ARG:HG3 | 3:N:674:ARG:HH11 | 1.74 | 0.52 |
| 5:P:367:MET:HA | 5:P:370:LYS:HG2 | 1.91 | 0.52 |
| 3:D:1167:SER:HB3 | 3:D:1170:ASP:OD2 | 2.09 | 0.52 |
| 3:D:1381:VAL:HG22 | 3:D:1382:THR:N | 2.24 | 0.52 |
| 3:D:1400:VAL:HB | 3:D:1401:GLU:OE1 | 2.09 | 0.52 |
| 3:D:164:GLY:HA3 | 3:D:447:VAL:CG1 | 2.40 | 0.52 |
| 2:M:1039:ALA:CB | 3:N:713:ILE:HD12 | 2.39 | 0.52 |
| 3:N:1442:ASN:HD21 | 3:N:1445:HIS:HB2 | 1.75 | 0.52 |
| 1:L:175:ARG:N | 1:L:200:TRP:O | 2.42 | 0.52 |
| 2:M:691:SER:O | 2:M:693:GLU:N | 2.43 | 0.52 |
| 3:D:28:LYS:O | 3:D:43:GLY:HA2 | 2.10 | 0.52 |
| 3:N:662:GLU:HG2 | 3:N:663:GLU:N | 2.25 | 0.52 |
| 1:K:209:GLU:HA | 1:K:212:ASN:ND2 | 2.25 | 0.52 |
| 2:M:513:VAL:N | 2:M:524:VAL:O | 2.42 | 0.52 |
| 3:D:219:GLU:HG2 | 3:D:220:ARG:N | 2.23 | 0.52 |
| 5:P:117:SER:CB | 5:P:124:PRO:HG3 | 2.40 | 0.52 |
| 2:M:193:LEU:O | 2:M:196:LEU:HG | 2.08 | 0.52 |
| 2:M:228:ALA:C | 2:M:229:MET:HG3 | 2.30 | 0.52 |
| 2:M:263:ASP:HB2 | 2:M:264:PRO:HD3 | 1.91 | 0.52 |
| 2:C:180:GLY:HA2 | 2:C:223:ASP:CG | 2.30 | 0.52 |
| 2:C:285:LEU:HD11 | 2:C:288:ARG:C | 2.30 | 0.52 |
| 3:N:129:PHE:O | 3:N:130:SER:HB2 | 2.10 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:86:ARG:NH1 | 3:N:522:PRO:HB2 | 2.24 | 0.52 |
| 3:N:90:MET:HE2 | 3:N:519:VAL:O | 2.09 | 0.52 |
| 5:P:211:ASP:O | 5:P:215:GLU:HG2 | 2.10 | 0.52 |
| 2:C:1102:LEU:HD23 | 2:C:1108:PRO:HA | 1.91 | 0.52 |
| 2:C:1090:LYS:HE2 | 2:C:1112:PHE:CZ | 2.45 | 0.52 |
| 3:D:1479:ASP:CA | 3:D:1482:ARG:HG3 | 2.40 | 0.52 |
| 3:D:1491:THR:O | 3:D:1494:ALA:HB3 | 2.10 | 0.52 |
| 3:D:566:ILE:O | 3:D:570:GLU:N | 2.37 | 0.52 |
| 3:D:567:ILE:O | 3:D:570:GLU:HB3 | 2.09 | 0.52 |
| 3:D:607:LEU:HG | 3:D:608:SER:N | 2.24 | 0.52 |
| 4:E:26:ARG:O | 4:E:30:LEU:CB | 2.58 | 0.52 |
| 3:D:665:GLY:O | 3:D:667:ALA:N | 2.43 | 0.52 |
| 2:C:41:ASN:O | 2:C:46:ALA:HB2 | 2.09 | 0.52 |
| 3:D:1381:VAL:HG13 | 3:D:1389:LEU:O | 2.10 | 0.52 |
| 2:M:6:PHE:HB2 | 2:M:902:ILE:O | 2.09 | 0.52 |
| 3:D:82:LYS:HB3 | 3:D:84:ILE:HG22 | 1.92 | 0.52 |
| 3:D:798:GLU:CG | 3:D:799:LYS:N | 2.73 | 0.52 |
| 1:B:76:VAL:O | 1:B:79:ILE:HB | 2.10 | 0.52 |
| 2:M:854:PRO:O | 2:M:856:GLU:N | 2.42 | 0.52 |
| 2:C:23:VAL:HA | 2:C:121:MET:HE3 | 1.86 | 0.52 |
| 1:K:74:ASP:O | 1:K:78:ILE:HG13 | 2.10 | 0.52 |
| 5:F:319:THR:O | 5:F:328:PHE:HA | 2.10 | 0.52 |
| 5:F:235:PHE:O | 5:F:236:SER:C | 2.47 | 0.52 |
| 3:N:1102:THR:HB | 3:N:1105:ILE:HD12 | 1.91 | 0.52 |
| 2:M:863:ASP:OD2 | 2:M:865:THR:HG23 | 2.09 | 0.52 |
| 3:D:970:LYS:O | 3:D:973:GLN:HB2 | 2.09 | 0.52 |
| 3:D:1165:TYR:CE2 | 3:D:1206:GLY:HA2 | 2.45 | 0.52 |
| 3:D:1047:LYS:HG2 | 3:D:1053:PHE:CZ | 2.44 | 0.52 |
| 2:M:799:ILE:O | 2:M:799:ILE:HG13 | 2.09 | 0.52 |
| 2:M:421:GLU:HG2 | 2:M:421:GLU:O | 2.09 | 0.52 |
| 2:M:816:LYS:HD2 | 2:M:816:LYS:H | 1.73 | 0.52 |
| 2:M:104:ASP:N | 2:M:104:ASP:OD1 | 2.42 | 0.52 |
| 2:M:141:HIS:HE1 | 2:M:144:PRO:HD3 | 1.74 | 0.52 |
| 5:P:224:VAL:O | 5:P:225:GLU:C | 2.48 | 0.52 |
| 3:D:1483:PHE:O | 3:D:1484:THR:C | 2.48 | 0.52 |
| 3:D:1497:GLU:O | 3:D:1501:GLU:HB2 | 2.10 | 0.52 |
| 3:D:412:GLY:N | 3:D:435:VAL:HB | 2.22 | 0.52 |
| 3:D:560:GLN:O | 3:D:561:GLY:C | 2.45 | 0.52 |
| 5:F:132:ARG:HB3 | 5:F:136:LEU:CD1 | 2.40 | 0.52 |
| 2:M:112:GLU:OE1 | 2:M:112:GLU:HA | 2.09 | 0.52 |
| 3:D:729:HIS:HD2 | 3:D:731:LEU:H | 1.58 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:606:VAL:HG12 | 2:M:611:ILE:HG12 | 1.92 | 0.52 |
| 5:F:288:TYR:O | 5:F:292:ALA:N | 2.32 | 0.52 |
| 3:N:1304:LYS:HG2 | 3:N:1305:LEU:N | 2.24 | 0.52 |
| 3:N:266:GLU:OE2 | 3:N:315:ARG:NH1 | 2.41 | 0.52 |
| 3:D:1379:VAL:O | 3:D:1392:GLY:HA2 | 2.09 | 0.52 |
| 1:L:104:GLU:HB3 | 1:L:137:ARG:CG | 2.28 | 0.52 |
| 2:C:676:ILE:CG1 | 2:C:873:PRO:HG3 | 2.40 | 0.52 |
| 3:D:945:SER:OG | 3:D:947:ILE:CG2 | 2.57 | 0.52 |
| 2:C:885:ILE:HG22 | 2:C:886:LEU:N | 2.25 | 0.52 |
| 3:N:711:LEU:HD23 | 3:N:735:ALA:HB2 | 1.92 | 0.52 |
| 2:C:857:ASP:HB3 | 2:C:978:ARG:HG2 | 1.92 | 0.52 |
| 3:N:584:ASN:OD1 | 3:N:590:PRO:CD | 2.47 | 0.52 |
| 3:N:1147:ARG:HB2 | 3:N:1166:LEU:CD1 | 2.36 | 0.52 |
| 3:N:1152:GLU:HG2 | 3:N:1153:VAL:N | 2.25 | 0.52 |
| 2:C:649:VAL:HG13 | 2:C:653:ASP:CG | 2.29 | 0.52 |
| 3:D:631:ILE:CG2 | 3:D:745:MET:HG3 | 2.32 | 0.52 |
| 2:C:727:PRO:HG2 | 2:C:785:VAL:O | 2.10 | 0.52 |
| 3:N:1401:GLU:OE1 | 3:N:1401:GLU:N | 2.42 | 0.52 |
| 3:N:1208:ASP:OD1 | 3:N:1210:SER:N | 2.32 | 0.52 |
| 3:D:966:GLU:O | 3:D:969:ARG:HG2 | 2.09 | 0.52 |
| 2:M:802:ARG:HG2 | 2:M:803:THR:N | 2.24 | 0.52 |
| 3:N:638:LYS:O | 3:N:640:HIS:N | 2.43 | 0.52 |
| 3:N:1296:SER:O | 3:N:1298:GLY:N | 2.43 | 0.52 |
| 2:M:202:TYR:HB2 | 2:M:207:LEU:HD21 | 1.92 | 0.52 |
| 2:C:300:ASP:C | 2:C:302:VAL:H | 2.14 | 0.52 |
| 2:C:520:GLU:HA | 2:C:520:GLU:OE1 | 2.08 | 0.52 |
| 3:N:409:VAL:CG1 | 3:N:413:ASP:OD2 | 2.57 | 0.52 |
| 3:N:527:MET:HA | 3:N:537:THR:HG22 | 1.91 | 0.52 |
| 5:F:117:SER:CB | 5:F:124:PRO:HG3 | 2.40 | 0.52 |
| 3:D:259:VAL:O | 3:D:260:GLU:HG3 | 2.10 | 0.52 |
| 3:N:355:VAL:CG1 | 3:N:359:ALA:HB3 | 2.40 | 0.52 |
| 3:D:241:ILE:HD11 | 3:D:310:LEU:HD22 | 1.91 | 0.52 |
| 5:P:351:SER:HA | 5:P:354:LEU:HD12 | 1.91 | 0.52 |
| 5:P:353:GLU:CG | 5:P:417:LYS:HD3 | 2.40 | 0.52 |
| 5:P:353:GLU:HG3 | 5:P:356:LYS:HD2 | 1.92 | 0.52 |
| 2:M:157:ARG:HH11 | 2:M:314:THR:HA | 1.74 | 0.52 |
| 2:M:311:PHE:HA | 2:M:314:THR:HG1 | 1.74 | 0.52 |
| 5:P:256:ARG:HG2 | 5:P:256:ARG:HH11 | 1.75 | 0.52 |
| 3:D:1380:GLU:O | 3:D:1417:TRP:HB2 | 2.10 | 0.52 |
| 3:N:142:LEU:HB2 | 3:N:145:VAL:O | 2.10 | 0.52 |
| 3:D:800:LYS:CE | 3:D:826:PRO:HD3 | 2.39 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:N:1467:ILE:HD11 | 9:N:1528:NE6:C19 | 2.40 | 0.52 |
| 3:N:909:ASN:HA | 3:N:912:LYS:NZ | 2.25 | 0.52 |
| 3:D:166:GLN:HA | 3:D:395:VAL:O | 2.10 | 0.52 |
| 2:M:1056:LYS:HD3 | 3:N:623:VAL:CG1 | 2.35 | 0.52 |
| 1:L:216:GLU:O | 1:L:217:ILE:C | 2.48 | 0.52 |
| 2:C:472:ARG:NH2 | 2:C:479:VAL:HG12 | 2.25 | 0.52 |
| 1:A:229:GLN:O | 1:B:13:VAL:N | 2.43 | 0.52 |
| 1:B:26:GLU:OE1 | 1:B:194:LYS:HG3 | 2.10 | 0.52 |
| 3:N:988:ARG:O | 3:N:989:TYR:C | 2.47 | 0.52 |
| 3:N:951:ILE:HG23 | 3:N:952:ASP:N | 2.25 | 0.52 |
| 3:N:1336:LEU:HD12 | 3:N:1340:GLY:C | 2.31 | 0.52 |
| 2:M:789:SER:HB2 | 2:M:791:ARG:HE | 1.75 | 0.52 |
| 2:C:250:ARG:HB3 | 2:C:253:ALA:HB2 | 1.92 | 0.52 |
| 3:D:135:LEU:CD2 | 3:D:135:LEU:N | 2.64 | 0.52 |
| 3:D:527:MET:SD | 3:D:537:THR:CG2 | 2.98 | 0.52 |
| 3:D:560:GLN:C | 5:F:132:ARG:NH1 | 2.64 | 0.52 |
| 3:D:348:GLN:HB2 | 3:D:351:MET:SD | 2.50 | 0.52 |
| 3:D:443:VAL:HG12 | 3:D:444:VAL:N | 2.25 | 0.52 |
| 5:P:380:GLU:HA | 5:P:385:GLU:OE1 | 2.10 | 0.52 |
| 1:A:36:LEU:O | 1:A:39:PRO:HD2 | 2.09 | 0.52 |
| 2:M:640:ARG:O | 2:M:656:ALA:HA | 2.09 | 0.52 |
| 2:M:108:ILE:CG2 | 2:M:368:THR:HG21 | 2.40 | 0.52 |
| 2:M:373:VAL:CG1 | 2:M:374:ASN:H | 2.18 | 0.52 |
| 5:P:279:GLN:HA | 5:P:284:ARG:O | 2.10 | 0.52 |
| 2:M:807:ARG:C | 2:M:809:GLY:H | 2.12 | 0.52 |
| 1:L:61:VAL:CG2 | 1:L:163:ASN:HB3 | 2.39 | 0.52 |
| 2:M:907:ASP:CG | 2:M:908:GLY:H | 2.12 | 0.52 |
| 3:D:953:ASP:C | 3:D:955:VAL:H | 2.12 | 0.52 |
| 2:C:674:VAL:HA | 2:C:869:VAL:O | 2.09 | 0.52 |
| 3:N:787:LEU:O | 3:N:788:GLY:C | 2.48 | 0.52 |
| 3:N:851:LEU:O | 3:N:854:ALA:HB3 | 2.10 | 0.52 |
| 3:N:937:TYR:H | 3:N:937:TYR:HD1 | 1.56 | 0.52 |
| 1:A:50:GLY:N | 1:A:147:GLY:O | 2.42 | 0.52 |
| 3:N:1118:ILE:HG23 | 3:N:1190:SER:HB3 | 1.91 | 0.52 |
| 5:F:79:ASP:O | 5:F:80:PRO:C | 2.46 | 0.52 |
| 2:C:572:ILE:HD11 | 2:C:701:THR:HB | 1.92 | 0.52 |
| 3:N:484:PRO:O | 3:N:489:ARG:CB | 2.51 | 0.52 |
| 3:N:664:LYS:O | 3:N:666:ILE:HG12 | 2.09 | 0.52 |
| 1:A:81:ASN:N | 1:A:81:ASN:HD22 | 2.08 | 0.52 |
| 3:N:177:ALA:HB3 | 3:N:191:LEU:O | 2.09 | 0.52 |
| 2:M:514:VAL:O | 2:M:514:VAL:HG23 | 2.10 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:998:GLU:O | 3:D:1001:GLU:HB3 | 2.09 | 0.52 |
| 5:P:145:PRO:CB | 5:P:150:THR:H | 2.23 | 0.52 |
| 2:M:715:THR:HG22 | 2:M:717:LEU:N | 2.23 | 0.52 |
| 4:E:80:VAL:HB | 4:E:81:PRO:CD | 2.39 | 0.52 |
| 1:K:178:ALA:HB2 | 2:M:864:GLY:CA | 2.40 | 0.52 |
| 3:N:1299:PHE:N | 3:N:1299:PHE:CD1 | 2.77 | 0.52 |
| 1:A:88:ARG:HG3 | 1:A:204:SER:O | 2.10 | 0.52 |
| 2:M:202:TYR:HB2 | 2:M:207:LEU:HD11 | 1.92 | 0.51 |
| 2:M:267:TYR:CD2 | 2:M:271:GLU:HB2 | 2.45 | 0.51 |
| 2:M:193:LEU:HD11 | 2:M:303:PHE:CD2 | 2.45 | 0.51 |
| 2:C:277:ALA:O | 2:C:281:LEU:N | 2.43 | 0.51 |
| 2:C:282:GLY:O | 2:C:283:ILE:HD13 | 2.09 | 0.51 |
| 2:C:580:MET:HB3 | 2:C:584:GLU:CD | 2.29 | 0.51 |
| 3:N:22:SER:OG | 3:N:92:HIS:ND1 | 2.42 | 0.51 |
| 3:N:465:LEU:HD13 | 3:N:509:PRO:O | 2.09 | 0.51 |
| 3:N:558:LEU:C | 3:N:560:GLN:N | 2.62 | 0.51 |
| 3:N:566:ILE:CA | 3:N:569:ASN:HB3 | 2.40 | 0.51 |
| 3:N:570:GLU:HB2 | 5:P:214:GLN:NE2 | 2.25 | 0.51 |
| 3:D:104:PHE:O | 3:D:112:ILE:HG12 | 2.10 | 0.51 |
| 3:D:1099:VAL:HG12 | 9:D:1529:NE6:H14 | 1.91 | 0.51 |
| 3:D:209:ARG:O | 3:D:347:VAL:N | 2.39 | 0.51 |
| 3:D:324:ALA:HB1 | 3:D:331:VAL:HG11 | 1.91 | 0.51 |
| 5:F:378:GLY:HA3 | 5:F:381:HIS:NE2 | 2.24 | 0.51 |
| 5:F:381:HIS:O | 5:F:384:GLU:N | 2.37 | 0.51 |
| 1:B:32:PHE:HA | 1:B:35:THR:OG1 | 2.10 | 0.51 |
| 3:N:1428:ALA:C | 3:N:1430:SER:H | 2.14 | 0.51 |
| 5:P:368:VAL:O | 5:P:371:LEU:HB2 | 2.10 | 0.51 |
| 2:M:759:THR:HB | 2:M:785:VAL:HG11 | 1.92 | 0.51 |
| 3:D:1378:TYR:OH | 3:D:1431:THR:HA | 2.09 | 0.51 |
| 2:M:554:ASP:HA | 3:N:1061:PHE:CZ | 2.45 | 0.51 |
| 2:C:589:ARG:HA | 2:C:596:TYR:OH | 2.10 | 0.51 |
| 2:M:526:PRO:O | 2:M:529:VAL:HG23 | 2.10 | 0.51 |
| 2:C:713:ARG:H | 2:C:720:GLU:CD | 2.13 | 0.51 |
| 3:N:701:LEU:O | 3:N:747:VAL:HA | 2.09 | 0.51 |
| 2:M:122:THR:HG22 | 2:M:123:GLU:H | 1.74 | 0.51 |
| 5:F:169:GLU:CD | 5:F:169:GLU:H | 2.12 | 0.51 |
| 3:D:1295:GLU:HG2 | 3:D:1300:SER:OG | 2.09 | 0.51 |
| 4:O:86:GLN:O | 4:O:90:GLU:HG3 | 2.10 | 0.51 |
| 2:C:480:THR:HG22 | 2:C:482:GLU:H | 1.73 | 0.51 |
| 4:O:26:ARG:O | 4:O:29:GLN:HG2 | 2.10 | 0.51 |
| 2:M:8:ARG:HG3 | 2:M:8:ARG:HH11 | 1.76 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:263:ASP:HB2 | 2:M:264:PRO:CD | 2.40 | 0.51 |
| 2:M:405:ARG:HD2 | 2:M:442:GLU:OE2 | 2.10 | 0.51 |
| 3:N:249:TYR:CD2 | 3:N:288:MET:HE1 | 2.45 | 0.51 |
| 2:C:308:ARG:O | 2:C:311:PHE:HB2 | 2.10 | 0.51 |
| 2:C:513:VAL:HG12 | 2:C:514:VAL:N | 2.24 | 0.51 |
| 2:C:513:VAL:N | 2:C:524:VAL:O | 2.42 | 0.51 |
| 3:N:562:ALA:HB3 | 3:N:567:ILE:CD1 | 2.36 | 0.51 |
| 3:D:1094:LEU:O | 3:D:1095:THR:C | 2.49 | 0.51 |
| 3:D:1103:HIS:HD2 | 3:D:1462:LEU:HB2 | 1.75 | 0.51 |
| 3:D:583:ASP:OD2 | 3:D:586:ARG:HG2 | 2.10 | 0.51 |
| 5:F:135:ILE:HD11 | 5:F:178:ARG:HA | 1.92 | 0.51 |
| 2:M:73:LEU:HB3 | 2:M:94:LEU:HA | 1.93 | 0.51 |
| 5:P:382:THR:HG22 | 5:P:397:ILE:HD12 | 1.91 | 0.51 |
| 2:C:54:ILE:HD13 | 2:C:355:VAL:CG1 | 2.39 | 0.51 |
| 2:M:371:LYS:HA | 5:P:280:GLN:OE1 | 2.09 | 0.51 |
| 3:D:36:THR:C | 3:D:37:LEU:HG | 2.31 | 0.51 |
| 3:D:1398:TRP:HA | 3:D:1402:ALA:H | 1.76 | 0.51 |
| 5:F:358:LEU:HG | 5:F:359:SER:N | 2.25 | 0.51 |
| 2:C:983:ILE:O | 2:C:985:GLY:N | 2.43 | 0.51 |
| 3:N:1380:GLU:O | 3:N:1417:TRP:HB2 | 2.10 | 0.51 |
| 2:C:914:ILE:C | 2:C:916:GLU:N | 2.62 | 0.51 |
| 2:M:678:PRO:O | 3:N:943:THR:HG23 | 2.10 | 0.51 |
| 2:C:689:VAL:HG21 | 2:C:870:ILE:HB | 1.92 | 0.51 |
| 2:C:861:LEU:CB | 2:C:862:PRO:HD2 | 2.40 | 0.51 |
| 2:M:1072:LYS:C | 3:N:659:LYS:HE3 | 2.31 | 0.51 |
| 1:L:34:VAL:C | 1:L:36:LEU:N | 2.60 | 0.51 |
| 3:N:807:ALA:H | 3:N:809:PRO:HD2 | 1.73 | 0.51 |
| 3:N:1402:ALA:HA | 3:N:1415:VAL:CG2 | 2.40 | 0.51 |
| 2:M:1007:ALA:HB2 | 3:N:648:MET:HE2 | 1.92 | 0.51 |
| 5:F:321:ILE:CG2 | 5:F:322:GLY:N | 2.73 | 0.51 |
| 3:N:470:LEU:O | 3:N:471:GLU:C | 2.48 | 0.51 |
| 2:M:726:ILE:HG13 | 2:M:728:HIS:HB3 | 1.91 | 0.51 |
| 3:D:900:ILE:HG22 | 3:D:902:LEU:N | 2.25 | 0.51 |
| 5:P:203:THR:HG22 | 5:P:204:GLY:N | 2.25 | 0.51 |
| 3:N:1183:ILE:C | 3:N:1184:GLN:HG3 | 2.29 | 0.51 |
| 3:N:1025:GLN:OE1 | 3:N:1025:GLN:HA | 2.09 | 0.51 |
| 3:N:916:TYR:HH | 3:N:1145:TYR:HH | 1.56 | 0.51 |
| 3:D:39:PRO:HG2 | 3:D:53:ILE:HD11 | 1.92 | 0.51 |
| 2:C:240:THR:O | 2:C:242:LEU:N | 2.44 | 0.51 |
| 3:N:131:LYS:CB | 3:N:456:MET:HE2 | 2.41 | 0.51 |
| 3:D:156:GLU:CD | 3:D:156:GLU:H | 2.12 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:F:118:GLU:O | 5:F:120:THR:N | 2.44 | 0.51 |
| 3:D:223:LEU:O | 3:D:224:ARG:HD2 | 2.09 | 0.51 |
| 3:D:241:ILE:CG2 | 3:D:242:LEU:N | 2.73 | 0.51 |
| 5:P:271:LEU:O | 5:P:274:THR:N | 2.41 | 0.51 |
| 5:P:300:ASP:O | 5:P:303:ARG:HB3 | 2.11 | 0.51 |
| 5:F:261:PRO:HB2 | 5:F:264:MET:CG | 2.40 | 0.51 |
| 2:C:773:LEU:CD1 | 2:C:777:ILE:HD11 | 2.40 | 0.51 |
| 3:D:1006:ALA:O | 3:D:1010:ASN:N | 2.30 | 0.51 |
| 3:D:798:GLU:HG3 | 3:D:799:LYS:HB2 | 1.92 | 0.51 |
| 3:D:907:GLU:O | 3:D:908:LYS:C | 2.48 | 0.51 |
| 3:D:1277:ILE:CG2 | 3:D:1278:ASP:H | 2.11 | 0.51 |
| 2:C:599:GLU:HB3 | 2:C:615:TYR:HD2 | 1.72 | 0.51 |
| 3:D:41:ARG:HE | 3:D:48:ARG:NE | 2.09 | 0.51 |
| 3:D:629:SER:O | 3:D:744:GLN:HG2 | 2.11 | 0.51 |
| 2:M:928:LYS:O | 2:M:931:GLY:N | 2.44 | 0.51 |
| 5:P:145:PRO:CG | 5:P:150:THR:H | 2.23 | 0.51 |
| 1:K:1:MET:N | 1:K:6:LEU:HD22 | 2.24 | 0.51 |
| 5:P:81:VAL:CG2 | 5:P:82:ARG:N | 2.73 | 0.51 |
| 3:N:986:ARG:O | 3:N:989:TYR:HB3 | 2.11 | 0.51 |
| 5:P:244:ARG:O | 5:P:248:ASN:ND2 | 2.44 | 0.51 |
| 3:D:709:HIS:O | 3:D:712:GLY:N | 2.40 | 0.51 |
| 5:P:126:LEU:O | 5:P:129:GLU:HB3 | 2.09 | 0.51 |
| 3:N:186:VAL:O | 3:N:189:GLN:HB2 | 2.10 | 0.51 |
| 2:C:724:ARG:HH21 | 2:C:734:LEU:HB3 | 1.74 | 0.51 |
| 5:P:376:ILE:HG22 | 5:P:377:ASP:N | 2.26 | 0.51 |
| 2:M:343:GLN:O | 2:M:346:VAL:HG22 | 2.10 | 0.51 |
| 2:C:195:LEU:HD12 | 2:C:238:LEU:CD2 | 2.41 | 0.51 |
| 2:C:145:GLY:HA3 | 2:C:276:LYS:CD | 2.40 | 0.51 |
| 2:C:512:ARG:HB3 | 2:C:523:ILE:HD11 | 1.93 | 0.51 |
| 3:N:128:TYR:CE1 | 3:N:461:ILE:HG13 | 2.45 | 0.51 |
| 3:D:1108:ARG:HE | 3:D:1199:GLY:CA | 2.22 | 0.51 |
| 2:C:1046:ALA:CA | 3:D:1472:ILE:HB | 2.40 | 0.51 |
| 3:D:566:ILE:CG1 | 3:D:567:ILE:N | 2.74 | 0.51 |
| 5:P:353:GLU:C | 5:P:356:LYS:HB2 | 2.30 | 0.51 |
| 1:B:57:TYR:O | 1:B:140:MET:HB2 | 2.10 | 0.51 |
| 3:D:674:ARG:HG3 | 3:D:674:ARG:HH11 | 1.76 | 0.51 |
| 3:D:33:ASN:O | 3:D:37:LEU:CA | 2.59 | 0.51 |
| 5:F:358:LEU:HD21 | 5:F:370:LYS:NZ | 2.25 | 0.51 |
| 5:F:370:LYS:CG | 5:F:371:LEU:N | 2.73 | 0.51 |
| 2:C:966:LEU:HD21 | 2:C:986:PRO:HG3 | 1.93 | 0.51 |
| 3:N:768:ASN:C | 3:N:769:LEU:HD12 | 2.29 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:1005:MET:CE | 3:D:648:MET:HB2 | 2.41 | 0.51 |
| 2:C:20:GLU:HA | 2:C:23:VAL:HG22 | 1.91 | 0.51 |
| 1:K:5:LYS:NZ | 1:K:29:GLU:N | 2.59 | 0.51 |
| 2:M:41:ASN:O | 2:M:46:ALA:N | 2.43 | 0.51 |
| 3:N:591:VAL:HG21 | 3:N:597:ASP:HA | 1.92 | 0.51 |
| 3:N:592:THR:HG23 | 3:N:600:LEU:CD2 | 2.36 | 0.51 |
| 3:N:1403:LEU:HD23 | 3:N:1408:ILE:HD11 | 1.91 | 0.51 |
| 3:D:1237:THR:O | 3:D:1255:GLY:HA3 | 2.10 | 0.51 |
| 2:M:328:LEU:HG | 2:M:433:THR:OG1 | 2.11 | 0.51 |
| 3:D:880:ILE:O | 3:D:883:ALA:HB3 | 2.10 | 0.51 |
| 3:D:792:ILE:HG21 | 3:D:941:PHE:CE1 | 2.46 | 0.51 |
| 1:L:91:ASN:ND2 | 1:L:93:SER:H | 2.08 | 0.51 |
| 5:F:328:PHE:O | 5:F:329:TYR:C | 2.49 | 0.51 |
| 2:C:380:ALA:O | 2:C:384:GLU:N | 2.42 | 0.51 |
| 2:C:747:ALA:O | 2:C:799:ILE:HA | 2.10 | 0.51 |
| 3:N:767:HIS:HA | 3:N:924:MET:CE | 2.41 | 0.51 |
| 1:B:144:VAL:HG12 | 1:B:145:ASP:N | 2.25 | 0.51 |
| 1:B:226:SER:O | 1:B:228:PRO:HD3 | 2.10 | 0.51 |
| 3:N:95:LEU:CD1 | 3:N:99:ALA:HB2 | 2.41 | 0.51 |
| 5:P:361:LEU:CD1 | 5:P:362:SER:H | 2.24 | 0.51 |
| 2:C:834:GLN:HB2 | 11:C:1128:HOH:O | 2.10 | 0.51 |
| 2:M:183:SER:HB3 | 2:M:185:LYS:HE2 | 1.92 | 0.51 |
| 1:A:14:ARG:CB | 1:B:233:VAL:HA | 2.20 | 0.51 |
| 2:C:205:GLU:N | 2:C:209:ARG:NH1 | 2.58 | 0.51 |
| 3:D:136:ASP:N | 3:D:453:ASP:O | 2.41 | 0.51 |
| 3:D:523:ASP:CA | 3:D:526:PRO:HG3 | 2.39 | 0.51 |
| 3:N:421:LEU:HD11 | 3:N:429:SER:N | 2.25 | 0.51 |
| 3:D:403:PHE:HB2 | 3:D:423:ASP:OD1 | 2.10 | 0.51 |
| 3:D:244:GLU:HA | 3:D:309:GLY:C | 2.31 | 0.51 |
| 5:P:355:GLU:HA | 5:P:358:LEU:HD23 | 1.92 | 0.51 |
| 5:P:386:VAL:CG2 | 5:P:387:GLY:H | 2.22 | 0.51 |
| 5:F:343:ASP:C | 5:F:347:GLN:NE2 | 2.64 | 0.51 |
| 2:C:377:PRO:HG2 | 2:C:378:LEU:H | 1.75 | 0.51 |
| 2:C:881:ASN:N | 2:C:881:ASN:ND2 | 2.45 | 0.51 |
| 2:M:677:MET:N | 2:M:871:LEU:O | 2.40 | 0.51 |
| 3:N:653:PHE:HD1 | 3:N:653:PHE:N | 2.07 | 0.51 |
| 3:N:658:LEU:HA | 3:N:661:MET:CE | 2.34 | 0.51 |
| 1:K:101:LEU:C | 1:K:102:LYS:HG3 | 2.30 | 0.51 |
| 1:K:38:ASN:HB3 | 1:K:39:PRO:CD | 2.40 | 0.51 |
| 2:M:945:ARG:O | 2:M:949:LYS:HG3 | 2.11 | 0.51 |
| 1:A:104:GLU:HG2 | 1:A:105:GLY:N | 2.25 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:185:LYS:CA | 2:C:190:LYS:HB3 | 2.38 | 0.51 |
| 3:D:1269:LYS:CE | 3:D:1269:LYS:H | 2.23 | 0.51 |
| 3:D:1367:HIS:O | 3:D:1370:ILE:HB | 2.10 | 0.51 |
| 2:C:152:PRO:HG2 | 2:C:153:ALA:H | 1.74 | 0.51 |
| 3:N:960:LYS:HG2 | 3:N:964:LEU:HD11 | 1.92 | 0.51 |
| 2:C:129:ILE:HG12 | 2:C:134:ARG:HB2 | 1.91 | 0.51 |
| 1:K:170:VAL:HG23 | 1:K:170:VAL:O | 2.10 | 0.51 |
| 2:M:260:LEU:CD1 | 2:M:288:ARG:HG2 | 2.41 | 0.51 |
| 3:N:228:ALA:HA | 3:N:326:GLU:OE1 | 2.11 | 0.51 |
| 2:C:266:ARG:HD2 | 2:C:273:GLY:CA | 2.40 | 0.51 |
| 3:N:411:THR:HA | 3:N:435:VAL:HG12 | 1.91 | 0.51 |
| 3:N:83:SER:O | 3:N:86:ARG:HB2 | 2.11 | 0.51 |
| 3:N:87:ARG:CB | 3:N:523:ASP:HB2 | 2.41 | 0.51 |
| 3:N:89:ARG:O | 3:N:521:PRO:HG3 | 2.11 | 0.51 |
| 3:D:135:LEU:CD2 | 3:D:135:LEU:H | 2.16 | 0.51 |
| 2:C:1102:LEU:O | 3:D:7:LYS:O | 2.29 | 0.51 |
| 5:P:382:THR:HG22 | 5:P:394:ARG:CB | 2.40 | 0.51 |
| 5:P:393:THR:HG22 | 5:P:394:ARG:N | 2.26 | 0.51 |
| 2:M:599:GLU:HA | 2:M:599:GLU:OE1 | 2.10 | 0.51 |
| 3:D:671:LYS:O | 3:D:674:ARG:HB2 | 2.11 | 0.51 |
| 5:P:262:VAL:C | 5:P:264:MET:H | 2.13 | 0.51 |
| 2:C:774:LEU:HD13 | 2:C:775:ARG:N | 2.26 | 0.51 |
| 3:D:85:VAL:CG2 | 3:D:89:ARG:NE | 2.73 | 0.51 |
| 3:D:957:PRO:CG | 3:D:1010:ASN:HD22 | 2.07 | 0.51 |
| 3:D:1126:ASP:HA | 3:D:1128:VAL:O | 2.10 | 0.51 |
| 3:N:1035:ILE:O | 3:N:1036:ARG:C | 2.49 | 0.51 |
| 3:N:1445:HIS:O | 3:N:1449:GLU:OE2 | 2.27 | 0.51 |
| 3:N:1464:GLU:CG | 3:N:1465:ASN:N | 2.74 | 0.51 |
| 3:N:828:LYS:CD | 3:N:828:LYS:H | 2.23 | 0.51 |
| 3:N:1150:ALA:O | 3:N:1151:ARG:HD3 | 2.10 | 0.51 |
| 3:N:686:GLU:H | 3:N:686:GLU:CD | 2.14 | 0.51 |
| 3:N:936:TYR:C | 3:N:936:TYR:CD2 | 2.84 | 0.51 |
| 3:N:807:ALA:HB2 | 3:N:833:GLU:OE1 | 2.10 | 0.51 |
| 3:N:173:PRO:HA | 3:N:209:ARG:HH11 | 1.76 | 0.51 |
| 1:B:175:ARG:NH1 | 1:B:175:ARG:HG2 | 2.26 | 0.51 |
| 2:C:346:VAL:CG2 | 2:C:347:GLY:H | 2.19 | 0.51 |
| 2:M:626:ARG:HH11 | 2:M:626:ARG:HG3 | 1.76 | 0.51 |
| 3:D:969:ARG:O | 3:D:972:LEU:HB2 | 2.11 | 0.51 |
| 3:N:961:LYS:O | 3:N:964:LEU:HB2 | 2.11 | 0.51 |
| 2:M:745:ILE:CG2 | 2:M:746:GLY:N | 2.73 | 0.51 |
| 2:C:142:ARG:HD3 | 2:C:163:ILE:CD1 | 2.41 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:184:MET:CG | 2:C:193:LEU:HD13 | 2.40 | 0.51 |
| 2:C:444:PRO:HD2 | 2:C:452:ILE:O | 2.09 | 0.51 |
| 3:N:22:SER:HB2 | 3:N:24:GLY:O | 2.10 | 0.51 |
| 3:N:555:LYS:CA | 3:N:558:LEU:HD12 | 2.37 | 0.51 |
| 3:D:1451:ALA:O | 3:D:1454:GLY:N | 2.41 | 0.51 |
| 3:N:399:ARG:O | 3:N:401:TYR:HD1 | 1.94 | 0.51 |
| 5:P:401:GLU:HG2 | 5:P:402:ASN:N | 2.25 | 0.51 |
| 2:M:643:VAL:HG23 | 2:M:647:GLN:NE2 | 2.26 | 0.51 |
| 5:P:306:GLU:OE1 | 5:P:306:GLU:HA | 2.11 | 0.51 |
| 5:P:368:VAL:CG2 | 5:P:369:LEU:H | 1.95 | 0.51 |
| 3:N:1492:LEU:HD11 | 4:O:74:VAL:HG21 | 1.93 | 0.51 |
| 4:O:40:LEU:CG | 4:O:44:GLU:HB2 | 2.40 | 0.51 |
| 3:D:1374:GLN:HA | 3:D:1377:LYS:HB2 | 1.92 | 0.51 |
| 3:D:1015:TYR:N | 3:D:1016:PRO:CD | 2.74 | 0.51 |
| 2:C:946:ARG:HE | 3:D:796:ARG:NH2 | 2.09 | 0.51 |
| 2:C:987:ILE:HD13 | 3:D:948:THR:HG23 | 1.92 | 0.51 |
| 3:D:1040:GLY:O | 3:D:1060:SER:HB3 | 2.10 | 0.51 |
| 3:N:826:PRO:HB3 | 3:N:828:LYS:NZ | 2.26 | 0.51 |
| 3:N:274:ARG:CB | 3:N:279:VAL:HG21 | 2.31 | 0.51 |
| 2:M:1015:LEU:O | 2:M:1018:GLN:NE2 | 2.44 | 0.51 |
| 3:D:1296:SER:HB3 | 3:D:1299:PHE:CD1 | 2.46 | 0.51 |
| 1:B:43:ILE:HG23 | 1:B:47:SER:HB2 | 1.93 | 0.51 |
| 1:B:43:ILE:HA | 1:B:46:SER:OG | 2.11 | 0.51 |
| 3:D:703:ASN:HB3 | 3:D:746:ALA:HB3 | 1.93 | 0.51 |
| 5:P:330:GLY:CA | 5:P:333:ILE:HD13 | 2.40 | 0.51 |
| 1:B:175:ARG:HH11 | 1:B:175:ARG:HG2 | 1.74 | 0.51 |
| 5:P:156:VAL:HG23 | 5:P:157:GLU:CD | 2.30 | 0.51 |
| 2:C:628:PHE:CD1 | 2:C:628:PHE:N | 2.77 | 0.51 |
| 5:P:92:PRO:C | 5:P:94:LEU:H | 2.13 | 0.51 |
| 3:D:756:GLN:O | 3:D:759:ALA:HB3 | 2.11 | 0.51 |
| 5:P:236:SER:O | 5:P:238:TYR:N | 2.44 | 0.51 |
| 3:D:769:LEU:CD1 | 3:D:769:LEU:N | 2.73 | 0.51 |
| 3:N:760:ARG:O | 3:N:764:LEU:HB2 | 2.11 | 0.51 |
| 4:O:29:GLN:C | 4:O:31:LEU:H | 2.13 | 0.51 |
| 2:C:888:THR:HA | 2:C:991:GLN:O | 2.11 | 0.51 |
| 2:M:205:GLU:HA | 2:M:209:ARG:HD3 | 1.92 | 0.51 |
| 2:C:200:LEU:HB3 | 2:C:202:TYR:CE2 | 2.46 | 0.51 |
| 5:P:207:LEU:O | 5:P:212:LEU:HD21 | 2.11 | 0.51 |
| 3:D:617:ASN:HB3 | 3:D:619:LEU:HG | 1.92 | 0.51 |
| 5:F:213:ILE:HG22 | 5:F:217:ASN:ND2 | 2.25 | 0.51 |
| 3:D:367:ILE:HB | 3:D:377:VAL:HG11 | 1.87 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:441:ARG:HD3 | 3:D:443:VAL:CG2 | 2.40 | 0.51 |
| 3:D:936:TYR:CD2 | 3:D:936:TYR:C | 2.84 | 0.51 |
| 1:B:58:ILE:HG23 | 1:B:61:VAL:HB | 1.88 | 0.51 |
| 5:F:408:LEU:HG | 5:F:409:LYS:N | 2.26 | 0.51 |
| 5:P:256:ARG:HH21 | 5:P:311:ALA:HA | 1.75 | 0.51 |
| 3:D:23:TYR:CD2 | 3:D:89:ARG:HD3 | 2.46 | 0.51 |
| 2:M:987:ILE:HD12 | 3:N:948:THR:CG2 | 2.41 | 0.51 |
| 2:M:186:VAL:CG1 | 2:M:187:ASN:H | 2.10 | 0.51 |
| 3:N:584:ASN:OD1 | 3:N:585:GLY:N | 2.44 | 0.51 |
| 2:C:695:LEU:HD22 | 2:C:832:LYS:HG2 | 1.93 | 0.51 |
| 2:M:1099:VAL:HA | 3:N:9:ARG:O | 2.10 | 0.51 |
| 1:K:40:LEU:O | 1:K:41:ARG:C | 2.48 | 0.51 |
| 3:D:1288:GLU:N | 3:D:1288:GLU:OE1 | 2.44 | 0.51 |
| 3:D:59:ALA:HB3 | 3:D:76:CYS:HB2 | 1.93 | 0.51 |
| 5:P:172:ARG:O | 5:P:176:ILE:HG13 | 2.11 | 0.51 |
| 3:N:1254:GLN:HG2 | 3:N:1255:GLY:H | 1.75 | 0.51 |
| 3:N:1485:GLN:N | 4:O:76:GLY:O | 2.35 | 0.51 |
| 3:D:701:LEU:HD21 | 3:D:715:ALA:HB2 | 1.92 | 0.51 |
| 1:B:87:VAL:HG12 | 1:B:122:ILE:HA | 1.91 | 0.51 |
| 3:N:470:LEU:HB2 | 3:N:503:LEU:CG | 2.41 | 0.51 |
| 2:M:578:VAL:HG13 | 2:M:671:ASN:CG | 2.32 | 0.51 |
| 3:N:1282:ARG:HB3 | 3:N:1293:PHE:HB3 | 1.92 | 0.51 |
| 3:D:1336:LEU:O | 3:D:1340:GLY:N | 2.43 | 0.51 |
| 5:P:359:SER:C | 5:P:361:LEU:H | 2.14 | 0.51 |
| 2:M:768:THR:HG22 | 2:M:770:GLU:H | 1.75 | 0.51 |
| 5:F:231:ARG:CB | 5:F:233:PHE:CE2 | 2.94 | 0.51 |
| 2:C:129:ILE:HG12 | 2:C:134:ARG:CB | 2.41 | 0.51 |
| 3:N:1125:PRO:HA | 3:N:1131:SER:O | 2.10 | 0.51 |
| 2:M:725:ASP:OD2 | 2:M:783:ARG:NH1 | 2.41 | 0.51 |
| 2:M:343:GLN:HG2 | 2:M:385:PHE:CB | 2.41 | 0.51 |
| 2:C:906:PHE:CE2 | 3:D:1067:VAL:HA | 2.46 | 0.51 |
| 3:D:1067:VAL:HG13 | 3:D:1068:LEU:H | 1.74 | 0.51 |
| 3:N:411:THR:HG21 | 5:P:179:GLU:HG2 | 1.92 | 0.51 |
| 3:D:1106:VAL:CG1 | 3:D:1107:VAL:N | 2.74 | 0.51 |
| 4:E:20:THR:O | 4:E:21:VAL:C | 2.49 | 0.51 |
| 4:E:87:LYS:HE3 | 4:E:91:ARG:HH22 | 1.76 | 0.51 |
| 3:D:295:GLY:O | 3:D:296:GLU:HG3 | 2.10 | 0.51 |
| 3:D:425:GLY:C | 3:D:427:VAL:H | 2.14 | 0.51 |
| 5:F:269:ASN:O | 5:F:270:LYS:C | 2.49 | 0.51 |
| 3:N:1495:ILE:CG2 | 3:N:1496:GLU:N | 2.71 | 0.51 |
| 4:O:40:LEU:HG | 4:O:44:GLU:HB2 | 1.93 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:1406:ARG:HG2 | 3:N:1412:LYS:CD | 2.41 | 0.51 |
| 1:L:57:TYR:O | 1:L:140:MET:HB2 | 2.11 | 0.51 |
| 3:D:1011:PHE:HE1 | 3:D:1018:ASN:ND2 | 2.09 | 0.51 |
| 3:N:971:LEU:O | 3:N:974:ILE:HB | 2.11 | 0.51 |
| 3:N:561:GLY:HA2 | 5:P:140:ARG:HH21 | 1.75 | 0.51 |
| 2:C:987:ILE:HG23 | 3:D:948:THR:HG21 | 1.91 | 0.51 |
| 3:N:490:ALA:O | 3:N:493:ARG:HG2 | 2.11 | 0.51 |
| 2:C:910:LYS:C | 2:C:914:ILE:HD13 | 2.31 | 0.51 |
| 2:M:675:ALA:O | 2:M:677:MET:HG2 | 2.10 | 0.51 |
| 1:L:176:ARG:HD3 | 3:N:884:ARG:NH2 | 2.26 | 0.51 |
| 2:M:243:ARG:CG | 2:M:244:PRO:CA | 2.88 | 0.51 |
| 1:A:178:ALA:HB2 | 2:C:864:GLY:CA | 2.39 | 0.51 |
| 3:N:1083:ASP:O | 3:N:1086:LEU:HB2 | 2.10 | 0.51 |
| 3:N:191:LEU:HB3 | 3:N:195:VAL:O | 2.10 | 0.51 |
| 2:C:395:LYS:HD3 | 2:C:397:GLU:OE1 | 2.11 | 0.51 |
| 2:M:18:LEU:C | 2:M:20:GLU:H | 2.15 | 0.51 |
| 3:N:406:ASP:N | 3:N:423:ASP:OD1 | 2.44 | 0.51 |
| 3:D:1367:HIS:O | 3:D:1371:VAL:HG23 | 2.11 | 0.51 |
| 2:M:12:VAL:HG23 | 2:M:13:ILE:N | 2.26 | 0.51 |
| 3:D:999:THR:O | 3:D:1003:VAL:HG23 | 2.11 | 0.51 |
| 1:L:12:THR:OG1 | 1:L:24:VAL:HB | 2.11 | 0.51 |
| 1:K:219:ARG:HH11 | 1:K:219:ARG:HG2 | 1.74 | 0.51 |
| 2:M:203:ASP:OD1 | 2:M:205:GLU:HB3 | 2.11 | 0.51 |
| 2:C:151:ASP:N | 2:C:158:TYR:HA | 2.18 | 0.51 |
| 2:C:157:ARG:NH1 | 2:C:158:TYR:OH | 2.44 | 0.51 |
| 2:C:144:PRO:CB | 2:C:266:ARG:HB3 | 2.40 | 0.51 |
| 3:N:521:PRO:C | 3:N:525:ARG:HH12 | 2.14 | 0.51 |
| 3:N:562:ALA:CB | 3:N:567:ILE:HD11 | 2.37 | 0.51 |
| 3:D:444:VAL:HG23 | 3:D:444:VAL:O | 2.11 | 0.51 |
| 2:M:73:LEU:CB | 2:M:93:PRO:O | 2.59 | 0.51 |
| 2:M:73:LEU:O | 2:M:73:LEU:HD12 | 2.11 | 0.51 |
| 3:D:322:VAL:HG22 | 3:D:333:LEU:HD22 | 1.93 | 0.51 |
| 5:P:380:GLU:HA | 5:P:385:GLU:CD | 2.31 | 0.51 |
| 1:A:34:VAL:C | 1:A:36:LEU:H | 2.14 | 0.51 |
| 3:N:1422:MET:SD | 3:N:1427:SER:HA | 2.51 | 0.51 |
| 5:P:291:ILE:O | 5:P:292:ALA:C | 2.49 | 0.51 |
| 1:L:56:VAL:HG12 | 1:L:57:TYR:H | 1.76 | 0.51 |
| 3:N:1472:ILE:HD13 | 3:N:1473:PRO:CD | 2.41 | 0.51 |
| 3:N:911:LEU:O | 3:N:912:LYS:C | 2.49 | 0.51 |
| 2:M:470:PRO:HG3 | 2:M:485:TYR:OH | 2.09 | 0.51 |
| 3:D:27:GLU:C | 3:D:28:LYS:HD3 | 2.30 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:1286:THR:CB | 3:D:1289:LYS:H | 2.23 | 0.51 |
| 3:N:648:MET:O | 3:N:649:ALA:C | 2.50 | 0.51 |
| 1:L:89:PHE:HD2 | 1:L:94:LEU:HB2 | 1.75 | 0.51 |
| 5:P:150:THR:O | 5:P:152:ASP:N | 2.44 | 0.51 |
| 2:C:628:PHE:HD1 | 2:C:628:PHE:N | 2.09 | 0.51 |
| 5:P:111:GLU:HA | 5:P:114:LYS:CG | 2.41 | 0.51 |
| 3:D:14:SER:O | 3:D:18:ILE:N | 2.30 | 0.51 |
| 5:F:235:PHE:O | 5:F:238:TYR:HB3 | 2.11 | 0.51 |
| 3:N:995:LEU:HG | 3:N:996:TRP:N | 2.25 | 0.51 |
| 3:N:582:LEU:HA | 3:N:603:LEU:HD12 | 1.92 | 0.51 |
| 2:C:687:ALA:HB1 | 2:C:850:ALA:HB2 | 1.92 | 0.51 |
| 3:N:961:LYS:HA | 3:N:964:LEU:HD12 | 1.93 | 0.51 |
| 4:O:30:LEU:O | 4:O:34:GLY:O | 2.29 | 0.51 |
| 2:M:211:LEU:O | 2:M:213:ALA:N | 2.44 | 0.50 |
| 3:N:319:ALA:HA | 3:N:336:PHE:O | 2.10 | 0.50 |
| 3:D:583:ASP:HA | 3:D:602:SER:OG | 2.11 | 0.50 |
| 3:N:402:PRO:CB | 3:N:443:VAL:HG22 | 2.41 | 0.50 |
| 1:B:112:ARG:HH22 | 1:B:125:PRO:HB2 | 1.76 | 0.50 |
| 1:B:112:ARG:NH2 | 1:B:125:PRO:HB2 | 2.25 | 0.50 |
| 3:D:653:PHE:O | 3:D:654:LYS:C | 2.48 | 0.50 |
| 5:F:350:LEU:O | 5:F:352:GLU:N | 2.44 | 0.50 |
| 2:C:115:LEU:N | 2:C:115:LEU:HD23 | 2.25 | 0.50 |
| 2:C:45:GLN:HA | 2:C:48:PHE:HD1 | 1.76 | 0.50 |
| 3:N:610:LYS:NZ | 3:N:1441:GLN:HA | 2.26 | 0.50 |
| 1:L:19:GLU:HA | 1:L:201:THR:OG1 | 2.10 | 0.50 |
| 1:L:88:ARG:O | 1:L:120:VAL:HA | 2.10 | 0.50 |
| 2:M:1036:GLU:O | 2:M:1037:VAL:C | 2.50 | 0.50 |
| 3:N:1344:VAL:HG13 | 3:N:1345:GLU:N | 2.26 | 0.50 |
| 1:K:56:VAL:HG21 | 1:K:82:LEU:HD12 | 1.93 | 0.50 |
| 1:K:9:PRO:HD2 | 1:L:224:TYR:CD1 | 2.45 | 0.50 |
| 3:N:598:ARG:HG2 | 3:N:598:ARG:NH1 | 2.27 | 0.50 |
| 2:C:1012:PRO:HB2 | 2:C:1021:LEU:O | 2.11 | 0.50 |
| 3:N:618:LEU:N | 3:N:618:LEU:HD23 | 2.25 | 0.50 |
| 3:N:605:ASP:N | 3:N:605:ASP:OD1 | 2.34 | 0.50 |
| 5:F:251:ILE:O | 5:F:255:ALA:CB | 2.59 | 0.50 |
| 3:D:349:PRO:CB | 5:F:97:GLU:HG2 | 2.41 | 0.50 |
| 5:F:138:SER:HA | 5:F:141:VAL:HG13 | 1.93 | 0.50 |
| 3:N:283:PHE:O | 3:N:284:LEU:HD23 | 2.11 | 0.50 |
| 2:C:151:ASP:HB2 | 2:C:158:TYR:HA | 1.93 | 0.50 |
| 2:C:266:ARG:HD2 | 2:C:273:GLY:HA3 | 1.93 | 0.50 |
| 3:N:437:VAL:HG12 | 3:N:438:ASP:O | 2.10 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:N:560:GLN:HG3 | 5:P:184:ARG:NH2 | 2.27 | 0.50 |
| 3:D:1466:VAL:C | 3:D:1468:LEU:N | 2.65 | 0.50 |
| 3:D:1478:SER:O | 3:D:1482:ARG:HG3 | 2.11 | 0.50 |
| 3:D:510:GLU:O | 3:D:513:ILE:HG22 | 2.12 | 0.50 |
| 5:F:116:LEU:O | 5:F:117:SER:C | 2.50 | 0.50 |
| 5:F:132:ARG:O | 5:F:133:ALA:C | 2.49 | 0.50 |
| 5:F:382:THR:HG23 | 5:F:397:ILE:HG21 | 1.92 | 0.50 |
| 2:C:94:LEU:N | 2:C:116:GLY:O | 2.43 | 0.50 |
| 2:M:355:VAL:C | 2:M:358:ARG:HG3 | 2.32 | 0.50 |
| 2:C:773:LEU:HD11 | 2:C:777:ILE:HD11 | 1.92 | 0.50 |
| 5:F:358:LEU:CD2 | 5:F:370:LYS:HZ2 | 2.23 | 0.50 |
| 1:B:186:LEU:C | 1:B:188:GLN:H | 2.15 | 0.50 |
| 2:C:874:LEU:HB3 | 3:D:1029:ARG:CD | 2.41 | 0.50 |
| 3:N:1465:ASN:HD22 | 3:N:1472:ILE:HA | 1.76 | 0.50 |
| 3:N:820:GLU:HA | 3:N:825:ALA:H | 1.76 | 0.50 |
| 3:N:1341:PRO:O | 3:N:1345:GLU:HG3 | 2.11 | 0.50 |
| 1:K:220:GLU:O | 1:K:223:THR:HB | 2.11 | 0.50 |
| 2:M:943:VAL:O | 2:M:944:LEU:C | 2.49 | 0.50 |
| 2:C:759:THR:HG22 | 2:C:787:ASP:HA | 1.93 | 0.50 |
| 1:B:151:VAL:O | 1:B:168:ASP:HA | 2.11 | 0.50 |
| 3:N:1404:ASN:HB3 | 3:N:1409:ALA:HB3 | 1.92 | 0.50 |
| 1:L:83:LYS:NZ | 1:L:168:ASP:HB2 | 2.26 | 0.50 |
| 2:C:569:VAL:HG12 | 2:C:996:LYS:O | 2.12 | 0.50 |
| 2:M:998:TYR:CE2 | 2:M:1000:MET:HA | 2.47 | 0.50 |
| 2:M:550:LEU:HD23 | 2:M:905:ILE:HD11 | 1.92 | 0.50 |
| 1:L:13:VAL:HG22 | 1:L:14:ARG:N | 2.26 | 0.50 |
| 2:M:897:LEU:HD21 | 2:M:920:GLN:HB3 | 1.92 | 0.50 |
| 2:C:249:LYS:O | 2:C:251:ASP:N | 2.44 | 0.50 |
| 2:M:261:ILE:HG22 | 2:M:262:ALA:H | 1.75 | 0.50 |
| 2:M:398:THR:N | 2:M:633:GLN:HG3 | 2.27 | 0.50 |
| 3:N:261:LEU:HD21 | 3:N:290:PRO:HB2 | 1.94 | 0.50 |
| 2:C:233:GLU:HB2 | 2:C:237:ARG:CZ | 2.41 | 0.50 |
| 2:C:3:ILE:CD1 | 2:C:5:ARG:HE | 2.25 | 0.50 |
| 3:N:141:ILE:CD1 | 3:N:450:TYR:H | 2.23 | 0.50 |
| 3:N:432:TYR:N | 3:N:432:TYR:CD1 | 2.79 | 0.50 |
| 3:N:462:GLN:O | 3:N:466:LYS:HG3 | 2.11 | 0.50 |
| 3:D:1103:HIS:CG | 3:D:1104:GLU:N | 2.79 | 0.50 |
| 3:D:256:GLU:HA | 3:D:272:LEU:HD13 | 1.92 | 0.50 |
| 3:D:355:VAL:HG13 | 3:D:359:ALA:HB3 | 1.92 | 0.50 |
| 5:P:412:GLU:C | 5:P:414:ARG:N | 2.63 | 0.50 |
| 2:M:606:VAL:CG1 | 2:M:611:ILE:HG23 | 2.39 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:605:LYS:O | 2:M:606:VAL:HG13 | 2.11 | 0.50 |
| 5:P:282:LEU:O | 5:P:284:ARG:N | 2.41 | 0.50 |
| 3:D:1101:VAL:HA | 3:D:1428:ALA:HB2 | 1.92 | 0.50 |
| 3:D:70:GLY:HA2 | 3:D:80:VAL:HG23 | 1.92 | 0.50 |
| 3:N:298:VAL:O | 3:N:298:VAL:HG12 | 2.11 | 0.50 |
| 1:A:41:ARG:HG2 | 1:A:45:LEU:HD11 | 1.93 | 0.50 |
| 3:N:1476:THR:HB | 4:O:21:VAL:CG2 | 2.40 | 0.50 |
| 3:N:1404:ASN:OD1 | 3:N:1409:ALA:HB2 | 2.11 | 0.50 |
| 3:N:1409:ALA:C | 3:N:1411:GLY:N | 2.64 | 0.50 |
| 3:D:1286:THR:C | 3:D:1288:GLU:H | 2.13 | 0.50 |
| 3:D:1342:GLU:H | 3:D:1342:GLU:CD | 2.14 | 0.50 |
| 2:M:486:MET:HG3 | 2:M:490:GLU:HB2 | 1.91 | 0.50 |
| 5:P:101:GLU:HA | 5:P:104:ARG:HH12 | 1.72 | 0.50 |
| 2:C:1008:ARG:NH2 | 2:C:1012:PRO:O | 2.44 | 0.50 |
| 3:N:1196:THR:HB | 3:N:1199:GLY:C | 2.32 | 0.50 |
| 2:C:1031:ARG:CB | 3:D:622:ARG:HH12 | 2.25 | 0.50 |
| 2:M:1110:ASP:OD1 | 2:M:1113:GLU:N | 2.44 | 0.50 |
| 2:M:726:ILE:C | 2:M:728:HIS:N | 2.65 | 0.50 |
| 3:D:1291:SER:HA | 3:D:1305:LEU:CD2 | 2.41 | 0.50 |
| 3:N:1483:PHE:N | 3:N:1483:PHE:CD1 | 2.78 | 0.50 |
| 5:P:119:ILE:O | 5:P:119:ILE:HG22 | 2.10 | 0.50 |
| 1:A:23:PHE:N | 1:A:23:PHE:CD1 | 2.79 | 0.50 |
| 2:M:483:VAL:HG22 | 2:M:484:VAL:N | 2.26 | 0.50 |
| 3:N:928:ALA:O | 3:N:929:ARG:C | 2.50 | 0.50 |
| 2:M:224:GLU:CB | 2:M:227:PHE:HB2 | 2.42 | 0.50 |
| 3:N:455:ARG:CB | 3:N:460:ALA:HB2 | 2.41 | 0.50 |
| 3:N:536:ALA:HA | 5:P:315:VAL:O | 2.11 | 0.50 |
| 3:D:1103:HIS:HA | 3:D:1223:ILE:CD1 | 2.41 | 0.50 |
| 3:D:113:GLY:HA3 | 3:D:124:GLU:CD | 2.31 | 0.50 |
| 4:E:75:PHE:C | 4:E:79:LEU:HD11 | 2.31 | 0.50 |
| 3:D:225:LEU:CD1 | 3:D:242:LEU:HD11 | 2.37 | 0.50 |
| 2:M:157:ARG:HG3 | 2:M:158:TYR:H | 1.75 | 0.50 |
| 3:D:807:ALA:N | 3:D:809:PRO:HD2 | 2.26 | 0.50 |
| 5:F:397:ILE:O | 5:F:398:ARG:C | 2.49 | 0.50 |
| 2:M:654:LEU:HD12 | 2:M:655:LEU:N | 2.22 | 0.50 |
| 5:F:343:ASP:O | 5:F:344:ALA:C | 2.50 | 0.50 |
| 2:M:100:LEU:HD23 | 2:M:368:THR:CG2 | 2.39 | 0.50 |
| 3:D:33:ASN:O | 3:D:37:LEU:HA | 2.12 | 0.50 |
| 3:D:1424:VAL:CG2 | 3:D:1425:THR:N | 2.75 | 0.50 |
| 1:L:100:LEU:HB3 | 1:L:115:LEU:HD22 | 1.92 | 0.50 |
| 3:N:1099:VAL:O | 3:N:1103:HIS:HB3 | 2.12 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:M:470:PRO:HG3 | 2:M:485:TYR:CE2 | 2.45 | 0.50 |
| 5:F:81:VAL:HG23 | 5:F:82:ARG:HG3 | 1.93 | 0.50 |
| 3:N:656:PHE:HD1 | 3:N:656:PHE:H | 1.56 | 0.50 |
| 3:N:655:PRO:O | 3:N:658:LEU:HB2 | 2.11 | 0.50 |
| 2:C:23:VAL:CA | 2:C:121:MET:HE1 | 2.37 | 0.50 |
| 3:N:812:ALA:HA | 3:N:816:HIS:H | 1.77 | 0.50 |
| 2:M:781:LYS:CA | 2:M:781:LYS:HE2 | 2.35 | 0.50 |
| 3:D:1341:PRO:O | 3:D:1344:VAL:N | 2.44 | 0.50 |
| 2:C:838:LYS:HE3 | 2:C:997:LEU:CB | 2.41 | 0.50 |
| 3:D:993:LEU:O | 3:D:994:GLN:C | 2.50 | 0.50 |
| 3:N:264:LEU:HB2 | 3:N:267:GLY:CA | 2.41 | 0.50 |
| 2:M:1055:LEU:CD1 | 2:M:1079:PRO:HG3 | 2.40 | 0.50 |
| 3:D:1269:LYS:CD | 3:D:1269:LYS:H | 2.25 | 0.50 |
| 3:N:986:ARG:HD3 | 3:N:989:TYR:HD2 | 1.76 | 0.50 |
| 2:M:728:HIS:NE2 | 2:M:730:SER:HB3 | 2.26 | 0.50 |
| 2:M:685:GLU:O | 2:M:686:ASP:HB2 | 2.10 | 0.50 |
| 1:L:151:VAL:HG21 | 1:L:171:PHE:HE1 | 1.76 | 0.50 |
| 3:D:1294:VAL:C | 3:D:1295:GLU:HG3 | 2.32 | 0.50 |
| 1:A:18:ARG:NE | 1:A:88:ARG:NH2 | 2.59 | 0.50 |
| 2:M:890:LEU:O | 2:M:893:ALA:HB3 | 2.12 | 0.50 |
| 2:M:138:SER:O | 2:M:410:ILE:HA | 2.12 | 0.50 |
| 4:E:40:LEU:HD21 | 4:E:44:GLU:HB2 | 1.94 | 0.50 |
| 3:N:217:LYS:CD | 3:N:262:LYS:NZ | 2.74 | 0.50 |
| 3:N:269:PHE:HD1 | 3:N:283:PHE:HB2 | 1.77 | 0.50 |
| 2:C:328:LEU:HD11 | 2:C:434:HIS:HA | 1.93 | 0.50 |
| 2:C:437:ARG:HA | 2:C:459:ALA:HB2 | 1.94 | 0.50 |
| 3:D:356:PRO:O | 3:D:385:VAL:HG11 | 2.12 | 0.50 |
| 2:M:95:TYR:CE2 | 2:M:114:PHE:HB3 | 2.46 | 0.50 |
| 3:D:925:GLU:OE2 | 4:E:6:ILE:HG22 | 2.11 | 0.50 |
| 5:F:403:LYS:O | 5:F:407:LYS:HB2 | 2.10 | 0.50 |
| 5:P:273:ARG:O | 5:P:277:GLN:HG3 | 2.12 | 0.50 |
| 2:M:817:PRO:HB3 | 5:P:309:LYS:HE2 | 1.93 | 0.50 |
| 3:N:1305:LEU:N | 3:N:1305:LEU:CD2 | 2.74 | 0.50 |
| 3:N:965:GLU:C | 3:N:965:GLU:CD | 2.70 | 0.50 |
| 2:C:882:LEU:HD12 | 3:D:1061:PHE:HB3 | 1.94 | 0.50 |
| 3:N:785:ILE:HG12 | 3:N:939:PHE:HE2 | 1.75 | 0.50 |
| 3:N:676:MET:O | 3:N:676:MET:SD | 2.70 | 0.50 |
| 1:K:100:LEU:HD13 | 1:K:115:LEU:HD12 | 1.93 | 0.50 |
| 1:K:53:VAL:HG21 | 1:K:82:LEU:HB3 | 1.94 | 0.50 |
| 3:N:1394:VAL:O | 3:N:1398:TRP:NE1 | 2.44 | 0.50 |
| 3:D:1335:LEU:HD21 | 3:D:1344:VAL:HA | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:M:1007:ALA:HB1 | 3:N:648:MET:HG3 | 1.92 | 0.50 |
| 2:C:1052:MET:SD | 3:D:623:VAL:HG21 | 2.52 | 0.50 |
| 5:P:155:THR:O | 5:P:159:ILE:HG12 | 2.11 | 0.50 |
| 1:L:112:ARG:HH21 | 1:L:126:ASP:CG | 2.14 | 0.50 |
| 2:M:567:GLN:HB2 | 2:M:997:LEU:HD22 | 1.93 | 0.50 |
| 3:N:995:LEU:O | 3:N:998:GLU:HB3 | 2.11 | 0.50 |
| 3:D:968:ASP:O | 3:D:971:LEU:HB2 | 2.12 | 0.50 |
| 1:A:56:VAL:HG13 | 1:A:141:GLU:O | 2.10 | 0.50 |
| 2:C:928:LYS:O | 2:C:931:GLY:N | 2.43 | 0.50 |
| 2:M:227:PHE:CD1 | 2:M:227:PHE:N | 2.79 | 0.50 |
| 2:M:233:GLU:CD | 2:M:234:ALA:H | 2.15 | 0.50 |
| 2:M:261:ILE:C | 2:M:288:ARG:NH2 | 2.65 | 0.50 |
| 2:M:303:PHE:O | 2:M:304:LEU:C | 2.49 | 0.50 |
| 3:N:336:PHE:C | 3:N:337:LEU:HD23 | 2.31 | 0.50 |
| 3:D:1068:LEU:HG | 3:D:1072:ILE:HD11 | 1.94 | 0.50 |
| 3:D:1079:LYS:HA | 3:D:1082:ALA:HB3 | 1.93 | 0.50 |
| 3:N:133:ILE:HD13 | 3:N:456:MET:CE | 2.41 | 0.50 |
| 3:N:36:THR:HG22 | 3:N:38:LYS:HE2 | 1.93 | 0.50 |
| 3:N:41:ARG:HG3 | 3:N:41:ARG:HH11 | 1.76 | 0.50 |
| 3:N:412:GLY:N | 3:N:435:VAL:O | 2.40 | 0.50 |
| 3:D:121:THR:O | 3:D:122:GLU:C | 2.50 | 0.50 |
| 3:D:411:THR:HG23 | 3:D:411:THR:O | 2.12 | 0.50 |
| 3:D:90:MET:HE3 | 3:D:520:LEU:HA | 1.93 | 0.50 |
| 3:D:564:GLU:C | 3:D:567:ILE:HB | 2.31 | 0.50 |
| 5:F:203:THR:HG22 | 5:F:204:GLY:N | 2.26 | 0.50 |
| 5:F:98:GLU:O | 5:F:99:GLU:C | 2.50 | 0.50 |
| 3:D:370:ALA:N | 3:D:376:GLU:OE2 | 2.44 | 0.50 |
| 3:D:266:GLU:HB3 | 3:D:286:VAL:CG2 | 2.42 | 0.50 |
| 5:P:356:LYS:HD3 | 5:P:417:LYS:HZ1 | 1.76 | 0.50 |
| 3:N:1488:ASP:OD1 | 3:N:1491:THR:CB | 2.59 | 0.50 |
| 2:C:772:ARG:HD3 | 5:F:373:LYS:CD | 2.41 | 0.50 |
| 2:C:94:LEU:HB3 | 2:C:116:GLY:O | 2.11 | 0.50 |
| 1:B:38:ASN:O | 1:B:41:ARG:HB3 | 2.12 | 0.50 |
| 2:C:47:ALA:O | 2:C:50:GLU:HG2 | 2.11 | 0.50 |
| 5:P:288:TYR:HA | 5:P:291:ILE:HG23 | 1.92 | 0.50 |
| 5:F:287:THR:HG23 | 5:F:290:GLU:OE1 | 2.12 | 0.50 |
| 5:P:379:ARG:HH11 | 5:P:379:ARG:CB | 2.24 | 0.50 |
| 3:D:829:VAL:N | 3:D:835:SER:OG | 2.38 | 0.50 |
| 2:C:971:LYS:HA | 2:C:988:VAL:HA | 1.93 | 0.50 |
| 1:A:49:PRO:HA | 1:A:147:GLY:O | 2.12 | 0.50 |
| 2:M:984:GLU:HG3 | 3:N:944:THR:O | 2.12 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:1276:GLU:O | 3:N:1277:ILE:HD13 | 2.12 | 0.50 |
| 3:D:1375:MET:HB2 | 3:D:1376:MET:HE3 | 1.92 | 0.50 |
| 2:M:1007:ALA:HA | 3:N:627:GLY:CA | 2.41 | 0.50 |
| 2:C:384:GLU:OE2 | 2:C:388:ARG:NH2 | 2.42 | 0.50 |
| 1:L:5:LYS:O | 1:L:7:LYS:N | 2.45 | 0.50 |
| 2:M:172:ILE:HG22 | 2:M:173:ASP:H | 1.77 | 0.50 |
| 1:L:52:ALA:HB1 | 1:L:170:VAL:N | 2.26 | 0.50 |
| 3:D:770:LEU:HD11 | 3:D:919:PHE:CD1 | 2.47 | 0.50 |
| 5:P:109:GLY:O | 5:P:112:ALA:HB3 | 2.11 | 0.50 |
| 2:M:139:GLN:C | 2:M:333:ILE:HD12 | 2.32 | 0.50 |
| 2:C:300:ASP:CG | 2:C:302:VAL:HB | 2.31 | 0.50 |
| 2:C:499:ALA:HA | 2:C:532:MET:HE3 | 1.94 | 0.50 |
| 3:N:127:LEU:CD2 | 3:N:128:TYR:N | 2.65 | 0.50 |
| 3:N:458:ALA:HB2 | 3:N:513:ILE:HD11 | 1.90 | 0.50 |
| 3:D:135:LEU:CD1 | 3:D:148:GLU:HB2 | 2.41 | 0.50 |
| 3:D:1494:ALA:O | 3:D:1497:GLU:HG2 | 2.11 | 0.50 |
| 3:D:520:LEU:HD12 | 3:D:521:PRO:HD2 | 1.94 | 0.50 |
| 3:D:359:ALA:N | 3:D:385:VAL:HB | 2.27 | 0.50 |
| 3:D:407:VAL:CG2 | 3:D:408:GLU:H | 2.23 | 0.50 |
| 3:D:422:ALA:H | 3:D:427:VAL:HB | 1.76 | 0.50 |
| 3:D:247:GLU:HA | 3:D:308:LYS:NZ | 2.25 | 0.50 |
| 4:E:10:PHE:C | 4:E:12:MET:H | 2.15 | 0.50 |
| 3:D:818:ARG:O | 3:D:822:ALA:N | 2.39 | 0.50 |
| 1:A:36:LEU:O | 1:A:37:GLY:C | 2.49 | 0.50 |
| 2:M:602:GLU:CG | 2:M:646:GLY:HA2 | 2.41 | 0.50 |
| 3:D:676:MET:SD | 3:D:676:MET:O | 2.70 | 0.50 |
| 2:C:987:ILE:CD1 | 3:D:948:THR:HG23 | 2.41 | 0.50 |
| 3:D:434:ARG:NE | 3:D:449:SER:O | 2.45 | 0.50 |
| 2:M:1102:LEU:O | 3:N:6:ARG:N | 2.43 | 0.50 |
| 3:N:1038:LEU:HD23 | 3:N:1061:PHE:HB2 | 1.94 | 0.50 |
| 2:M:691:SER:OG | 2:M:693:GLU:HB3 | 2.11 | 0.50 |
| 2:M:1014:SER:OG | 2:M:1017:THR:HG23 | 2.11 | 0.50 |
| 2:C:695:LEU:CD2 | 2:C:832:LYS:HE2 | 2.42 | 0.50 |
| 2:M:59:LYS:HD2 | 2:M:59:LYS:H | 1.74 | 0.50 |
| 2:M:1086:ARG:O | 2:M:1087:VAL:C | 2.48 | 0.50 |
| 1:K:110:LYS:N | 1:K:113:ASP:OD2 | 2.44 | 0.50 |
| 2:M:946:ARG:HH11 | 2:M:984:GLU:HB2 | 1.77 | 0.50 |
| 2:M:498:GLN:OE1 | 3:N:1068:LEU:HB2 | 2.12 | 0.50 |
| 2:C:807:ARG:CB | 2:C:807:ARG:NH1 | 2.75 | 0.50 |
| 2:C:394:PHE:HB3 | 2:C:632:ASN:ND2 | 2.27 | 0.50 |
| 3:D:711:LEU:C | 3:D:713:ILE:H | 2.13 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:68:ILE:HB | 1:L:71:VAL:HB | 1.94 | 0.50 |
| 3:N:960:LYS:HE3 | 3:N:964:LEU:HD11 | 1.94 | 0.50 |
| 2:C:718:GLY:O | 2:C:761:PHE:HE1 | 1.95 | 0.50 |
| 2:M:768:THR:HG22 | 2:M:770:GLU:HG2 | 1.93 | 0.50 |
| 5:F:231:ARG:HB3 | 5:F:233:PHE:CE2 | 2.47 | 0.50 |
| 2:C:722:ILE:HA | 2:C:757:GLY:O | 2.11 | 0.50 |
| 2:M:193:LEU:HD21 | 2:M:307:LEU:HD22 | 1.92 | 0.50 |
| 2:M:631:SER:C | 2:M:634:GLY:H | 2.14 | 0.50 |
| 3:N:324:ALA:CB | 3:N:331:VAL:HG11 | 2.42 | 0.50 |
| 2:C:274:ARG:CZ | 2:C:285:LEU:CD2 | 2.90 | 0.50 |
| 2:C:415:PRO:C | 2:C:417:GLY:H | 2.16 | 0.50 |
| 3:N:137:PRO:CG | 3:N:138:LYS:N | 2.74 | 0.50 |
| 3:N:411:THR:HA | 3:N:435:VAL:O | 2.12 | 0.50 |
| 5:P:181:GLU:O | 5:P:184:ARG:HB3 | 2.11 | 0.50 |
| 5:P:79:ASP:O | 5:P:79:ASP:OD1 | 2.29 | 0.50 |
| 3:N:572:ARG:HH12 | 5:P:84:TYR:CA | 2.24 | 0.50 |
| 3:D:140:ALA:N | 3:D:450:TYR:HE2 | 2.00 | 0.50 |
| 3:D:525:ARG:HH11 | 3:D:525:ARG:HG2 | 1.77 | 0.50 |
| 5:P:355:GLU:HA | 5:P:358:LEU:HB3 | 1.93 | 0.50 |
| 1:L:79:ILE:CA | 1:L:82:LEU:HG | 2.40 | 0.50 |
| 2:C:348:LEU:N | 2:C:378:LEU:HD13 | 2.27 | 0.50 |
| 2:C:55:GLU:HG2 | 2:C:57:GLU:N | 2.26 | 0.50 |
| 5:P:269:ASN:O | 5:P:270:LYS:C | 2.50 | 0.50 |
| 3:D:1011:PHE:HE1 | 3:D:1018:ASN:CG | 2.15 | 0.50 |
| 3:D:911:LEU:O | 3:D:912:LYS:C | 2.50 | 0.50 |
| 2:M:690:ILE:N | 2:M:851:LYS:O | 2.45 | 0.50 |
| 2:M:911:GLU:HB2 | 2:M:912:PRO:HD3 | 1.92 | 0.50 |
| 2:M:1032:PHE:CZ | 2:M:1036:GLU:HB3 | 2.47 | 0.50 |
| 3:N:477:LEU:O | 3:N:481:MET:N | 2.44 | 0.50 |
| 2:M:509:ALA:O | 2:M:510:ALA:HB2 | 2.10 | 0.50 |
| 3:N:1208:ASP:O | 3:N:1209:LEU:CB | 2.60 | 0.50 |
| 1:K:90:LEU:HB2 | 1:K:119:ASP:HB3 | 1.94 | 0.50 |
| 5:P:151:LEU:HB2 | 5:P:155:THR:CB | 2.42 | 0.50 |
| 2:C:813:VAL:HG12 | 2:C:815:LEU:HG | 1.94 | 0.50 |
| 1:A:215:VAL:O | 1:A:216:GLU:C | 2.50 | 0.50 |
| 3:N:921:ARG:C | 3:N:922:LEU:HD23 | 2.32 | 0.50 |
| 3:N:530:VAL:HG23 | 3:N:531:ASP:N | 2.24 | 0.50 |
| 1:K:1:MET:H1 | 1:K:6:LEU:CD1 | 2.21 | 0.50 |
| 2:M:861:LEU:CB | 2:M:862:PRO:HD2 | 2.40 | 0.50 |
| 3:N:957:PRO:CG | 3:N:1007:VAL:HA | 2.41 | 0.50 |
| 2:M:145:GLY:HA3 | 2:M:276:LYS:HD2 | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:M:405:ARG:HH22 | 2:M:409:ARG:CZ | 2.25 | 0.50 |
| 2:M:455:LEU:HD12 | 2:M:456:ALA:H | 1.77 | 0.50 |
| 2:C:230:ARG:HG2 | 2:C:230:ARG:O | 2.11 | 0.50 |
| 2:C:141:HIS:NE2 | 2:C:332:ARG:HB3 | 2.27 | 0.50 |
| 3:N:36:THR:CB | 3:N:38:LYS:HG2 | 2.24 | 0.50 |
| 3:D:238:PRO:CD | 3:D:318:ARG:HA | 2.42 | 0.50 |
| 3:D:402:PRO:HA | 3:D:443:VAL:HA | 1.94 | 0.50 |
| 5:F:372:ARG:CG | 5:F:378:GLY:O | 2.55 | 0.50 |
| 1:A:38:ASN:O | 1:A:39:PRO:C | 2.49 | 0.50 |
| 3:D:674:ARG:HG3 | 3:D:674:ARG:NH1 | 2.27 | 0.50 |
| 2:C:102:HIS:O | 2:C:105:THR:N | 2.44 | 0.50 |
| 2:M:807:ARG:CZ | 2:M:807:ARG:CB | 2.90 | 0.50 |
| 3:N:1269:LYS:C | 3:N:1271:LYS:N | 2.66 | 0.50 |
| 3:D:1031:ASN:HB2 | 3:D:1032:PRO:CD | 2.40 | 0.50 |
| 3:D:397:LYS:HE3 | 3:D:448:GLU:CD | 2.32 | 0.50 |
| 3:N:60:CYS:CB | 3:N:62:LYS:HE2 | 2.36 | 0.50 |
| 2:C:910:LYS:HE3 | 2:C:912:PRO:HG2 | 1.94 | 0.50 |
| 3:N:1229:ILE:C | 3:N:1232:PRO:HD2 | 2.32 | 0.50 |
| 2:C:689:VAL:O | 2:C:690:ILE:HD13 | 2.12 | 0.50 |
| 2:M:1036:GLU:CD | 2:M:1036:GLU:H | 2.14 | 0.50 |
| 2:M:1048:THR:HA | 3:N:755:ALA:HB1 | 1.94 | 0.50 |
| 2:C:601:GLY:HA3 | 2:C:614:ARG:O | 2.12 | 0.50 |
| 2:M:948:GLU:CB | 2:M:953:VAL:HG23 | 2.42 | 0.50 |
| 3:N:729:HIS:CG | 3:N:730:PRO:HD2 | 2.47 | 0.50 |
| 1:K:64:GLU:CA | 1:K:165:ILE:HD13 | 2.42 | 0.50 |
| 2:M:41:ASN:O | 2:M:46:ALA:CB | 2.60 | 0.50 |
| 2:M:41:ASN:O | 2:M:42:VAL:C | 2.50 | 0.50 |
| 3:N:592:THR:CG2 | 3:N:598:ARG:HH12 | 2.24 | 0.50 |
| 3:N:586:ARG:O | 3:N:587:ARG:CG | 2.60 | 0.50 |
| 1:B:182:GLU:HG3 | 1:B:194:LYS:HD3 | 1.94 | 0.50 |
| 2:C:389:SER:HB3 | 2:C:392:SER:HB3 | 1.94 | 0.50 |
| 3:N:174:GLY:HA2 | 3:N:389:GLU:CD | 2.32 | 0.50 |
| 1:A:15:THR:CB | 1:A:21:GLY:HA3 | 2.39 | 0.50 |
| 2:M:833:LEU:CD1 | 2:M:837:ASP:HB2 | 2.42 | 0.50 |
| 3:N:160:GLU:O | 3:N:164:GLY:O | 2.29 | 0.50 |
| 3:D:192:ALA:O | 3:D:193:PRO:C | 2.48 | 0.50 |
| 3:D:500:ARG:O | 3:D:504:ASP:N | 2.33 | 0.50 |
| 3:D:710:ARG:C | 3:D:712:GLY:H | 2.15 | 0.50 |
| 3:D:1363:LEU:HD23 | 3:D:1364:HIS:N | 2.27 | 0.50 |
| 1:A:98:THR:CG2 | 1:A:141:GLU:HB3 | 2.42 | 0.50 |
| 3:D:757:ALA:O | 3:D:758:GLU:C | 2.49 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:1004:LYS:HB3 | 2:M:1006:HIS:CE1 | 2.47 | 0.50 |
| 3:D:1360:GLY:O | 3:D:1362:LYS:HE2 | 2.12 | 0.50 |
| 3:D:291:LEU:HB3 | 3:D:294:HIS:HB2 | 1.94 | 0.50 |
| 2:M:1042:ALA:HB3 | 3:N:710:ARG:HB2 | 1.94 | 0.50 |
| 2:M:170:PRO:HD2 | 2:M:263:ASP:O | 2.12 | 0.49 |
| 3:N:29:PRO:HG3 | 3:N:548:ILE:CB | 2.41 | 0.49 |
| 2:C:1015:LEU:CB | 5:F:333:ILE:HG22 | 2.42 | 0.49 |
| 5:F:127:ILE:O | 5:F:130:VAL:HB | 2.11 | 0.49 |
| 3:D:297:ILE:HG23 | 3:D:298:VAL:H | 1.76 | 0.49 |
| 3:N:443:VAL:CG1 | 3:N:444:VAL:N | 2.75 | 0.49 |
| 3:D:932:ASP:O | 3:D:935:LYS:HB3 | 2.11 | 0.49 |
| 1:B:99:LEU:HB3 | 1:B:114:PHE:CD2 | 2.47 | 0.49 |
| 2:M:606:VAL:HG12 | 2:M:611:ILE:CG2 | 2.39 | 0.49 |
| 3:D:673:ALA:O | 3:D:676:MET:HB3 | 2.11 | 0.49 |
| 2:C:65:VAL:HB | 2:C:101:ILE:HB | 1.94 | 0.49 |
| 2:M:101:ILE:CG2 | 2:M:102:HIS:N | 2.67 | 0.49 |
| 3:N:1495:ILE:CG2 | 3:N:1496:GLU:H | 2.22 | 0.49 |
| 2:M:689:VAL:HG22 | 2:M:870:ILE:HB | 1.93 | 0.49 |
| 2:C:862:PRO:C | 2:C:864:GLY:H | 2.15 | 0.49 |
| 3:N:1155:VAL:O | 3:N:1158:VAL:HG12 | 2.12 | 0.49 |
| 5:F:82:ARG:HH11 | 5:F:82:ARG:HG3 | 1.76 | 0.49 |
| 2:M:1008:ARG:O | 3:N:652:LEU:HD23 | 2.12 | 0.49 |
| 2:C:504:GLU:OE2 | 2:C:507:ARG:HD3 | 2.12 | 0.49 |
| 5:F:282:LEU:C | 5:F:284:ARG:H | 2.15 | 0.49 |
| 2:C:312:ALA:O | 2:C:318:PRO:HB2 | 2.12 | 0.49 |
| 2:C:721:ARG:O | 2:C:758:ARG:HA | 2.13 | 0.49 |
| 1:B:171:PHE:O | 1:B:172:SER:C | 2.50 | 0.49 |
| 2:M:430:VAL:HA | 2:M:434:HIS:CD2 | 2.47 | 0.49 |
| 3:N:393:ILE:HG22 | 3:N:394:LEU:N | 2.27 | 0.49 |
| 5:F:320:PRO:HA | 5:F:327:SER:O | 2.12 | 0.49 |
| 2:M:861:LEU:HD23 | 2:M:861:LEU:N | 2.26 | 0.49 |
| 3:D:965:GLU:CD | 3:D:965:GLU:C | 2.71 | 0.49 |
| 3:D:625:TYR:CD1 | 3:D:625:TYR:N | 2.80 | 0.49 |
| 5:P:194:LEU:HD13 | 5:P:194:LEU:O | 2.12 | 0.49 |
| 3:D:1460:ILE:HG13 | 3:D:1461:GLY:N | 2.26 | 0.49 |
| 2:M:496:ILE:HA | 2:M:531:PHE:O | 2.12 | 0.49 |
| 5:P:146:GLY:N | 5:P:149:GLU:HB2 | 2.27 | 0.49 |
| 2:M:211:LEU:C | 2:M:213:ALA:N | 2.64 | 0.49 |
| 4:E:49:GLN:HG3 | 4:E:54:LEU:HD23 | 1.93 | 0.49 |
| 4:E:67:GLU:O | 4:E:70:THR:O | 2.30 | 0.49 |
| 2:C:273:GLY:HA2 | 2:C:276:LYS:HG3 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:47:GLU:CB | 3:N:51:GLY:O | 2.60 | 0.49 |
| 3:D:560:GLN:HA | 3:D:560:GLN:OE1 | 2.11 | 0.49 |
| 3:D:598:ARG:HH11 | 3:D:598:ARG:HG2 | 1.76 | 0.49 |
| 3:D:257:GLY:CA | 3:D:274:ARG:HA | 2.28 | 0.49 |
| 5:P:349:LEU:HA | 5:P:352:GLU:CD | 2.33 | 0.49 |
| 5:P:402:ASN:HD22 | 5:P:402:ASN:N | 2.09 | 0.49 |
| 1:B:58:ILE:HD13 | 1:B:58:ILE:C | 2.32 | 0.49 |
| 2:M:313:LEU:C | 2:M:315:ALA:N | 2.65 | 0.49 |
| 3:D:657:LEU:O | 3:D:658:LEU:C | 2.50 | 0.49 |
| 2:C:41:ASN:OD1 | 2:C:46:ALA:HA | 2.13 | 0.49 |
| 5:F:288:TYR:HB3 | 5:F:301:ALA:CB | 2.42 | 0.49 |
| 3:N:671:LYS:O | 3:N:674:ARG:HB2 | 2.11 | 0.49 |
| 3:N:1229:ILE:O | 3:N:1232:PRO:HD2 | 2.11 | 0.49 |
| 3:N:1364:HIS:ND1 | 3:N:1366:LYS:HG3 | 2.27 | 0.49 |
| 3:D:171:LEU:CD1 | 3:D:390:PRO:HB2 | 2.41 | 0.49 |
| 3:N:1117:TYR:HA | 3:N:1193:THR:HG21 | 1.94 | 0.49 |
| 2:M:1012:PRO:HD2 | 2:M:1021:LEU:O | 2.12 | 0.49 |
| 2:C:599:GLU:HB3 | 2:C:615:TYR:CE2 | 2.47 | 0.49 |
| 1:A:151:VAL:HG13 | 1:A:155:LYS:HG2 | 1.94 | 0.49 |
| 1:K:44:LEU:CD2 | 1:K:214:ALA:HB2 | 2.42 | 0.49 |
| 1:B:151:VAL:HG21 | 1:B:171:PHE:CE1 | 2.48 | 0.49 |
| 1:K:29:GLU:O | 1:K:30:ARG:C | 2.51 | 0.49 |
| 1:K:11:PHE:CE2 | 1:L:225:PHE:O | 2.65 | 0.49 |
| 3:D:1335:LEU:O | 3:D:1335:LEU:HD12 | 2.12 | 0.49 |
| 3:N:1311:LEU:HD21 | 3:N:1313:VAL:O | 2.12 | 0.49 |
| 3:N:703:ASN:HD22 | 3:N:704:ARG:N | 2.11 | 0.49 |
| 5:F:145:PRO:HB3 | 5:F:152:ASP:OD2 | 2.11 | 0.49 |
| 3:N:1130:ARG:NH2 | 3:N:1323:GLN:NE2 | 2.57 | 0.49 |
| 2:C:579:VAL:HA | 2:C:901:TYR:O | 2.12 | 0.49 |
| 1:A:217:ILE:HG22 | 1:A:221:HIS:CD2 | 2.47 | 0.49 |
| 4:O:46:PRO:O | 4:O:57:ASP:N | 2.38 | 0.49 |
| 2:C:494:TYR:HB3 | 2:C:530:GLU:OE2 | 2.12 | 0.49 |
| 2:C:731:GLU:O | 2:C:734:LEU:N | 2.42 | 0.49 |
| 2:M:754:ILE:HG12 | 2:M:791:ARG:HD2 | 1.93 | 0.49 |
| 3:N:414:ARG:O | 3:N:415:VAL:HG13 | 2.11 | 0.49 |
| 2:M:193:LEU:O | 2:M:195:LEU:N | 2.45 | 0.49 |
| 2:M:396:ASP:O | 2:M:403:SER:CA | 2.60 | 0.49 |
| 2:M:591:SER:O | 2:M:592:LEU:HB2 | 2.12 | 0.49 |
| 2:C:157:ARG:CG | 2:C:158:TYR:H | 2.13 | 0.49 |
| 2:C:332:ARG:HG2 | 2:C:333:ILE:N | 2.27 | 0.49 |
| 2:C:543:ASN:HA | 2:C:546:LEU:CD1 | 2.41 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1084:THR:HG23 | 3:D:1085:ALA:H | 1.76 | 0.49 |
| 3:N:42:ASP:OD1 | 3:N:48:ARG:NH2 | 2.45 | 0.49 |
| 3:D:605:ASP:OD1 | 3:D:605:ASP:N | 2.45 | 0.49 |
| 3:D:605:ASP:O | 3:D:609:GLY:HA2 | 2.12 | 0.49 |
| 5:F:225:GLU:OE1 | 5:F:226:LYS:NZ | 2.44 | 0.49 |
| 3:D:243:ALA:HB3 | 3:D:311:LEU:CD1 | 2.34 | 0.49 |
| 3:D:248:PRO:HB3 | 3:D:308:LYS:NZ | 2.26 | 0.49 |
| 3:D:227:LEU:HG | 3:D:326:GLU:OE1 | 2.12 | 0.49 |
| 3:D:932:ASP:HA | 3:D:935:LYS:HE2 | 1.94 | 0.49 |
| 2:M:611:ILE:HD11 | 2:M:641:PRO:HB3 | 1.93 | 0.49 |
| 3:D:660:LYS:O | 3:D:663:GLU:HB2 | 2.12 | 0.49 |
| 2:C:115:LEU:CD1 | 2:C:373:VAL:CG1 | 2.73 | 0.49 |
| 5:F:271:LEU:CD1 | 5:F:307:THR:HG21 | 2.40 | 0.49 |
| 2:M:815:LEU:HD21 | 2:M:822:VAL:HG22 | 1.92 | 0.49 |
| 3:N:1418:LYS:O | 3:N:1420:LEU:HD13 | 2.11 | 0.49 |
| 3:N:302:GLN:N | 3:N:303:PRO:CD | 2.75 | 0.49 |
| 3:N:712:GLY:O | 3:N:713:ILE:HG13 | 2.12 | 0.49 |
| 2:M:676:ILE:CG1 | 2:M:873:PRO:HG3 | 2.40 | 0.49 |
| 3:N:1117:TYR:HD1 | 3:N:1118:ILE:O | 1.95 | 0.49 |
| 3:N:758:GLU:HG2 | 4:O:20:THR:HG21 | 1.94 | 0.49 |
| 3:D:853:VAL:O | 3:D:856:GLY:N | 2.41 | 0.49 |
| 3:N:483:HIS:CB | 3:N:484:PRO:CD | 2.79 | 0.49 |
| 2:M:1085:PHE:O | 2:M:1089:VAL:HG23 | 2.12 | 0.49 |
| 1:K:199:ILE:HG21 | 1:K:207:PRO:HA | 1.94 | 0.49 |
| 2:M:504:GLU:OE2 | 2:M:507:ARG:HD3 | 2.12 | 0.49 |
| 2:M:317:VAL:HG13 | 2:M:320:HIS:CE1 | 2.47 | 0.49 |
| 2:M:486:MET:HG2 | 2:M:487:THR:O | 2.11 | 0.49 |
| 3:D:59:ALA:HB3 | 3:D:76:CYS:CB | 2.42 | 0.49 |
| 2:M:18:LEU:C | 2:M:20:GLU:N | 2.65 | 0.49 |
| 2:C:1039:ALA:HA | 3:D:1227:GLN:NE2 | 2.27 | 0.49 |
| 2:M:728:HIS:CG | 2:M:729:LEU:N | 2.80 | 0.49 |
| 2:C:757:GLY:HA2 | 2:C:789:SER:HB3 | 1.93 | 0.49 |
| 1:B:6:LEU:C | 1:B:8:ALA:H | 2.15 | 0.49 |
| 3:D:155:ASP:O | 3:D:158:TYR:N | 2.45 | 0.49 |
| 2:M:268:ASP:O | 2:M:288:ARG:HD2 | 2.12 | 0.49 |
| 2:M:382:ILE:O | 2:M:385:PHE:HB3 | 2.12 | 0.49 |
| 2:M:543:ASN:HA | 2:M:546:LEU:CD1 | 2.39 | 0.49 |
| 2:C:178:PRO:HB2 | 2:C:220:GLY:HA3 | 1.94 | 0.49 |
| 3:D:1066:THR:O | 3:D:1070:TYR:N | 2.39 | 0.49 |
| 3:N:413:ASP:O | 3:N:435:VAL:N | 2.45 | 0.49 |
| 5:P:135:ILE:C | 5:P:137:GLY:H | 2.15 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:D:1464:GLU:HG2 | 3:D:1465:ASN:H | 1.77 | 0.49 |
| 5:F:112:ALA:O | 5:F:116:LEU:HG | 2.12 | 0.49 |
| 5:F:135:ILE:HD12 | 5:F:181:GLU:HB3 | 1.95 | 0.49 |
| 3:D:358:GLY:HA2 | 3:D:385:VAL:C | 2.32 | 0.49 |
| 2:M:355:VAL:HA | 2:M:358:ARG:CG | 2.41 | 0.49 |
| 5:P:367:MET:CB | 5:P:370:LYS:HE2 | 2.38 | 0.49 |
| 3:D:1379:VAL:O | 3:D:1393:GLN:N | 2.44 | 0.49 |
| 3:D:1007:VAL:O | 3:D:1010:ASN:HB3 | 2.11 | 0.49 |
| 3:N:1166:LEU:HA | 3:N:1170:ASP:OD2 | 2.12 | 0.49 |
| 2:C:617:ASP:OD2 | 2:C:619:ARG:HG3 | 2.13 | 0.49 |
| 2:C:594:ALA:HB1 | 2:C:654:LEU:HD11 | 1.94 | 0.49 |
| 2:M:1061:GLU:HA | 2:M:1064:ASN:HD22 | 1.78 | 0.49 |
| 1:K:173:PRO:HG3 | 1:K:205:VAL:HG21 | 1.92 | 0.49 |
| 3:N:1165:TYR:HE2 | 3:N:1206:GLY:HA2 | 1.77 | 0.49 |
| 2:M:146:VAL:HG22 | 2:M:162:ILE:CG1 | 2.36 | 0.49 |
| 3:N:169:TYR:O | 3:N:392:SER:HB3 | 2.13 | 0.49 |
| 5:P:152:ASP:HA | 5:P:156:VAL:HG11 | 1.94 | 0.49 |
| 5:P:156:VAL:HG23 | 5:P:157:GLU:H | 1.77 | 0.49 |
| 3:N:210:ARG:HB3 | 3:N:388:HIS:HB2 | 1.94 | 0.49 |
| 2:M:742:VAL:HG12 | 2:M:743:VAL:N | 2.27 | 0.49 |
| 1:B:219:ARG:HG2 | 1:B:219:ARG:NH1 | 2.23 | 0.49 |
| 1:B:158:ILE:C | 1:B:159:LYS:HG3 | 2.33 | 0.49 |
| 3:D:960:LYS:HG2 | 3:D:964:LEU:HD12 | 1.93 | 0.49 |
| 3:D:500:ARG:O | 3:D:504:ASP:HB2 | 2.12 | 0.49 |
| 1:K:89:PHE:CB | 1:K:146:ARG:HH21 | 2.23 | 0.49 |
| 2:M:730:SER:OG | 2:M:731:GLU:N | 2.45 | 0.49 |
| 3:D:1293:PHE:HD1 | 3:D:1302:GLU:HA | 1.75 | 0.49 |
| 2:M:800:VAL:HG12 | 2:M:801:VAL:H | 1.78 | 0.49 |
| 3:N:1306:PRO:HB2 | 3:N:1308:GLU:HG3 | 1.93 | 0.49 |
| 2:M:426:ASP:O | 2:M:429:ASP:HB2 | 2.12 | 0.49 |
| 2:M:894:GLY:HA2 | 2:M:901:TYR:OH | 2.11 | 0.49 |
| 2:M:569:VAL:HG23 | 2:M:570:PRO:HD2 | 1.95 | 0.49 |
| 1:L:134:GLU:C | 1:L:136:GLY:H | 2.16 | 0.49 |
| 2:M:541:SER:O | 2:M:544:THR:HB | 2.13 | 0.49 |
| 3:N:323:GLU:CB | 3:N:334:THR:HB | 2.39 | 0.49 |
| 2:C:176:VAL:HG12 | 2:C:182:VAL:HA | 1.94 | 0.49 |
| 2:C:214:TYR:OH | 2:C:308:ARG:HB2 | 2.12 | 0.49 |
| 3:D:558:LEU:C | 3:D:560:GLN:N | 2.64 | 0.49 |
| 5:F:209:PHE:O | 5:F:212:LEU:HB2 | 2.13 | 0.49 |
| 3:D:258:VAL:HG23 | 3:D:273:ARG:O | 2.13 | 0.49 |
| 2:C:36:PRO:HG2 | 2:C:38:LYS:HB3 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:678:GLU:HG3 | 3:D:679:ARG:CG | 2.38 | 0.49 |
| 2:M:63:GLY:H | 2:M:103:LYS:CB | 2.26 | 0.49 |
| 3:D:32:ILE:CG2 | 3:D:37:LEU:HA | 2.42 | 0.49 |
| 5:P:367:MET:HE1 | 5:P:371:LEU:HD21 | 1.94 | 0.49 |
| 5:P:370:LYS:HA | 5:P:374:GLY:CA | 2.42 | 0.49 |
| 3:N:1487:VAL:O | 4:O:74:VAL:HG22 | 2.12 | 0.49 |
| 1:B:5:LYS:HZ3 | 1:B:189:ARG:CZ | 2.25 | 0.49 |
| 3:D:206:ARG:HB3 | 3:D:207:PHE:CD1 | 2.48 | 0.49 |
| 3:N:1155:VAL:O | 3:N:1158:VAL:CG1 | 2.60 | 0.49 |
| 3:N:1167:SER:N | 3:N:1170:ASP:OD2 | 2.46 | 0.49 |
| 2:M:1050:GLN:O | 2:M:1053:LEU:N | 2.40 | 0.49 |
| 1:B:64:GLU:O | 1:B:76:VAL:HG23 | 2.13 | 0.49 |
| 3:N:1350:GLU:O | 3:N:1354:LYS:HG3 | 2.12 | 0.49 |
| 3:D:28:LYS:HG2 | 3:D:42:ASP:O | 2.13 | 0.49 |
| 1:A:170:VAL:O | 1:A:170:VAL:HG23 | 2.13 | 0.49 |
| 2:M:926:PHE:O | 2:M:927:GLY:C | 2.50 | 0.49 |
| 1:A:103:ALA:O | 1:A:104:GLU:HB2 | 2.11 | 0.49 |
| 1:K:9:PRO:HA | 1:K:26:GLU:O | 2.12 | 0.49 |
| 2:M:428:ARG:NH2 | 2:M:451:LEU:HD11 | 2.27 | 0.49 |
| 1:B:182:GLU:CG | 1:B:194:LYS:HD3 | 2.42 | 0.49 |
| 5:P:156:VAL:O | 5:P:159:ILE:HB | 2.12 | 0.49 |
| 2:C:630:ARG:HD2 | 2:C:705:ILE:HB | 1.93 | 0.49 |
| 5:P:111:GLU:CG | 5:P:114:LYS:HZ2 | 2.23 | 0.49 |
| 2:M:297:GLU:H | 2:M:297:GLU:CD | 2.15 | 0.49 |
| 3:D:15:PRO:HA | 3:D:18:ILE:HD12 | 1.94 | 0.49 |
| 2:M:512:ARG:HD2 | 2:M:523:ILE:CG1 | 2.39 | 0.49 |
| 2:C:896:PHE:C | 2:C:898:GLY:N | 2.66 | 0.49 |
| 1:A:222:LEU:HA | 1:A:225:PHE:CE1 | 2.47 | 0.49 |
| 3:D:172:PRO:HB2 | 3:D:175:VAL:HG23 | 1.93 | 0.49 |
| 3:D:775:GLY:HA2 | 3:D:1209:LEU:O | 2.12 | 0.49 |
| 3:N:188:GLY:H | 3:N:197:SER:C | 2.15 | 0.49 |
| 2:M:410:ILE:N | 2:M:410:ILE:HD12 | 2.28 | 0.49 |
| 2:C:471:TYR:CE2 | 2:C:496:ILE:HG21 | 2.48 | 0.49 |
| 3:N:520:LEU:HD12 | 3:N:521:PRO:HD2 | 1.95 | 0.49 |
| 5:F:118:GLU:C | 5:F:120:THR:N | 2.63 | 0.49 |
| 5:F:408:LEU:O | 5:F:411:HIS:N | 2.42 | 0.49 |
| 2:C:73:LEU:O | 2:C:73:LEU:HD12 | 2.11 | 0.49 |
| 2:C:96:ALA:HB3 | 2:C:113:VAL:HG23 | 1.95 | 0.49 |
| 2:M:63:GLY:O | 2:M:102:HIS:HA | 2.13 | 0.49 |
| 2:M:65:VAL:HG12 | 2:M:66:LEU:N | 2.27 | 0.49 |
| 5:F:291:ILE:O | 5:F:295:MET:N | 2.33 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:N:959:GLU:N | 3:N:959:GLU:CD | 2.65 | 0.49 |
| 3:D:912:LYS:O | 3:D:915:VAL:HB | 2.12 | 0.49 |
| 3:N:1092:GLY:O | 3:N:1093:TYR:C | 2.50 | 0.49 |
| 3:N:1472:ILE:HD13 | 3:N:1473:PRO:HD3 | 1.93 | 0.49 |
| 3:N:789:LEU:HG | 3:N:938:GLY:HA2 | 1.95 | 0.49 |
| 2:M:971:LYS:HZ1 | 3:N:950:GLY:HA3 | 1.78 | 0.49 |
| 1:A:177:VAL:HG12 | 1:A:178:ALA:N | 2.27 | 0.49 |
| 2:M:1060:ILE:HG13 | 2:M:1083:GLU:HG3 | 1.94 | 0.49 |
| 1:A:150:TYR:HA | 1:A:169:ALA:O | 2.12 | 0.49 |
| 1:K:122:ILE:CG2 | 1:K:123:MET:N | 2.76 | 0.49 |
| 3:N:812:ALA:O | 3:N:814:ALA:N | 2.45 | 0.49 |
| 1:A:111:ALA:C | 1:A:113:ASP:N | 2.65 | 0.49 |
| 1:A:124:ASN:HB2 | 1:A:127:LEU:CB | 2.43 | 0.49 |
| 2:M:37:GLU:CG | 2:M:71:TYR:HE2 | 2.23 | 0.49 |
| 2:M:431:HIS:ND1 | 2:M:432:ARG:HG2 | 2.28 | 0.49 |
| 5:P:151:LEU:HB2 | 5:P:155:THR:HB | 1.94 | 0.49 |
| 5:P:107:GLU:OE1 | 5:P:230:LYS:HE3 | 2.11 | 0.49 |
| 1:A:222:LEU:HD12 | 1:B:219:ARG:HA | 1.94 | 0.49 |
| 3:D:1488:ASP:HA | 4:E:73:LEU:HD13 | 1.94 | 0.49 |
| 5:P:216:GLY:CA | 5:P:243:ILE:HG23 | 2.42 | 0.49 |
| 3:D:254:GLU:CD | 3:D:299:GLU:O | 2.51 | 0.49 |
| 2:M:322:VAL:HG12 | 2:M:323:ASP:N | 2.20 | 0.49 |
| 2:C:175:GLU:HG2 | 2:C:176:VAL:H | 1.76 | 0.49 |
| 2:C:138:SER:O | 2:C:410:ILE:HA | 2.12 | 0.49 |
| 3:N:135:LEU:H | 3:N:135:LEU:HD23 | 1.75 | 0.49 |
| 3:N:154:THR:HG23 | 3:N:157:GLU:H | 1.77 | 0.49 |
| 5:P:132:ARG:CZ | 5:P:184:ARG:HH12 | 2.25 | 0.49 |
| 5:P:206:GLY:O | 5:P:207:LEU:HB2 | 2.11 | 0.49 |
| 2:C:1102:LEU:HD11 | 3:D:9:ARG:HB2 | 1.95 | 0.49 |
| 3:D:1470:ARG:HG2 | 3:D:1471:LEU:N | 2.28 | 0.49 |
| 3:D:509:PRO:HG2 | 3:D:510:GLU:OE2 | 2.13 | 0.49 |
| 5:P:383:LEU:HD23 | 5:P:394:ARG:HD3 | 1.93 | 0.49 |
| 5:P:416:ARG:HD2 | 5:P:419:ARG:CG | 2.40 | 0.49 |
| 3:D:814:ALA:O | 3:D:818:ARG:HG3 | 2.11 | 0.49 |
| 5:F:386:VAL:CG1 | 5:F:394:ARG:N | 2.76 | 0.49 |
| 2:M:650:ARG:HE | 2:M:650:ARG:CA | 2.22 | 0.49 |
| 5:P:288:TYR:CA | 5:P:291:ILE:HG23 | 2.42 | 0.49 |
| 5:P:302:LYS:O | 5:P:306:GLU:OE2 | 2.30 | 0.49 |
| 3:D:33:ASN:O | 3:D:37:LEU:N | 2.46 | 0.49 |
| 3:D:1160:LEU:O | 3:D:1161:GLU:C | 2.50 | 0.49 |
| 3:D:1398:TRP:O | 3:D:1402:ALA:HB3 | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:1095:THR:O | 3:N:1096:ARG:C | 2.51 | 0.49 |
| 3:N:1447:LEU:O | 3:N:1448:THR:C | 2.49 | 0.49 |
| 2:M:869:VAL:CG2 | 2:M:870:ILE:N | 2.76 | 0.49 |
| 3:N:1112:CYS:N | 3:N:1201:CYS:HB2 | 2.28 | 0.49 |
| 1:A:29:GLU:O | 1:A:193:ASP:OD2 | 2.30 | 0.49 |
| 3:N:16:GLU:N | 3:N:16:GLU:CD | 2.61 | 0.49 |
| 3:N:18:ILE:HG21 | 3:N:518:PRO:HG3 | 1.95 | 0.49 |
| 1:A:76:VAL:O | 1:A:77:GLU:C | 2.51 | 0.49 |
| 2:M:946:ARG:NH1 | 2:M:984:GLU:HB2 | 2.28 | 0.49 |
| 1:A:68:ILE:HG23 | 1:A:69:PRO:HD2 | 1.95 | 0.49 |
| 3:N:207:PHE:CB | 3:N:391:ALA:HB3 | 2.41 | 0.49 |
| 5:F:321:ILE:CG2 | 5:F:322:GLY:H | 2.26 | 0.49 |
| 1:L:85:LEU:HD11 | 1:L:87:VAL:HG13 | 1.94 | 0.49 |
| 5:F:300:ASP:CG | 5:F:302:LYS:HE3 | 2.32 | 0.49 |
| 3:D:1434:TRP:CZ3 | 3:D:1457:ASP:HB2 | 2.48 | 0.49 |
| 4:E:55:PHE:CD1 | 4:E:55:PHE:N | 2.81 | 0.49 |
| 2:M:1114:GLY:C | 2:M:1116:ALA:N | 2.65 | 0.49 |
| 2:C:428:ARG:NH2 | 2:C:451:LEU:HD11 | 2.28 | 0.49 |
| 3:D:1078:ARG:O | 3:D:1080:GLY:N | 2.46 | 0.49 |
| 3:N:356:PRO:HB3 | 3:N:440:VAL:CG2 | 2.41 | 0.49 |
| 3:D:408:GLU:CD | 3:D:421:LEU:HG | 2.32 | 0.49 |
| 3:D:248:PRO:CA | 3:D:308:LYS:NZ | 2.73 | 0.49 |
| 3:D:785:ILE:HG23 | 3:D:938:GLY:HA3 | 1.95 | 0.49 |
| 3:D:806:PHE:CZ | 3:D:816:HIS:CE1 | 3.01 | 0.49 |
| 5:F:381:HIS:N | 5:F:385:GLU:CD | 2.66 | 0.49 |
| 5:F:393:THR:CG2 | 5:F:394:ARG:N | 2.75 | 0.49 |
| 2:M:65:VAL:O | 2:M:100:LEU:CD1 | 2.60 | 0.49 |
| 3:N:1107:VAL:HG21 | 3:N:1219:GLU:HB3 | 1.95 | 0.49 |
| 3:N:59:ALA:C | 3:N:61:GLY:N | 2.65 | 0.49 |
| 3:N:62:LYS:HE3 | 3:N:75:ARG:HH11 | 1.78 | 0.49 |
| 3:N:1442:ASN:O | 3:N:1446:VAL:HG23 | 2.12 | 0.49 |
| 3:N:859:ASP:O | 3:N:862:ASP:HB2 | 2.13 | 0.49 |
| 2:C:691:SER:HB2 | 2:C:868:ASP:HA | 1.93 | 0.49 |
| 3:N:1161:GLU:OE2 | 3:N:1164:ARG:HB2 | 2.11 | 0.49 |
| 3:N:756:GLN:O | 3:N:759:ALA:HB3 | 2.12 | 0.49 |
| 2:M:1040:LEU:HD23 | 3:N:763:MET:HE1 | 1.94 | 0.49 |
| 3:D:844:ALA:N | 3:D:848:GLU:OE1 | 2.45 | 0.49 |
| 3:N:14:SER:O | 3:N:17:LYS:HB3 | 2.13 | 0.49 |
| 3:N:676:MET:C | 3:N:677:LEU:HD23 | 2.33 | 0.49 |
| 3:N:696:HIS:CD2 | 4:O:48:MET:HG2 | 2.48 | 0.49 |
| 3:D:736:PHE:O | 3:D:737:ASN:C | 2.51 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:K:20:TYR:CG | 1:K:21:GLY:N | 2.81 | 0.49 |
| 1:L:37:GLY:O | 1:L:38:ASN:C | 2.51 | 0.49 |
| 3:N:634:GLY:HA3 | 3:N:637:LEU:CD1 | 2.43 | 0.49 |
| 3:N:1397:LYS:O | 3:N:1398:TRP:CD1 | 2.66 | 0.49 |
| 3:D:1253:THR:HG22 | 3:D:1254:GLN:N | 2.28 | 0.49 |
| 3:D:1339:LYS:HB3 | 3:D:1343:ALA:CB | 2.41 | 0.49 |
| 3:N:1311:LEU:HG | 3:N:1312:LEU:N | 2.28 | 0.49 |
| 3:D:1207:TYR:HA | 3:D:1213:ARG:O | 2.11 | 0.49 |
| 2:C:630:ARG:HG3 | 2:C:631:SER:N | 2.27 | 0.49 |
| 1:A:63:HIS:HB2 | 2:C:799:ILE:HD11 | 1.93 | 0.49 |
| 3:D:16:GLU:N | 3:D:16:GLU:OE1 | 2.46 | 0.49 |
| 5:F:304:VAL:HG12 | 5:F:308:LEU:HD21 | 1.94 | 0.49 |
| 2:C:918:LEU:CD1 | 2:C:968:LEU:HA | 2.42 | 0.49 |
| 3:N:984:THR:HG22 | 3:N:987:GLU:CD | 2.33 | 0.49 |
| 2:C:731:GLU:C | 2:C:733:ALA:N | 2.64 | 0.49 |
| 5:F:86:HIS:C | 5:F:88:ILE:N | 2.65 | 0.49 |
| 1:B:240:LYS:HD2 | 1:B:240:LYS:N | 2.28 | 0.49 |
| 3:D:68:PHE:HZ | 5:F:376:ILE:HG12 | 1.77 | 0.49 |
| 3:D:926:LYS:HE2 | 3:D:929:ARG:NH1 | 2.28 | 0.49 |
| 1:K:151:VAL:O | 1:K:169:ALA:N | 2.43 | 0.49 |
| 3:D:277:GLU:HG3 | 3:D:278:PRO:N | 2.27 | 0.49 |
| 2:M:237:ARG:O | 2:M:240:THR:HB | 2.12 | 0.49 |
| 2:M:254:VAL:HB | 2:M:258:TYR:OH | 2.12 | 0.49 |
| 2:C:267:TYR:CB | 2:C:272:ALA:H | 2.26 | 0.49 |
| 2:C:273:GLY:O | 2:C:276:LYS:HB2 | 2.12 | 0.49 |
| 2:C:471:TYR:HB3 | 2:C:531:PHE:HD2 | 1.77 | 0.49 |
| 3:N:130:SER:HB3 | 3:N:132:TYR:HE1 | 1.72 | 0.49 |
| 3:N:565:ILE:HG23 | 3:N:566:ILE:N | 2.13 | 0.49 |
| 5:P:132:ARG:O | 5:P:135:ILE:N | 2.44 | 0.49 |
| 3:D:87:ARG:CB | 3:D:523:ASP:HB2 | 2.43 | 0.49 |
| 3:D:584:ASN:OD1 | 3:D:590:PRO:CD | 2.55 | 0.49 |
| 3:D:591:VAL:O | 3:D:592:THR:C | 2.50 | 0.49 |
| 2:M:94:LEU:C | 2:M:114:PHE:HA | 2.33 | 0.49 |
| 5:P:350:LEU:C | 5:P:352:GLU:N | 2.65 | 0.49 |
| 3:N:1497:GLU:HB2 | 4:O:88:GLU:OE2 | 2.12 | 0.49 |
| 3:D:806:PHE:HZ | 3:D:816:HIS:CE1 | 2.30 | 0.49 |
| 3:D:811:GLU:HB3 | 3:D:815:ALA:CB | 2.42 | 0.49 |
| 2:C:32:ALA:O | 2:C:35:PRO:HD2 | 2.13 | 0.49 |
| 2:C:92:ALA:C | 2:C:117:HIS:HB3 | 2.32 | 0.49 |
| 1:A:36:LEU:C | 1:A:39:PRO:HD2 | 2.33 | 0.49 |
| 1:B:32:PHE:O | 1:B:33:GLY:C | 2.50 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:M:589:ARG:HG2 | 2:M:596:TYR:OH | 2.12 | 0.49 |
| 2:M:610:ARG:HE | 2:M:612:VAL:HG23 | 1.77 | 0.49 |
| 5:F:418:LEU:N | 5:F:418:LEU:HD12 | 2.11 | 0.49 |
| 2:C:344:PHE:CE2 | 2:C:348:LEU:HD13 | 2.48 | 0.49 |
| 5:P:296:GLY:C | 5:P:299:TRP:HD1 | 2.17 | 0.49 |
| 3:N:1489:GLN:HA | 3:N:1492:LEU:CG | 2.43 | 0.49 |
| 3:N:1406:ARG:CB | 3:N:1412:LYS:HE2 | 2.40 | 0.49 |
| 1:L:56:VAL:N | 1:L:165:ILE:O | 2.44 | 0.49 |
| 3:D:1020:LEU:O | 3:D:1021:TYR:C | 2.51 | 0.49 |
| 3:N:972:LEU:HD23 | 3:N:972:LEU:H | 1.78 | 0.49 |
| 2:C:971:LYS:HZ1 | 3:D:950:GLY:HA3 | 1.76 | 0.49 |
| 2:M:874:LEU:HD13 | 3:N:783:ARG:HB3 | 1.94 | 0.49 |
| 3:N:881:LEU:O | 3:N:884:ARG:HB3 | 2.13 | 0.49 |
| 2:M:1017:THR:HB | 2:M:1019:GLN:NE2 | 2.28 | 0.49 |
| 1:A:152:PRO:O | 1:A:155:LYS:HB3 | 2.13 | 0.49 |
| 1:K:138:LEU:HD21 | 1:K:140:MET:CE | 2.42 | 0.49 |
| 2:M:41:ASN:O | 2:M:43:GLY:N | 2.46 | 0.49 |
| 2:M:37:GLU:OE2 | 2:M:71:TYR:O | 2.29 | 0.49 |
| 5:P:145:PRO:HG3 | 5:P:150:THR:O | 2.12 | 0.49 |
| 5:F:308:LEU:HD23 | 5:F:308:LEU:N | 2.27 | 0.49 |
| 2:C:493:ARG:HB2 | 2:C:494:TYR:CD1 | 2.48 | 0.49 |
| 3:D:1291:SER:HA | 3:D:1305:LEU:HD23 | 1.95 | 0.49 |
| 3:D:1137:ARG:O | 3:D:1138:ALA:C | 2.51 | 0.49 |
| 2:C:1050:GLN:NE2 | 3:D:1469:GLY:O | 2.40 | 0.49 |
| 2:M:208:ALA:O | 2:M:212:GLY:HA3 | 2.12 | 0.49 |
| 3:N:322:VAL:HA | 3:N:335:LEU:CD1 | 2.42 | 0.49 |
| 2:C:178:PRO:HA | 2:C:181:VAL:O | 2.13 | 0.49 |
| 2:C:269:LEU:HA | 2:C:288:ARG:CB | 2.42 | 0.49 |
| 3:N:100:ALA:HB3 | 3:N:575:GLN:HE22 | 1.77 | 0.49 |
| 3:N:521:PRO:C | 3:N:525:ARG:NH1 | 2.66 | 0.49 |
| 3:D:127:LEU:CD1 | 3:D:134:VAL:HG22 | 2.43 | 0.49 |
| 4:E:92:ILE:HB | 4:E:93:TYR:CD1 | 2.47 | 0.49 |
| 3:N:401:TYR:HB2 | 3:N:444:VAL:HG23 | 1.95 | 0.49 |
| 3:N:421:LEU:HD11 | 3:N:429:SER:HB3 | 1.95 | 0.49 |
| 3:N:441:ARG:O | 3:N:442:ASN:C | 2.51 | 0.49 |
| 3:D:442:ASN:HD22 | 3:D:442:ASN:H | 1.61 | 0.49 |
| 2:M:95:TYR:HA | 2:M:113:VAL:O | 2.13 | 0.49 |
| 1:B:112:ARG:CZ | 1:B:125:PRO:HB2 | 2.42 | 0.49 |
| 1:A:208:LEU:O | 1:A:209:GLU:C | 2.51 | 0.49 |
| 3:D:1398:TRP:CB | 3:D:1402:ALA:HB3 | 2.43 | 0.49 |
| 3:N:1445:HIS:O | 3:N:1446:VAL:C | 2.49 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:M:1049:LEU:O | 2:M:1053:LEU:HG | 2.13 | 0.49 |
| 1:B:73:GLU:CB | 1:B:78:ILE:HD11 | 2.43 | 0.49 |
| 3:D:857:ILE:HG13 | 3:D:858:VAL:HG23 | 1.94 | 0.49 |
| 3:N:1341:PRO:HG2 | 3:N:1342:GLU:CD | 2.30 | 0.49 |
| 3:N:657:LEU:O | 3:N:658:LEU:C | 2.51 | 0.49 |
| 1:K:36:LEU:C | 1:K:39:PRO:HD2 | 2.33 | 0.49 |
| 3:N:806:PHE:CE2 | 3:N:812:ALA:HB3 | 2.47 | 0.49 |
| 3:N:1394:VAL:HG11 | 3:N:1397:LYS:HE3 | 1.94 | 0.49 |
| 3:D:1346:ARG:HH11 | 3:D:1346:ARG:CG | 2.25 | 0.49 |
| 3:D:1376:MET:CE | 3:D:1421:LEU:HA | 2.43 | 0.49 |
| 3:N:1048:PRO:CG | 3:N:1075:HIS:HD2 | 2.22 | 0.49 |
| 5:F:161:GLN:O | 5:F:165:SER:HB3 | 2.13 | 0.49 |
| 3:D:983:LEU:CD2 | 3:D:987:GLU:HB3 | 2.41 | 0.49 |
| 1:A:220:GLU:O | 1:A:223:THR:HB | 2.12 | 0.49 |
| 3:N:187:LYS:N | 3:N:200:ASP:OD2 | 2.46 | 0.49 |
| 3:N:1026:SER:C | 3:N:1028:ALA:H | 2.17 | 0.49 |
| 3:N:1046:GLN:HB2 | 3:N:1052:THR:HA | 1.93 | 0.49 |
| 3:D:234:GLU:O | 3:D:236:TYR:N | 2.41 | 0.49 |
| 2:C:726:ILE:HG13 | 2:C:728:HIS:HB3 | 1.94 | 0.49 |
| 3:N:895:VAL:O | 3:N:899:LEU:HG | 2.12 | 0.49 |
| 5:P:115:LYS:O | 5:P:119:ILE:HG13 | 2.13 | 0.49 |
| 2:M:916:GLU:O | 2:M:919:ALA:HB3 | 2.12 | 0.49 |
| 2:M:705:ILE:O | 2:M:705:ILE:HG23 | 2.13 | 0.49 |
| 2:M:176:VAL:HG12 | 2:M:181:VAL:O | 2.12 | 0.48 |
| 2:M:230:ARG:O | 2:M:230:ARG:HG2 | 2.13 | 0.48 |
| 3:N:225:LEU:O | 3:N:330:THR:HA | 2.13 | 0.48 |
| 3:N:317:VAL:HG23 | 3:N:338:GLU:O | 2.13 | 0.48 |
| 1:A:16:GLN:CD | 1:B:235:ALA:HB1 | 2.33 | 0.48 |
| 2:C:424:GLY:O | 2:C:428:ARG:HG3 | 2.13 | 0.48 |
| 2:C:498:GLN:HB3 | 2:C:500:ASN:OD1 | 2.13 | 0.48 |
| 2:C:499:ALA:HB2 | 2:C:533:ASP:O | 2.13 | 0.48 |
| 3:N:22:SER:HB2 | 3:N:92:HIS:ND1 | 2.28 | 0.48 |
| 3:D:1466:VAL:O | 3:D:1468:LEU:N | 2.46 | 0.48 |
| 5:F:130:VAL:O | 5:F:131:VAL:C | 2.52 | 0.48 |
| 3:D:226:PRO:HB2 | 3:D:231:VAL:HG21 | 1.94 | 0.48 |
| 2:C:48:PHE:CE1 | 2:C:71:TYR:HB3 | 2.48 | 0.48 |
| 5:P:300:ASP:OD1 | 5:P:302:LYS:HG3 | 2.12 | 0.48 |
| 3:D:827:ILE:CA | 3:D:836:VAL:HB | 2.38 | 0.48 |
| 2:C:874:LEU:HB3 | 3:D:1029:ARG:HD3 | 1.95 | 0.48 |
| 3:D:783:ARG:CZ | 3:D:1029:ARG:NH1 | 2.76 | 0.48 |
| 2:M:554:ASP:OD2 | 2:M:556:ASN:HB2 | 2.12 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:N:712:GLY:C | 3:N:713:ILE:HG13 | 2.33 | 0.48 |
| 3:N:1161:GLU:CG | 3:N:1164:ARG:HB2 | 2.39 | 0.48 |
| 2:C:833:LEU:HD12 | 2:C:837:ASP:OD2 | 2.13 | 0.48 |
| 1:K:100:LEU:HD23 | 1:K:101:LEU:N | 2.23 | 0.48 |
| 2:C:20:GLU:C | 2:C:23:VAL:HG22 | 2.33 | 0.48 |
| 1:K:152:PRO:HA | 1:K:168:ASP:OD1 | 2.13 | 0.48 |
| 1:A:57:TYR:CE1 | 1:A:163:ASN:HB2 | 2.46 | 0.48 |
| 2:M:498:GLN:CD | 3:N:1068:LEU:HB2 | 2.33 | 0.48 |
| 1:L:91:ASN:CB | 1:L:94:LEU:HG | 2.39 | 0.48 |
| 2:C:800:VAL:HG12 | 2:C:801:VAL:N | 2.28 | 0.48 |
| 1:A:213:GLN:O | 1:A:214:ALA:C | 2.51 | 0.48 |
| 1:L:83:LYS:CE | 1:L:168:ASP:HB2 | 2.43 | 0.48 |
| 3:N:967:ALA:HB2 | 3:N:999:THR:HG21 | 1.95 | 0.48 |
| 3:D:470:LEU:HB2 | 3:D:503:LEU:CD2 | 2.42 | 0.48 |
| 2:C:939:ARG:HD2 | 2:C:982:PRO:HD3 | 1.94 | 0.48 |
| 3:N:98:PRO:CA | 3:N:514:LEU:O | 2.60 | 0.48 |
| 4:E:86:GLN:O | 4:E:90:GLU:HG3 | 2.13 | 0.48 |
| 3:D:1117:TYR:HD1 | 3:D:1118:ILE:O | 1.96 | 0.48 |
| 3:N:1137:ARG:O | 3:N:1138:ALA:C | 2.49 | 0.48 |
| 4:O:29:GLN:O | 4:O:31:LEU:N | 2.45 | 0.48 |
| 1:K:153:ALA:HA | 1:K:156:HIS:CE1 | 2.48 | 0.48 |
| 2:M:198:ARG:HH21 | 2:M:231:PRO:CD | 2.24 | 0.48 |
| 2:M:193:LEU:CD2 | 2:M:307:LEU:HD13 | 2.43 | 0.48 |
| 2:M:385:PHE:CD1 | 2:M:385:PHE:C | 2.84 | 0.48 |
| 3:N:259:VAL:HG21 | 3:N:292:VAL:CA | 2.43 | 0.48 |
| 2:C:258:TYR:CD2 | 2:C:258:TYR:N | 2.79 | 0.48 |
| 2:C:313:LEU:C | 2:C:315:ALA:N | 2.65 | 0.48 |
| 2:C:471:TYR:CD1 | 2:C:486:MET:HE2 | 2.48 | 0.48 |
| 3:N:119:SER:HB3 | 3:N:123:LEU:N | 2.23 | 0.48 |
| 3:N:573:MET:CE | 5:P:211:ASP:OD1 | 2.61 | 0.48 |
| 5:P:76:SER:C | 5:P:78:SER:N | 2.65 | 0.48 |
| 5:P:75:ILE:CG1 | 5:P:76:SER:H | 2.10 | 0.48 |
| 3:D:318:ARG:CZ | 3:D:338:GLU:OE2 | 2.61 | 0.48 |
| 3:D:1098:LEU:N | 3:D:1098:LEU:HD12 | 2.27 | 0.48 |
| 3:D:1440:PHE:HE2 | 3:D:1463:LYS:HZ3 | 1.60 | 0.48 |
| 3:D:1465:ASN:ND2 | 3:D:1471:LEU:O | 2.42 | 0.48 |
| 3:N:355:VAL:CG1 | 3:N:356:PRO:HD2 | 2.43 | 0.48 |
| 3:D:438:ASP:C | 3:D:439:LEU:HD23 | 2.34 | 0.48 |
| 3:D:223:LEU:O | 3:D:332:TYR:CD1 | 2.66 | 0.48 |
| 1:A:43:ILE:CG2 | 1:A:47:SER:HB2 | 2.42 | 0.48 |
| 5:P:288:TYR:C | 5:P:291:ILE:HG23 | 2.32 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:M:712:ALA:HA | 2:M:720:GLU:OE1 | 2.13 | 0.48 |
| 3:D:1105:ILE:HD11 | 3:D:1374:GLN:CD | 2.32 | 0.48 |
| 3:D:55:ASP:OD2 | 5:F:337:HIS:NE2 | 2.46 | 0.48 |
| 3:N:1379:VAL:HA | 3:N:1420:LEU:HB2 | 1.95 | 0.48 |
| 2:M:690:ILE:HB | 2:M:852:ILE:HG12 | 1.95 | 0.48 |
| 3:N:844:ALA:HB1 | 3:N:867:ARG:NH1 | 2.28 | 0.48 |
| 2:M:914:ILE:HD12 | 2:M:914:ILE:H | 1.75 | 0.48 |
| 2:M:1033:GLY:O | 2:M:1036:GLU:HB2 | 2.13 | 0.48 |
| 2:C:612:VAL:HA | 2:C:622:GLU:HA | 1.95 | 0.48 |
| 1:A:101:LEU:HD13 | 1:A:113:ASP:O | 2.13 | 0.48 |
| 3:N:1415:VAL:HG23 | 3:N:1415:VAL:O | 2.13 | 0.48 |
| 3:N:702:LEU:O | 3:N:736:PHE:HZ | 1.95 | 0.48 |
| 3:D:989:TYR:O | 3:D:992:ILE:HB | 2.13 | 0.48 |
| 1:L:10:VAL:O | 1:L:10:VAL:HG23 | 2.12 | 0.48 |
| 3:D:175:VAL:HG11 | 3:D:192:ALA:HB1 | 1.93 | 0.48 |
| 3:D:1041:LEU:HD21 | 3:D:1043:GLY:HA2 | 1.95 | 0.48 |
| 3:N:896:ALA:O | 3:N:900:ILE:HG13 | 2.12 | 0.48 |
| 2:M:557:ARG:O | 2:M:844:GLY:HA3 | 2.13 | 0.48 |
| 1:L:72:LYS:C | 1:L:72:LYS:HD3 | 2.33 | 0.48 |
| 2:M:212:GLY:HA3 | 2:M:218:VAL:CG1 | 2.42 | 0.48 |
| 2:M:203:ASP:CA | 2:M:228:ALA:HB1 | 2.43 | 0.48 |
| 2:M:309:TYR:CZ | 2:M:321:GLU:HG3 | 2.47 | 0.48 |
| 3:N:245:LEU:HA | 3:N:309:GLY:N | 2.04 | 0.48 |
| 2:C:182:VAL:CG2 | 2:C:221:LEU:HA | 2.43 | 0.48 |
| 3:N:105:VAL:HG13 | 3:N:124:GLU:OE2 | 2.13 | 0.48 |
| 3:N:39:PRO:HB3 | 3:N:45:PHE:O | 2.12 | 0.48 |
| 2:C:1095:LEU:HG | 3:D:603:LEU:HD13 | 1.93 | 0.48 |
| 3:D:152:LEU:CG | 3:D:153:LEU:N | 2.77 | 0.48 |
| 3:D:522:PRO:N | 3:D:525:ARG:HH12 | 2.12 | 0.48 |
| 3:D:128:TYR:OH | 3:D:575:GLN:CD | 2.51 | 0.48 |
| 5:F:120:THR:CG2 | 5:F:122:LEU:HG | 2.43 | 0.48 |
| 3:D:355:VAL:HG23 | 3:D:367:ILE:HG23 | 1.93 | 0.48 |
| 3:D:241:ILE:HD13 | 3:D:310:LEU:HD22 | 1.93 | 0.48 |
| 3:D:324:ALA:CB | 3:D:331:VAL:HG11 | 2.44 | 0.48 |
| 3:D:662:GLU:N | 3:D:667:ALA:HB3 | 2.28 | 0.48 |
| 2:M:808:ARG:O | 2:M:810:ASP:N | 2.46 | 0.48 |
| 3:D:1397:LYS:CB | 3:D:1398:TRP:CZ3 | 2.93 | 0.48 |
| 3:D:793:THR:HG21 | 3:D:906:GLN:CG | 2.41 | 0.48 |
| 3:D:162:ARG:HA | 3:D:449:SER:OG | 2.13 | 0.48 |
| 3:N:1092:GLY:O | 3:N:1096:ARG:N | 2.35 | 0.48 |
| 2:M:691:SER:C | 2:M:693:GLU:N | 2.63 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:N:757:ALA:O | 3:N:758:GLU:C | 2.51 | 0.48 |
| 4:O:19:LEU:O | 4:O:20:THR:C | 2.51 | 0.48 |
| 2:M:1015:LEU:CD1 | 5:P:335:ASP:HB2 | 2.42 | 0.48 |
| 3:D:41:ARG:NH2 | 3:D:48:ARG:NH1 | 2.61 | 0.48 |
| 1:K:206:THR:HB | 1:K:209:GLU:OE1 | 2.13 | 0.48 |
| 2:M:946:ARG:HH11 | 2:M:984:GLU:CB | 2.26 | 0.48 |
| 3:N:1208:ASP:HB3 | 3:N:1211:MET:O | 2.13 | 0.48 |
| 3:N:1372:VAL:O | 3:N:1373:ARG:C | 2.51 | 0.48 |
| 2:C:389:SER:HB3 | 2:C:392:SER:CB | 2.44 | 0.48 |
| 2:M:17:PRO:O | 2:M:20:GLU:HB2 | 2.14 | 0.48 |
| 2:M:764:GLU:HB3 | 2:M:766:GLU:OE2 | 2.12 | 0.48 |
| 1:L:5:LYS:HZ3 | 1:L:189:ARG:NE | 2.12 | 0.48 |
| 3:N:502:PHE:O | 3:N:503:LEU:C | 2.51 | 0.48 |
| 2:M:380:ALA:CA | 2:M:384:GLU:HG2 | 2.44 | 0.48 |
| 2:M:685:GLU:C | 2:M:687:ALA:H | 2.16 | 0.48 |
| 2:M:685:GLU:HB3 | 3:N:740:PHE:HD1 | 1.77 | 0.48 |
| 2:M:769:PRO:HG2 | 3:N:65:ARG:NH1 | 2.28 | 0.48 |
| 3:N:69:GLU:CD | 3:N:71:LYS:HZ1 | 2.17 | 0.48 |
| 2:M:198:ARG:NH1 | 2:M:203:ASP:HB3 | 2.28 | 0.48 |
| 2:M:230:ARG:CG | 2:M:233:GLU:HG2 | 2.42 | 0.48 |
| 2:M:321:GLU:H | 2:M:321:GLU:CD | 2.15 | 0.48 |
| 4:E:40:LEU:HD13 | 4:E:72:ARG:HH12 | 1.78 | 0.48 |
| 3:D:135:LEU:HG | 3:D:151:GLN:O | 2.13 | 0.48 |
| 4:E:29:GLN:CG | 4:E:30:LEU:N | 2.76 | 0.48 |
| 5:F:125:ASP:CG | 5:F:126:LEU:N | 2.67 | 0.48 |
| 3:D:266:GLU:OE1 | 3:D:314:PRO:HB3 | 2.14 | 0.48 |
| 3:D:661:MET:HE1 | 3:D:677:LEU:HD11 | 1.93 | 0.48 |
| 3:N:1405:GLU:O | 3:N:1410:GLU:C | 2.52 | 0.48 |
| 3:D:1381:VAL:HG11 | 3:D:1388:ARG:O | 2.13 | 0.48 |
| 3:D:491:LYS:O | 3:D:494:LYS:HB2 | 2.13 | 0.48 |
| 3:N:795:VAL:HA | 3:N:861:GLN:O | 2.13 | 0.48 |
| 2:C:589:ARG:HG2 | 2:C:596:TYR:CZ | 2.48 | 0.48 |
| 1:L:235:ALA:HB3 | 1:L:236:PRO:CD | 2.35 | 0.48 |
| 3:D:630:VAL:HG12 | 3:D:631:ILE:N | 2.27 | 0.48 |
| 1:K:124:ASN:O | 1:K:127:LEU:HB3 | 2.13 | 0.48 |
| 1:A:111:ALA:O | 1:A:114:PHE:HD1 | 1.97 | 0.48 |
| 2:C:603:VAL:HG11 | 2:C:644:VAL:C | 2.34 | 0.48 |
| 3:D:1345:GLU:O | 3:D:1346:ARG:C | 2.52 | 0.48 |
| 2:C:958:THR:O | 2:C:959:PRO:C | 2.52 | 0.48 |
| 5:P:157:GLU:CD | 5:P:157:GLU:N | 2.66 | 0.48 |
| 2:C:809:GLY:N | 2:C:813:VAL:HB | 2.28 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:L:167:VAL:HG12 | 1:L:168:ASP:N | 2.27 | 0.48 |
| 2:M:560:MET:HB3 | 2:M:564:MET:HE1 | 1.94 | 0.48 |
| 3:N:984:THR:CG2 | 3:N:987:GLU:H | 2.26 | 0.48 |
| 3:N:1108:ARG:HD2 | 3:N:1199:GLY:HA3 | 1.95 | 0.48 |
| 2:M:549:PHE:CE2 | 2:M:886:LEU:CB | 2.96 | 0.48 |
| 2:C:250:ARG:O | 2:C:252:LYS:N | 2.47 | 0.48 |
| 5:P:361:LEU:CG | 5:P:362:SER:H | 2.25 | 0.48 |
| 3:D:1046:GLN:CB | 3:D:1052:THR:HA | 2.44 | 0.48 |
| 5:P:146:GLY:HA3 | 5:P:149:GLU:OE2 | 2.14 | 0.48 |
| 2:C:550:LEU:HD22 | 2:C:905:ILE:HD11 | 1.96 | 0.48 |
| 3:N:1047:LYS:HG2 | 3:N:1053:PHE:CZ | 2.47 | 0.48 |
| 2:M:1118:LYS:HG3 | 2:M:1119:ARG:N | 2.28 | 0.48 |
| 2:M:343:GLN:HG2 | 2:M:385:PHE:CG | 2.49 | 0.48 |
| 2:C:234:ALA:HA | 2:C:237:ARG:HD2 | 1.94 | 0.48 |
| 3:N:573:MET:HE3 | 5:P:210:LEU:HB2 | 1.96 | 0.48 |
| 3:D:217:LYS:O | 3:D:339:TRP:HD1 | 1.96 | 0.48 |
| 3:D:1443:THR:HG23 | 9:D:1529:NE6:H24 | 1.96 | 0.48 |
| 3:D:406:ASP:CB | 3:D:423:ASP:HA | 2.42 | 0.48 |
| 3:D:225:LEU:HD11 | 3:D:242:LEU:CD1 | 2.40 | 0.48 |
| 3:D:932:ASP:O | 3:D:935:LYS:HE2 | 2.13 | 0.48 |
| 3:D:186:VAL:O | 3:D:189:GLN:HB2 | 2.13 | 0.48 |
| 3:D:692:GLU:O | 3:D:693:GLU:C | 2.52 | 0.48 |
| 3:D:692:GLU:O | 3:D:695:ILE:HB | 2.14 | 0.48 |
| 2:C:1067:TYR:CB | 5:F:341:PRO:HB3 | 2.43 | 0.48 |
| 2:C:112:GLU:OE1 | 2:C:112:GLU:HA | 2.14 | 0.48 |
| 2:M:108:ILE:HB | 2:M:368:THR:CG2 | 2.27 | 0.48 |
| 5:P:367:MET:O | 5:P:370:LYS:CG | 2.61 | 0.48 |
| 3:D:493:ARG:HG3 | 3:D:494:LYS:N | 2.27 | 0.48 |
| 3:D:914:LEU:HD12 | 3:D:914:LEU:C | 2.33 | 0.48 |
| 2:M:909:ALA:O | 2:M:910:LYS:HD2 | 2.13 | 0.48 |
| 2:C:742:VAL:CG1 | 2:C:743:VAL:N | 2.77 | 0.48 |
| 5:F:75:ILE:C | 5:F:77:THR:H | 2.15 | 0.48 |
| 2:M:1008:ARG:NH2 | 2:M:1012:PRO:O | 2.47 | 0.48 |
| 3:N:673:ALA:C | 3:N:676:MET:HB3 | 2.34 | 0.48 |
| 2:M:944:LEU:HD11 | 2:M:963:LEU:HD21 | 1.96 | 0.48 |
| 1:K:38:ASN:HB2 | 2:M:980:GLY:HA3 | 1.95 | 0.48 |
| 1:K:73:GLU:CD | 1:K:73:GLU:H | 2.17 | 0.48 |
| 3:N:703:ASN:HD22 | 3:N:704:ARG:H | 1.60 | 0.48 |
| 3:N:631:ILE:HG12 | 3:N:743:ASP:O | 2.13 | 0.48 |
| 2:C:838:LYS:HE3 | 2:C:997:LEU:HB3 | 1.95 | 0.48 |
| 1:A:211:LEU:O | 1:A:214:ALA:HB3 | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:D:756:GLN:HE22 | 3:D:760:ARG:HD2 | 1.78 | 0.48 |
| 1:B:55:SER:HA | 1:B:167:VAL:HG23 | 1.95 | 0.48 |
| 4:O:46:PRO:HG2 | 4:O:63:TRP:CD1 | 2.49 | 0.48 |
| 2:C:529:VAL:HG12 | 2:C:530:GLU:N | 2.29 | 0.48 |
| 2:C:292:ARG:HE | 2:C:295:ASP:CB | 2.27 | 0.48 |
| 3:D:622:ARG:HG2 | 3:D:622:ARG:HH11 | 1.77 | 0.48 |
| 3:D:1117:TYR:O | 3:D:1193:THR:HG21 | 2.13 | 0.48 |
| 3:D:926:LYS:O | 3:D:929:ARG:HB2 | 2.13 | 0.48 |
| 2:M:916:GLU:OE1 | 2:M:916:GLU:C | 2.52 | 0.48 |
| 2:M:916:GLU:O | 2:M:919:ALA:N | 2.46 | 0.48 |
| 3:N:1359:GLN:HG3 | 3:N:1359:GLN:O | 2.12 | 0.48 |
| 2:M:176:VAL:HG12 | 2:M:182:VAL:HA | 1.95 | 0.48 |
| 2:C:230:ARG:HH11 | 2:C:230:ARG:CG | 2.24 | 0.48 |
| 2:C:157:ARG:NH1 | 2:C:314:THR:HA | 2.28 | 0.48 |
| 3:N:522:PRO:N | 3:N:525:ARG:NH1 | 2.60 | 0.48 |
| 3:D:45:PHE:HB3 | 3:D:86:ARG:NH2 | 2.28 | 0.48 |
| 3:D:564:GLU:HA | 5:F:140:ARG:NH1 | 2.28 | 0.48 |
| 3:D:571:LYS:O | 3:D:574:LEU:HB3 | 2.13 | 0.48 |
| 3:N:357:GLU:O | 3:N:358:GLY:C | 2.52 | 0.48 |
| 3:D:208:PRO:O | 3:D:209:ARG:HG3 | 2.13 | 0.48 |
| 3:D:408:GLU:OE2 | 3:D:422:ALA:CB | 2.62 | 0.48 |
| 3:D:285:PRO:O | 3:D:286:VAL:C | 2.52 | 0.48 |
| 1:B:68:ILE:HD12 | 1:B:71:VAL:CB | 2.42 | 0.48 |
| 5:F:295:MET:HG3 | 5:F:299:TRP:CE2 | 2.49 | 0.48 |
| 3:D:1404:ASN:OD1 | 3:D:1409:ALA:HB2 | 2.13 | 0.48 |
| 3:D:69:GLU:CG | 3:D:70:GLY:H | 2.27 | 0.48 |
| 2:C:971:LYS:HZ2 | 3:D:950:GLY:HA3 | 1.78 | 0.48 |
| 2:M:751:PRO:CB | 2:M:794:PRO:HA | 2.29 | 0.48 |
| 3:N:1231:GLU:HB3 | 3:N:1232:PRO:HD3 | 1.95 | 0.48 |
| 1:L:80:LEU:HB3 | 3:N:844:ALA:CB | 2.40 | 0.48 |
| 3:N:799:LYS:N | 3:N:829:VAL:HG12 | 2.28 | 0.48 |
| 3:N:860:LEU:O | 3:N:877:PRO:HD2 | 2.13 | 0.48 |
| 2:C:854:PRO:O | 2:C:857:ASP:OD2 | 2.31 | 0.48 |
| 5:F:92:PRO:C | 5:F:94:LEU:H | 2.16 | 0.48 |
| 1:A:167:VAL:CG1 | 1:A:168:ASP:N | 2.77 | 0.48 |
| 1:L:34:VAL:O | 1:L:36:LEU:N | 2.46 | 0.48 |
| 3:N:806:PHE:H | 3:N:809:PRO:HG2 | 1.79 | 0.48 |
| 1:K:162:ILE:HG13 | 1:K:163:ASN:N | 2.27 | 0.48 |
| 1:B:151:VAL:O | 1:B:169:ALA:N | 2.47 | 0.48 |
| 1:B:176:ARG:HD3 | 3:D:884:ARG:NH2 | 2.28 | 0.48 |
| 3:N:1068:LEU:O | 3:N:1069:GLU:C | 2.52 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:632:VAL:O | 3:N:727:GLN:HA | 2.14 | 0.48 |
| 3:D:234:GLU:C | 3:D:236:TYR:N | 2.66 | 0.48 |
| 3:D:475:LYS:HA | 3:D:478:LEU:HB2 | 1.95 | 0.48 |
| 3:D:1336:LEU:HD12 | 3:D:1340:GLY:C | 2.32 | 0.48 |
| 5:P:103:ALA:HB1 | 5:P:229:TYR:HB3 | 1.95 | 0.48 |
| 2:M:154:ARG:HG2 | 2:M:156:GLY:H | 1.78 | 0.48 |
| 5:P:202:TYR:CD2 | 5:P:205:ARG:NH1 | 2.82 | 0.48 |
| 1:K:99:LEU:HB3 | 1:K:114:PHE:CD2 | 2.47 | 0.48 |
| 3:D:1458:GLU:O | 3:D:1459:LEU:HD23 | 2.14 | 0.48 |
| 2:M:304:LEU:CB | 2:M:305:PRO:CD | 2.85 | 0.48 |
| 1:B:239:ALA:C | 1:B:241:GLU:N | 2.67 | 0.48 |
| 2:C:157:ARG:HD3 | 2:C:158:TYR:CE1 | 2.49 | 0.48 |
| 2:C:446:GLY:O | 2:C:448:ASN:N | 2.46 | 0.48 |
| 2:C:409:ARG:HA | 2:C:453:THR:O | 2.13 | 0.48 |
| 3:N:113:GLY:C | 3:N:115:LEU:N | 2.67 | 0.48 |
| 3:N:458:ALA:HB1 | 3:N:513:ILE:CD1 | 2.38 | 0.48 |
| 3:D:1098:LEU:O | 3:D:1102:THR:N | 2.46 | 0.48 |
| 3:D:543:LEU:O | 3:D:546:ARG:CG | 2.50 | 0.48 |
| 5:P:418:LEU:O | 5:P:421:PHE:HA | 2.13 | 0.48 |
| 1:B:216:GLU:O | 1:B:217:ILE:C | 2.52 | 0.48 |
| 2:M:610:ARG:HD2 | 2:M:622:GLU:CG | 2.44 | 0.48 |
| 2:C:65:VAL:CG2 | 2:C:101:ILE:HB | 2.43 | 0.48 |
| 2:M:100:LEU:CD2 | 2:M:368:THR:HG23 | 2.41 | 0.48 |
| 5:P:287:THR:HG23 | 5:P:289:GLU:OE1 | 2.14 | 0.48 |
| 5:P:288:TYR:HB2 | 5:P:289:GLU:OE2 | 2.14 | 0.48 |
| 3:N:1290:LEU:O | 3:N:1305:LEU:HD23 | 2.13 | 0.48 |
| 3:D:55:ASP:HA | 3:D:83:SER:N | 2.29 | 0.48 |
| 3:D:96:ALA:O | 5:F:144:ILE:HD11 | 2.14 | 0.48 |
| 3:N:493:ARG:HG3 | 3:N:494:LYS:N | 2.29 | 0.48 |
| 3:N:1233:GLY:O | 3:N:1235:GLN:N | 2.47 | 0.48 |
| 2:C:753:ASP:O | 2:C:791:ARG:HA | 2.13 | 0.48 |
| 1:A:41:ARG:O | 1:A:45:LEU:HG | 2.14 | 0.48 |
| 3:N:761:ILE:CD1 | 4:O:20:THR:HA | 2.43 | 0.48 |
| 1:A:5:LYS:HZ3 | 1:A:192:LEU:HD22 | 1.77 | 0.48 |
| 3:N:477:LEU:C | 3:N:479:GLU:N | 2.67 | 0.48 |
| 1:A:167:VAL:HG12 | 1:A:168:ASP:H | 1.75 | 0.48 |
| 3:D:1353:GLN:HB3 | 3:D:1357:ARG:CZ | 2.43 | 0.48 |
| 2:M:979:THR:C | 2:M:981:GLU:N | 2.67 | 0.48 |
| 3:N:811:GLU:HB3 | 3:N:815:ALA:HB3 | 1.94 | 0.48 |
| 2:C:1000:MET:HB3 | 2:C:1002:GLU:CG | 2.34 | 0.48 |
| 5:P:321:ILE:CG1 | 5:P:332:PHE:HE1 | 2.24 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:41:ASN:HB2 | 2:M:46:ALA:CA | 2.43 | 0.48 |
| 3:N:1277:ILE:CG2 | 3:N:1278:ASP:N | 2.75 | 0.48 |
| 3:D:1178:ALA:HB2 | 3:D:1183:ILE:HG23 | 1.95 | 0.48 |
| 3:D:1335:LEU:HD11 | 3:D:1343:ALA:HB1 | 1.95 | 0.48 |
| 3:N:1313:VAL:HG22 | 3:N:1314:LYS:H | 1.78 | 0.48 |
| 3:N:173:PRO:CA | 3:N:209:ARG:NH1 | 2.76 | 0.48 |
| 2:M:881:ASN:ND2 | 2:M:881:ASN:H | 1.97 | 0.48 |
| 3:D:792:ILE:O | 3:D:878:GLY:HA3 | 2.13 | 0.48 |
| 3:N:767:HIS:HA | 3:N:924:MET:HE2 | 1.96 | 0.48 |
| 3:D:14:SER:C | 3:D:16:GLU:N | 2.65 | 0.48 |
| 3:D:1216:SER:HB2 | 4:E:16:LYS:H | 1.76 | 0.48 |
| 3:N:997:THR:O | 3:N:1000:THR:HB | 2.14 | 0.48 |
| 3:D:769:LEU:O | 3:D:778:LEU:N | 2.45 | 0.48 |
| 2:M:614:ARG:HA | 2:M:619:ARG:O | 2.14 | 0.48 |
| 2:M:174:LEU:CD2 | 2:M:184:MET:HG2 | 2.43 | 0.48 |
| 5:F:361:LEU:CG | 5:F:362:SER:N | 2.77 | 0.48 |
| 2:C:930:LYS:C | 2:C:932:GLU:N | 2.66 | 0.48 |
| 5:P:117:SER:O | 5:P:121:GLY:N | 2.45 | 0.48 |
| 2:C:1075:ASP:OD1 | 2:C:1076:VAL:N | 2.41 | 0.48 |
| 2:M:218:VAL:HG11 | 2:M:222:MET:HE2 | 1.96 | 0.48 |
| 2:M:439:CYS:SG | 2:M:441:VAL:CG1 | 3.02 | 0.48 |
| 2:M:455:LEU:HD11 | 2:M:459:ALA:CB | 2.43 | 0.48 |
| 1:B:235:ALA:O | 1:B:237:GLU:N | 2.46 | 0.48 |
| 2:C:198:ARG:HE | 2:C:231:PRO:HD3 | 1.77 | 0.48 |
| 2:C:413:LEU:HA | 2:C:419:THR:HG23 | 1.94 | 0.48 |
| 3:N:27:GLU:O | 3:N:28:LYS:HD3 | 2.13 | 0.48 |
| 3:N:433:GLY:CA | 3:N:447:VAL:O | 2.56 | 0.48 |
| 3:N:540:LEU:O | 3:N:543:LEU:HB2 | 2.14 | 0.48 |
| 3:N:548:ILE:O | 3:N:549:ASN:C | 2.52 | 0.48 |
| 3:N:557:LEU:HG | 3:N:557:LEU:H | 1.33 | 0.48 |
| 2:C:1033:GLY:O | 2:C:1037:VAL:HG23 | 2.13 | 0.48 |
| 3:D:1481:VAL:O | 3:D:1483:PHE:N | 2.47 | 0.48 |
| 3:D:355:VAL:CG1 | 3:D:359:ALA:HB3 | 2.44 | 0.48 |
| 3:D:352:ASN:N | 3:D:369:ALA:O | 2.44 | 0.48 |
| 1:B:63:HIS:CD2 | 3:D:813:LEU:HD13 | 2.48 | 0.48 |
| 5:P:287:THR:HG23 | 5:P:290:GLU:OE1 | 2.13 | 0.48 |
| 3:D:1378:TYR:O | 3:D:1420:LEU:HB2 | 2.13 | 0.48 |
| 3:D:828:LYS:HE2 | 3:D:828:LYS:O | 2.13 | 0.48 |
| 3:D:906:GLN:HA | 3:D:906:GLN:NE2 | 2.28 | 0.48 |
| 2:M:672:VAL:HG23 | 2:M:868:ASP:HB2 | 1.96 | 0.48 |
| 3:N:790:TYR:HA | 3:N:793:THR:OG1 | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:N:1167:SER:HB3 | 3:N:1170:ASP:OD1 | 2.14 | 0.48 |
| 2:C:648:ARG:O | 2:C:649:VAL:HG23 | 2.14 | 0.48 |
| 2:C:625:LEU:CD1 | 2:C:639:GLN:HB2 | 2.31 | 0.48 |
| 2:C:832:LYS:HG2 | 2:C:833:LEU:H | 1.79 | 0.48 |
| 2:C:926:PHE:O | 2:C:927:GLY:C | 2.52 | 0.48 |
| 2:C:923:GLU:O | 2:C:927:GLY:N | 2.46 | 0.48 |
| 2:M:1060:ILE:O | 2:M:1062:GLY:N | 2.47 | 0.48 |
| 3:D:630:VAL:HG22 | 3:D:744:GLN:HG3 | 1.96 | 0.48 |
| 2:M:930:LYS:C | 2:M:932:GLU:N | 2.67 | 0.48 |
| 2:C:317:VAL:H | 2:C:318:PRO:HD3 | 1.74 | 0.48 |
| 2:M:38:LYS:CG | 2:M:39:ARG:H | 2.12 | 0.48 |
| 2:C:603:VAL:HG21 | 2:C:644:VAL:O | 2.14 | 0.48 |
| 2:M:432:ARG:CG | 2:M:433:THR:N | 2.77 | 0.48 |
| 3:N:169:TYR:O | 3:N:392:SER:HA | 2.14 | 0.48 |
| 2:M:564:MET:HA | 2:M:567:GLN:NE2 | 2.29 | 0.48 |
| 3:D:969:ARG:CG | 3:D:970:LYS:N | 2.76 | 0.48 |
| 3:D:181:ASP:C | 3:D:183:GLU:N | 2.61 | 0.48 |
| 2:M:462:ASP:O | 2:M:464:LEU:N | 2.47 | 0.48 |
| 2:M:75:GLU:O | 2:M:77:PRO:CD | 2.61 | 0.48 |
| 2:M:757:GLY:HA2 | 2:M:789:SER:CB | 2.43 | 0.48 |
| 3:D:1059:SER:HB2 | 3:D:1065:LEU:CD2 | 2.44 | 0.48 |
| 1:L:154:GLU:HG2 | 3:N:840:LYS:HE3 | 1.95 | 0.48 |
| 2:M:230:ARG:HD3 | 2:M:230:ARG:H | 1.76 | 0.48 |
| 4:E:40:LEU:HD21 | 4:E:44:GLU:HB3 | 1.96 | 0.48 |
| 3:N:259:VAL:O | 3:N:260:GLU:CG | 2.62 | 0.48 |
| 2:C:144:PRO:HB3 | 2:C:163:ILE:O | 2.13 | 0.48 |
| 2:C:198:ARG:HE | 2:C:231:PRO:HG3 | 1.78 | 0.48 |
| 2:C:436:GLY:O | 2:C:459:ALA:HB2 | 2.13 | 0.48 |
| 3:D:1078:ARG:HG3 | 3:D:1078:ARG:NH1 | 2.29 | 0.48 |
| 3:N:131:LYS:HB3 | 3:N:131:LYS:NZ | 2.28 | 0.48 |
| 3:N:136:ASP:HB2 | 3:N:137:PRO:CD | 2.35 | 0.48 |
| 3:N:41:ARG:HH21 | 3:N:48:ARG:CZ | 2.27 | 0.48 |
| 3:D:318:ARG:CG | 3:D:319:ALA:N | 2.76 | 0.48 |
| 3:D:1106:VAL:HG11 | 3:D:1474:ALA:HB2 | 1.95 | 0.48 |
| 3:D:1472:ILE:CD1 | 3:D:1473:PRO:HD2 | 2.38 | 0.48 |
| 3:D:564:GLU:HA | 3:D:567:ILE:HG13 | 1.95 | 0.48 |
| 5:F:115:LYS:HB3 | 5:F:119:ILE:CD1 | 2.44 | 0.48 |
| 3:N:1488:ASP:OD1 | 3:N:1491:THR:HB | 2.14 | 0.48 |
| 2:M:604:ALA:HB3 | 2:M:612:VAL:C | 2.33 | 0.48 |
| 5:F:291:ILE:HD11 | 5:F:295:MET:HB2 | 1.96 | 0.48 |
| 2:C:773:LEU:O | 2:C:776:SER:OG | 2.26 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1128:VAL:HG21 | 3:D:1131:SER:CB | 2.34 | 0.48 |
| 2:M:1101:THR:CB | 3:N:5:VAL:HG21 | 2.28 | 0.48 |
| 2:C:914:ILE:O | 2:C:916:GLU:N | 2.46 | 0.48 |
| 1:K:186:LEU:C | 1:K:188:GLN:N | 2.59 | 0.48 |
| 3:N:1223:ILE:HD11 | 9:N:1528:NE6:H14B | 1.96 | 0.48 |
| 3:N:1223:ILE:O | 3:N:1224:VAL:C | 2.51 | 0.48 |
| 2:M:575:GLN:HE21 | 2:M:670:GLN:CB | 2.24 | 0.48 |
| 3:N:1481:VAL:HG11 | 4:O:18:ARG:HA | 1.96 | 0.48 |
| 2:M:1083:GLU:O | 2:M:1084:SER:C | 2.52 | 0.48 |
| 1:K:138:LEU:HD12 | 1:K:139:ASN:N | 2.26 | 0.48 |
| 1:K:107:LYS:CE | 1:K:108:GLU:O | 2.62 | 0.48 |
| 1:B:151:VAL:HG21 | 1:B:171:PHE:HE1 | 1.79 | 0.48 |
| 2:C:644:VAL:O | 2:C:647:GLN:CB | 2.62 | 0.48 |
| 1:L:128:HIS:CE1 | 1:L:131:THR:HG23 | 2.49 | 0.48 |
| 3:D:1311:LEU:HD12 | 3:D:1312:LEU:N | 2.23 | 0.48 |
| 1:K:1:MET:CA | 1:K:6:LEU:HD22 | 2.43 | 0.48 |
| 1:K:176:ARG:HB3 | 1:K:200:TRP:CD1 | 2.48 | 0.48 |
| 3:D:965:GLU:O | 3:D:966:GLU:C | 2.50 | 0.48 |
| 3:N:951:ILE:HD11 | 3:N:1062:ARG:HG3 | 1.95 | 0.48 |
| 3:N:630:VAL:HG22 | 3:N:744:GLN:HG2 | 1.95 | 0.48 |
| 2:C:848:VAL:HG12 | 2:C:849:VAL:N | 2.27 | 0.48 |
| 3:N:1257:PRO:HA | 3:N:1260:ILE:HD12 | 1.96 | 0.48 |
| 5:F:362:SER:O | 5:F:366:ALA:N | 2.44 | 0.48 |
| 1:K:103:ALA:C | 1:K:104:GLU:HG3 | 2.34 | 0.48 |
| 2:M:1023:GLY:N | 2:M:1026:GLN:O | 2.46 | 0.48 |
| 2:C:191:PHE:CZ | 2:C:196:LEU:HD21 | 2.49 | 0.48 |
| 2:C:178:PRO:C | 2:C:220:GLY:HA2 | 2.25 | 0.48 |
| 2:C:483:VAL:CG2 | 2:C:484:VAL:N | 2.77 | 0.48 |
| 2:C:542:VAL:O | 2:C:545:ASN:HB2 | 2.14 | 0.48 |
| 3:D:1066:THR:HG22 | 3:D:1068:LEU:N | 2.28 | 0.48 |
| 3:N:570:GLU:CA | 5:P:214:GLN:HE21 | 2.27 | 0.48 |
| 3:N:565:ILE:HD11 | 5:P:87:GLU:OE2 | 2.13 | 0.48 |
| 3:D:1106:VAL:O | 3:D:1108:ARG:HG3 | 2.14 | 0.48 |
| 3:D:110:SER:O | 3:D:111:LYS:C | 2.52 | 0.48 |
| 4:E:24:ALA:O | 4:E:27:ALA:HB3 | 2.14 | 0.48 |
| 4:E:33:HIS:HB2 | 4:E:37:ASN:OD1 | 2.14 | 0.48 |
| 3:D:368:VAL:O | 3:D:377:VAL:HB | 2.14 | 0.48 |
| 3:N:361:VAL:HG11 | 3:N:367:ILE:HD11 | 1.96 | 0.48 |
| 3:D:288:MET:HE1 | 3:D:307:ALA:HB2 | 1.95 | 0.48 |
| 5:F:399:GLN:O | 5:F:402:ASN:HB2 | 2.14 | 0.48 |
| 2:M:643:VAL:HG23 | 2:M:647:GLN:OE1 | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:664:LYS:O | 3:D:665:GLY:C | 2.53 | 0.48 |
| 3:D:1380:GLU:HA | 3:D:1392:GLY:HA2 | 1.95 | 0.48 |
| 3:N:1364:HIS:CE1 | 3:N:1366:LYS:HG3 | 2.49 | 0.48 |
| 3:N:884:ARG:O | 3:N:888:GLU:HG2 | 2.13 | 0.48 |
| 2:C:673:LEU:HA | 2:C:673:LEU:HD23 | 1.73 | 0.48 |
| 3:N:1118:ILE:HG23 | 3:N:1193:THR:HG23 | 1.96 | 0.48 |
| 2:M:1048:THR:O | 2:M:1051:GLU:HG3 | 2.14 | 0.48 |
| 4:O:18:ARG:O | 4:O:19:LEU:C | 2.51 | 0.48 |
| 2:C:599:GLU:HG3 | 2:C:600:ASP:N | 2.28 | 0.48 |
| 2:C:698:ASP:HA | 2:C:832:LYS:HE3 | 1.96 | 0.48 |
| 1:A:29:GLU:HB3 | 1:A:32:PHE:CD1 | 2.49 | 0.48 |
| 3:N:685:ASP:O | 3:N:686:GLU:C | 2.52 | 0.48 |
| 3:D:1353:GLN:HB3 | 3:D:1357:ARG:NE | 2.29 | 0.48 |
| 1:K:41:ARG:CG | 1:K:45:LEU:HD11 | 2.41 | 0.48 |
| 2:M:68:PHE:HZ | 2:M:71:TYR:N | 2.11 | 0.48 |
| 5:P:111:GLU:HA | 5:P:114:LYS:HG3 | 1.96 | 0.48 |
| 3:D:191:LEU:HD23 | 3:D:195:VAL:HG12 | 1.96 | 0.48 |
| 5:P:235:PHE:O | 5:P:236:SER:C | 2.52 | 0.48 |
| 3:D:178:LEU:HG | 3:D:181:ASP:CG | 2.34 | 0.48 |
| 5:P:361:LEU:HG | 5:P:366:ALA:HB2 | 1.94 | 0.48 |
| 2:C:722:ILE:O | 2:C:722:ILE:HG13 | 2.13 | 0.48 |
| 3:N:414:ARG:C | 3:N:415:VAL:HG13 | 2.35 | 0.48 |
| 2:M:340:MET:C | 2:M:340:MET:SD | 2.92 | 0.48 |
| 2:M:252:LYS:O | 2:M:255:ALA:HB3 | 2.14 | 0.47 |
| 2:M:252:LYS:HD3 | 2:M:298:PHE:HE1 | 1.79 | 0.47 |
| 2:C:257:VAL:CA | 2:C:261:ILE:HD12 | 2.28 | 0.47 |
| 2:C:428:ARG:NH2 | 2:C:447:ALA:O | 2.44 | 0.47 |
| 2:C:463:GLU:CD | 2:C:463:GLU:N | 2.67 | 0.47 |
| 2:C:430:VAL:HB | 3:D:1078:ARG:NH1 | 2.29 | 0.47 |
| 3:D:1078:ARG:O | 3:D:1079:LYS:C | 2.53 | 0.47 |
| 3:D:1085:ALA:CA | 3:D:1088:THR:HG22 | 2.43 | 0.47 |
| 3:N:409:VAL:HG12 | 3:N:410:SER:N | 2.28 | 0.47 |
| 5:P:77:THR:C | 5:P:79:ASP:N | 2.66 | 0.47 |
| 5:F:132:ARG:O | 5:F:135:ILE:N | 2.47 | 0.47 |
| 3:D:270:LEU:HD12 | 3:D:271:VAL:N | 2.28 | 0.47 |
| 3:N:361:VAL:HG13 | 3:N:365:ASP:CB | 2.21 | 0.47 |
| 3:N:368:VAL:N | 3:N:377:VAL:HB | 2.29 | 0.47 |
| 3:D:225:LEU:O | 3:D:331:VAL:N | 2.47 | 0.47 |
| 3:D:313:MET:SD | 3:D:314:PRO:CD | 2.95 | 0.47 |
| 5:P:409:LYS:HG3 | 5:P:410:TYR:H | 1.78 | 0.47 |
| 1:B:97:VAL:CG1 | 1:B:98:THR:N | 2.74 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:N:1378:TYR:HB2 | 3:N:1422:MET:HE3 | 1.96 | 0.47 |
| 5:P:288:TYR:O | 5:P:292:ALA:N | 2.33 | 0.47 |
| 3:D:36:THR:HB | 3:D:38:LYS:CG | 2.38 | 0.47 |
| 5:F:261:PRO:CD | 5:F:264:MET:HG3 | 2.39 | 0.47 |
| 5:P:370:LYS:HA | 5:P:374:GLY:N | 2.28 | 0.47 |
| 3:D:65:ARG:HD2 | 3:D:66:GLN:H | 1.79 | 0.47 |
| 1:B:186:LEU:HG | 1:B:188:GLN:OE1 | 2.14 | 0.47 |
| 3:N:252:ARG:HG3 | 3:N:300:LYS:O | 2.14 | 0.47 |
| 3:N:1366:LYS:O | 3:N:1369:GLU:N | 2.47 | 0.47 |
| 3:D:168:THR:HB | 3:D:206:ARG:NH1 | 2.29 | 0.47 |
| 2:C:572:ILE:HG13 | 2:C:573:ARG:HG3 | 1.96 | 0.47 |
| 2:C:595:LEU:O | 2:C:655:LEU:N | 2.47 | 0.47 |
| 3:N:676:MET:HG3 | 3:N:677:LEU:HD21 | 1.95 | 0.47 |
| 1:L:106:PRO:CA | 1:L:133:GLU:HA | 2.36 | 0.47 |
| 3:D:1287:GLU:N | 3:D:1288:GLU:OE1 | 2.47 | 0.47 |
| 3:N:703:ASN:ND2 | 3:N:704:ARG:N | 2.62 | 0.47 |
| 2:M:430:VAL:HG12 | 3:N:1075:HIS:HA | 1.95 | 0.47 |
| 5:P:104:ARG:HG3 | 5:P:105:LYS:N | 2.29 | 0.47 |
| 3:N:622:ARG:HG2 | 3:N:622:ARG:NH1 | 2.28 | 0.47 |
| 3:D:760:ARG:NH1 | 4:E:59:ASN:OD1 | 2.40 | 0.47 |
| 3:N:984:THR:HG22 | 3:N:987:GLU:HG3 | 1.93 | 0.47 |
| 3:N:202:VAL:O | 3:N:395:VAL:HA | 2.14 | 0.47 |
| 2:M:685:GLU:HB3 | 3:N:740:PHE:CE1 | 2.48 | 0.47 |
| 3:N:69:GLU:CG | 3:N:71:LYS:HZ3 | 2.27 | 0.47 |
| 2:M:1076:VAL:HG12 | 2:M:1077:PRO:N | 2.29 | 0.47 |
| 2:M:237:ARG:O | 2:M:240:THR:OG1 | 2.29 | 0.47 |
| 2:M:273:GLY:HA2 | 2:M:276:LYS:NZ | 2.30 | 0.47 |
| 2:M:274:ARG:HH21 | 2:M:284:ARG:CB | 2.10 | 0.47 |
| 2:C:198:ARG:O | 2:C:201:GLY:N | 2.46 | 0.47 |
| 2:C:419:THR:O | 2:C:420:ARG:HG3 | 2.15 | 0.47 |
| 3:D:1066:THR:CB | 3:D:1069:GLU:HG3 | 2.44 | 0.47 |
| 3:N:43:GLY:H | 3:N:46:ASP:HB2 | 1.78 | 0.47 |
| 3:N:87:ARG:CA | 3:N:523:ASP:HB2 | 2.43 | 0.47 |
| 3:D:1094:LEU:CD2 | 3:D:1230:GLY:HA2 | 2.37 | 0.47 |
| 3:D:118:LEU:CA | 3:D:123:LEU:HD12 | 2.33 | 0.47 |
| 3:D:591:VAL:HG12 | 3:D:599:PRO:CA | 2.43 | 0.47 |
| 3:D:614:PHE:CD2 | 3:D:617:ASN:ND2 | 2.82 | 0.47 |
| 3:N:368:VAL:HB | 3:N:377:VAL:CB | 2.44 | 0.47 |
| 5:P:353:GLU:HA | 5:P:356:LYS:HB2 | 1.95 | 0.47 |
| 2:M:615:TYR:O | 2:M:618:GLY:N | 2.45 | 0.47 |
| 4:O:70:THR:C | 4:O:72:ARG:N | 2.68 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:874:LEU:O | 3:D:1029:ARG:HD3 | 2.14 | 0.47 |
| 3:N:73:CYS:C | 3:N:75:ARG:H | 2.18 | 0.47 |
| 3:N:1434:TRP:C | 3:N:1434:TRP:CD1 | 2.86 | 0.47 |
| 3:N:1436:SER:O | 3:N:1439:SER:HB3 | 2.14 | 0.47 |
| 3:N:497:GLU:HA | 3:N:497:GLU:OE1 | 2.13 | 0.47 |
| 3:N:1223:ILE:O | 3:N:1226:ALA:N | 2.47 | 0.47 |
| 3:N:1224:VAL:O | 3:N:1225:ALA:C | 2.52 | 0.47 |
| 1:A:41:ARG:NH1 | 1:A:177:VAL:O | 2.46 | 0.47 |
| 2:M:1063:ARG:O | 2:M:1066:ALA:HB3 | 2.14 | 0.47 |
| 1:A:153:ALA:HA | 1:A:156:HIS:CE1 | 2.48 | 0.47 |
| 1:K:205:VAL:HG12 | 1:K:206:THR:N | 2.29 | 0.47 |
| 1:K:22:GLU:OE1 | 2:M:934:PHE:CZ | 2.67 | 0.47 |
| 1:A:128:HIS:HE1 | 1:A:131:THR:HG23 | 1.77 | 0.47 |
| 3:D:1286:THR:HB | 3:D:1289:LYS:O | 2.13 | 0.47 |
| 5:F:156:VAL:HG23 | 5:F:157:GLU:N | 2.25 | 0.47 |
| 1:A:220:GLU:O | 1:A:223:THR:CB | 2.62 | 0.47 |
| 4:O:46:PRO:C | 4:O:57:ASP:H | 2.16 | 0.47 |
| 3:N:1221:VAL:HG12 | 3:N:1370:ILE:HD13 | 1.96 | 0.47 |
| 2:C:708:TYR:N | 2:C:708:TYR:CD1 | 2.82 | 0.47 |
| 1:A:1:MET:N | 1:A:6:LEU:HD13 | 2.29 | 0.47 |
| 3:D:473:LEU:O | 3:D:476:GLU:HB3 | 2.13 | 0.47 |
| 2:M:1001:VAL:HG23 | 2:M:1002:GLU:N | 2.29 | 0.47 |
| 3:N:1296:SER:C | 3:N:1298:GLY:N | 2.66 | 0.47 |
| 5:F:91:VAL:C | 5:F:93:LEU:H | 2.18 | 0.47 |
| 1:L:105:GLY:O | 1:L:107:LYS:HG2 | 2.15 | 0.47 |
| 1:B:111:ALA:HA | 1:B:129:ILE:HD11 | 1.95 | 0.47 |
| 2:M:408:ARG:O | 2:M:454:SER:HA | 2.15 | 0.47 |
| 2:M:540:PHE:CD1 | 2:M:540:PHE:N | 2.82 | 0.47 |
| 3:N:227:LEU:HD11 | 3:N:326:GLU:HA | 1.95 | 0.47 |
| 2:C:191:PHE:HB2 | 2:C:192:PRO:CD | 2.45 | 0.47 |
| 2:C:334:ARG:HB2 | 2:C:339:LEU:CD2 | 2.42 | 0.47 |
| 2:C:431:HIS:HE1 | 2:C:432:ARG:HG2 | 1.77 | 0.47 |
| 2:C:471:TYR:O | 2:C:484:VAL:N | 2.47 | 0.47 |
| 2:C:401:LEU:CD1 | 2:C:543:ASN:HB3 | 2.38 | 0.47 |
| 3:D:1095:THR:O | 3:D:1096:ARG:C | 2.53 | 0.47 |
| 3:D:505:SER:CB | 3:D:1453:ALA:O | 2.62 | 0.47 |
| 3:D:1465:ASN:ND2 | 3:D:1473:PRO:HD3 | 2.29 | 0.47 |
| 3:D:459:GLU:O | 3:D:463:GLN:HG2 | 2.15 | 0.47 |
| 3:D:582:LEU:HA | 3:D:603:LEU:CD1 | 2.18 | 0.47 |
| 5:F:124:PRO:O | 5:F:127:ILE:HB | 2.14 | 0.47 |
| 5:F:127:ILE:HG22 | 5:F:128:ARG:N | 2.29 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:F:209:PHE:CD2 | 5:F:213:ILE:HD11 | 2.50 | 0.47 |
| 5:F:411:HIS:C | 5:F:413:SER:H | 2.16 | 0.47 |
| 3:D:656:PHE:H | 3:D:656:PHE:HD1 | 1.62 | 0.47 |
| 5:F:343:ASP:HB2 | 5:F:347:GLN:HE22 | 1.78 | 0.47 |
| 3:N:1378:TYR:HB2 | 3:N:1422:MET:CE | 2.43 | 0.47 |
| 2:C:367:LEU:HG | 2:C:372:LEU:CD2 | 2.38 | 0.47 |
| 5:P:370:LYS:CG | 5:P:371:LEU:N | 2.70 | 0.47 |
| 3:N:1489:GLN:O | 3:N:1492:LEU:HB2 | 2.14 | 0.47 |
| 1:L:58:ILE:O | 1:L:59:GLU:C | 2.51 | 0.47 |
| 3:D:55:ASP:HB3 | 3:D:82:LYS:HA | 1.96 | 0.47 |
| 3:D:1016:PRO:O | 3:D:1021:TYR:HD1 | 1.98 | 0.47 |
| 1:B:5:LYS:HA | 1:B:5:LYS:HD3 | 1.58 | 0.47 |
| 3:N:73:CYS:CB | 3:N:76:CYS:SG | 3.02 | 0.47 |
| 3:N:843:PHE:HD1 | 3:N:848:GLU:OE2 | 1.96 | 0.47 |
| 2:C:615:TYR:OH | 2:C:623:TYR:OH | 2.26 | 0.47 |
| 2:C:575:GLN:HB2 | 2:C:670:GLN:HA | 1.96 | 0.47 |
| 3:N:10:ILE:HG12 | 3:N:1451:ALA:HA | 1.97 | 0.47 |
| 2:M:976:ASP:C | 2:M:978:ARG:H | 2.17 | 0.47 |
| 2:M:47:ALA:O | 2:M:50:GLU:HG2 | 2.13 | 0.47 |
| 2:C:603:VAL:HG12 | 2:C:645:VAL:HA | 1.96 | 0.47 |
| 3:N:207:PHE:HB2 | 3:N:391:ALA:H | 1.79 | 0.47 |
| 2:C:1048:THR:O | 2:C:1052:MET:CB | 2.62 | 0.47 |
| 2:C:78:PHE:HB3 | 2:C:79:PRO:HD2 | 1.95 | 0.47 |
| 3:D:315:ARG:N | 3:D:315:ARG:HD2 | 2.27 | 0.47 |
| 3:N:1042:ARG:HB3 | 3:N:1057:VAL:CG1 | 2.44 | 0.47 |
| 2:C:588:VAL:HG21 | 2:C:664:GLY:O | 2.14 | 0.47 |
| 5:F:95:THR:HG22 | 5:F:96:LEU:N | 2.29 | 0.47 |
| 2:C:246:ASP:CG | 2:C:247:PRO:HD2 | 2.34 | 0.47 |
| 1:K:133:GLU:HG2 | 1:K:134:GLU:N | 2.29 | 0.47 |
| 2:M:141:HIS:HE1 | 2:M:143:SER:HA | 1.80 | 0.47 |
| 2:M:209:ARG:HD2 | 2:M:209:ARG:N | 2.28 | 0.47 |
| 2:M:208:ALA:O | 2:M:218:VAL:HG11 | 2.14 | 0.47 |
| 2:M:276:LYS:CA | 2:M:280:LYS:HE3 | 2.45 | 0.47 |
| 2:M:322:VAL:O | 2:M:323:ASP:CG | 2.53 | 0.47 |
| 2:M:544:THR:C | 2:M:546:LEU:H | 2.17 | 0.47 |
| 3:N:238:PRO:HB3 | 3:N:318:ARG:HA | 1.96 | 0.47 |
| 3:N:325:GLU:N | 3:N:331:VAL:HG13 | 2.29 | 0.47 |
| 2:C:159:ILE:HG22 | 2:C:175:GLU:HB2 | 1.96 | 0.47 |
| 2:C:327:HIS:ND1 | 2:C:329:GLY:N | 2.62 | 0.47 |
| 2:C:512:ARG:CB | 2:C:523:ILE:HD11 | 2.45 | 0.47 |
| 3:N:508:ARG:HD3 | 3:N:510:GLU:OE1 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:N:29:PRO:HG3 | 3:N:548:ILE:CG2 | 2.45 | 0.47 |
| 2:C:1090:LYS:HE3 | 3:D:88:TYR:O | 2.15 | 0.47 |
| 3:D:401:TYR:HB2 | 3:D:444:VAL:HG23 | 1.95 | 0.47 |
| 2:C:52:PHE:CD1 | 2:C:67:ASP:HA | 2.48 | 0.47 |
| 2:C:97:ARG:HG2 | 2:C:111:ASP:HB3 | 1.96 | 0.47 |
| 5:P:264:MET:O | 5:P:267:THR:OG1 | 2.28 | 0.47 |
| 3:N:1489:GLN:HA | 3:N:1492:LEU:HB2 | 1.96 | 0.47 |
| 3:D:397:LYS:HG3 | 3:D:448:GLU:OE1 | 2.15 | 0.47 |
| 3:N:58:CYS:SG | 3:N:63:TYR:N | 2.67 | 0.47 |
| 1:L:88:ARG:HB2 | 1:L:121:GLU:HB3 | 1.96 | 0.47 |
| 2:M:693:GLU:HG3 | 2:M:697:ARG:HH11 | 1.79 | 0.47 |
| 3:N:937:TYR:O | 3:N:938:GLY:C | 2.52 | 0.47 |
| 2:M:1008:ARG:NH1 | 3:N:624:ASP:OD1 | 2.48 | 0.47 |
| 1:B:78:ILE:HG22 | 1:B:82:LEU:HD21 | 1.96 | 0.47 |
| 2:M:839:LEU:CD2 | 2:M:996:LYS:HA | 2.32 | 0.47 |
| 2:C:1004:LYS:HB3 | 2:C:1006:HIS:HE1 | 1.80 | 0.47 |
| 1:K:173:PRO:O | 1:K:201:THR:HA | 2.14 | 0.47 |
| 2:C:504:GLU:HG3 | 2:C:504:GLU:O | 2.15 | 0.47 |
| 3:N:812:ALA:C | 3:N:814:ALA:H | 2.16 | 0.47 |
| 2:C:185:LYS:CG | 2:C:190:LYS:HD3 | 2.36 | 0.47 |
| 3:D:1253:THR:HG22 | 3:D:1254:GLN:H | 1.80 | 0.47 |
| 1:A:57:TYR:CE2 | 1:A:161:ARG:NH1 | 2.82 | 0.47 |
| 5:F:154:LYS:O | 5:F:158:GLU:HG3 | 2.14 | 0.47 |
| 3:D:1001:GLU:CA | 3:D:1001:GLU:OE2 | 2.56 | 0.47 |
| 3:N:644:LEU:HD12 | 3:N:645:PRO:CD | 2.41 | 0.47 |
| 4:O:46:PRO:HB3 | 4:O:57:ASP:HB3 | 1.94 | 0.47 |
| 3:D:473:LEU:HA | 3:D:476:GLU:HB3 | 1.96 | 0.47 |
| 2:M:753:ASP:O | 2:M:791:ARG:HA | 2.14 | 0.47 |
| 4:O:61:GLU:O | 4:O:65:MET:HG3 | 2.14 | 0.47 |
| 1:K:143:ARG:NH1 | 1:K:158:ILE:HG23 | 2.29 | 0.47 |
| 2:C:527:GLU:N | 2:C:527:GLU:OE1 | 2.47 | 0.47 |
| 2:M:405:ARG:NH2 | 2:M:409:ARG:NE | 2.63 | 0.47 |
| 2:C:189:ARG:HH21 | 2:C:242:LEU:HD23 | 1.78 | 0.47 |
| 2:C:431:HIS:HE1 | 2:C:433:THR:HG23 | 1.80 | 0.47 |
| 2:C:448:ASN:HB3 | 2:C:452:ILE:HD12 | 1.95 | 0.47 |
| 2:C:523:ILE:HG12 | 2:C:524:VAL:N | 2.30 | 0.47 |
| 3:N:93:ILE:N | 3:N:517:VAL:O | 2.47 | 0.47 |
| 2:C:1100:GLN:O | 3:D:9:ARG:HB3 | 2.14 | 0.47 |
| 3:D:102:ILE:C | 3:D:104:PHE:N | 2.68 | 0.47 |
| 3:D:358:GLY:CA | 3:D:385:VAL:O | 2.59 | 0.47 |
| 2:M:777:ILE:HG22 | 5:P:409:LYS:HB3 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:F:379:ARG:C | 5:F:379:ARG:HD3 | 2.35 | 0.47 |
| 2:M:605:LYS:HB2 | 2:M:610:ARG:HH21 | 1.79 | 0.47 |
| 1:A:206:THR:O | 1:A:207:PRO:C | 2.50 | 0.47 |
| 5:P:373:LYS:HZ2 | 5:P:373:LYS:CB | 2.26 | 0.47 |
| 3:D:1397:LYS:CG | 3:D:1398:TRP:HZ3 | 2.26 | 0.47 |
| 3:N:970:LYS:HG3 | 3:N:974:ILE:CD1 | 2.44 | 0.47 |
| 3:N:1103:HIS:CG | 3:N:1104:GLU:N | 2.82 | 0.47 |
| 2:M:673:LEU:HD21 | 2:M:895:TYR:CD1 | 2.49 | 0.47 |
| 3:N:866:VAL:N | 3:N:873:LEU:O | 2.40 | 0.47 |
| 3:N:1121:PRO:O | 3:N:1122:LEU:HD23 | 2.14 | 0.47 |
| 1:A:76:VAL:O | 1:A:80:LEU:HG | 2.15 | 0.47 |
| 1:L:34:VAL:C | 1:L:36:LEU:H | 2.18 | 0.47 |
| 5:F:368:VAL:CG2 | 5:F:369:LEU:N | 2.71 | 0.47 |
| 3:N:79:GLU:CG | 3:N:80:VAL:H | 2.19 | 0.47 |
| 3:N:1401:GLU:C | 3:N:1403:LEU:H | 2.17 | 0.47 |
| 2:M:428:ARG:NH2 | 2:M:447:ALA:O | 2.47 | 0.47 |
| 2:M:489:THR:O | 2:M:490:GLU:C | 2.53 | 0.47 |
| 3:N:207:PHE:HD1 | 3:N:391:ALA:HB3 | 1.80 | 0.47 |
| 5:P:94:LEU:HD11 | 5:P:190:ALA:HB3 | 1.95 | 0.47 |
| 2:C:893:ALA:HB1 | 2:C:897:LEU:HD12 | 1.96 | 0.47 |
| 3:D:709:HIS:NE2 | 3:D:711:LEU:HB2 | 2.29 | 0.47 |
| 3:D:1293:PHE:HD1 | 3:D:1302:GLU:CA | 2.27 | 0.47 |
| 3:D:254:GLU:OE1 | 3:D:299:GLU:HB2 | 2.15 | 0.47 |
| 2:C:1118:LYS:HG3 | 2:C:1119:ARG:N | 2.29 | 0.47 |
| 3:D:1025:GLN:C | 3:D:1027:GLY:N | 2.68 | 0.47 |
| 2:M:141:HIS:ND1 | 2:M:141:HIS:C | 2.68 | 0.47 |
| 2:M:396:ASP:O | 2:M:403:SER:N | 2.47 | 0.47 |
| 3:N:572:ARG:CD | 5:P:80:PRO:HB3 | 2.44 | 0.47 |
| 3:D:135:LEU:HD11 | 3:D:148:GLU:CB | 2.44 | 0.47 |
| 3:D:139:GLY:HA2 | 3:D:450:TYR:HE2 | 1.79 | 0.47 |
| 3:D:545:ARG:O | 3:D:546:ARG:C | 2.52 | 0.47 |
| 4:E:29:GLN:HG3 | 4:E:30:LEU:N | 2.30 | 0.47 |
| 3:D:358:GLY:HA2 | 3:D:385:VAL:CA | 2.44 | 0.47 |
| 3:D:833:GLU:O | 3:D:834:THR:CG2 | 2.63 | 0.47 |
| 3:D:186:VAL:CG1 | 3:D:187:LYS:N | 2.74 | 0.47 |
| 2:M:650:ARG:CZ | 2:M:653:ASP:OD1 | 2.63 | 0.47 |
| 2:M:596:TYR:O | 2:M:655:LEU:HD11 | 2.15 | 0.47 |
| 3:D:661:MET:HB3 | 3:D:667:ALA:HB2 | 1.95 | 0.47 |
| 5:F:338:LEU:HA | 5:F:339:PRO:HD3 | 1.75 | 0.47 |
| 2:M:65:VAL:O | 2:M:100:LEU:HD12 | 2.15 | 0.47 |
| 5:P:300:ASP:HB3 | 5:P:302:LYS:HE3 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:L:159:LYS:HB2 | 1:L:164:ALA:HB3 | 1.97 | 0.47 |
| 3:D:828:LYS:HE2 | 3:D:828:LYS:C | 2.34 | 0.47 |
| 1:B:186:LEU:O | 1:B:188:GLN:NE2 | 2.48 | 0.47 |
| 3:N:1169:ASP:O | 3:N:1170:ASP:C | 2.51 | 0.47 |
| 2:M:941:VAL:O | 2:M:942:GLU:C | 2.52 | 0.47 |
| 1:K:74:ASP:HB3 | 1:K:77:GLU:HB2 | 1.97 | 0.47 |
| 3:N:1313:VAL:CG2 | 3:N:1314:LYS:N | 2.78 | 0.47 |
| 3:D:142:LEU:HB3 | 3:D:146:PRO:CA | 2.37 | 0.47 |
| 4:O:56:ASP:HB3 | 4:O:63:TRP:HZ2 | 1.79 | 0.47 |
| 3:N:200:ASP:OD1 | 3:N:201:GLY:N | 2.47 | 0.47 |
| 3:N:954:ALA:HA | 3:N:1039:CYS:SG | 2.55 | 0.47 |
| 2:M:726:ILE:O | 2:M:728:HIS:N | 2.47 | 0.47 |
| 4:O:90:GLU:O | 4:O:94:PRO:HA | 2.14 | 0.47 |
| 3:N:1426:LYS:O | 3:N:1429:LEU:N | 2.47 | 0.47 |
| 2:M:208:ALA:HB2 | 2:M:221:LEU:CD2 | 2.38 | 0.47 |
| 2:M:252:LYS:CD | 2:M:298:PHE:HE1 | 2.28 | 0.47 |
| 2:M:342:ASP:O | 2:M:346:VAL:HG13 | 2.15 | 0.47 |
| 3:N:307:ALA:HB1 | 3:N:311:LEU:CD1 | 2.43 | 0.47 |
| 3:N:329:GLU:HG2 | 3:N:330:THR:CG2 | 2.41 | 0.47 |
| 2:C:431:HIS:CE1 | 2:C:433:THR:HG23 | 2.50 | 0.47 |
| 3:D:1067:VAL:HG22 | 3:D:1068:LEU:N | 2.29 | 0.47 |
| 2:C:523:ILE:O | 2:C:524:VAL:CG1 | 2.62 | 0.47 |
| 3:N:554:LEU:CD1 | 3:N:558:LEU:HD11 | 2.45 | 0.47 |
| 5:P:220:LEU:O | 5:P:220:LEU:HD12 | 2.14 | 0.47 |
| 3:D:111:LYS:O | 3:D:115:LEU:HB2 | 2.15 | 0.47 |
| 3:D:511:TRP:HA | 3:D:511:TRP:CE3 | 2.49 | 0.47 |
| 5:F:130:VAL:O | 5:F:132:ARG:N | 2.47 | 0.47 |
| 3:D:1462:LEU:O | 3:D:1463:LYS:C | 2.53 | 0.47 |
| 4:E:84:ARG:HG2 | 4:E:88:GLU:CG | 2.45 | 0.47 |
| 3:D:441:ARG:O | 3:D:443:VAL:HG23 | 2.15 | 0.47 |
| 4:E:5:GLY:O | 4:E:9:LEU:N | 2.36 | 0.47 |
| 1:B:112:ARG:CG | 1:B:113:ASP:N | 2.78 | 0.47 |
| 1:B:58:ILE:HG22 | 1:B:61:VAL:HB | 1.96 | 0.47 |
| 3:D:833:GLU:C | 3:D:834:THR:HG23 | 2.34 | 0.47 |
| 3:D:833:GLU:O | 3:D:834:THR:HG23 | 2.15 | 0.47 |
| 5:F:269:ASN:O | 5:F:271:LEU:N | 2.47 | 0.47 |
| 2:M:727:PRO:HG2 | 2:M:785:VAL:O | 2.15 | 0.47 |
| 3:N:1489:GLN:HA | 3:N:1492:LEU:CD1 | 2.41 | 0.47 |
| 3:D:1172:HIS:O | 3:D:1173:LEU:C | 2.51 | 0.47 |
| 3:D:1397:LYS:C | 3:D:1398:TRP:HE3 | 2.17 | 0.47 |
| 3:D:1426:LYS:O | 3:D:1429:LEU:HB3 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1009:LYS:O | 3:D:1013:GLU:HG2 | 2.14 | 0.47 |
| 3:D:1019:PRO:O | 3:D:1020:LEU:C | 2.52 | 0.47 |
| 2:C:948:GLU:CB | 2:C:953:VAL:HG23 | 2.44 | 0.47 |
| 1:L:18:ARG:O | 1:L:207:PRO:HD3 | 2.15 | 0.47 |
| 2:M:988:VAL:HG23 | 11:M:1123:HOH:O | 2.15 | 0.47 |
| 3:N:783:ARG:HG2 | 3:N:783:ARG:HH11 | 1.79 | 0.47 |
| 3:N:857:ILE:O | 3:N:858:VAL:CG2 | 2.63 | 0.47 |
| 2:C:737:LEU:HD22 | 2:C:754:ILE:CG2 | 2.44 | 0.47 |
| 3:N:1174:LEU:O | 3:N:1175:ILE:C | 2.53 | 0.47 |
| 3:N:1111:ASP:HA | 3:N:1201:CYS:SG | 2.54 | 0.47 |
| 2:M:1038:TRP:HD1 | 2:M:1041:GLU:OE1 | 1.97 | 0.47 |
| 1:B:74:ASP:OD2 | 1:B:75:VAL:N | 2.47 | 0.47 |
| 3:N:1352:ILE:O | 3:N:1353:GLN:C | 2.53 | 0.47 |
| 1:L:30:ARG:HA | 1:L:193:ASP:OD1 | 2.14 | 0.47 |
| 3:N:815:ALA:O | 3:N:818:ARG:HB2 | 2.15 | 0.47 |
| 1:K:66:SER:HB2 | 1:K:75:VAL:HG21 | 1.97 | 0.47 |
| 1:K:56:VAL:HG12 | 1:K:57:TYR:N | 2.29 | 0.47 |
| 2:C:762:LYS:O | 2:C:765:SER:N | 2.47 | 0.47 |
| 1:A:229:GLN:O | 1:B:12:THR:HA | 2.14 | 0.47 |
| 3:N:1400:VAL:HA | 3:N:1408:ILE:HD12 | 1.95 | 0.47 |
| 3:N:1211:MET:HG3 | 3:N:1213:ARG:HH11 | 1.79 | 0.47 |
| 3:N:1011:PHE:HB3 | 3:N:1021:TYR:CD1 | 2.49 | 0.47 |
| 1:B:70:GLY:HA2 | 1:B:133:GLU:CG | 2.45 | 0.47 |
| 2:M:431:HIS:ND1 | 2:M:432:ARG:N | 2.62 | 0.47 |
| 3:N:1066:THR:HG22 | 3:N:1068:LEU:H | 1.78 | 0.47 |
| 5:F:329:TYR:O | 5:F:332:PHE:HD1 | 1.97 | 0.47 |
| 3:D:1280:VAL:HG13 | 3:D:1317:ASP:C | 2.34 | 0.47 |
| 3:D:1280:VAL:HG13 | 3:D:1317:ASP:N | 2.30 | 0.47 |
| 3:D:988:ARG:NH2 | 3:D:1054:GLU:OE2 | 2.48 | 0.47 |
| 3:N:924:MET:HG3 | 3:N:925:GLU:N | 2.30 | 0.47 |
| 4:O:6:ILE:HG23 | 4:O:7:ASP:N | 2.30 | 0.47 |
| 2:M:716:LYS:C | 2:M:718:GLY:H | 2.18 | 0.47 |
| 5:P:234:LYS:HE2 | 5:P:236:SER:HB2 | 1.97 | 0.47 |
| 3:N:1124:GLN:O | 3:N:1133:ARG:N | 2.48 | 0.47 |
| 2:M:1046:ALA:HB1 | 3:N:1471:LEU:CD1 | 2.43 | 0.47 |
| 1:L:5:LYS:NZ | 1:L:189:ARG:CZ | 2.77 | 0.47 |
| 2:C:731:GLU:C | 2:C:733:ALA:H | 2.17 | 0.47 |
| 1:B:117:VAL:CG1 | 1:B:118:ALA:H | 2.27 | 0.47 |
| 2:C:250:ARG:HB2 | 2:C:253:ALA:HB2 | 1.96 | 0.47 |
| 1:A:22:GLU:C | 1:A:23:PHE:CD1 | 2.88 | 0.47 |
| 2:C:588:VAL:HG13 | 2:C:593:ALA:HB3 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:1118:LYS:HG3 | 2:C:1119:ARG:HG3 | 1.97 | 0.47 |
| 2:M:1105:LYS:HB3 | 2:M:1107:ASN:ND2 | 2.29 | 0.47 |
| 3:D:1194:CYS:HB2 | 3:D:1204:CYS:CB | 2.45 | 0.47 |
| 2:M:262:ALA:O | 2:M:265:ARG:HG2 | 2.15 | 0.47 |
| 3:N:225:LEU:O | 3:N:331:VAL:N | 2.34 | 0.47 |
| 2:C:157:ARG:HH11 | 2:C:314:THR:HA | 1.79 | 0.47 |
| 2:C:191:PHE:HE2 | 2:C:196:LEU:HD21 | 1.76 | 0.47 |
| 2:C:517:ARG:HB2 | 2:C:520:GLU:CB | 2.41 | 0.47 |
| 3:N:554:LEU:HA | 3:N:557:LEU:HD12 | 1.97 | 0.47 |
| 3:D:1462:LEU:O | 3:D:1466:VAL:HG23 | 2.15 | 0.47 |
| 3:D:592:THR:O | 3:D:593:ASN:C | 2.53 | 0.47 |
| 3:D:351:MET:HA | 3:D:369:ALA:O | 2.15 | 0.47 |
| 5:P:382:THR:CG2 | 5:P:397:ILE:HB | 2.45 | 0.47 |
| 5:P:353:GLU:HG3 | 5:P:417:LYS:HD3 | 1.96 | 0.47 |
| 3:D:832:ARG:C | 3:D:834:THR:N | 2.67 | 0.47 |
| 5:F:386:VAL:HG12 | 5:F:394:ARG:N | 2.30 | 0.47 |
| 2:C:41:ASN:C | 2:C:41:ASN:ND2 | 2.68 | 0.47 |
| 2:M:246:ASP:OD2 | 2:M:250:ARG:NH2 | 2.47 | 0.47 |
| 3:D:1149:LEU:HG | 3:D:1151:ARG:O | 2.14 | 0.47 |
| 3:D:944:THR:O | 3:D:946:GLY:N | 2.48 | 0.47 |
| 2:M:1014:SER:O | 2:M:1018:GLN:N | 2.46 | 0.47 |
| 3:N:1476:THR:CG2 | 4:O:20:THR:HB | 2.45 | 0.47 |
| 3:D:843:PHE:CE1 | 3:D:849:ALA:HA | 2.50 | 0.47 |
| 3:N:1342:GLU:O | 3:N:1346:ARG:N | 2.40 | 0.47 |
| 1:K:22:GLU:OE1 | 2:M:934:PHE:HZ | 1.97 | 0.47 |
| 3:D:1330:ILE:HD12 | 3:D:1347:TYR:CZ | 2.49 | 0.47 |
| 3:N:1311:LEU:CG | 3:N:1312:LEU:N | 2.78 | 0.47 |
| 2:C:1008:ARG:HD2 | 2:C:1028:GLY:C | 2.36 | 0.47 |
| 3:N:1109:GLU:HG3 | 3:N:1196:THR:HG23 | 1.97 | 0.47 |
| 3:D:212:ARG:HD3 | 3:D:342:PRO:HB3 | 1.97 | 0.47 |
| 2:M:728:HIS:CD2 | 2:M:734:LEU:HD21 | 2.49 | 0.47 |
| 3:N:601:ARG:HH11 | 3:N:601:ARG:HG2 | 1.79 | 0.47 |
| 2:M:164:PRO:HD3 | 2:M:266:ARG:HH21 | 1.78 | 0.47 |
| 2:M:257:VAL:HA | 2:M:261:ILE:CD1 | 2.33 | 0.47 |
| 2:M:264:PRO:C | 2:M:289:THR:HG21 | 2.36 | 0.47 |
| 2:M:439:CYS:HB2 | 2:M:541:SER:CB | 2.43 | 0.47 |
| 3:N:249:TYR:CG | 3:N:307:ALA:HB3 | 2.49 | 0.47 |
| 3:N:224:ARG:HD2 | 3:N:332:TYR:HB2 | 1.97 | 0.47 |
| 2:C:172:ILE:HG22 | 2:C:173:ASP:N | 2.30 | 0.47 |
| 2:C:176:VAL:O | 2:C:178:PRO:HD3 | 2.14 | 0.47 |
| 2:C:239:PHE:O | 2:C:242:LEU:N | 2.39 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:261:ILE:C | 2:C:288:ARG:NH2 | 2.68 | 0.47 |
| 2:C:264:PRO:CB | 2:C:289:THR:HG21 | 2.42 | 0.47 |
| 2:C:517:ARG:N | 2:C:520:GLU:HB2 | 2.30 | 0.47 |
| 2:C:3:ILE:HD11 | 2:C:5:ARG:HH21 | 1.79 | 0.47 |
| 3:N:126:VAL:HG12 | 3:N:127:LEU:N | 2.29 | 0.47 |
| 3:N:137:PRO:HD3 | 3:N:453:ASP:HB3 | 1.94 | 0.47 |
| 3:N:508:ARG:HA | 3:N:509:PRO:HD2 | 1.63 | 0.47 |
| 3:N:564:GLU:O | 3:N:567:ILE:HB | 2.15 | 0.47 |
| 2:C:1090:LYS:O | 2:C:1091:GLU:C | 2.53 | 0.47 |
| 3:D:1442:ASN:ND2 | 3:D:1442:ASN:O | 2.48 | 0.47 |
| 3:D:1444:THR:O | 3:D:1445:HIS:C | 2.52 | 0.47 |
| 5:F:102:LEU:CD1 | 5:F:183:ALA:HB1 | 2.45 | 0.47 |
| 5:F:313:GLU:CD | 5:F:313:GLU:H | 2.18 | 0.47 |
| 2:M:73:LEU:HB2 | 2:M:93:PRO:O | 2.14 | 0.47 |
| 1:B:67:THR:OG1 | 1:B:68:ILE:N | 2.47 | 0.47 |
| 2:C:65:VAL:O | 2:C:100:LEU:HD12 | 2.15 | 0.47 |
| 2:C:41:ASN:CA | 2:C:45:GLN:HB3 | 2.28 | 0.47 |
| 5:F:290:GLU:O | 5:F:293:GLU:HB2 | 2.15 | 0.47 |
| 2:M:760:SER:O | 2:M:785:VAL:HG13 | 2.15 | 0.47 |
| 3:N:1496:GLU:OE2 | 3:N:1499:ARG:HB3 | 2.15 | 0.47 |
| 3:D:1171:VAL:O | 3:D:1172:HIS:C | 2.52 | 0.47 |
| 3:D:826:PRO:HB3 | 3:D:828:LYS:NZ | 2.29 | 0.47 |
| 3:D:164:GLY:HA3 | 3:D:447:VAL:HG12 | 1.97 | 0.47 |
| 3:N:297:ILE:HB | 3:N:302:GLN:HE22 | 1.80 | 0.47 |
| 2:M:909:ALA:HA | 2:M:913:GLU:OE1 | 2.15 | 0.47 |
| 2:C:650:ARG:H | 2:C:650:ARG:HE | 0.79 | 0.47 |
| 1:A:30:ARG:HH21 | 1:A:191:ASP:HB2 | 1.79 | 0.47 |
| 3:N:1344:VAL:O | 3:N:1347:TYR:HB3 | 2.14 | 0.47 |
| 2:C:24:GLU:O | 2:C:25:SER:C | 2.54 | 0.47 |
| 3:N:806:PHE:HA | 3:N:809:PRO:CG | 2.44 | 0.47 |
| 3:N:1213:ARG:CG | 3:N:1213:ARG:NH1 | 2.73 | 0.47 |
| 3:N:1274:ILE:HA | 3:N:1325:LEU:HG | 1.96 | 0.47 |
| 3:N:207:PHE:HE1 | 5:P:95:THR:HB | 1.80 | 0.47 |
| 3:N:170:PRO:HA | 3:N:391:ALA:O | 2.14 | 0.47 |
| 2:M:906:PHE:HZ | 3:N:1070:TYR:CG | 2.33 | 0.47 |
| 2:C:1056:LYS:HB3 | 3:D:623:VAL:HG13 | 1.97 | 0.47 |
| 3:D:1213:ARG:NH1 | 3:D:1213:ARG:HG2 | 2.23 | 0.47 |
| 2:C:807:ARG:HH11 | 2:C:807:ARG:HB3 | 1.79 | 0.47 |
| 1:L:111:ALA:HB3 | 1:L:125:PRO:CA | 2.40 | 0.47 |
| 1:L:87:VAL:HG12 | 1:L:122:ILE:HG12 | 1.96 | 0.47 |
| 2:M:493:ARG:HB2 | 2:M:494:TYR:CD1 | 2.49 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:P:247:ILE:O | 5:P:248:ASN:C | 2.51 | 0.47 |
| 3:D:775:GLY:CA | 3:D:1209:LEU:HD22 | 2.44 | 0.47 |
| 3:N:188:GLY:N | 3:N:198:ARG:HA | 2.27 | 0.47 |
| 1:B:238:GLU:HB3 | 1:B:240:LYS:NZ | 2.29 | 0.47 |
| 2:M:1105:LYS:CB | 2:M:1107:ASN:ND2 | 2.78 | 0.47 |
| 2:M:175:GLU:C | 2:M:183:SER:HB2 | 2.35 | 0.47 |
| 2:M:175:GLU:CG | 2:M:176:VAL:H | 2.11 | 0.47 |
| 2:M:399:ASN:O | 2:M:402:SER:OG | 2.28 | 0.47 |
| 3:D:416:ALA:CB | 3:D:432:TYR:CG | 2.97 | 0.47 |
| 4:E:42:PRO:O | 4:E:43:GLU:C | 2.54 | 0.47 |
| 2:C:240:THR:C | 2:C:242:LEU:N | 2.68 | 0.47 |
| 2:C:302:VAL:HB | 2:C:303:PHE:HD1 | 1.79 | 0.47 |
| 2:C:441:VAL:O | 2:C:559:LEU:HD13 | 2.15 | 0.47 |
| 3:D:615:ARG:O | 3:D:1096:ARG:NH2 | 2.48 | 0.47 |
| 3:D:87:ARG:HG3 | 3:D:88:TYR:CD2 | 2.50 | 0.47 |
| 5:F:111:GLU:O | 5:F:114:LYS:HB2 | 2.15 | 0.47 |
| 3:D:932:ASP:CA | 3:D:935:LYS:HE2 | 2.45 | 0.47 |
| 5:P:352:GLU:C | 5:P:354:LEU:N | 2.66 | 0.47 |
| 5:F:393:THR:HG22 | 5:F:395:GLU:H | 1.80 | 0.47 |
| 2:C:93:PRO:HB3 | 2:C:114:PHE:HD1 | 1.80 | 0.47 |
| 5:P:271:LEU:O | 5:P:272:SER:C | 2.52 | 0.47 |
| 3:D:1404:ASN:HB3 | 3:D:1409:ALA:HB3 | 1.97 | 0.47 |
| 2:C:889:HIS:CE1 | 3:D:951:ILE:H | 2.24 | 0.47 |
| 2:C:6:PHE:CB | 2:C:908:GLY:HA2 | 2.44 | 0.47 |
| 3:N:1380:GLU:HA | 3:N:1392:GLY:HA2 | 1.97 | 0.47 |
| 3:N:1104:GLU:OE1 | 3:N:1104:GLU:N | 2.47 | 0.47 |
| 3:N:274:ARG:HD3 | 3:N:279:VAL:HG11 | 1.97 | 0.47 |
| 3:D:1296:SER:HB3 | 3:D:1299:PHE:HD1 | 1.80 | 0.47 |
| 3:N:692:GLU:CD | 3:N:692:GLU:C | 2.74 | 0.47 |
| 2:M:928:LYS:O | 2:M:929:ARG:C | 2.54 | 0.47 |
| 2:M:918:LEU:CD1 | 2:M:968:LEU:HA | 2.45 | 0.47 |
| 5:P:321:ILE:HD11 | 5:P:329:TYR:CA | 2.45 | 0.47 |
| 3:N:1084:THR:O | 3:N:1085:ALA:C | 2.53 | 0.47 |
| 5:P:102:LEU:HD21 | 5:P:187:LEU:N | 2.30 | 0.47 |
| 5:P:145:PRO:HB2 | 5:P:150:THR:H | 1.79 | 0.47 |
| 2:C:346:VAL:O | 2:C:350:ARG:HG3 | 2.15 | 0.47 |
| 3:N:1041:LEU:HG | 3:N:1043:GLY:N | 2.29 | 0.47 |
| 3:N:403:PHE:HD1 | 3:N:423:ASP:OD1 | 1.96 | 0.47 |
| 1:K:200:TRP:CD1 | 1:K:200:TRP:N | 2.83 | 0.47 |
| 2:C:1043:TYR:CD1 | 3:D:710:ARG:HB2 | 2.50 | 0.47 |
| 2:C:408:ARG:HD3 | 11:C:1122:HOH:O | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:M:800:VAL:HG12 | 2:M:801:VAL:N | 2.30 | 0.47 |
| 3:N:114:THR:O | 3:N:114:THR:HG22 | 2.15 | 0.47 |
| 2:M:200:LEU:HB2 | 2:M:202:TYR:CE2 | 2.50 | 0.46 |
| 2:M:304:LEU:O | 2:M:308:ARG:HG2 | 2.15 | 0.46 |
| 2:M:583:LEU:O | 2:M:587:VAL:HG23 | 2.15 | 0.46 |
| 2:C:191:PHE:CD2 | 2:C:192:PRO:O | 2.68 | 0.46 |
| 2:C:144:PRO:O | 2:C:266:ARG:HD3 | 2.14 | 0.46 |
| 3:N:131:LYS:C | 3:N:456:MET:HE3 | 2.36 | 0.46 |
| 3:N:87:ARG:HA | 3:N:523:ASP:HB2 | 1.97 | 0.46 |
| 5:F:112:ALA:O | 5:F:113:ILE:C | 2.53 | 0.46 |
| 3:N:440:VAL:HG23 | 3:N:441:ARG:N | 2.30 | 0.46 |
| 3:D:368:VAL:N | 3:D:377:VAL:HB | 2.27 | 0.46 |
| 1:B:217:ILE:HG22 | 1:B:221:HIS:NE2 | 2.30 | 0.46 |
| 5:P:282:LEU:C | 5:P:284:ARG:N | 2.69 | 0.46 |
| 5:P:279:GLN:HA | 5:P:286:PRO:HD3 | 1.97 | 0.46 |
| 5:P:300:ASP:CB | 5:P:302:LYS:HE3 | 2.45 | 0.46 |
| 4:O:40:LEU:HD13 | 4:O:72:ARG:CZ | 2.45 | 0.46 |
| 3:D:1403:LEU:HB3 | 3:D:1408:ILE:HD12 | 1.97 | 0.46 |
| 1:B:179:PHE:CB | 1:B:197:LEU:HD13 | 2.28 | 0.46 |
| 3:N:1033:GLN:O | 3:N:1034:GLN:C | 2.52 | 0.46 |
| 3:N:788:GLY:N | 3:N:942:SER:HB3 | 2.30 | 0.46 |
| 3:N:879:ARG:HB3 | 3:N:902:LEU:HD12 | 1.97 | 0.46 |
| 3:N:257:GLY:CA | 3:N:274:ARG:CA | 2.92 | 0.46 |
| 5:F:90:GLN:OE1 | 5:F:189:GLU:HB3 | 2.15 | 0.46 |
| 3:N:750:PRO:HG2 | 3:N:756:GLN:NE2 | 2.31 | 0.46 |
| 4:O:19:LEU:O | 4:O:23:VAL:HG23 | 2.15 | 0.46 |
| 2:M:1090:LYS:O | 2:M:1094:ALA:N | 2.35 | 0.46 |
| 1:L:95:GLN:O | 1:L:145:ASP:OD1 | 2.32 | 0.46 |
| 3:N:1079:LYS:HB3 | 3:N:1239:ARG:NH2 | 2.30 | 0.46 |
| 2:C:548:PRO:HG2 | 2:C:843:HIS:CE1 | 2.50 | 0.46 |
| 1:A:71:VAL:HG22 | 1:A:132:LEU:CD2 | 2.45 | 0.46 |
| 3:N:470:LEU:HB2 | 3:N:503:LEU:HG | 1.97 | 0.46 |
| 3:D:739:ASP:N | 3:D:739:ASP:OD1 | 2.42 | 0.46 |
| 2:M:550:LEU:C | 2:M:552:HIS:H | 2.18 | 0.46 |
| 5:P:216:GLY:HA3 | 5:P:243:ILE:HG23 | 1.97 | 0.46 |
| 3:D:747:VAL:HG22 | 3:D:748:HIS:N | 2.30 | 0.46 |
| 1:B:24:VAL:HG12 | 1:B:25:LEU:N | 2.30 | 0.46 |
| 2:M:305:PRO:CA | 2:M:308:ARG:HG2 | 2.44 | 0.46 |
| 2:M:141:HIS:HD2 | 2:M:334:ARG:HG3 | 1.80 | 0.46 |
| 1:B:233:VAL:C | 1:B:235:ALA:N | 2.68 | 0.46 |
| 2:C:204:GLN:HE22 | 2:C:225:SER:HB3 | 1.81 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:260:LEU:HD12 | 2:C:288:ARG:NE | 2.30 | 0.46 |
| 2:C:1102:LEU:CD2 | 2:C:1108:PRO:HA | 2.45 | 0.46 |
| 2:C:1112:PHE:C | 2:C:1113:GLU:HG2 | 2.35 | 0.46 |
| 3:D:126:VAL:CG1 | 3:D:132:TYR:HB2 | 2.45 | 0.46 |
| 3:D:511:TRP:HA | 3:D:511:TRP:HE3 | 1.79 | 0.46 |
| 3:D:567:ILE:O | 3:D:568:ARG:C | 2.53 | 0.46 |
| 5:F:110:MET:CE | 5:F:111:GLU:HG3 | 2.45 | 0.46 |
| 5:P:386:VAL:CG1 | 5:P:394:ARG:N | 2.77 | 0.46 |
| 2:C:769:PRO:HA | 2:C:772:ARG:HB2 | 1.96 | 0.46 |
| 5:P:260:ILE:CG1 | 5:P:261:PRO:HD2 | 2.44 | 0.46 |
| 5:P:306:GLU:CD | 5:P:306:GLU:N | 2.69 | 0.46 |
| 5:P:308:LEU:O | 5:P:311:ALA:N | 2.41 | 0.46 |
| 5:P:373:LYS:HD2 | 5:P:374:GLY:CA | 2.44 | 0.46 |
| 3:D:1399:ASP:O | 3:D:1403:LEU:CB | 2.63 | 0.46 |
| 1:L:161:ARG:HB2 | 1:L:164:ALA:CB | 2.29 | 0.46 |
| 3:D:414:ARG:NH1 | 3:D:451:ASP:OD2 | 2.48 | 0.46 |
| 2:C:910:LYS:CG | 2:C:913:GLU:HG3 | 2.34 | 0.46 |
| 2:C:916:GLU:C | 2:C:916:GLU:OE1 | 2.54 | 0.46 |
| 3:N:1092:GLY:O | 3:N:1096:ARG:HB2 | 2.15 | 0.46 |
| 3:N:1147:ARG:HD2 | 3:N:1188:VAL:HG21 | 1.97 | 0.46 |
| 3:N:932:ASP:O | 3:N:933:ALA:C | 2.54 | 0.46 |
| 3:N:528:VAL:O | 3:N:535:PHE:HB3 | 2.14 | 0.46 |
| 1:K:107:LYS:HE3 | 1:K:107:LYS:HB2 | 1.65 | 0.46 |
| 2:C:1000:MET:O | 2:C:1003:ASP:N | 2.47 | 0.46 |
| 1:K:11:PHE:CD1 | 1:L:225:PHE:HA | 2.50 | 0.46 |
| 3:N:1400:VAL:O | 3:N:1408:ILE:HD12 | 2.15 | 0.46 |
| 3:D:1122:LEU:O | 3:D:1135:ARG:N | 2.47 | 0.46 |
| 3:N:1048:PRO:HA | 3:N:1079:LYS:CE | 2.45 | 0.46 |
| 1:B:175:ARG:O | 1:B:176:ARG:HB2 | 2.13 | 0.46 |
| 1:A:218:LEU:O | 1:A:221:HIS:HB2 | 2.15 | 0.46 |
| 1:B:54:THR:O | 1:B:167:VAL:N | 2.48 | 0.46 |
| 5:P:392:VAL:CG1 | 5:P:396:ARG:HD3 | 2.42 | 0.46 |
| 3:N:740:PHE:N | 3:N:740:PHE:CD1 | 2.82 | 0.46 |
| 3:N:1339:LYS:HB3 | 3:N:1343:ALA:HB2 | 1.96 | 0.46 |
| 3:D:1434:TRP:CZ3 | 3:D:1457:ASP:N | 2.82 | 0.46 |
| 2:M:551:GLU:O | 3:N:1064:GLY:HA2 | 2.15 | 0.46 |
| 1:L:152:PRO:HG2 | 1:L:155:LYS:CB | 2.45 | 0.46 |
| 2:M:305:PRO:O | 2:M:306:THR:C | 2.53 | 0.46 |
| 4:E:39:VAL:HG23 | 4:E:67:GLU:OE2 | 2.15 | 0.46 |
| 3:N:224:ARG:CG | 3:N:330:THR:OG1 | 2.63 | 0.46 |
| 2:C:186:VAL:HG22 | 2:C:189:ARG:O | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:448:ASN:HA | 2:C:451:LEU:HD12 | 1.96 | 0.46 |
| 2:C:517:ARG:O | 2:C:520:GLU:CG | 2.63 | 0.46 |
| 3:N:149:LYS:CG | 3:N:150:ARG:N | 2.78 | 0.46 |
| 3:D:558:LEU:C | 3:D:560:GLN:H | 2.18 | 0.46 |
| 4:E:19:LEU:HD12 | 4:E:19:LEU:O | 2.16 | 0.46 |
| 5:F:100:VAL:O | 5:F:103:ALA:HB3 | 2.15 | 0.46 |
| 3:D:274:ARG:HE | 3:D:279:VAL:CG1 | 2.27 | 0.46 |
| 3:D:246:PRO:HD2 | 3:D:308:LYS:HA | 1.96 | 0.46 |
| 5:P:381:HIS:C | 5:P:385:GLU:HG3 | 2.36 | 0.46 |
| 1:B:32:PHE:O | 1:B:36:LEU:N | 2.47 | 0.46 |
| 2:C:71:TYR:CD2 | 2:C:71:TYR:N | 2.69 | 0.46 |
| 5:P:265:VAL:O | 5:P:268:ILE:HB | 2.14 | 0.46 |
| 3:D:1426:LYS:O | 3:D:1427:SER:C | 2.54 | 0.46 |
| 1:L:161:ARG:N | 1:L:164:ALA:HB2 | 2.29 | 0.46 |
| 3:N:1363:LEU:HD23 | 3:N:1364:HIS:N | 2.30 | 0.46 |
| 1:L:18:ARG:NH1 | 1:L:88:ARG:HH22 | 2.04 | 0.46 |
| 3:N:864:VAL:CG1 | 3:N:865:THR:H | 2.19 | 0.46 |
| 3:D:168:THR:HB | 3:D:206:ARG:CZ | 2.45 | 0.46 |
| 3:N:759:ALA:HA | 3:N:763:MET:SD | 2.55 | 0.46 |
| 3:D:866:VAL:HG12 | 3:D:867:ARG:N | 2.30 | 0.46 |
| 2:C:594:ALA:C | 2:C:595:LEU:HD23 | 2.35 | 0.46 |
| 2:C:832:LYS:CG | 2:C:833:LEU:H | 2.28 | 0.46 |
| 1:L:208:LEU:O | 1:L:209:GLU:C | 2.54 | 0.46 |
| 3:N:1353:GLN:O | 3:N:1354:LYS:C | 2.53 | 0.46 |
| 1:A:169:ALA:HB1 | 1:A:171:PHE:CZ | 2.50 | 0.46 |
| 1:K:202:ASP:OD1 | 1:K:203:GLY:N | 2.48 | 0.46 |
| 1:K:206:THR:N | 1:K:209:GLU:OE1 | 2.47 | 0.46 |
| 2:C:243:ARG:HG2 | 2:C:244:PRO:HG3 | 1.96 | 0.46 |
| 5:F:323:ASP:O | 5:F:325:LYS:HG3 | 2.14 | 0.46 |
| 3:D:991:GLN:HA | 3:D:994:GLN:HG2 | 1.98 | 0.46 |
| 3:N:765:SER:C | 3:N:767:HIS:H | 2.18 | 0.46 |
| 4:E:61:GLU:O | 4:E:62:THR:C | 2.53 | 0.46 |
| 2:M:562:SER:O | 2:M:565:GLN:N | 2.48 | 0.46 |
| 3:N:264:LEU:HB2 | 3:N:267:GLY:H | 1.77 | 0.46 |
| 2:M:757:GLY:HA2 | 2:M:789:SER:HB3 | 1.96 | 0.46 |
| 3:D:1290:LEU:O | 3:D:1305:LEU:HD23 | 2.14 | 0.46 |
| 3:N:760:ARG:NH1 | 4:O:59:ASN:OD1 | 2.48 | 0.46 |
| 2:M:1118:LYS:O | 2:M:1119:ARG:HB2 | 2.13 | 0.46 |
| 4:O:68:LEU:O | 4:O:69:LEU:C | 2.52 | 0.46 |
| 1:B:28:LEU:HA | 1:B:28:LEU:HD23 | 1.69 | 0.46 |
| 2:M:261:ILE:CA | 2:M:288:ARG:HH21 | 2.29 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:M:143:SER:HB3 | 2:M:332:ARG:HB2 | 1.97 | 0.46 |
| 2:M:631:SER:HB2 | 2:M:637:LEU:HD11 | 1.96 | 0.46 |
| 3:N:324:ALA:HA | 3:N:333:LEU:HD23 | 1.97 | 0.46 |
| 2:C:141:HIS:HD2 | 2:C:334:ARG:HG2 | 1.81 | 0.46 |
| 2:C:233:GLU:O | 2:C:237:ARG:HG3 | 2.16 | 0.46 |
| 2:C:453:THR:OG1 | 2:C:454:SER:N | 2.48 | 0.46 |
| 2:C:543:ASN:HB2 | 2:C:565:GLN:HE21 | 1.80 | 0.46 |
| 3:D:1066:THR:HG22 | 3:D:1067:VAL:N | 2.30 | 0.46 |
| 3:N:149:LYS:N | 3:N:149:LYS:CD | 2.76 | 0.46 |
| 2:C:1017:THR:O | 2:C:1018:GLN:HB2 | 2.15 | 0.46 |
| 3:D:1098:LEU:CD1 | 3:D:1098:LEU:N | 2.76 | 0.46 |
| 3:D:22:SER:C | 3:D:24:GLY:H | 2.19 | 0.46 |
| 3:D:562:ALA:HB1 | 3:D:566:ILE:HD11 | 1.97 | 0.46 |
| 3:D:592:THR:HG22 | 3:D:600:LEU:HD21 | 1.98 | 0.46 |
| 4:E:27:ALA:O | 4:E:28:GLN:C | 2.54 | 0.46 |
| 4:E:30:LEU:CD1 | 4:E:37:ASN:HB2 | 2.45 | 0.46 |
| 3:D:379:ALA:C | 3:D:380:GLU:HG3 | 2.35 | 0.46 |
| 5:P:352:GLU:O | 5:P:355:GLU:CD | 2.54 | 0.46 |
| 3:D:692:GLU:O | 3:D:695:ILE:N | 2.49 | 0.46 |
| 5:F:371:LEU:HD23 | 5:F:375:LEU:CD1 | 2.46 | 0.46 |
| 3:N:490:ALA:HA | 3:N:493:ARG:HH21 | 1.80 | 0.46 |
| 1:L:200:TRP:CD1 | 1:L:200:TRP:N | 2.83 | 0.46 |
| 3:D:206:ARG:NE | 3:D:394:LEU:HB2 | 2.10 | 0.46 |
| 2:M:1045:ALA:HB1 | 2:M:1048:THR:OG1 | 2.15 | 0.46 |
| 3:N:1481:VAL:O | 3:N:1482:ARG:C | 2.53 | 0.46 |
| 3:N:1258:ARG:HH21 | 3:N:1351:GLU:HG3 | 1.81 | 0.46 |
| 3:N:1466:VAL:C | 3:N:1468:LEU:N | 2.69 | 0.46 |
| 1:A:154:GLU:N | 1:A:154:GLU:CD | 2.62 | 0.46 |
| 1:K:125:PRO:HG2 | 1:K:126:ASP:H | 1.80 | 0.46 |
| 1:K:34:VAL:CG1 | 1:L:42:ARG:NH1 | 2.78 | 0.46 |
| 1:K:41:ARG:HA | 1:K:177:VAL:HG11 | 1.97 | 0.46 |
| 1:K:41:ARG:HG2 | 1:K:45:LEU:CD1 | 2.45 | 0.46 |
| 1:L:30:ARG:HD3 | 2:M:854:PRO:HG3 | 1.98 | 0.46 |
| 5:F:274:THR:HG22 | 5:F:278:LEU:CG | 2.45 | 0.46 |
| 1:K:56:VAL:O | 1:K:165:ILE:N | 2.49 | 0.46 |
| 1:K:75:VAL:HA | 1:K:78:ILE:HD12 | 1.97 | 0.46 |
| 1:L:143:ARG:HG3 | 1:L:143:ARG:HH11 | 1.81 | 0.46 |
| 2:M:48:PHE:O | 2:M:50:GLU:N | 2.48 | 0.46 |
| 2:M:53:PRO:HB3 | 2:M:67:ASP:OD2 | 2.15 | 0.46 |
| 3:N:1206:GLY:O | 3:N:1214:PRO:HA | 2.15 | 0.46 |
| 3:D:1341:PRO:O | 3:D:1342:GLU:C | 2.53 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:N:1079:LYS:HA | 3:N:1082:ALA:HB3 | 1.98 | 0.46 |
| 3:N:1048:PRO:HA | 3:N:1079:LYS:HZ1 | 1.79 | 0.46 |
| 3:N:172:PRO:O | 3:N:173:PRO:C | 2.54 | 0.46 |
| 3:D:142:LEU:CB | 3:D:146:PRO:HA | 2.39 | 0.46 |
| 3:N:1236:LEU:O | 3:N:1237:THR:C | 2.53 | 0.46 |
| 3:D:499:VAL:HG12 | 3:D:503:LEU:CD1 | 2.45 | 0.46 |
| 1:K:182:GLU:HG2 | 1:K:194:LYS:O | 2.15 | 0.46 |
| 4:O:60:ALA:O | 4:O:61:GLU:C | 2.53 | 0.46 |
| 3:N:234:GLU:C | 3:N:236:TYR:H | 2.19 | 0.46 |
| 5:P:319:THR:HA | 5:P:320:PRO:HD3 | 1.82 | 0.46 |
| 1:L:180:GLN:O | 1:L:180:GLN:HG2 | 2.15 | 0.46 |
| 3:N:438:ASP:CG | 3:N:439:LEU:H | 2.19 | 0.46 |
| 3:N:539:ASP:O | 3:N:540:LEU:C | 2.54 | 0.46 |
| 3:D:567:ILE:HG22 | 3:D:571:LYS:CE | 2.43 | 0.46 |
| 3:D:1498:ALA:HB3 | 4:E:84:ARG:CZ | 2.45 | 0.46 |
| 1:B:208:LEU:O | 1:B:211:LEU:N | 2.48 | 0.46 |
| 2:C:1070:ILE:HG21 | 3:D:656:PHE:CE1 | 2.51 | 0.46 |
| 3:D:656:PHE:O | 3:D:659:LYS:HB3 | 2.16 | 0.46 |
| 2:C:56:GLU:O | 2:C:359:MET:HE1 | 2.16 | 0.46 |
| 5:P:291:ILE:O | 5:P:294:ALA:N | 2.49 | 0.46 |
| 5:F:265:VAL:N | 5:F:268:ILE:HD12 | 2.30 | 0.46 |
| 5:F:288:TYR:O | 5:F:289:GLU:C | 2.53 | 0.46 |
| 3:D:1018:ASN:C | 3:D:1018:ASN:OD1 | 2.53 | 0.46 |
| 3:D:917:GLN:O | 3:D:918:ALA:C | 2.54 | 0.46 |
| 3:D:434:ARG:HH21 | 3:D:451:ASP:HA | 1.81 | 0.46 |
| 3:N:1038:LEU:O | 3:N:1060:SER:HB2 | 2.16 | 0.46 |
| 3:N:1091:SER:O | 3:N:1092:GLY:C | 2.54 | 0.46 |
| 3:N:799:LYS:HB2 | 3:N:826:PRO:CD | 2.46 | 0.46 |
| 2:M:1056:LYS:CE | 3:N:625:TYR:HB2 | 2.32 | 0.46 |
| 1:A:195:LEU:HD12 | 1:A:195:LEU:C | 2.35 | 0.46 |
| 1:L:217:ILE:HG22 | 1:L:221:HIS:CD2 | 2.51 | 0.46 |
| 2:M:1085:PHE:CZ | 3:N:1468:LEU:HG | 2.50 | 0.46 |
| 3:N:661:MET:CE | 3:N:677:LEU:HD11 | 2.44 | 0.46 |
| 3:N:637:LEU:HD13 | 3:N:642:CYS:HA | 1.97 | 0.46 |
| 1:A:110:LYS:HA | 1:A:127:LEU:O | 2.15 | 0.46 |
| 3:D:1341:PRO:HB2 | 3:D:1342:GLU:OE1 | 2.14 | 0.46 |
| 3:D:1344:VAL:CG1 | 3:D:1345:GLU:H | 2.28 | 0.46 |
| 3:N:1311:LEU:HG | 3:N:1313:VAL:H | 1.80 | 0.46 |
| 3:D:1312:LEU:HG | 3:D:1312:LEU:O | 2.16 | 0.46 |
| 3:D:995:LEU:O | 3:D:998:GLU:HB3 | 2.15 | 0.46 |
| 2:C:807:ARG:O | 2:C:809:GLY:N | 2.49 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:765:SER:O | 3:N:767:HIS:N | 2.47 | 0.46 |
| 5:P:223:ALA:HB2 | 5:P:242:TRP:CG | 2.50 | 0.46 |
| 5:F:353:GLU:HA | 5:F:356:LYS:HB2 | 1.97 | 0.46 |
| 1:A:91:ASN:O | 1:A:94:LEU:HB2 | 2.16 | 0.46 |
| 3:D:680:GLN:HA | 3:D:683:ILE:CG1 | 2.45 | 0.46 |
| 2:M:172:ILE:CG2 | 2:M:173:ASP:N | 2.78 | 0.46 |
| 2:M:539:VAL:O | 2:M:539:VAL:HG12 | 2.15 | 0.46 |
| 3:D:1137:ARG:C | 3:D:1141:GLU:HG3 | 2.36 | 0.46 |
| 4:E:50:THR:O | 4:E:51:LEU:HB2 | 2.15 | 0.46 |
| 2:C:75:GLU:O | 2:C:77:PRO:HD3 | 2.16 | 0.46 |
| 2:M:415:PRO:C | 2:M:417:GLY:H | 2.19 | 0.46 |
| 2:C:218:VAL:O | 2:C:221:LEU:HB3 | 2.16 | 0.46 |
| 2:C:238:LEU:O | 2:C:241:LEU:CG | 2.52 | 0.46 |
| 2:C:239:PHE:O | 2:C:240:THR:C | 2.53 | 0.46 |
| 2:C:1015:LEU:HD12 | 5:F:335:ASP:CB | 2.46 | 0.46 |
| 3:D:1480:PHE:HD2 | 3:D:1481:VAL:HG23 | 1.72 | 0.46 |
| 5:F:207:LEU:C | 5:F:212:LEU:HD21 | 2.35 | 0.46 |
| 3:D:246:PRO:O | 3:D:248:PRO:HA | 2.15 | 0.46 |
| 1:A:209:GLU:CA | 1:A:212:ASN:ND2 | 2.79 | 0.46 |
| 2:M:370:ALA:O | 2:M:373:VAL:N | 2.38 | 0.46 |
| 3:D:32:ILE:HG23 | 3:D:38:LYS:N | 2.31 | 0.46 |
| 5:F:270:LYS:HA | 5:F:273:ARG:HD2 | 1.98 | 0.46 |
| 3:N:671:LYS:C | 3:N:674:ARG:HB2 | 2.36 | 0.46 |
| 3:D:1155:VAL:O | 3:D:1158:VAL:N | 2.28 | 0.46 |
| 3:D:1172:HIS:CA | 3:D:1175:ILE:HD12 | 2.33 | 0.46 |
| 1:B:195:LEU:HD12 | 1:B:196:THR:N | 2.30 | 0.46 |
| 2:C:674:VAL:CA | 2:C:869:VAL:HG13 | 2.46 | 0.46 |
| 3:D:907:GLU:H | 3:D:910:SER:HG | 1.64 | 0.46 |
| 2:C:984:GLU:CG | 3:D:944:THR:O | 2.64 | 0.46 |
| 2:C:910:LYS:HE3 | 2:C:912:PRO:CB | 2.45 | 0.46 |
| 3:N:1444:THR:O | 3:N:1445:HIS:C | 2.54 | 0.46 |
| 3:N:853:VAL:O | 3:N:856:GLY:N | 2.43 | 0.46 |
| 3:D:418:GLY:O | 3:D:428:LYS:CE | 2.63 | 0.46 |
| 2:M:946:ARG:NH1 | 2:M:984:GLU:CB | 2.79 | 0.46 |
| 1:B:52:ALA:HB3 | 1:B:171:PHE:CD2 | 2.51 | 0.46 |
| 5:P:328:PHE:O | 5:P:329:TYR:C | 2.54 | 0.46 |
| 2:C:626:ARG:HH11 | 2:C:626:ARG:CG | 2.26 | 0.46 |
| 1:B:70:GLY:C | 1:B:133:GLU:HG2 | 2.36 | 0.46 |
| 3:N:106:LYS:O | 3:N:108:VAL:HG12 | 2.15 | 0.46 |
| 3:N:209:ARG:HH21 | 3:N:391:ALA:CB | 2.29 | 0.46 |
| 2:M:906:PHE:CZ | 3:N:1070:TYR:CD2 | 3.04 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:808:ARG:O | 2:C:809:GLY:C | 2.53 | 0.46 |
| 4:O:7:ASP:O | 4:O:10:PHE:HB2 | 2.16 | 0.46 |
| 1:B:144:VAL:HG12 | 1:B:145:ASP:H | 1.81 | 0.46 |
| 3:N:615:ARG:HG3 | 3:N:616:GLN:N | 2.30 | 0.46 |
| 3:D:1114:THR:O | 3:D:1114:THR:HG23 | 2.16 | 0.46 |
| 2:C:707:ARG:NH2 | 2:C:709:GLU:OE2 | 2.48 | 0.46 |
| 3:D:1041:LEU:HG | 3:D:1043:GLY:H | 1.76 | 0.46 |
| 3:D:470:LEU:C | 3:D:472:ALA:N | 2.67 | 0.46 |
| 3:D:769:LEU:HD12 | 3:D:769:LEU:N | 2.30 | 0.46 |
| 2:C:941:VAL:O | 2:C:942:GLU:C | 2.53 | 0.46 |
| 3:N:603:LEU:O | 3:N:604:THR:C | 2.54 | 0.46 |
| 3:D:1120:VAL:CB | 3:D:1144:LEU:HD21 | 2.45 | 0.46 |
| 5:F:361:LEU:HG | 5:F:362:SER:H | 1.79 | 0.46 |
| 2:C:12:VAL:HG12 | 2:C:481:ASP:OD1 | 2.15 | 0.46 |
| 5:P:359:SER:O | 5:P:361:LEU:N | 2.49 | 0.46 |
| 2:M:135:VAL:HG23 | 2:M:395:LYS:HB2 | 1.96 | 0.46 |
| 2:M:193:LEU:HD23 | 2:M:307:LEU:HD22 | 1.97 | 0.46 |
| 2:M:333:ILE:HG21 | 2:M:461:VAL:HG21 | 1.98 | 0.46 |
| 3:N:212:ARG:N | 3:N:386:HIS:O | 2.40 | 0.46 |
| 2:C:261:ILE:HG22 | 2:C:262:ALA:N | 2.29 | 0.46 |
| 2:C:400:PRO:O | 2:C:401:LEU:C | 2.54 | 0.46 |
| 2:C:435:TYR:CE2 | 2:C:516:ARG:CZ | 2.98 | 0.46 |
| 2:C:512:ARG:HD3 | 2:C:512:ARG:HA | 1.82 | 0.46 |
| 3:N:550:ARG:CZ | 3:N:573:MET:HB3 | 2.44 | 0.46 |
| 3:N:84:ILE:C | 3:N:86:ARG:N | 2.69 | 0.46 |
| 3:N:545:ARG:HE | 5:P:257:THR:HA | 1.81 | 0.46 |
| 3:D:115:LEU:O | 3:D:116:LEU:HD23 | 2.16 | 0.46 |
| 3:D:1462:LEU:HD22 | 3:D:1472:ILE:CD1 | 2.46 | 0.46 |
| 3:D:159:ARG:C | 3:D:161:LEU:H | 2.19 | 0.46 |
| 3:D:295:GLY:HA3 | 3:D:303:PRO:HD3 | 1.98 | 0.46 |
| 5:F:402:ASN:H | 5:F:402:ASN:HD22 | 1.61 | 0.46 |
| 1:B:41:ARG:NH1 | 1:B:41:ARG:HG3 | 2.31 | 0.46 |
| 3:D:690:ALA:O | 3:D:691:LEU:C | 2.54 | 0.46 |
| 5:F:296:GLY:HA3 | 5:F:297:PRO:HD2 | 1.53 | 0.46 |
| 3:D:1388:ARG:HG2 | 3:D:1391:GLU:HG3 | 1.97 | 0.46 |
| 1:B:195:LEU:HD12 | 1:B:196:THR:H | 1.81 | 0.46 |
| 3:N:847:ASP:O | 3:N:848:GLU:C | 2.54 | 0.46 |
| 5:F:92:PRO:O | 5:F:94:LEU:N | 2.49 | 0.46 |
| 3:D:858:VAL:CG1 | 3:D:859:ASP:N | 2.77 | 0.46 |
| 1:B:77:GLU:HB2 | 3:D:872:ARG:NH2 | 2.30 | 0.46 |
| 2:C:641:PRO:HA | 2:C:655:LEU:O | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:N:468:LEU:HD11 | 3:N:473:LEU:HD13 | 1.97 | 0.46 |
| 3:D:417:PRO:CB | 3:D:429:SER:C | 2.84 | 0.46 |
| 2:M:479:VAL:HG21 | 2:M:503:LEU:HD21 | 1.97 | 0.46 |
| 1:A:109:VAL:HB | 1:A:130:ALA:N | 2.29 | 0.46 |
| 3:N:704:ARG:NE | 3:N:738:ALA:HB2 | 2.31 | 0.46 |
| 3:N:736:PHE:O | 3:N:737:ASN:C | 2.53 | 0.46 |
| 2:C:607:ASP:OD1 | 2:C:608:GLY:N | 2.49 | 0.46 |
| 3:D:60:CYS:SG | 3:D:62:LYS:HG2 | 2.55 | 0.46 |
| 1:B:175:ARG:N | 1:B:200:TRP:O | 2.33 | 0.46 |
| 2:C:1009:SER:CB | 3:D:651:GLU:OE2 | 2.63 | 0.46 |
| 2:C:808:ARG:H | 2:C:815:LEU:CD1 | 2.29 | 0.46 |
| 2:C:385:PHE:CG | 2:C:386:PHE:N | 2.82 | 0.46 |
| 2:C:630:ARG:NE | 2:C:705:ILE:O | 2.48 | 0.46 |
| 1:A:65:PHE:CD1 | 1:A:65:PHE:N | 2.83 | 0.46 |
| 2:M:715:THR:HB | 2:M:718:GLY:O | 2.16 | 0.46 |
| 4:O:57:ASP:O | 4:O:63:TRP:NE1 | 2.40 | 0.46 |
| 1:A:71:VAL:HG22 | 1:A:132:LEU:HD22 | 1.98 | 0.46 |
| 3:D:1499:ARG:C | 3:D:1499:ARG:HD3 | 2.36 | 0.46 |
| 3:N:1108:ARG:HE | 3:N:1199:GLY:CA | 2.29 | 0.46 |
| 3:D:178:LEU:CG | 3:D:181:ASP:HB2 | 2.44 | 0.46 |
| 2:M:536:PRO:HB2 | 2:M:905:ILE:CG2 | 2.46 | 0.46 |
| 3:D:1292:VAL:O | 3:D:1303:TYR:N | 2.44 | 0.46 |
| 3:D:1360:GLY:HA2 | 3:D:1362:LYS:HZ1 | 1.80 | 0.46 |
| 3:D:1124:GLN:HA | 3:D:1125:PRO:HD3 | 1.64 | 0.46 |
| 3:D:633:VAL:O | 3:D:635:PRO:HD3 | 2.16 | 0.46 |
| 2:M:202:TYR:O | 2:M:207:LEU:HD11 | 2.16 | 0.46 |
| 3:N:211:VAL:HA | 3:N:386:HIS:O | 2.15 | 0.46 |
| 3:N:337:LEU:C | 3:N:338:GLU:HG3 | 2.35 | 0.46 |
| 3:N:558:LEU:C | 3:N:560:GLN:H | 2.17 | 0.46 |
| 3:D:1231:GLU:C | 3:D:1231:GLU:CD | 2.75 | 0.46 |
| 3:D:1481:VAL:HG21 | 4:E:18:ARG:HB2 | 1.98 | 0.46 |
| 3:D:135:LEU:HD11 | 3:D:148:GLU:HG3 | 1.98 | 0.46 |
| 3:D:575:GLN:OE1 | 3:D:575:GLN:HA | 2.16 | 0.46 |
| 3:N:441:ARG:C | 3:N:443:VAL:H | 2.19 | 0.46 |
| 2:M:97:ARG:C | 2:M:98:LEU:HD23 | 2.36 | 0.46 |
| 3:D:262:LYS:HG2 | 3:D:263:GLU:N | 2.31 | 0.46 |
| 2:M:773:LEU:O | 2:M:777:ILE:HG13 | 2.16 | 0.46 |
| 5:P:385:GLU:HA | 5:P:388:ALA:CB | 2.45 | 0.46 |
| 5:F:401:GLU:CG | 5:F:405:LEU:HD11 | 2.46 | 0.46 |
| 2:C:94:LEU:O | 2:C:114:PHE:HA | 2.16 | 0.46 |
| 2:C:341:THR:O | 2:C:345:ARG:HG3 | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:P:276:ARG:O | 5:P:278:LEU:N | 2.48 | 0.46 |
| 3:D:1388:ARG:N | 3:D:1391:GLU:OE2 | 2.43 | 0.46 |
| 3:D:1030:GLY:HA2 | 3:D:1034:GLN:NE2 | 2.30 | 0.46 |
| 3:N:1380:GLU:HB3 | 3:N:1418:LYS:HB3 | 1.96 | 0.46 |
| 3:N:855:HIS:O | 3:N:857:ILE:HG23 | 2.15 | 0.46 |
| 3:N:881:LEU:O | 3:N:882:PHE:C | 2.54 | 0.46 |
| 2:M:1040:LEU:HD13 | 2:M:1049:LEU:HB2 | 1.97 | 0.46 |
| 1:B:79:ILE:O | 1:B:82:LEU:HG | 2.15 | 0.46 |
| 2:C:625:LEU:HD12 | 2:C:639:GLN:OE1 | 2.16 | 0.46 |
| 3:N:661:MET:HE2 | 3:N:677:LEU:HD11 | 1.97 | 0.46 |
| 2:M:922:PHE:O | 2:M:923:GLU:C | 2.54 | 0.46 |
| 2:M:930:LYS:O | 2:M:932:GLU:N | 2.39 | 0.46 |
| 1:L:70:GLY:HA2 | 1:L:133:GLU:CG | 2.46 | 0.46 |
| 3:D:1283:ILE:HG13 | 3:D:1315:ASP:OD1 | 2.15 | 0.46 |
| 2:C:386:PHE:HD1 | 2:C:386:PHE:H | 1.64 | 0.46 |
| 3:D:18:ILE:HD12 | 3:D:516:ALA:HB3 | 1.97 | 0.46 |
| 3:N:182:GLY:HA2 | 3:N:203:ALA:CB | 2.42 | 0.46 |
| 3:D:962:GLN:O | 3:D:965:GLU:N | 2.48 | 0.46 |
| 3:N:179:VAL:C | 3:N:181:ASP:N | 2.67 | 0.46 |
| 4:O:92:ILE:HB | 4:O:93:TYR:CD1 | 2.51 | 0.46 |
| 3:D:8:VAL:HG12 | 3:D:1434:TRP:CH2 | 2.51 | 0.46 |
| 2:M:768:THR:HB | 2:M:771:GLU:HB3 | 1.98 | 0.46 |
| 2:M:1006:HIS:HA | 2:M:1027:PHE:CE1 | 2.51 | 0.46 |
| 3:N:1025:GLN:C | 3:N:1027:GLY:H | 2.18 | 0.46 |
| 2:C:550:LEU:CD2 | 2:C:905:ILE:HD11 | 2.45 | 0.46 |
| 1:B:91:ASN:HD22 | 1:B:92:PRO:N | 2.14 | 0.46 |
| 2:M:213:ALA:C | 2:M:215:GLY:N | 2.68 | 0.46 |
| 2:M:274:ARG:O | 2:M:275:TYR:C | 2.53 | 0.46 |
| 3:N:259:VAL:HG23 | 3:N:270:LEU:CD1 | 2.44 | 0.46 |
| 2:C:335:THR:C | 2:C:339:LEU:HD12 | 2.36 | 0.46 |
| 2:C:432:ARG:CG | 2:C:433:THR:N | 2.79 | 0.46 |
| 3:N:566:ILE:C | 3:N:569:ASN:HB3 | 2.35 | 0.46 |
| 2:C:1100:GLN:O | 3:D:9:ARG:N | 2.39 | 0.46 |
| 3:D:1091:SER:O | 3:D:1093:TYR:N | 2.49 | 0.46 |
| 3:D:535:PHE:CD1 | 3:D:535:PHE:N | 2.84 | 0.46 |
| 3:D:256:GLU:HB2 | 3:D:296:GLU:HG2 | 1.98 | 0.46 |
| 5:P:401:GLU:O | 5:P:402:ASN:C | 2.54 | 0.46 |
| 1:B:210:ALA:O | 1:B:213:GLN:N | 2.49 | 0.46 |
| 1:L:64:GLU:HA | 1:L:75:VAL:HG11 | 1.96 | 0.46 |
| 5:F:392:VAL:CG1 | 5:F:396:ARG:HB3 | 2.46 | 0.46 |
| 5:F:400:ILE:O | 5:F:401:GLU:C | 2.54 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:D:655:PRO:O | 3:D:658:LEU:HB2 | 2.16 | 0.46 |
| 2:C:1067:TYR:HB2 | 5:F:341:PRO:HB3 | 1.97 | 0.46 |
| 3:D:1383:ASP:CB | 3:D:1416:ALA:HB3 | 2.46 | 0.46 |
| 3:D:916:TYR:OH | 3:D:1168:MET:HB2 | 2.15 | 0.46 |
| 3:N:1094:LEU:O | 3:N:1097:LYS:N | 2.48 | 0.46 |
| 3:N:1232:PRO:O | 3:N:1235:GLN:HG2 | 2.16 | 0.46 |
| 3:N:1103:HIS:CD2 | 3:N:1463:LYS:H | 2.34 | 0.46 |
| 1:L:19:GLU:HG2 | 1:L:203:GLY:N | 2.31 | 0.46 |
| 2:M:693:GLU:HA | 2:M:696:LYS:HD2 | 1.97 | 0.46 |
| 3:N:846:PRO:O | 3:N:847:ASP:C | 2.53 | 0.46 |
| 3:D:169:TYR:N | 3:D:393:ILE:O | 2.48 | 0.46 |
| 4:O:48:MET:O | 4:O:54:LEU:HA | 2.16 | 0.46 |
| 3:N:372:ASP:C | 3:N:374:GLU:H | 2.19 | 0.46 |
| 2:M:701:THR:OG1 | 2:M:832:LYS:HG3 | 2.16 | 0.46 |
| 3:N:1404:ASN:OD1 | 3:N:1408:ILE:HG22 | 2.15 | 0.46 |
| 2:C:243:ARG:HG3 | 2:C:244:PRO:CA | 2.38 | 0.46 |
| 3:D:988:ARG:O | 3:D:989:TYR:C | 2.54 | 0.46 |
| 3:D:990:ASP:O | 3:D:994:GLN:NE2 | 2.47 | 0.46 |
| 1:L:110:LYS:HD2 | 1:L:126:ASP:CA | 2.45 | 0.46 |
| 3:D:14:SER:HB2 | 3:D:17:LYS:CB | 2.44 | 0.46 |
| 2:M:833:LEU:HD12 | 2:M:837:ASP:CG | 2.35 | 0.46 |
| 3:D:775:GLY:HA3 | 3:D:1209:LEU:HD22 | 1.97 | 0.46 |
| 3:D:1363:LEU:C | 3:D:1363:LEU:HD23 | 2.36 | 0.46 |
| 3:N:630:VAL:HA | 3:N:744:GLN:HA | 1.98 | 0.46 |
| 2:C:1031:ARG:N | 3:D:622:ARG:NH1 | 2.63 | 0.46 |
| 2:M:1103:ASP:OD1 | 2:M:1105:LYS:HB2 | 2.15 | 0.46 |
| 1:B:91:ASN:HB2 | 1:B:119:ASP:OD2 | 2.15 | 0.46 |
| 1:L:6:LEU:O | 1:L:8:ALA:N | 2.45 | 0.46 |
| 2:M:401:LEU:O | 2:M:402:SER:C | 2.54 | 0.46 |
| 3:N:259:VAL:HG22 | 3:N:260:GLU:N | 2.31 | 0.46 |
| 2:C:191:PHE:CD2 | 2:C:195:LEU:HD11 | 2.49 | 0.46 |
| 2:C:219:GLN:C | 2:C:221:LEU:N | 2.65 | 0.46 |
| 2:C:3:ILE:HD11 | 2:C:5:ARG:HE | 1.80 | 0.46 |
| 3:N:104:PHE:O | 3:N:112:ILE:HD11 | 2.16 | 0.46 |
| 5:P:207:LEU:HB3 | 5:P:212:LEU:CD2 | 2.46 | 0.46 |
| 3:D:113:GLY:O | 3:D:115:LEU:N | 2.49 | 0.46 |
| 3:D:522:PRO:CA | 3:D:525:ARG:NH1 | 2.79 | 0.46 |
| 3:D:548:ILE:O | 3:D:549:ASN:C | 2.54 | 0.46 |
| 5:P:382:THR:O | 5:P:386:VAL:HG13 | 2.16 | 0.46 |
| 1:B:206:THR:O | 1:B:207:PRO:C | 2.54 | 0.46 |
| 1:B:208:LEU:O | 1:B:209:GLU:C | 2.54 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:313:LEU:O | 2:M:315:ALA:N | 2.49 | 0.46 |
| 5:F:406:ARG:HA | 5:F:409:LYS:HE3 | 1.98 | 0.46 |
| 2:M:645:VAL:C | 2:M:647:GLN:H | 2.19 | 0.46 |
| 3:D:695:ILE:O | 3:D:696:HIS:C | 2.54 | 0.46 |
| 2:M:352:ALA:O | 2:M:356:ARG:HG3 | 2.16 | 0.46 |
| 3:D:1153:VAL:O | 3:D:1159:ARG:HA | 2.15 | 0.46 |
| 3:D:96:ALA:HB3 | 3:D:554:LEU:CD2 | 2.46 | 0.46 |
| 3:N:1348:LEU:O | 3:N:1349:VAL:C | 2.53 | 0.46 |
| 3:D:42:ASP:OD1 | 3:D:48:ARG:NH2 | 2.49 | 0.46 |
| 3:N:660:LYS:CG | 3:N:694:VAL:HG22 | 2.46 | 0.46 |
| 1:K:108:GLU:HG3 | 1:K:131:THR:HG22 | 1.96 | 0.46 |
| 5:P:102:LEU:HD11 | 5:P:183:ALA:C | 2.36 | 0.46 |
| 3:D:59:ALA:C | 3:D:61:GLY:N | 2.70 | 0.46 |
| 2:C:712:ALA:C | 2:C:820:ARG:HG3 | 2.36 | 0.46 |
| 3:N:990:ASP:HA | 3:N:993:LEU:CG | 2.46 | 0.46 |
| 3:D:709:HIS:O | 3:D:710:ARG:C | 2.54 | 0.46 |
| 3:N:471:GLU:O | 3:N:474:GLU:HB3 | 2.15 | 0.46 |
| 3:N:630:VAL:HG22 | 3:N:744:GLN:CG | 2.46 | 0.46 |
| 2:M:790:LEU:HD12 | 2:M:791:ARG:N | 2.30 | 0.46 |
| 2:C:717:LEU:HD21 | 2:C:764:GLU:HG3 | 1.97 | 0.46 |
| 3:D:1260:ILE:O | 3:D:1261:GLU:C | 2.54 | 0.46 |
| 2:M:682:TYR:C | 2:M:684:PHE:H | 2.19 | 0.46 |
| 2:C:275:TYR:CE1 | 2:C:279:GLU:OE1 | 2.69 | 0.46 |
| 2:M:261:ILE:O | 2:M:264:PRO:HD2 | 2.16 | 0.45 |
| 2:C:192:PRO:O | 2:C:195:LEU:CG | 2.61 | 0.45 |
| 2:C:285:LEU:HD11 | 2:C:288:ARG:O | 2.15 | 0.45 |
| 2:C:323:ASP:O | 2:C:325:ILE:HD12 | 2.15 | 0.45 |
| 2:C:499:ALA:HA | 2:C:532:MET:HG2 | 1.98 | 0.45 |
| 3:N:162:ARG:NH1 | 3:N:434:ARG:HH22 | 2.14 | 0.45 |
| 2:C:1089:VAL:O | 2:C:1092:LEU:HB2 | 2.15 | 0.45 |
| 4:E:92:ILE:HG13 | 4:E:92:ILE:H | 1.57 | 0.45 |
| 5:F:110:MET:HE3 | 5:F:111:GLU:HG3 | 1.98 | 0.45 |
| 5:F:140:ARG:O | 5:F:140:ARG:HG2 | 2.16 | 0.45 |
| 3:D:259:VAL:HG21 | 3:D:292:VAL:C | 2.35 | 0.45 |
| 3:D:302:GLN:O | 3:D:304:LEU:HG | 2.16 | 0.45 |
| 5:P:382:THR:HG22 | 5:P:394:ARG:CA | 2.46 | 0.45 |
| 5:P:403:LYS:HD2 | 5:P:407:LYS:HE2 | 1.97 | 0.45 |
| 5:P:412:GLU:C | 5:P:414:ARG:H | 2.18 | 0.45 |
| 1:K:69:PRO:HA | 2:M:607:ASP:OD1 | 2.16 | 0.45 |
| 2:C:943:VAL:O | 2:C:946:ARG:HB3 | 2.17 | 0.45 |
| 1:K:186:LEU:HD23 | 1:K:188:GLN:HE21 | 1.81 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:577:PRO:HG3 | 2:C:993:PHE:CD2 | 2.51 | 0.45 |
| 2:C:754:ILE:HG12 | 2:C:791:ARG:HD3 | 1.97 | 0.45 |
| 3:N:274:ARG:CD | 3:N:279:VAL:HG11 | 2.46 | 0.45 |
| 3:D:885:ILE:O | 3:D:888:GLU:HB2 | 2.16 | 0.45 |
| 5:F:174:LEU:HD12 | 5:F:174:LEU:C | 2.37 | 0.45 |
| 2:C:383:ARG:O | 2:C:387:SER:OG | 2.32 | 0.45 |
| 2:M:512:ARG:HB3 | 2:M:523:ILE:HG13 | 1.98 | 0.45 |
| 5:F:238:TYR:CD2 | 5:F:239:ALA:N | 2.84 | 0.45 |
| 3:N:887:ALA:CA | 3:N:890:VAL:HG22 | 2.46 | 0.45 |
| 3:N:989:TYR:CE2 | 3:N:993:LEU:HD11 | 2.51 | 0.45 |
| 5:F:168:LYS:O | 5:F:172:ARG:N | 2.42 | 0.45 |
| 2:M:350:ARG:HA | 2:M:353:ARG:CD | 2.46 | 0.45 |
| 3:N:1282:ARG:NH2 | 3:N:1293:PHE:CD2 | 2.84 | 0.45 |
| 3:D:685:ASP:C | 3:D:687:VAL:N | 2.69 | 0.45 |
| 3:N:56:TYR:CE2 | 3:N:66:GLN:HG3 | 2.51 | 0.45 |
| 1:L:44:LEU:O | 1:L:174:VAL:HG21 | 2.16 | 0.45 |
| 4:O:55:PHE:N | 4:O:55:PHE:CD1 | 2.84 | 0.45 |
| 2:M:397:GLU:CG | 2:M:632:ASN:HB2 | 2.43 | 0.45 |
| 2:C:543:ASN:HA | 2:C:546:LEU:HD12 | 1.98 | 0.45 |
| 3:N:152:LEU:CG | 3:N:153:LEU:N | 2.79 | 0.45 |
| 3:N:154:THR:HG22 | 3:N:157:GLU:HB2 | 1.97 | 0.45 |
| 5:P:209:PHE:CA | 5:P:212:LEU:HG | 2.47 | 0.45 |
| 3:D:520:LEU:CG | 3:D:524:LEU:HB2 | 2.46 | 0.45 |
| 5:F:123:ASP:HB2 | 5:F:126:LEU:HB2 | 1.98 | 0.45 |
| 5:F:134:LYS:HB3 | 5:F:178:ARG:HH12 | 1.81 | 0.45 |
| 5:F:209:PHE:CA | 5:F:212:LEU:HG | 2.46 | 0.45 |
| 5:F:214:GLN:HA | 5:F:217:ASN:ND2 | 2.11 | 0.45 |
| 3:D:355:VAL:CG1 | 3:D:356:PRO:HD2 | 2.46 | 0.45 |
| 4:O:88:GLU:HA | 4:O:91:ARG:HD2 | 1.99 | 0.45 |
| 3:D:808:THR:OG1 | 3:D:809:PRO:HD3 | 2.17 | 0.45 |
| 2:M:615:TYR:O | 2:M:616:GLU:C | 2.55 | 0.45 |
| 5:F:287:THR:OG1 | 5:F:288:TYR:N | 2.48 | 0.45 |
| 3:N:674:ARG:NH2 | 5:P:342:VAL:HG13 | 2.31 | 0.45 |
| 3:D:1173:LEU:O | 3:D:1176:LYS:N | 2.49 | 0.45 |
| 3:D:1380:GLU:N | 3:D:1420:LEU:HG | 2.31 | 0.45 |
| 3:D:493:ARG:HB2 | 3:D:1388:ARG:HD2 | 1.97 | 0.45 |
| 3:D:828:LYS:CD | 3:D:828:LYS:N | 2.79 | 0.45 |
| 2:C:903:SER:OG | 2:C:908:GLY:HA3 | 2.16 | 0.45 |
| 2:C:910:LYS:CG | 2:C:912:PRO:HD2 | 2.29 | 0.45 |
| 2:C:976:ASP:OD2 | 2:C:979:THR:HG23 | 2.16 | 0.45 |
| 3:N:372:ASP:OD2 | 3:N:374:GLU:O | 2.34 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:918:LEU:HD12 | 2:M:968:LEU:CA | 2.44 | 0.45 |
| 2:M:32:ALA:C | 2:M:35:PRO:HD2 | 2.36 | 0.45 |
| 2:M:41:ASN:ND2 | 2:M:42:VAL:N | 2.64 | 0.45 |
| 2:C:645:VAL:C | 2:C:647:GLN:H | 2.18 | 0.45 |
| 2:C:243:ARG:CG | 2:C:244:PRO:CA | 2.92 | 0.45 |
| 1:A:159:LYS:NZ | 1:A:164:ALA:O | 2.40 | 0.45 |
| 3:N:1018:ASN:OD1 | 3:N:1020:LEU:N | 2.49 | 0.45 |
| 3:D:884:ARG:C | 3:D:888:GLU:HG2 | 2.36 | 0.45 |
| 2:C:1014:SER:N | 2:C:1021:LEU:HB2 | 2.32 | 0.45 |
| 2:C:395:LYS:CE | 2:C:403:SER:HB2 | 2.44 | 0.45 |
| 2:M:23:VAL:HG12 | 2:M:121:MET:CE | 2.46 | 0.45 |
| 2:C:799:ILE:O | 2:C:801:VAL:HG13 | 2.17 | 0.45 |
| 2:M:627:ARG:O | 2:M:629:TYR:CD1 | 2.70 | 0.45 |
| 3:D:699:VAL:CG1 | 3:D:717:GLN:HG2 | 2.42 | 0.45 |
| 3:N:1336:LEU:HB3 | 3:N:1337:GLU:OE1 | 2.16 | 0.45 |
| 2:M:728:HIS:CD2 | 2:M:730:SER:O | 2.69 | 0.45 |
| 3:N:839:LEU:O | 3:N:840:LYS:C | 2.54 | 0.45 |
| 3:D:646:LYS:HG2 | 3:D:720:LEU:HB3 | 1.98 | 0.45 |
| 2:M:267:TYR:CE2 | 2:M:271:GLU:HB2 | 2.51 | 0.45 |
| 2:M:274:ARG:HH21 | 2:M:284:ARG:CD | 2.29 | 0.45 |
| 2:C:441:VAL:HG11 | 2:C:544:THR:HG21 | 1.98 | 0.45 |
| 2:C:462:ASP:O | 2:C:465:GLY:N | 2.42 | 0.45 |
| 2:C:441:VAL:CG1 | 2:C:544:THR:HG21 | 2.46 | 0.45 |
| 3:N:465:LEU:HD22 | 3:N:509:PRO:HB2 | 1.98 | 0.45 |
| 2:C:1082:PRO:O | 2:C:1083:GLU:C | 2.53 | 0.45 |
| 3:D:127:LEU:HA | 3:D:132:TYR:O | 2.16 | 0.45 |
| 3:D:540:LEU:O | 3:D:543:LEU:N | 2.49 | 0.45 |
| 3:D:185:VAL:HG23 | 3:D:203:ALA:N | 2.30 | 0.45 |
| 5:F:410:TYR:HA | 5:F:413:SER:OG | 2.15 | 0.45 |
| 1:K:68:ILE:CG2 | 1:K:69:PRO:HD2 | 2.43 | 0.45 |
| 2:M:603:VAL:HG12 | 2:M:645:VAL:HA | 1.96 | 0.45 |
| 1:A:206:THR:HG21 | 1:A:208:LEU:HB3 | 1.96 | 0.45 |
| 5:P:271:LEU:H | 5:P:271:LEU:HD23 | 1.80 | 0.45 |
| 5:P:364:ARG:HB3 | 5:P:389:PHE:HZ | 1.81 | 0.45 |
| 2:M:88:LEU:O | 2:M:131:GLY:N | 2.34 | 0.45 |
| 3:D:1379:VAL:HA | 3:D:1420:LEU:HG | 1.98 | 0.45 |
| 3:N:297:ILE:HB | 3:N:302:GLN:NE2 | 2.32 | 0.45 |
| 1:K:186:LEU:N | 1:K:189:ARG:O | 2.49 | 0.45 |
| 2:C:854:PRO:O | 2:C:856:GLU:N | 2.49 | 0.45 |
| 2:M:1017:THR:O | 2:M:1018:GLN:HB2 | 2.15 | 0.45 |
| 1:A:181:VAL:CG1 | 1:A:193:ASP:HB3 | 2.46 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:7:LYS:HD3 | 1:A:7:LYS:HA | 1.66 | 0.45 |
| 3:N:1468:LEU:CD2 | 3:N:1468:LEU:C | 2.85 | 0.45 |
| 3:N:1468:LEU:HD22 | 3:N:1470:ARG:N | 2.31 | 0.45 |
| 2:C:503:LEU:HD11 | 2:C:506:ASN:O | 2.16 | 0.45 |
| 3:N:731:LEU:CD1 | 3:N:931:LEU:HB3 | 2.47 | 0.45 |
| 1:B:176:ARG:HD2 | 1:B:200:TRP:NE1 | 2.32 | 0.45 |
| 3:D:884:ARG:O | 3:D:886:VAL:N | 2.50 | 0.45 |
| 1:B:26:GLU:HB2 | 1:B:27:PRO:HA | 1.98 | 0.45 |
| 3:D:959:GLU:HB3 | 3:D:963:TYR:CZ | 2.50 | 0.45 |
| 2:C:839:LEU:CD2 | 2:C:996:LYS:HA | 2.45 | 0.45 |
| 3:N:1127:GLU:OE2 | 3:N:1133:ARG:HD2 | 2.17 | 0.45 |
| 2:C:728:HIS:CE1 | 2:C:730:SER:N | 2.85 | 0.45 |
| 2:C:12:VAL:HG23 | 2:C:13:ILE:CD1 | 2.46 | 0.45 |
| 3:D:823:LEU:O | 3:D:823:LEU:HG | 2.16 | 0.45 |
| 4:O:64:ALA:O | 4:O:65:MET:C | 2.55 | 0.45 |
| 5:P:231:ARG:HB3 | 5:P:233:PHE:CE2 | 2.51 | 0.45 |
| 3:D:770:LEU:HD11 | 3:D:919:PHE:CE1 | 2.52 | 0.45 |
| 1:A:51:THR:HA | 1:A:145:ASP:O | 2.17 | 0.45 |
| 2:M:57:GLU:HG3 | 2:M:62:GLY:O | 2.16 | 0.45 |
| 2:M:198:ARG:NE | 2:M:231:PRO:HD3 | 2.30 | 0.45 |
| 2:M:241:LEU:N | 2:M:241:LEU:HD23 | 2.32 | 0.45 |
| 2:M:408:ARG:NH2 | 2:M:457:ALA:O | 2.49 | 0.45 |
| 2:C:471:TYR:HB3 | 2:C:531:PHE:CD2 | 2.50 | 0.45 |
| 3:D:1081:GLY:O | 3:D:1084:THR:HG23 | 2.15 | 0.45 |
| 3:D:1088:THR:HG23 | 3:D:1089:ALA:N | 2.31 | 0.45 |
| 3:N:460:ALA:O | 3:N:463:GLN:HB2 | 2.16 | 0.45 |
| 3:N:84:ILE:O | 3:N:86:ARG:N | 2.49 | 0.45 |
| 3:D:550:ARG:HH11 | 3:D:573:MET:C | 2.20 | 0.45 |
| 5:F:206:GLY:O | 5:F:207:LEU:HB2 | 2.16 | 0.45 |
| 3:D:227:LEU:CD2 | 3:D:326:GLU:OE2 | 2.65 | 0.45 |
| 3:D:766:ALA:O | 3:D:767:HIS:HD2 | 1.99 | 0.45 |
| 4:E:10:PHE:O | 4:E:12:MET:N | 2.50 | 0.45 |
| 2:M:774:LEU:HA | 2:M:777:ILE:CD1 | 2.40 | 0.45 |
| 5:P:393:THR:HG22 | 5:P:395:GLU:H | 1.81 | 0.45 |
| 2:C:34:VAL:O | 2:C:36:PRO:HD3 | 2.17 | 0.45 |
| 1:B:41:ARG:CA | 1:B:44:LEU:HD12 | 2.35 | 0.45 |
| 2:M:600:ASP:CA | 2:M:650:ARG:HA | 2.46 | 0.45 |
| 2:C:376:ARG:N | 2:C:377:PRO:HD2 | 2.31 | 0.45 |
| 4:O:40:LEU:HD12 | 4:O:41:GLU:HG2 | 1.97 | 0.45 |
| 3:N:614:PHE:CZ | 9:N:1528:NE6:H23 | 2.51 | 0.45 |
| 3:N:709:HIS:NE2 | 3:N:711:LEU:HB2 | 2.32 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:N:879:ARG:HB3 | 3:N:902:LEU:CD1 | 2.46 | 0.45 |
| 1:A:41:ARG:CG | 1:A:45:LEU:HD11 | 2.46 | 0.45 |
| 3:D:843:PHE:HB2 | 3:D:866:VAL:HG22 | 1.97 | 0.45 |
| 3:D:862:ASP:O | 3:D:876:SER:HB2 | 2.16 | 0.45 |
| 2:M:1090:LYS:O | 2:M:1093:GLN:HB2 | 2.17 | 0.45 |
| 1:L:38:ASN:O | 1:L:42:ARG:HG3 | 2.15 | 0.45 |
| 1:L:30:ARG:HD3 | 2:M:854:PRO:HB3 | 1.98 | 0.45 |
| 2:M:31:GLN:O | 2:M:35:PRO:HB2 | 2.17 | 0.45 |
| 2:C:643:VAL:HG22 | 2:C:644:VAL:N | 2.31 | 0.45 |
| 3:D:1342:GLU:N | 3:D:1342:GLU:CD | 2.69 | 0.45 |
| 3:D:1342:GLU:OE1 | 3:D:1342:GLU:N | 2.40 | 0.45 |
| 1:B:10:VAL:N | 1:B:26:GLU:O | 2.43 | 0.45 |
| 2:C:135:VAL:HG23 | 2:C:395:LYS:CA | 2.44 | 0.45 |
| 5:P:251:ILE:O | 5:P:255:ALA:CB | 2.64 | 0.45 |
| 2:C:87:ASP:CG | 2:C:824:ARG:HH22 | 2.20 | 0.45 |
| 3:D:970:LYS:HA | 3:D:973:GLN:HE21 | 1.81 | 0.45 |
| 1:A:143:ARG:HH11 | 1:A:158:ILE:HG23 | 1.82 | 0.45 |
| 1:A:54:THR:CG2 | 1:A:158:ILE:HG13 | 2.46 | 0.45 |
| 2:M:681:GLY:O | 2:M:684:PHE:HB2 | 2.16 | 0.45 |
| 3:N:373:PRO:O | 3:N:376:GLU:OE1 | 2.35 | 0.45 |
| 5:F:285:GLU:OE1 | 5:F:285:GLU:HA | 2.15 | 0.45 |
| 2:M:235:LEU:HD22 | 2:M:236:ILE:CG1 | 2.47 | 0.45 |
| 2:M:546:LEU:C | 2:M:581:THR:HG21 | 2.37 | 0.45 |
| 2:C:151:ASP:CB | 2:C:158:TYR:HA | 2.47 | 0.45 |
| 2:C:187:ASN:C | 2:C:188:LYS:HG2 | 2.36 | 0.45 |
| 2:C:205:GLU:HA | 2:C:209:ARG:HH11 | 1.82 | 0.45 |
| 2:C:227:PHE:H | 2:C:227:PHE:HD1 | 1.65 | 0.45 |
| 2:C:399:ASN:CB | 2:C:400:PRO:CD | 2.95 | 0.45 |
| 3:N:438:ASP:O | 3:N:439:LEU:HD23 | 2.16 | 0.45 |
| 5:P:132:ARG:O | 5:P:133:ALA:C | 2.55 | 0.45 |
| 3:D:1103:HIS:CD2 | 3:D:1463:LYS:N | 2.79 | 0.45 |
| 3:D:1479:ASP:HA | 3:D:1482:ARG:CG | 2.46 | 0.45 |
| 3:D:463:GLN:HA | 3:D:463:GLN:NE2 | 2.32 | 0.45 |
| 3:D:575:GLN:CA | 3:D:575:GLN:OE1 | 2.65 | 0.45 |
| 3:D:584:ASN:H | 3:D:602:SER:CB | 2.29 | 0.45 |
| 3:D:274:ARG:HE | 3:D:279:VAL:HG21 | 1.82 | 0.45 |
| 2:M:73:LEU:C | 2:M:73:LEU:HD12 | 2.37 | 0.45 |
| 5:P:402:ASN:O | 5:P:406:ARG:HG3 | 2.16 | 0.45 |
| 1:B:56:VAL:HG13 | 1:B:142:VAL:HA | 1.99 | 0.45 |
| 2:C:36:PRO:HG2 | 2:C:38:LYS:CG | 2.47 | 0.45 |
| 2:M:607:ASP:O | 2:M:609:ASN:N | 2.50 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:63:GLY:O | 2:C:102:HIS:HA | 2.17 | 0.45 |
| 5:P:261:PRO:C | 5:P:264:MET:HB2 | 2.37 | 0.45 |
| 5:P:306:GLU:O | 5:P:310:ILE:HG13 | 2.16 | 0.45 |
| 5:F:256:ARG:HG2 | 5:F:258:ILE:H | 1.81 | 0.45 |
| 2:M:712:ALA:CB | 2:M:821:GLU:HG2 | 2.46 | 0.45 |
| 4:O:40:LEU:HD21 | 4:O:44:GLU:CB | 2.47 | 0.45 |
| 3:D:1105:ILE:HA | 3:D:1198:TYR:O | 2.17 | 0.45 |
| 2:C:986:PRO:O | 2:C:987:ILE:HD13 | 2.17 | 0.45 |
| 3:N:491:LYS:O | 3:N:492:ALA:C | 2.55 | 0.45 |
| 2:C:910:LYS:HE3 | 2:C:912:PRO:CG | 2.46 | 0.45 |
| 3:N:1034:GLN:O | 3:N:1037:GLN:HB2 | 2.17 | 0.45 |
| 1:K:189:ARG:HB2 | 1:K:192:LEU:HD11 | 1.98 | 0.45 |
| 1:K:183:ASP:OD1 | 1:K:190:THR:O | 2.33 | 0.45 |
| 2:C:691:SER:HB3 | 2:C:868:ASP:HA | 1.97 | 0.45 |
| 2:C:577:PRO:HG3 | 2:C:993:PHE:CD1 | 2.52 | 0.45 |
| 3:N:1194:CYS:HA | 3:N:1204:CYS:SG | 2.56 | 0.45 |
| 2:C:604:ALA:HB3 | 2:C:612:VAL:O | 2.16 | 0.45 |
| 2:M:961:GLU:O | 2:M:962:GLN:C | 2.54 | 0.45 |
| 2:C:20:GLU:HA | 2:C:23:VAL:CG2 | 2.47 | 0.45 |
| 2:M:479:VAL:HB | 2:M:506:ASN:OD1 | 2.16 | 0.45 |
| 1:A:112:ARG:HE | 1:A:125:PRO:HB2 | 1.81 | 0.45 |
| 2:C:1094:ALA:HA | 3:D:518:PRO:HB2 | 1.98 | 0.45 |
| 3:N:1048:PRO:CG | 3:N:1075:HIS:CD2 | 2.95 | 0.45 |
| 3:D:1211:MET:CB | 3:D:1213:ARG:NH1 | 2.79 | 0.45 |
| 2:C:714:ASP:OD2 | 2:C:820:ARG:NE | 2.50 | 0.45 |
| 2:C:385:PHE:O | 2:C:386:PHE:C | 2.54 | 0.45 |
| 3:D:966:GLU:HA | 3:D:969:ARG:NH2 | 2.31 | 0.45 |
| 2:M:728:HIS:NE2 | 2:M:733:ALA:HB3 | 2.32 | 0.45 |
| 2:C:275:TYR:O | 2:C:279:GLU:HB3 | 2.17 | 0.45 |
| 3:N:215:TYR:HD1 | 3:N:381:ALA:O | 1.99 | 0.45 |
| 1:K:58:ILE:O | 1:K:59:GLU:C | 2.55 | 0.45 |
| 2:M:148:PHE:CZ | 2:M:309:TYR:HD2 | 2.35 | 0.45 |
| 2:M:199:VAL:HG21 | 2:M:238:LEU:HD12 | 1.96 | 0.45 |
| 2:M:138:SER:HB2 | 2:M:333:ILE:HD11 | 1.98 | 0.45 |
| 2:M:335:THR:O | 2:M:339:LEU:HG | 2.16 | 0.45 |
| 3:N:320:ALA:O | 3:N:335:LEU:HB3 | 2.16 | 0.45 |
| 2:C:175:GLU:O | 2:C:176:VAL:CG1 | 2.59 | 0.45 |
| 2:C:432:ARG:NH1 | 2:C:518:LYS:O | 2.50 | 0.45 |
| 3:N:153:LEU:HG | 3:N:154:THR:N | 2.31 | 0.45 |
| 3:N:438:ASP:HA | 3:N:445:ARG:HH22 | 1.82 | 0.45 |
| 3:N:462:GLN:HB2 | 3:N:513:ILE:HG12 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:N:570:GLU:HB2 | 5:P:214:GLN:HE21 | 1.81 | 0.45 |
| 3:D:109:PRO:O | 3:D:111:LYS:N | 2.49 | 0.45 |
| 3:D:569:ASN:HD21 | 5:F:214:GLN:NE2 | 2.15 | 0.45 |
| 5:F:110:MET:HE3 | 5:F:111:GLU:N | 2.32 | 0.45 |
| 5:F:220:LEU:O | 5:F:223:ALA:HB3 | 2.17 | 0.45 |
| 3:D:441:ARG:CB | 3:D:443:VAL:HG23 | 2.47 | 0.45 |
| 5:P:386:VAL:HG11 | 5:P:394:ARG:H | 1.82 | 0.45 |
| 1:B:212:ASN:OD1 | 1:B:212:ASN:N | 2.47 | 0.45 |
| 2:C:771:GLU:O | 2:C:772:ARG:C | 2.54 | 0.45 |
| 1:B:40:LEU:O | 1:B:41:ARG:C | 2.54 | 0.45 |
| 2:C:54:ILE:O | 2:C:54:ILE:HG23 | 2.16 | 0.45 |
| 5:P:367:MET:HB2 | 5:P:371:LEU:HD11 | 1.98 | 0.45 |
| 3:D:1396:GLU:O | 3:D:1397:LYS:CD | 2.65 | 0.45 |
| 3:N:1364:HIS:ND1 | 3:N:1365:ASP:N | 2.64 | 0.45 |
| 1:L:120:VAL:HG12 | 1:L:121:GLU:N | 2.31 | 0.45 |
| 2:M:672:VAL:HG23 | 2:M:673:LEU:H | 1.81 | 0.45 |
| 2:M:889:HIS:CE1 | 2:M:970:GLY:HA3 | 2.52 | 0.45 |
| 5:F:84:TYR:O | 5:F:87:GLU:HG2 | 2.17 | 0.45 |
| 1:A:29:GLU:O | 1:A:30:ARG:C | 2.54 | 0.45 |
| 1:K:18:ARG:O | 1:K:207:PRO:HD3 | 2.15 | 0.45 |
| 1:K:215:VAL:O | 1:K:218:LEU:HB3 | 2.15 | 0.45 |
| 1:L:28:LEU:HD22 | 1:L:29:GLU:H | 1.81 | 0.45 |
| 1:L:28:LEU:HD22 | 1:L:29:GLU:N | 2.32 | 0.45 |
| 1:A:105:GLY:O | 1:A:107:LYS:HG2 | 2.16 | 0.45 |
| 5:F:157:GLU:HB3 | 5:F:161:GLN:OE1 | 2.16 | 0.45 |
| 5:F:321:ILE:HD11 | 5:F:329:TYR:CA | 2.47 | 0.45 |
| 2:M:833:LEU:HD12 | 2:M:837:ASP:OD2 | 2.17 | 0.45 |
| 1:A:219:ARG:O | 1:A:220:GLU:C | 2.54 | 0.45 |
| 3:N:993:LEU:O | 3:N:994:GLN:C | 2.54 | 0.45 |
| 3:N:996:TRP:O | 3:N:997:THR:C | 2.55 | 0.45 |
| 3:D:773:ALA:HA | 3:D:1367:HIS:NE2 | 2.31 | 0.45 |
| 3:N:1334:GLN:O | 3:N:1337:GLU:HB2 | 2.17 | 0.45 |
| 3:N:1339:LYS:HB3 | 3:N:1343:ALA:CB | 2.47 | 0.45 |
| 1:K:143:ARG:HH11 | 1:K:158:ILE:CG2 | 2.29 | 0.45 |
| 5:P:361:LEU:CG | 5:P:362:SER:N | 2.80 | 0.45 |
| 3:N:3:LYS:HE2 | 3:N:3:LYS:HB3 | 1.77 | 0.45 |
| 2:M:164:PRO:HA | 2:M:266:ARG:HA | 1.98 | 0.45 |
| 2:M:395:LYS:HE2 | 2:M:403:SER:HB3 | 1.99 | 0.45 |
| 2:M:439:CYS:HB2 | 2:M:541:SER:N | 2.32 | 0.45 |
| 3:N:261:LEU:HD11 | 3:N:290:PRO:O | 2.17 | 0.45 |
| 2:C:162:ILE:HB | 2:C:172:ILE:HB | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:257:VAL:O | 2:C:261:ILE:HB | 2.17 | 0.45 |
| 2:C:268:ASP:OD2 | 2:C:268:ASP:N | 2.50 | 0.45 |
| 2:C:499:ALA:O | 2:C:501:THR:N | 2.50 | 0.45 |
| 2:C:583:LEU:O | 2:C:587:VAL:HG23 | 2.17 | 0.45 |
| 3:N:50:PHE:CD2 | 3:N:522:PRO:HD3 | 2.52 | 0.45 |
| 3:N:85:VAL:HG21 | 3:N:89:ARG:NH2 | 2.31 | 0.45 |
| 3:D:1436:SER:O | 3:D:1439:SER:N | 2.49 | 0.45 |
| 3:D:1486:VAL:HG22 | 4:E:75:PHE:CA | 2.45 | 0.45 |
| 3:D:460:ALA:O | 3:D:463:GLN:HB2 | 2.17 | 0.45 |
| 3:D:531:ASP:O | 3:D:532:GLY:C | 2.55 | 0.45 |
| 3:D:567:ILE:CD1 | 5:F:140:ARG:HH22 | 2.29 | 0.45 |
| 5:F:175:HIS:C | 5:F:178:ARG:HB2 | 2.37 | 0.45 |
| 3:D:812:ALA:HA | 3:D:816:HIS:CB | 2.26 | 0.45 |
| 2:M:99:GLN:HA | 2:M:109:LYS:HA | 1.98 | 0.45 |
| 5:P:285:GLU:HA | 5:P:286:PRO:HD2 | 1.79 | 0.45 |
| 3:N:1107:VAL:CG2 | 3:N:1219:GLU:HB3 | 2.46 | 0.45 |
| 3:D:1197:ARG:HG2 | 3:D:1198:TYR:CE2 | 2.52 | 0.45 |
| 3:D:65:ARG:CB | 5:F:375:LEU:O | 2.64 | 0.45 |
| 3:N:970:LYS:O | 3:N:971:LEU:C | 2.53 | 0.45 |
| 2:C:674:VAL:HG11 | 2:C:992:MET:CB | 2.46 | 0.45 |
| 2:C:674:VAL:HG21 | 2:C:871:LEU:CD1 | 2.45 | 0.45 |
| 2:C:910:LYS:HG2 | 2:C:913:GLU:CD | 2.37 | 0.45 |
| 3:N:1223:ILE:O | 3:N:1226:ALA:HB3 | 2.17 | 0.45 |
| 2:M:469:THR:HG22 | 2:M:470:PRO:O | 2.16 | 0.45 |
| 3:N:623:VAL:HG12 | 3:N:625:TYR:N | 2.32 | 0.45 |
| 2:C:596:TYR:N | 2:C:596:TYR:CD1 | 2.84 | 0.45 |
| 3:N:1345:GLU:CA | 3:N:1348:LEU:HD12 | 2.35 | 0.45 |
| 2:M:1091:GLU:O | 2:M:1095:LEU:HG | 2.17 | 0.45 |
| 2:M:1111:ILE:HG13 | 2:M:1112:PHE:CD1 | 2.52 | 0.45 |
| 2:M:945:ARG:O | 2:M:948:GLU:HG2 | 2.17 | 0.45 |
| 1:K:74:ASP:C | 1:K:74:ASP:OD1 | 2.55 | 0.45 |
| 3:N:1020:LEU:O | 3:N:1021:TYR:C | 2.54 | 0.45 |
| 3:N:586:ARG:O | 3:N:587:ARG:HG2 | 2.17 | 0.45 |
| 2:M:446:GLY:O | 2:M:448:ASN:N | 2.50 | 0.45 |
| 2:M:446:GLY:O | 2:M:449:ILE:N | 2.47 | 0.45 |
| 3:D:57:GLU:CG | 3:D:64:LYS:HA | 2.38 | 0.45 |
| 2:M:23:VAL:CA | 2:M:121:MET:HE1 | 2.42 | 0.45 |
| 2:C:578:VAL:CG2 | 2:C:579:VAL:HG12 | 2.44 | 0.45 |
| 3:N:1108:ARG:HE | 3:N:1198:TYR:C | 2.20 | 0.45 |
| 3:D:1323:GLN:HG3 | 3:D:1324:PRO:HD2 | 1.98 | 0.45 |
| 2:M:726:ILE:CG1 | 2:M:728:HIS:HB2 | 2.47 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:148:PHE:N | 2:M:148:PHE:CD1 | 2.84 | 0.45 |
| 2:C:176:VAL:HG11 | 2:C:182:VAL:HA | 1.99 | 0.45 |
| 3:N:411:THR:O | 3:N:411:THR:HG23 | 2.17 | 0.45 |
| 3:N:554:LEU:HG | 3:N:558:LEU:HD11 | 1.99 | 0.45 |
| 3:D:119:SER:H | 3:D:123:LEU:CB | 2.29 | 0.45 |
| 3:D:154:THR:HG23 | 3:D:157:GLU:H | 1.82 | 0.45 |
| 3:D:160:GLU:O | 3:D:161:LEU:HD23 | 2.17 | 0.45 |
| 3:D:568:ARG:O | 3:D:569:ASN:C | 2.55 | 0.45 |
| 4:E:19:LEU:O | 4:E:20:THR:C | 2.55 | 0.45 |
| 3:D:441:ARG:O | 3:D:442:ASN:C | 2.52 | 0.45 |
| 1:B:59:GLU:HB2 | 1:B:139:ASN:ND2 | 2.32 | 0.45 |
| 3:D:671:LYS:HE2 | 3:D:675:ARG:CD | 2.47 | 0.45 |
| 5:P:282:LEU:O | 5:P:284:ARG:HG2 | 2.17 | 0.45 |
| 5:P:370:LYS:O | 5:P:374:GLY:N | 2.49 | 0.45 |
| 2:M:759:THR:HA | 2:M:786:LYS:O | 2.17 | 0.45 |
| 3:N:1487:VAL:O | 4:O:73:LEU:HD12 | 2.17 | 0.45 |
| 4:O:71:GLY:C | 4:O:73:LEU:N | 2.68 | 0.45 |
| 3:D:1149:LEU:CD2 | 3:D:1160:LEU:O | 2.65 | 0.45 |
| 3:D:1151:ARG:C | 3:D:1162:GLU:CB | 2.80 | 0.45 |
| 3:N:1405:GLU:OE2 | 3:N:1407:LEU:HG | 2.16 | 0.45 |
| 3:N:1267:ARG:NE | 3:N:1271:LYS:NZ | 2.63 | 0.45 |
| 2:C:674:VAL:HG11 | 2:C:992:MET:HB3 | 1.99 | 0.45 |
| 2:C:953:VAL:HG13 | 2:C:966:LEU:HD13 | 1.99 | 0.45 |
| 3:N:614:PHE:CD2 | 3:N:617:ASN:ND2 | 2.85 | 0.45 |
| 1:L:19:GLU:HG2 | 1:L:203:GLY:CA | 2.47 | 0.45 |
| 3:N:796:ARG:HD2 | 3:N:862:ASP:OD2 | 2.16 | 0.45 |
| 3:N:1153:VAL:HG12 | 3:N:1155:VAL:HG23 | 1.99 | 0.45 |
| 1:L:185:ARG:NH2 | 3:N:692:GLU:HG3 | 2.32 | 0.45 |
| 3:N:351:MET:HG3 | 3:N:370:ALA:HB2 | 1.98 | 0.45 |
| 1:K:203:GLY:C | 1:K:205:VAL:H | 2.20 | 0.45 |
| 1:K:206:THR:HG23 | 1:K:207:PRO:HD2 | 1.99 | 0.45 |
| 1:K:23:PHE:N | 1:K:23:PHE:CD1 | 2.85 | 0.45 |
| 1:K:73:GLU:HG2 | 1:K:130:ALA:HA | 1.98 | 0.45 |
| 1:B:150:TYR:OH | 1:B:168:ASP:HB3 | 2.16 | 0.45 |
| 3:D:1254:GLN:HG2 | 3:D:1255:GLY:N | 2.31 | 0.45 |
| 5:P:104:ARG:HB2 | 5:P:108:GLU:OE2 | 2.16 | 0.45 |
| 3:D:880:ILE:O | 3:D:881:LEU:C | 2.55 | 0.45 |
| 2:M:91:GLN:HB3 | 2:M:119:PRO:HA | 1.99 | 0.45 |
| 5:P:241:TRP:O | 5:P:244:ARG:HB2 | 2.16 | 0.45 |
| 2:C:557:ARG:O | 2:C:560:MET:HB2 | 2.17 | 0.45 |
| 1:K:63:HIS:CD2 | 2:M:801:VAL:HA | 2.52 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:636:GLN:OE1 | 3:D:636:GLN:HA | 2.16 | 0.45 |
| 2:M:198:ARG:NE | 2:M:231:PRO:HG3 | 2.32 | 0.45 |
| 2:M:136:ILE:CD1 | 2:M:392:SER:HA | 2.42 | 0.45 |
| 2:C:274:ARG:CZ | 2:C:285:LEU:HD23 | 2.47 | 0.45 |
| 2:C:497:ALA:O | 2:C:532:MET:HG3 | 2.16 | 0.45 |
| 3:N:102:ILE:HD12 | 3:N:579:ASP:HB3 | 1.98 | 0.45 |
| 3:N:23:TYR:CZ | 3:N:89:ARG:NH1 | 2.85 | 0.45 |
| 3:D:113:GLY:N | 3:D:124:GLU:OE1 | 2.50 | 0.45 |
| 3:D:614:PHE:HA | 3:D:617:ASN:HD22 | 1.82 | 0.45 |
| 3:D:280:ALA:HB1 | 3:D:282:TYR:OH | 2.16 | 0.45 |
| 2:C:681:GLY:O | 2:C:684:PHE:HB2 | 2.16 | 0.45 |
| 5:P:350:LEU:C | 5:P:352:GLU:H | 2.19 | 0.45 |
| 5:P:405:LEU:HB2 | 5:P:406:ARG:H | 1.64 | 0.45 |
| 5:P:422:LEU:H | 5:P:422:LEU:HD23 | 1.81 | 0.45 |
| 1:A:43:ILE:HG23 | 1:A:47:SER:HB2 | 1.99 | 0.45 |
| 2:C:63:GLY:H | 2:C:103:LYS:HA | 1.81 | 0.45 |
| 2:M:365:ASP:C | 2:M:367:LEU:H | 2.19 | 0.45 |
| 5:F:288:TYR:HB3 | 5:F:301:ALA:HB1 | 1.99 | 0.45 |
| 2:M:720:GLU:HG3 | 2:M:720:GLU:H | 1.50 | 0.45 |
| 3:N:1465:ASN:CB | 3:N:1473:PRO:HD3 | 2.47 | 0.45 |
| 1:L:18:ARG:NH1 | 1:L:88:ARG:NH2 | 2.59 | 0.45 |
| 3:N:828:LYS:HA | 3:N:835:SER:OG | 2.17 | 0.45 |
| 3:N:797:LYS:HA | 3:N:828:LYS:O | 2.16 | 0.45 |
| 3:N:834:THR:HA | 3:N:838:ARG:HD2 | 1.98 | 0.45 |
| 3:N:793:THR:CG2 | 3:N:906:GLN:HG2 | 2.47 | 0.45 |
| 2:C:650:ARG:O | 2:C:653:ASP:OD2 | 2.34 | 0.45 |
| 1:L:218:LEU:O | 1:L:221:HIS:HB2 | 2.17 | 0.45 |
| 3:D:428:LYS:HG2 | 3:D:429:SER:N | 2.31 | 0.45 |
| 3:N:660:LYS:HD3 | 3:N:663:GLU:CD | 2.37 | 0.45 |
| 1:K:206:THR:HG22 | 1:K:208:LEU:HB3 | 1.99 | 0.45 |
| 2:M:984:GLU:CG | 3:N:944:THR:O | 2.65 | 0.45 |
| 2:C:477:GLY:O | 2:C:508:ILE:HG13 | 2.16 | 0.45 |
| 1:B:13:VAL:HG23 | 1:B:22:GLU:O | 2.17 | 0.45 |
| 2:M:572:ILE:HD12 | 2:M:701:THR:HB | 1.98 | 0.45 |
| 1:A:102:LYS:HA | 1:A:138:LEU:O | 2.17 | 0.45 |
| 3:D:881:LEU:O | 3:D:882:PHE:C | 2.55 | 0.45 |
| 5:P:163:LEU:O | 5:P:166:LEU:HB2 | 2.17 | 0.45 |
| 2:M:835:VAL:O | 2:M:835:VAL:HG13 | 2.16 | 0.45 |
| 3:D:958:GLU:OE2 | 3:D:961:LYS:CG | 2.65 | 0.45 |
| 3:D:1000:THR:CG2 | 3:D:1036:ARG:HD2 | 2.46 | 0.45 |
| 3:D:1305:LEU:CD2 | 3:D:1305:LEU:N | 2.79 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:K:54:THR:HG21 | 1:K:143:ARG:HD3 | 1.98 | 0.45 |
| 3:D:1087:ARG:NH2 | 3:D:1236:LEU:O | 2.50 | 0.45 |
| 4:O:24:ALA:O | 4:O:27:ALA:N | 2.50 | 0.45 |
| 2:M:205:GLU:N | 2:M:209:ARG:HH11 | 2.15 | 0.45 |
| 3:N:217:LYS:HD3 | 3:N:262:LYS:NZ | 2.31 | 0.45 |
| 1:B:233:VAL:C | 1:B:235:ALA:H | 2.20 | 0.45 |
| 2:C:327:HIS:CE1 | 2:C:329:GLY:HA3 | 2.52 | 0.45 |
| 2:C:141:HIS:CD2 | 2:C:334:ARG:CG | 2.99 | 0.45 |
| 2:C:428:ARG:NE | 2:C:451:LEU:HD21 | 2.31 | 0.45 |
| 2:C:5:ARG:HA | 2:C:902:ILE:HB | 1.99 | 0.45 |
| 3:N:152:LEU:HD12 | 3:N:153:LEU:H | 1.82 | 0.45 |
| 3:N:411:THR:H | 3:N:437:VAL:HG21 | 1.82 | 0.45 |
| 2:C:1092:LEU:O | 2:C:1095:LEU:HB2 | 2.17 | 0.45 |
| 3:D:1091:SER:O | 3:D:1092:GLY:C | 2.55 | 0.45 |
| 3:D:12:LEU:HD23 | 3:D:1451:ALA:HB1 | 1.99 | 0.45 |
| 3:D:5:VAL:O | 3:D:6:ARG:HG3 | 2.17 | 0.45 |
| 5:F:204:GLY:C | 5:F:206:GLY:N | 2.69 | 0.45 |
| 3:N:357:GLU:N | 3:N:357:GLU:CD | 2.68 | 0.45 |
| 3:N:355:VAL:HG11 | 3:N:385:VAL:HG21 | 1.99 | 0.45 |
| 3:N:441:ARG:HG3 | 3:N:443:VAL:HG21 | 1.96 | 0.45 |
| 3:D:288:MET:HG3 | 3:D:305:ALA:HB1 | 1.99 | 0.45 |
| 3:D:936:TYR:HE2 | 3:D:940:THR:HG21 | 1.82 | 0.45 |
| 2:C:1067:TYR:HB2 | 5:F:341:PRO:CB | 2.47 | 0.45 |
| 2:C:108:ILE:CG2 | 2:C:368:THR:HG21 | 2.47 | 0.45 |
| 2:M:56:GLU:HB3 | 2:M:359:MET:SD | 2.57 | 0.45 |
| 3:N:671:LYS:HE2 | 3:N:675:ARG:CG | 2.47 | 0.45 |
| 5:P:379:ARG:CG | 5:P:379:ARG:HH11 | 2.30 | 0.45 |
| 3:D:1378:TYR:CE2 | 3:D:1394:VAL:HG22 | 2.52 | 0.45 |
| 3:N:613:ARG:O | 3:N:614:PHE:C | 2.55 | 0.45 |
| 2:M:877:PRO:HD3 | 3:N:1023:MET:HE1 | 1.99 | 0.45 |
| 3:N:795:VAL:CG1 | 3:N:876:SER:HB3 | 2.47 | 0.45 |
| 3:D:480:GLU:O | 3:D:484:PRO:HD2 | 2.17 | 0.45 |
| 3:N:750:PRO:HG2 | 3:N:756:GLN:HE22 | 1.82 | 0.45 |
| 1:L:208:LEU:O | 1:L:211:LEU:HB3 | 2.16 | 0.45 |
| 2:M:1098:ASP:HB2 | 3:N:17:LYS:NZ | 2.31 | 0.45 |
| 3:D:630:VAL:CG1 | 3:D:631:ILE:N | 2.79 | 0.45 |
| 1:K:44:LEU:HD21 | 1:K:214:ALA:HB2 | 1.99 | 0.45 |
| 2:C:508:ILE:CD1 | 2:C:526:PRO:HB3 | 2.47 | 0.45 |
| 2:M:503:LEU:HD11 | 2:M:506:ASN:O | 2.17 | 0.45 |
| 3:N:596:SER:C | 3:N:598:ARG:H | 2.20 | 0.45 |
| 1:L:89:PHE:CD2 | 1:L:94:LEU:CB | 3.00 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:1129:THR:HG22 | 3:N:1130:ARG:N | 2.32 | 0.45 |
| 5:P:250:ALA:O | 5:P:253:ASP:HB2 | 2.17 | 0.45 |
| 2:M:522:VAL:CG1 | 2:M:523:ILE:N | 2.80 | 0.45 |
| 1:B:156:HIS:C | 1:B:158:ILE:H | 2.19 | 0.45 |
| 5:F:245:GLN:HA | 5:F:245:GLN:NE2 | 2.26 | 0.45 |
| 1:A:9:PRO:HB2 | 1:A:25:LEU:CD1 | 2.46 | 0.45 |
| 2:M:353:ARG:HH11 | 2:M:353:ARG:HG2 | 1.82 | 0.45 |
| 2:C:1031:ARG:CA | 3:D:622:ARG:NH1 | 2.80 | 0.45 |
| 3:D:1180:ALA:O | 3:D:1181:GLY:C | 2.55 | 0.45 |
| 3:N:1280:VAL:HG12 | 3:N:1281:VAL:N | 2.32 | 0.45 |
| 2:M:361:MET:N | 2:M:361:MET:SD | 2.73 | 0.45 |
| 2:C:842:ARG:NH2 | 2:C:887:GLU:OE2 | 2.46 | 0.45 |
| 2:M:235:LEU:O | 2:M:238:LEU:HB2 | 2.17 | 0.44 |
| 3:N:223:LEU:HG | 3:N:224:ARG:H | 1.82 | 0.44 |
| 2:C:439:CYS:SG | 2:C:442:GLU:HB2 | 2.57 | 0.44 |
| 2:C:512:ARG:NH1 | 2:C:524:VAL:HA | 2.28 | 0.44 |
| 3:N:130:SER:CA | 3:N:568:ARG:NH2 | 2.80 | 0.44 |
| 3:D:598:ARG:NH1 | 3:D:598:ARG:HG2 | 2.33 | 0.44 |
| 5:P:411:HIS:CE1 | 5:P:412:GLU:OE2 | 2.70 | 0.44 |
| 3:D:1171:VAL:HG12 | 3:D:1175:ILE:CD1 | 2.43 | 0.44 |
| 3:D:1173:LEU:HG | 3:D:1174:LEU:N | 2.31 | 0.44 |
| 3:D:1381:VAL:CG1 | 3:D:1389:LEU:O | 2.65 | 0.44 |
| 5:F:355:GLU:CB | 5:F:358:LEU:HD23 | 2.47 | 0.44 |
| 3:N:970:LYS:HE2 | 3:N:974:ILE:HG12 | 2.00 | 0.44 |
| 2:C:953:VAL:HA | 2:C:965:GLU:OE2 | 2.16 | 0.44 |
| 2:M:1101:THR:O | 2:M:1102:LEU:HD23 | 2.17 | 0.44 |
| 3:N:881:LEU:HG | 3:N:885:ILE:HD11 | 2.00 | 0.44 |
| 2:C:671:ASN:C | 2:C:672:VAL:HG12 | 2.37 | 0.44 |
| 2:C:675:ALA:HB2 | 2:C:867:VAL:HG11 | 1.98 | 0.44 |
| 5:F:77:THR:O | 5:F:79:ASP:N | 2.48 | 0.44 |
| 5:F:85:LEU:HA | 5:F:85:LEU:HD23 | 1.73 | 0.44 |
| 1:B:72:LYS:HD3 | 1:B:73:GLU:N | 2.32 | 0.44 |
| 2:C:600:ASP:CB | 2:C:650:ARG:HA | 2.41 | 0.44 |
| 3:N:1134:LEU:HD12 | 3:N:1135:ARG:H | 1.83 | 0.44 |
| 3:N:1258:ARG:HH21 | 3:N:1351:GLU:CG | 2.30 | 0.44 |
| 2:M:946:ARG:O | 2:M:949:LYS:HB2 | 2.16 | 0.44 |
| 2:C:18:LEU:O | 2:C:21:ILE:CD1 | 2.65 | 0.44 |
| 2:M:504:GLU:CG | 2:M:507:ARG:HB2 | 2.45 | 0.44 |
| 5:P:323:ASP:C | 5:P:323:ASP:OD1 | 2.55 | 0.44 |
| 3:N:1205:TYR:CD2 | 3:N:1215:VAL:HG11 | 2.50 | 0.44 |
| 2:M:424:GLY:O | 2:M:425:PHE:C | 2.55 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:P:159:ILE:O | 5:P:163:LEU:HG | 2.17 | 0.44 |
| 2:C:403:SER:O | 2:C:407:LYS:HG3 | 2.18 | 0.44 |
| 2:C:748:GLU:HA | 2:C:799:ILE:HG22 | 1.98 | 0.44 |
| 5:P:111:GLU:HG3 | 5:P:114:LYS:CE | 2.47 | 0.44 |
| 3:D:175:VAL:CG1 | 3:D:193:PRO:HD2 | 2.46 | 0.44 |
| 3:N:984:THR:N | 3:N:987:GLU:OE2 | 2.25 | 0.44 |
| 1:A:11:PHE:O | 1:B:229:GLN:CB | 2.63 | 0.44 |
| 1:A:9:PRO:HA | 1:A:27:PRO:HD2 | 1.99 | 0.44 |
| 3:D:214:GLU:HG2 | 3:D:342:PRO:HA | 2.00 | 0.44 |
| 4:O:25:LYS:O | 4:O:28:GLN:HB2 | 2.17 | 0.44 |
| 2:M:710:ILE:HG22 | 2:M:823:VAL:HB | 1.98 | 0.44 |
| 2:M:709:GLU:HA | 2:M:823:VAL:O | 2.17 | 0.44 |
| 1:A:18:ARG:CD | 1:A:88:ARG:NH2 | 2.80 | 0.44 |
| 1:B:184:THR:HG22 | 1:B:192:LEU:O | 2.17 | 0.44 |
| 2:M:175:GLU:O | 2:M:176:VAL:HG13 | 2.18 | 0.44 |
| 2:M:276:LYS:O | 2:M:280:LYS:HG3 | 2.17 | 0.44 |
| 2:C:164:PRO:HG3 | 2:C:170:PRO:HD2 | 1.98 | 0.44 |
| 2:C:176:VAL:HG12 | 2:C:182:VAL:CA | 2.48 | 0.44 |
| 2:C:405:ARG:HG3 | 2:C:543:ASN:OD1 | 2.17 | 0.44 |
| 3:D:318:ARG:HG2 | 3:D:319:ALA:H | 1.78 | 0.44 |
| 3:D:591:VAL:HG21 | 3:D:597:ASP:HA | 1.99 | 0.44 |
| 5:F:102:LEU:HD23 | 5:F:187:LEU:HB2 | 1.98 | 0.44 |
| 5:F:101:GLU:HG2 | 5:F:105:LYS:HE3 | 2.00 | 0.44 |
| 5:F:203:THR:CG2 | 5:F:204:GLY:N | 2.80 | 0.44 |
| 1:B:104:GLU:HA | 1:B:137:ARG:HA | 1.98 | 0.44 |
| 3:D:186:VAL:CG1 | 3:D:187:LYS:H | 2.29 | 0.44 |
| 2:C:95:TYR:CE2 | 2:C:114:PHE:HB3 | 2.53 | 0.44 |
| 2:M:657:ASP:CG | 2:M:664:GLY:H | 2.21 | 0.44 |
| 2:C:63:GLY:H | 2:C:103:LYS:CA | 2.28 | 0.44 |
| 2:C:61:LYS:O | 2:C:103:LYS:HB2 | 2.17 | 0.44 |
| 2:C:45:GLN:O | 2:C:48:PHE:HB2 | 2.17 | 0.44 |
| 2:C:98:LEU:HD11 | 2:C:113:VAL:HG21 | 1.99 | 0.44 |
| 3:D:1171:VAL:O | 3:D:1175:ILE:HG13 | 2.17 | 0.44 |
| 3:D:1390:LEU:O | 3:D:1390:LEU:HD12 | 2.17 | 0.44 |
| 2:M:1101:THR:C | 2:M:1102:LEU:HD23 | 2.38 | 0.44 |
| 2:C:914:ILE:CD1 | 2:C:914:ILE:H | 2.30 | 0.44 |
| 3:N:253:ALA:N | 3:N:301:GLY:CA | 2.74 | 0.44 |
| 3:N:1462:LEU:O | 3:N:1463:LYS:C | 2.54 | 0.44 |
| 3:N:787:LEU:HD12 | 3:N:787:LEU:HA | 1.73 | 0.44 |
| 3:N:841:TYR:HB3 | 3:N:843:PHE:CZ | 2.52 | 0.44 |
| 3:N:847:ASP:OD1 | 3:N:848:GLU:N | 2.46 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:168:THR:CB | 3:D:206:ARG:NH1 | 2.80 | 0.44 |
| 2:C:861:LEU:HB2 | 2:C:863:ASP:OD1 | 2.17 | 0.44 |
| 3:N:1149:LEU:HD23 | 3:N:1161:GLU:C | 2.37 | 0.44 |
| 3:N:1171:VAL:CA | 3:N:1174:LEU:HD12 | 2.32 | 0.44 |
| 1:A:31:GLY:O | 1:A:33:GLY:N | 2.50 | 0.44 |
| 3:N:1345:GLU:O | 3:N:1346:ARG:C | 2.55 | 0.44 |
| 3:D:29:PRO:O | 3:D:30:GLU:C | 2.55 | 0.44 |
| 3:D:30:GLU:CG | 3:D:40:GLU:HG2 | 2.47 | 0.44 |
| 1:L:54:THR:HB | 1:L:143:ARG:HD2 | 1.99 | 0.44 |
| 2:M:47:ALA:HA | 2:M:50:GLU:OE2 | 2.17 | 0.44 |
| 3:D:1376:MET:HE2 | 3:D:1421:LEU:HA | 1.98 | 0.44 |
| 3:N:1018:ASN:C | 3:N:1018:ASN:OD1 | 2.56 | 0.44 |
| 3:N:172:PRO:HB2 | 3:N:175:VAL:CG2 | 2.48 | 0.44 |
| 2:C:397:GLU:OE2 | 2:C:632:ASN:N | 2.50 | 0.44 |
| 2:M:443:THR:O | 2:M:559:LEU:HD11 | 2.18 | 0.44 |
| 3:N:1127:GLU:HG3 | 3:N:1128:VAL:N | 2.29 | 0.44 |
| 3:D:1324:PRO:C | 3:D:1325:LEU:HD23 | 2.37 | 0.44 |
| 3:D:821:VAL:HG22 | 3:D:840:LYS:HZ2 | 1.81 | 0.44 |
| 2:C:293:PHE:HD1 | 2:C:294:GLU:CG | 2.30 | 0.44 |
| 2:M:707:ARG:HG2 | 2:M:708:TYR:N | 2.32 | 0.44 |
| 5:P:361:LEU:HG | 5:P:362:SER:N | 2.31 | 0.44 |
| 2:M:385:PHE:O | 2:M:389:SER:HB2 | 2.17 | 0.44 |
| 3:N:284:LEU:HD12 | 3:N:290:PRO:CB | 2.48 | 0.44 |
| 2:C:178:PRO:C | 2:C:180:GLY:N | 2.69 | 0.44 |
| 2:C:499:ALA:C | 2:C:501:THR:H | 2.20 | 0.44 |
| 3:N:90:MET:HG2 | 3:N:521:PRO:HD3 | 1.98 | 0.44 |
| 3:N:527:MET:SD | 3:N:537:THR:CG2 | 3.05 | 0.44 |
| 3:D:112:ILE:HG13 | 3:D:124:GLU:OE1 | 2.17 | 0.44 |
| 2:M:69:LEU:HD22 | 2:M:97:ARG:HD3 | 2.00 | 0.44 |
| 3:D:325:GLU:OE2 | 3:D:332:TYR:HB3 | 2.17 | 0.44 |
| 3:D:930:LEU:O | 3:D:931:LEU:C | 2.54 | 0.44 |
| 5:P:382:THR:HG23 | 5:P:397:ILE:HB | 1.99 | 0.44 |
| 2:M:157:ARG:CG | 2:M:314:THR:HG22 | 2.47 | 0.44 |
| 2:C:38:LYS:CG | 2:C:39:ARG:N | 2.74 | 0.44 |
| 2:M:719:PRO:CB | 2:M:820:ARG:NH1 | 2.79 | 0.44 |
| 3:D:1383:ASP:HA | 3:D:1384:PRO:HD2 | 1.82 | 0.44 |
| 2:M:867:VAL:HG23 | 2:M:868:ASP:N | 2.31 | 0.44 |
| 3:N:796:ARG:HG3 | 3:N:861:GLN:O | 2.17 | 0.44 |
| 2:M:1021:LEU:HD12 | 2:M:1022:GLY:H | 1.82 | 0.44 |
| 3:D:853:VAL:HG11 | 3:D:860:LEU:CD2 | 2.47 | 0.44 |
| 3:N:1344:VAL:CG1 | 3:N:1345:GLU:N | 2.80 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:N:485:SER:O | 3:N:489:ARG:NH1 | 2.50 | 0.44 |
| 3:N:732:VAL:C | 3:N:734:GLU:H | 2.19 | 0.44 |
| 3:N:819:GLY:CA | 3:N:822:ALA:HB3 | 2.45 | 0.44 |
| 1:K:25:LEU:HD21 | 1:L:224:TYR:CB | 2.47 | 0.44 |
| 2:C:626:ARG:HG3 | 2:C:626:ARG:NH1 | 2.26 | 0.44 |
| 3:N:1404:ASN:HA | 3:N:1409:ALA:H | 1.82 | 0.44 |
| 3:N:1274:ILE:HG22 | 3:N:1324:PRO:HA | 1.98 | 0.44 |
| 2:C:385:PHE:CD1 | 2:C:389:SER:HB2 | 2.53 | 0.44 |
| 5:P:250:ALA:O | 5:P:251:ILE:C | 2.56 | 0.44 |
| 3:D:680:GLN:HA | 3:D:683:ILE:HG13 | 1.99 | 0.44 |
| 2:M:669:GLY:N | 2:M:993:PHE:CZ | 2.86 | 0.44 |
| 2:M:732:ALA:HA | 2:M:735:ARG:HG2 | 1.99 | 0.44 |
| 2:M:731:GLU:HA | 2:M:734:LEU:HD12 | 2.00 | 0.44 |
| 2:C:683:ASN:N | 2:C:683:ASN:HD22 | 2.11 | 0.44 |
| 5:P:362:SER:O | 5:P:363:GLU:C | 2.55 | 0.44 |
| 2:M:140:ILE:HA | 2:M:332:ARG:O | 2.17 | 0.44 |
| 2:M:240:THR:O | 2:M:242:LEU:N | 2.51 | 0.44 |
| 2:M:336:VAL:O | 2:M:337:GLY:C | 2.56 | 0.44 |
| 2:M:410:ILE:HG22 | 2:M:411:SER:N | 2.31 | 0.44 |
| 2:C:162:ILE:C | 2:C:163:ILE:HG13 | 2.38 | 0.44 |
| 2:C:546:LEU:CD2 | 2:C:583:LEU:HB2 | 2.47 | 0.44 |
| 3:D:1072:ILE:HG13 | 3:D:1072:ILE:H | 1.45 | 0.44 |
| 3:N:148:GLU:C | 3:N:149:LYS:HD3 | 2.36 | 0.44 |
| 3:N:545:ARG:CZ | 5:P:257:THR:HA | 2.48 | 0.44 |
| 3:N:563:PRO:CD | 3:N:566:ILE:HD11 | 2.42 | 0.44 |
| 3:N:563:PRO:C | 3:N:567:ILE:HG12 | 2.38 | 0.44 |
| 2:C:1096:ALA:C | 2:C:1097:LEU:HG | 2.37 | 0.44 |
| 4:E:19:LEU:C | 4:E:19:LEU:HD12 | 2.38 | 0.44 |
| 3:N:444:VAL:O | 3:N:444:VAL:HG23 | 2.17 | 0.44 |
| 5:P:346:THR:O | 5:P:349:LEU:N | 2.50 | 0.44 |
| 5:P:382:THR:HG22 | 5:P:394:ARG:HB2 | 1.98 | 0.44 |
| 5:P:397:ILE:HA | 5:P:400:ILE:HD12 | 1.98 | 0.44 |
| 1:B:61:VAL:HG13 | 1:B:163:ASN:HB3 | 2.00 | 0.44 |
| 2:M:310:LEU:HD12 | 2:M:310:LEU:O | 2.17 | 0.44 |
| 2:M:599:GLU:HG3 | 2:M:600:ASP:H | 1.80 | 0.44 |
| 5:F:354:LEU:HD23 | 5:F:418:LEU:HD23 | 1.98 | 0.44 |
| 5:P:305:GLU:CG | 5:P:309:LYS:HE3 | 2.38 | 0.44 |
| 5:F:296:GLY:C | 5:F:299:TRP:HD1 | 2.21 | 0.44 |
| 2:M:87:ASP:HA | 2:M:131:GLY:CA | 2.47 | 0.44 |
| 3:N:1496:GLU:OE2 | 3:N:1499:ARG:NE | 2.51 | 0.44 |
| 3:N:1286:THR:HB | 3:N:1289:LYS:O | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:N:827:ILE:HG23 | 3:N:837:GLY:CA | 2.47 | 0.44 |
| 3:N:885:ILE:H | 3:N:885:ILE:HG13 | 1.65 | 0.44 |
| 3:N:1353:GLN:HB3 | 3:N:1357:ARG:CZ | 2.47 | 0.44 |
| 1:L:185:ARG:HH22 | 3:N:692:GLU:CG | 2.30 | 0.44 |
| 3:N:664:LYS:HB2 | 3:N:666:ILE:CD1 | 2.47 | 0.44 |
| 1:K:212:ASN:O | 1:K:213:GLN:C | 2.55 | 0.44 |
| 2:M:930:LYS:HA | 2:M:930:LYS:HD3 | 1.64 | 0.44 |
| 1:K:9:PRO:HB2 | 1:K:25:LEU:CD1 | 2.46 | 0.44 |
| 3:N:1078:ARG:O | 3:N:1080:GLY:N | 2.50 | 0.44 |
| 5:F:159:ILE:HG22 | 5:F:163:LEU:HD11 | 2.00 | 0.44 |
| 2:C:807:ARG:C | 2:C:809:GLY:H | 2.19 | 0.44 |
| 2:C:136:ILE:HA | 2:C:136:ILE:HD13 | 1.84 | 0.44 |
| 2:M:457:ALA:N | 2:M:540:PHE:O | 2.50 | 0.44 |
| 2:M:396:ASP:HA | 2:M:633:GLN:NE2 | 2.32 | 0.44 |
| 3:D:431:VAL:HG12 | 3:D:432:TYR:N | 2.33 | 0.44 |
| 4:E:49:GLN:HG3 | 4:E:54:LEU:CD2 | 2.47 | 0.44 |
| 3:N:211:VAL:HG22 | 3:N:387:LEU:HG | 2.00 | 0.44 |
| 3:N:292:VAL:HG23 | 3:N:293:VAL:N | 2.23 | 0.44 |
| 2:C:227:PHE:CA | 2:C:237:ARG:HH12 | 2.22 | 0.44 |
| 3:N:28:LYS:HG2 | 3:N:42:ASP:HB3 | 1.98 | 0.44 |
| 3:N:416:ALA:HB3 | 3:N:432:TYR:CD2 | 2.51 | 0.44 |
| 3:D:520:LEU:HG | 3:D:524:LEU:HB2 | 1.99 | 0.44 |
| 3:D:564:GLU:CD | 3:D:564:GLU:C | 2.76 | 0.44 |
| 5:F:222:ARG:O | 5:F:225:GLU:HB3 | 2.17 | 0.44 |
| 3:N:408:GLU:CB | 3:N:421:LEU:O | 2.64 | 0.44 |
| 3:D:368:VAL:HB | 3:D:377:VAL:CB | 2.48 | 0.44 |
| 3:D:223:LEU:N | 3:D:333:LEU:O | 2.47 | 0.44 |
| 1:B:101:LEU:HB3 | 1:B:140:MET:CE | 2.46 | 0.44 |
| 1:B:98:THR:HA | 1:B:142:VAL:O | 2.17 | 0.44 |
| 1:B:215:VAL:CG2 | 1:B:216:GLU:H | 2.30 | 0.44 |
| 1:B:218:LEU:O | 1:B:221:HIS:N | 2.50 | 0.44 |
| 3:D:186:VAL:HA | 3:D:200:ASP:OD2 | 2.17 | 0.44 |
| 5:F:401:GLU:HG2 | 5:F:405:LEU:HD11 | 1.97 | 0.44 |
| 2:M:102:HIS:NE2 | 2:M:108:ILE:CD1 | 2.80 | 0.44 |
| 2:M:369:PRO:HB2 | 2:M:371:LYS:HG2 | 2.00 | 0.44 |
| 3:D:1115:THR:O | 3:D:1151:ARG:NH2 | 2.50 | 0.44 |
| 3:D:1387:SER:HB3 | 3:D:1391:GLU:OE2 | 2.18 | 0.44 |
| 2:C:674:VAL:CB | 2:C:869:VAL:HG13 | 2.48 | 0.44 |
| 3:N:878:GLY:O | 3:N:879:ARG:C | 2.56 | 0.44 |
| 3:N:792:ILE:HD12 | 3:N:881:LEU:HD23 | 1.99 | 0.44 |
| 3:D:417:PRO:HG2 | 3:D:428:LYS:CE | 2.48 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:658:LEU:HD23 | 3:N:661:MET:CE | 2.46 | 0.44 |
| 3:N:804:LEU:O | 3:N:805:GLU:HG2 | 2.17 | 0.44 |
| 3:N:819:GLY:O | 3:N:824:ASN:ND2 | 2.51 | 0.44 |
| 2:M:628:PHE:HA | 2:M:638:ASP:HB3 | 1.99 | 0.44 |
| 3:D:1372:VAL:HG13 | 3:D:1375:MET:HE3 | 1.98 | 0.44 |
| 3:N:1048:PRO:C | 3:N:1050:GLY:N | 2.70 | 0.44 |
| 2:M:532:MET:HG2 | 2:M:533:ASP:N | 2.33 | 0.44 |
| 2:C:843:HIS:C | 2:C:845:ASN:H | 2.21 | 0.44 |
| 3:N:502:PHE:O | 3:N:506:GLY:N | 2.51 | 0.44 |
| 2:M:79:PRO:HG2 | 2:M:82:GLU:CB | 2.47 | 0.44 |
| 4:O:81:PRO:O | 4:O:85:LEU:CD2 | 2.66 | 0.44 |
| 3:N:1310:ARG:HD3 | 3:N:1327:ARG:HD3 | 2.00 | 0.44 |
| 2:M:267:TYR:HB3 | 2:M:270:GLY:CA | 2.47 | 0.44 |
| 2:M:283:ILE:CG2 | 2:M:284:ARG:N | 2.59 | 0.44 |
| 2:M:540:PHE:HB3 | 2:M:544:THR:HG21 | 2.00 | 0.44 |
| 3:N:227:LEU:HD12 | 3:N:331:VAL:HG23 | 2.00 | 0.44 |
| 1:A:14:ARG:NH1 | 1:A:14:ARG:HG2 | 2.33 | 0.44 |
| 2:C:191:PHE:HD2 | 2:C:195:LEU:CD1 | 2.29 | 0.44 |
| 2:C:322:VAL:HG12 | 2:C:323:ASP:N | 2.31 | 0.44 |
| 3:D:1082:ALA:O | 3:D:1083:ASP:C | 2.56 | 0.44 |
| 3:D:1084:THR:O | 3:D:1085:ALA:C | 2.56 | 0.44 |
| 3:N:161:LEU:HD23 | 3:N:161:LEU:N | 2.31 | 0.44 |
| 3:D:108:VAL:HA | 3:D:110:SER:N | 2.32 | 0.44 |
| 3:D:465:LEU:HD13 | 3:D:509:PRO:O | 2.18 | 0.44 |
| 5:F:117:SER:N | 5:F:127:ILE:CD1 | 2.81 | 0.44 |
| 3:D:732:VAL:C | 3:D:734:GLU:N | 2.70 | 0.44 |
| 3:D:937:TYR:O | 3:D:938:GLY:C | 2.56 | 0.44 |
| 3:D:832:ARG:C | 3:D:834:THR:H | 2.19 | 0.44 |
| 1:A:205:VAL:HG12 | 1:A:206:THR:N | 2.32 | 0.44 |
| 5:P:300:ASP:HB3 | 5:P:302:LYS:CE | 2.48 | 0.44 |
| 5:F:307:THR:O | 5:F:311:ALA:N | 2.48 | 0.44 |
| 3:N:1492:LEU:HA | 3:N:1492:LEU:HD23 | 1.86 | 0.44 |
| 3:D:1149:LEU:HD21 | 3:D:1153:VAL:HG23 | 1.99 | 0.44 |
| 3:N:1405:GLU:O | 3:N:1410:GLU:CA | 2.65 | 0.44 |
| 3:D:1424:VAL:O | 3:D:1425:THR:C | 2.55 | 0.44 |
| 1:B:179:PHE:HB2 | 1:B:196:THR:O | 2.18 | 0.44 |
| 3:D:55:ASP:HA | 3:D:83:SER:H | 1.83 | 0.44 |
| 1:K:183:ASP:HA | 1:K:192:LEU:O | 2.18 | 0.44 |
| 1:L:241:GLU:N | 1:L:242:PRO:CD | 2.73 | 0.44 |
| 2:M:1008:ARG:HD2 | 2:M:1028:GLY:C | 2.38 | 0.44 |
| 1:K:23:PHE:CD2 | 1:K:211:LEU:HD23 | 2.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:L:96:THR:HB | 1:L:145:ASP:OD1 | 2.18 | 0.44 |
| 1:K:29:GLU:O | 1:K:32:PHE:HB2 | 2.17 | 0.44 |
| 3:D:1258:ARG:NH2 | 3:D:1351:GLU:CG | 2.81 | 0.44 |
| 1:B:106:PRO:HA | 1:B:133:GLU:CA | 2.38 | 0.44 |
| 3:D:984:THR:HG22 | 3:D:987:GLU:CD | 2.38 | 0.44 |
| 2:C:807:ARG:NH1 | 2:C:807:ARG:HB2 | 2.33 | 0.44 |
| 1:L:167:VAL:CG1 | 1:L:168:ASP:N | 2.80 | 0.44 |
| 5:P:238:TYR:CG | 5:P:239:ALA:N | 2.82 | 0.44 |
| 1:A:24:VAL:CG1 | 1:A:25:LEU:N | 2.80 | 0.44 |
| 2:C:1039:ALA:O | 2:C:1042:ALA:HB3 | 2.17 | 0.44 |
| 1:L:5:LYS:NZ | 1:L:189:ARG:NE | 2.66 | 0.44 |
| 5:P:229:TYR:O | 5:P:231:ARG:N | 2.51 | 0.44 |
| 3:N:900:ILE:HG22 | 3:N:901:GLN:N | 2.32 | 0.44 |
| 1:K:65:PHE:N | 1:K:65:PHE:CD1 | 2.85 | 0.44 |
| 2:M:136:ILE:HG22 | 2:M:336:VAL:HG22 | 1.99 | 0.44 |
| 2:M:194:VAL:HG13 | 2:M:197:LEU:HD12 | 1.99 | 0.44 |
| 2:M:208:ALA:HB1 | 2:M:218:VAL:HG21 | 1.99 | 0.44 |
| 4:E:39:VAL:HG12 | 4:E:72:ARG:HB3 | 1.98 | 0.44 |
| 2:C:148:PHE:N | 2:C:148:PHE:CD1 | 2.86 | 0.44 |
| 2:C:233:GLU:OE1 | 2:C:237:ARG:NH1 | 2.50 | 0.44 |
| 2:C:139:GLN:C | 2:C:333:ILE:HD12 | 2.38 | 0.44 |
| 3:D:1068:LEU:O | 3:D:1069:GLU:C | 2.56 | 0.44 |
| 3:N:553:ARG:HD3 | 5:P:215:GLU:OE1 | 2.18 | 0.44 |
| 3:D:139:GLY:O | 3:D:147:VAL:CB | 2.53 | 0.44 |
| 3:D:563:PRO:C | 3:D:565:ILE:N | 2.71 | 0.44 |
| 5:F:185:GLN:O | 5:F:188:ILE:HB | 2.17 | 0.44 |
| 5:F:213:ILE:HG13 | 5:F:213:ILE:H | 1.59 | 0.44 |
| 3:N:400:VAL:HG22 | 3:N:402:PRO:CD | 2.46 | 0.44 |
| 3:N:443:VAL:HG12 | 3:N:444:VAL:N | 2.32 | 0.44 |
| 3:D:934:LEU:HG | 3:D:934:LEU:H | 1.55 | 0.44 |
| 2:M:640:ARG:O | 2:M:657:ASP:N | 2.49 | 0.44 |
| 2:C:1068:GLU:O | 2:C:1071:ILE:HB | 2.17 | 0.44 |
| 3:D:660:LYS:CG | 3:D:694:VAL:HG22 | 2.27 | 0.44 |
| 2:C:115:LEU:CB | 2:C:375:SER:HB3 | 2.42 | 0.44 |
| 5:P:373:LYS:HZ1 | 5:P:373:LYS:HB3 | 1.77 | 0.44 |
| 2:M:807:ARG:HB3 | 2:M:807:ARG:CZ | 2.47 | 0.44 |
| 2:C:774:LEU:HA | 2:C:777:ILE:CD1 | 2.44 | 0.44 |
| 2:M:239:PHE:HE2 | 2:M:250:ARG:HD2 | 1.82 | 0.44 |
| 3:D:1155:VAL:O | 3:D:1156:LEU:C | 2.55 | 0.44 |
| 3:D:1160:LEU:HD22 | 3:D:1164:ARG:CD | 2.47 | 0.44 |
| 3:N:266:GLU:OE1 | 3:N:314:PRO:HA | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:N:1405:GLU:CD | 3:N:1406:ARG:HG3 | 2.37 | 0.44 |
| 3:D:1397:LYS:CB | 3:D:1398:TRP:HZ3 | 2.31 | 0.44 |
| 2:C:874:LEU:O | 2:C:877:PRO:HD2 | 2.17 | 0.44 |
| 3:D:910:SER:HG | 3:D:911:LEU:H | 1.65 | 0.44 |
| 2:C:984:GLU:O | 3:D:946:GLY:HA3 | 2.18 | 0.44 |
| 3:N:778:LEU:HA | 3:N:778:LEU:HD13 | 1.82 | 0.44 |
| 3:N:1172:HIS:O | 3:N:1173:LEU:C | 2.55 | 0.44 |
| 3:N:1191:PRO:C | 3:N:1193:THR:N | 2.70 | 0.44 |
| 2:M:1019:GLN:O | 2:M:1020:PRO:C | 2.55 | 0.44 |
| 2:C:720:GLU:HB3 | 2:C:760:SER:CB | 2.41 | 0.44 |
| 2:M:52:PHE:HB3 | 2:M:53:PRO:HA | 1.99 | 0.44 |
| 3:D:1253:THR:HG21 | 3:D:1258:ARG:N | 2.32 | 0.44 |
| 2:C:610:ARG:NH1 | 2:C:610:ARG:HG3 | 2.32 | 0.44 |
| 3:N:207:PHE:CD1 | 3:N:391:ALA:HB3 | 2.53 | 0.44 |
| 3:D:881:LEU:O | 3:D:884:ARG:HB3 | 2.18 | 0.44 |
| 3:D:884:ARG:HG3 | 3:D:888:GLU:OE2 | 2.18 | 0.44 |
| 3:D:890:VAL:HG23 | 3:D:892:ASP:H | 1.83 | 0.44 |
| 2:C:347:GLY:HA3 | 2:C:381:ALA:HB2 | 2.00 | 0.44 |
| 2:M:564:MET:O | 2:M:567:GLN:N | 2.51 | 0.44 |
| 3:N:984:THR:HG23 | 3:N:987:GLU:H | 1.83 | 0.44 |
| 2:M:462:ASP:C | 2:M:464:LEU:H | 2.21 | 0.44 |
| 2:M:473:ARG:NE | 2:M:482:GLU:OE1 | 2.41 | 0.44 |
| 1:A:26:GLU:OE1 | 1:A:194:LYS:HE3 | 2.17 | 0.44 |
| 2:C:154:ARG:C | 2:C:156:GLY:H | 2.21 | 0.44 |
| 3:N:960:LYS:O | 3:N:961:LYS:C | 2.56 | 0.44 |
| 5:P:118:GLU:HG2 | 5:P:119:ILE:N | 2.30 | 0.44 |
| 2:M:193:LEU:HD11 | 2:M:303:PHE:HD2 | 1.82 | 0.44 |
| 2:M:333:ILE:O | 2:M:333:ILE:HG23 | 2.18 | 0.44 |
| 2:C:302:VAL:C | 2:C:304:LEU:N | 2.71 | 0.44 |
| 2:C:280:LYS:O | 2:C:309:TYR:CZ | 2.71 | 0.44 |
| 2:C:554:ASP:OD2 | 2:C:556:ASN:HB2 | 2.17 | 0.44 |
| 2:C:580:MET:O | 2:C:902:ILE:HA | 2.17 | 0.44 |
| 2:C:906:PHE:HZ | 3:D:1070:TYR:CG | 2.36 | 0.44 |
| 3:N:521:PRO:HB2 | 3:N:524:LEU:HG | 2.00 | 0.44 |
| 3:D:127:LEU:HD23 | 3:D:128:TYR:HA | 2.00 | 0.44 |
| 3:D:125:GLN:NE2 | 3:D:587:ARG:HE | 2.12 | 0.44 |
| 3:D:258:VAL:O | 3:D:271:VAL:O | 2.35 | 0.44 |
| 3:D:274:ARG:NE | 3:D:279:VAL:CG1 | 2.80 | 0.44 |
| 3:N:362:GLU:O | 3:N:365:ASP:HB2 | 2.17 | 0.44 |
| 3:D:245:LEU:N | 3:D:309:GLY:N | 2.61 | 0.44 |
| 4:E:6:ILE:O | 4:E:10:PHE:CD1 | 2.70 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:811:GLU:CB | 3:D:815:ALA:HB3 | 2.47 | 0.44 |
| 5:F:354:LEU:HD23 | 5:F:418:LEU:CD2 | 2.48 | 0.44 |
| 2:M:727:PRO:HD2 | 2:M:787:ASP:HB2 | 1.99 | 0.44 |
| 2:M:1101:THR:HA | 3:N:5:VAL:HG11 | 1.99 | 0.44 |
| 3:N:1033:GLN:H | 3:N:1033:GLN:NE2 | 2.13 | 0.44 |
| 2:M:872:ASN:HA | 2:M:873:PRO:HD3 | 1.80 | 0.44 |
| 3:N:799:LYS:HB2 | 3:N:826:PRO:CG | 2.47 | 0.44 |
| 5:F:82:ARG:HA | 5:F:85:LEU:HB2 | 1.99 | 0.44 |
| 3:D:871:LYS:NZ | 3:D:897:TRP:CH2 | 2.85 | 0.44 |
| 2:C:575:GLN:HE21 | 2:C:670:GLN:HG2 | 1.81 | 0.44 |
| 1:L:185:ARG:HH22 | 3:N:692:GLU:HG3 | 1.83 | 0.44 |
| 1:K:57:TYR:CE1 | 1:K:163:ASN:HB2 | 2.52 | 0.44 |
| 1:K:11:PHE:HD2 | 1:L:227:ASN:C | 2.20 | 0.44 |
| 3:D:1122:LEU:C | 3:D:1135:ARG:HG3 | 2.37 | 0.44 |
| 1:A:69:PRO:HA | 2:C:607:ASP:CG | 2.39 | 0.44 |
| 3:D:1280:VAL:HA | 3:D:1317:ASP:O | 2.18 | 0.44 |
| 2:M:833:LEU:HD12 | 2:M:833:LEU:HA | 1.79 | 0.44 |
| 3:D:697:GLY:HA3 | 4:E:59:ASN:ND2 | 2.33 | 0.44 |
| 5:F:302:LYS:C | 5:F:302:LYS:HD2 | 2.38 | 0.44 |
| 5:F:361:LEU:CG | 5:F:362:SER:H | 2.31 | 0.44 |
| 5:P:233:PHE:HD1 | 5:P:233:PHE:O | 2.01 | 0.44 |
| 2:C:757:GLY:HA2 | 2:C:789:SER:CB | 2.48 | 0.44 |
| 3:D:372:ASP:C | 3:D:374:GLU:N | 2.69 | 0.44 |
| 2:M:206:THR:HA | 2:M:210:GLU:OE2 | 2.18 | 0.44 |
| 2:M:208:ALA:HB1 | 2:M:218:VAL:CG2 | 2.47 | 0.44 |
| 2:M:236:ILE:O | 2:M:237:ARG:C | 2.56 | 0.44 |
| 2:M:334:ARG:CB | 2:M:339:LEU:HD21 | 2.45 | 0.44 |
| 3:D:1489:GLN:HE22 | 4:E:72:ARG:HA | 1.83 | 0.44 |
| 4:E:39:VAL:O | 4:E:72:ARG:HD2 | 2.17 | 0.44 |
| 2:C:260:LEU:CB | 2:C:291:ALA:HB2 | 2.47 | 0.44 |
| 2:C:336:VAL:N | 2:C:339:LEU:HD12 | 2.32 | 0.44 |
| 3:N:122:GLU:O | 3:N:126:VAL:CG2 | 2.66 | 0.44 |
| 2:C:1104:GLU:C | 2:C:1106:ASP:N | 2.71 | 0.44 |
| 3:D:100:ALA:CB | 3:D:128:TYR:CE2 | 3.00 | 0.44 |
| 3:D:99:ALA:HB1 | 3:D:578:VAL:HG21 | 2.00 | 0.44 |
| 5:F:102:LEU:O | 5:F:105:LYS:HB2 | 2.18 | 0.44 |
| 5:F:184:ARG:O | 5:F:185:GLN:C | 2.55 | 0.44 |
| 3:D:931:LEU:O | 3:D:934:LEU:HB2 | 2.17 | 0.44 |
| 5:P:408:LEU:HD12 | 5:P:411:HIS:CE1 | 2.53 | 0.44 |
| 2:M:588:VAL:CG2 | 2:M:589:ARG:H | 2.29 | 0.44 |
| 5:F:348:SER:OG | 5:F:349:LEU:N | 2.51 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:60:GLY:C | 2:C:62:GLY:N | 2.68 | 0.44 |
| 5:P:291:ILE:O | 5:P:291:ILE:HD12 | 2.18 | 0.44 |
| 3:D:36:THR:CG2 | 3:D:38:LYS:HE2 | 2.48 | 0.44 |
| 3:D:35:ARG:HG3 | 3:D:36:THR:OG1 | 2.18 | 0.44 |
| 5:F:256:ARG:HH11 | 5:F:256:ARG:HG2 | 1.83 | 0.44 |
| 3:N:1267:ARG:NH2 | 3:N:1271:LYS:NZ | 2.53 | 0.44 |
| 3:D:800:LYS:HZ2 | 3:D:825:ALA:HA | 1.83 | 0.44 |
| 2:C:984:GLU:CD | 3:D:791:TYR:HE2 | 2.21 | 0.44 |
| 3:D:920:LEU:O | 3:D:921:ARG:C | 2.57 | 0.44 |
| 3:N:1091:SER:O | 3:N:1093:TYR:N | 2.50 | 0.44 |
| 2:M:677:MET:HB2 | 2:M:678:PRO:HD2 | 2.00 | 0.44 |
| 2:C:853:LEU:HA | 2:C:854:PRO:HD3 | 1.80 | 0.44 |
| 5:F:83:GLN:O | 5:F:84:TYR:C | 2.55 | 0.44 |
| 3:N:1476:THR:CG2 | 4:O:17:TYR:HB3 | 2.48 | 0.44 |
| 3:D:871:LYS:HG2 | 3:D:873:LEU:HD21 | 1.99 | 0.44 |
| 2:C:589:ARG:O | 2:C:592:LEU:HD23 | 2.18 | 0.44 |
| 2:C:832:LYS:HG2 | 2:C:833:LEU:N | 2.33 | 0.44 |
| 1:L:185:ARG:HB3 | 1:L:190:THR:HG23 | 2.00 | 0.44 |
| 2:M:1060:ILE:HG13 | 2:M:1083:GLU:CG | 2.48 | 0.44 |
| 3:N:664:LYS:O | 3:N:665:GLY:C | 2.56 | 0.44 |
| 2:M:477:GLY:O | 2:M:507:ARG:HA | 2.17 | 0.44 |
| 3:N:804:LEU:HD23 | 3:N:804:LEU:HA | 1.75 | 0.44 |
| 3:N:806:PHE:HE1 | 3:N:816:HIS:NE2 | 2.16 | 0.44 |
| 1:K:73:GLU:HB3 | 1:K:78:ILE:CG1 | 2.47 | 0.44 |
| 2:C:626:ARG:CG | 2:C:626:ARG:NH1 | 2.81 | 0.44 |
| 3:N:1404:ASN:CA | 3:N:1409:ALA:H | 2.31 | 0.44 |
| 3:D:1346:ARG:NH1 | 3:D:1346:ARG:HG3 | 2.32 | 0.44 |
| 1:A:139:ASN:O | 1:A:140:MET:HB3 | 2.17 | 0.44 |
| 5:P:100:VAL:O | 5:P:101:GLU:C | 2.55 | 0.44 |
| 3:N:1372:VAL:HG13 | 3:N:1375:MET:HE3 | 1.99 | 0.44 |
| 1:B:55:SER:HB3 | 1:B:166:PRO:HA | 2.00 | 0.44 |
| 1:A:1:MET:CA | 1:A:6:LEU:HD22 | 2.48 | 0.44 |
| 4:E:81:PRO:O | 4:E:85:LEU:HD21 | 2.17 | 0.44 |
| 3:N:1321:ALA:O | 3:N:1339:LYS:HE3 | 2.17 | 0.44 |
| 3:D:1059:SER:HB2 | 3:D:1065:LEU:HD22 | 2.00 | 0.44 |
| 2:M:264:PRO:HB2 | 2:M:289:THR:CB | 2.46 | 0.43 |
| 2:C:193:LEU:HD23 | 2:C:307:LEU:HD22 | 2.00 | 0.43 |
| 2:C:1015:LEU:HD13 | 5:F:335:ASP:HA | 1.99 | 0.43 |
| 3:D:566:ILE:HG13 | 3:D:567:ILE:N | 2.33 | 0.43 |
| 5:F:136:LEU:HB3 | 5:F:140:ARG:HD3 | 2.00 | 0.43 |
| 3:N:399:ARG:HD3 | 3:N:399:ARG:HA | 1.76 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:N:400:VAL:HG23 | 3:N:443:VAL:HG11 | 1.98 | 0.43 |
| 3:D:284:LEU:HD22 | 3:D:288:MET:HG2 | 1.99 | 0.43 |
| 3:D:244:GLU:CD | 3:D:310:LEU:HD23 | 2.38 | 0.43 |
| 5:P:380:GLU:HA | 5:P:385:GLU:OE2 | 2.17 | 0.43 |
| 1:B:38:ASN:HB3 | 1:B:39:PRO:CD | 2.34 | 0.43 |
| 5:P:267:THR:O | 5:P:270:LYS:HB3 | 2.18 | 0.43 |
| 5:P:268:ILE:HA | 5:P:271:LEU:HG | 1.99 | 0.43 |
| 5:P:370:LYS:O | 5:P:371:LEU:C | 2.55 | 0.43 |
| 1:L:104:GLU:HA | 1:L:132:LEU:HD13 | 2.00 | 0.43 |
| 3:D:953:ASP:C | 3:D:955:VAL:N | 2.72 | 0.43 |
| 3:D:1029:ARG:HH11 | 3:D:1029:ARG:CG | 2.14 | 0.43 |
| 3:D:921:ARG:HH11 | 3:D:921:ARG:HA | 1.82 | 0.43 |
| 3:N:492:ALA:O | 3:N:493:ARG:C | 2.55 | 0.43 |
| 3:D:1038:LEU:HD23 | 3:D:1061:PHE:CB | 2.47 | 0.43 |
| 1:K:186:LEU:O | 1:K:186:LEU:HG | 2.18 | 0.43 |
| 3:N:1091:SER:C | 3:N:1093:TYR:H | 2.18 | 0.43 |
| 3:N:1191:PRO:C | 3:N:1193:THR:H | 2.20 | 0.43 |
| 3:N:485:SER:C | 3:N:489:ARG:HD3 | 2.36 | 0.43 |
| 1:K:127:LEU:HD12 | 1:K:128:HIS:N | 2.33 | 0.43 |
| 3:N:803:GLY:C | 3:N:805:GLU:H | 2.21 | 0.43 |
| 2:C:713:ARG:NH2 | 2:C:758:ARG:HH12 | 2.15 | 0.43 |
| 1:B:13:VAL:HG21 | 1:B:23:PHE:CD2 | 2.53 | 0.43 |
| 1:L:54:THR:OG1 | 1:L:145:ASP:HB2 | 2.17 | 0.43 |
| 1:A:104:GLU:HA | 1:A:137:ARG:HA | 2.00 | 0.43 |
| 3:D:1286:THR:C | 3:D:1288:GLU:N | 2.70 | 0.43 |
| 3:D:1286:THR:HG22 | 3:D:1288:GLU:HB2 | 2.00 | 0.43 |
| 3:D:1347:TYR:CZ | 3:D:1351:GLU:HG2 | 2.53 | 0.43 |
| 3:D:142:LEU:HD13 | 3:D:144:GLY:N | 2.33 | 0.43 |
| 3:N:1126:ASP:OD1 | 3:N:1126:ASP:O | 2.35 | 0.43 |
| 3:D:985:ASP:N | 3:D:985:ASP:OD2 | 2.46 | 0.43 |
| 5:P:245:GLN:O | 5:P:246:ALA:C | 2.56 | 0.43 |
| 3:D:959:GLU:O | 3:D:962:GLN:HB2 | 2.18 | 0.43 |
| 3:D:1274:ILE:HA | 3:D:1325:LEU:HG | 2.00 | 0.43 |
| 1:L:13:VAL:CG2 | 1:L:14:ARG:N | 2.81 | 0.43 |
| 3:N:414:ARG:O | 3:N:415:VAL:CG1 | 2.66 | 0.43 |
| 1:K:99:LEU:CB | 1:K:114:PHE:CD2 | 3.00 | 0.43 |
| 3:D:579:ASP:O | 3:D:580:ALA:C | 2.56 | 0.43 |
| 3:N:919:PHE:CD1 | 3:N:919:PHE:C | 2.91 | 0.43 |
| 2:M:409:ARG:C | 2:M:410:ILE:HD12 | 2.38 | 0.43 |
| 2:C:157:ARG:CG | 2:C:158:TYR:N | 2.81 | 0.43 |
| 2:C:198:ARG:HE | 2:C:231:PRO:CG | 2.31 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:273:GLY:HA2 | 2:C:276:LYS:CG | 2.48 | 0.43 |
| 3:N:102:ILE:O | 3:N:105:VAL:N | 2.51 | 0.43 |
| 3:N:154:THR:HG23 | 3:N:156:GLU:HG2 | 2.00 | 0.43 |
| 3:N:437:VAL:HB | 5:P:179:GLU:OE2 | 2.18 | 0.43 |
| 5:P:188:ILE:O | 5:P:189:GLU:C | 2.56 | 0.43 |
| 2:C:1085:PHE:CD1 | 2:C:1085:PHE:C | 2.91 | 0.43 |
| 3:D:1443:THR:CG2 | 9:D:1529:NE6:H24 | 2.47 | 0.43 |
| 3:D:1450:ALA:HA | 3:D:1455:LYS:HG3 | 1.99 | 0.43 |
| 3:D:1467:ILE:HD11 | 9:D:1529:NE6:C19 | 2.48 | 0.43 |
| 3:D:241:ILE:CG1 | 3:D:312:ARG:HG2 | 2.48 | 0.43 |
| 5:P:355:GLU:HA | 5:P:358:LEU:CD2 | 2.48 | 0.43 |
| 5:P:410:TYR:HA | 5:P:413:SER:OG | 2.19 | 0.43 |
| 5:P:421:PHE:CD1 | 5:P:422:LEU:N | 2.86 | 0.43 |
| 4:O:39:VAL:HG12 | 4:O:39:VAL:O | 2.18 | 0.43 |
| 1:L:82:LEU:N | 1:L:82:LEU:HD23 | 2.33 | 0.43 |
| 3:D:815:ALA:O | 3:D:818:ARG:HB2 | 2.18 | 0.43 |
| 5:F:401:GLU:O | 5:F:402:ASN:C | 2.56 | 0.43 |
| 3:D:675:ARG:O | 3:D:677:LEU:N | 2.51 | 0.43 |
| 5:P:288:TYR:HB3 | 5:P:301:ALA:HA | 2.01 | 0.43 |
| 3:D:787:LEU:O | 3:D:788:GLY:C | 2.56 | 0.43 |
| 3:N:494:LYS:HA | 3:N:1388:ARG:NH1 | 2.23 | 0.43 |
| 2:M:750:LYS:O | 2:M:751:PRO:C | 2.55 | 0.43 |
| 3:N:912:LYS:HB3 | 3:N:912:LYS:NZ | 2.21 | 0.43 |
| 2:M:914:ILE:O | 2:M:917:LEU:N | 2.51 | 0.43 |
| 3:N:256:GLU:HB2 | 3:N:296:GLU:CG | 2.47 | 0.43 |
| 5:F:79:ASP:HB2 | 5:F:81:VAL:CG2 | 2.47 | 0.43 |
| 2:C:601:GLY:O | 2:C:648:ARG:HA | 2.17 | 0.43 |
| 2:C:833:LEU:HD12 | 2:C:833:LEU:HA | 1.81 | 0.43 |
| 1:L:208:LEU:CD1 | 1:L:212:ASN:HD21 | 2.31 | 0.43 |
| 3:N:692:GLU:O | 3:N:695:ILE:N | 2.51 | 0.43 |
| 2:M:854:PRO:HD2 | 2:M:857:ASP:OD1 | 2.18 | 0.43 |
| 2:M:928:LYS:O | 2:M:928:LYS:HG2 | 2.19 | 0.43 |
| 2:C:750:LYS:O | 2:C:751:PRO:C | 2.55 | 0.43 |
| 1:K:56:VAL:HG22 | 1:K:142:VAL:HG13 | 2.00 | 0.43 |
| 2:M:571:LEU:HD22 | 2:M:701:THR:N | 2.33 | 0.43 |
| 3:D:1286:THR:CG2 | 3:D:1288:GLU:HB2 | 2.48 | 0.43 |
| 1:A:161:ARG:H | 1:A:164:ALA:HB2 | 1.83 | 0.43 |
| 2:C:815:LEU:HD21 | 2:C:822:VAL:HG22 | 1.99 | 0.43 |
| 2:C:384:GLU:OE2 | 2:C:384:GLU:HA | 2.17 | 0.43 |
| 2:C:826:TYR:CD1 | 2:C:826:TYR:N | 2.87 | 0.43 |
| 1:L:86:VAL:HG22 | 1:L:123:MET:CG | 2.48 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:78:PHE:HD2 | 2:C:82:GLU:OE2 | 2.01 | 0.43 |
| 3:D:701:LEU:HD23 | 3:D:715:ALA:HB2 | 1.98 | 0.43 |
| 3:D:1209:LEU:HA | 3:D:1209:LEU:HD23 | 1.81 | 0.43 |
| 3:D:1000:THR:HG22 | 3:D:1036:ARG:HD2 | 1.99 | 0.43 |
| 3:D:711:LEU:C | 3:D:713:ILE:N | 2.71 | 0.43 |
| 1:L:5:LYS:HA | 1:L:5:LYS:HD3 | 1.81 | 0.43 |
| 3:D:1366:LYS:O | 3:D:1367:HIS:C | 2.56 | 0.43 |
| 3:N:1006:ALA:O | 3:N:1007:VAL:C | 2.57 | 0.43 |
| 4:E:73:LEU:HD12 | 4:E:74:VAL:N | 2.31 | 0.43 |
| 2:C:470:PRO:CB | 2:C:534:VAL:HG21 | 2.48 | 0.43 |
| 2:M:1000:MET:HB3 | 2:M:1002:GLU:HG3 | 2.00 | 0.43 |
| 2:M:576:ALA:HB3 | 2:M:900:ARG:HH12 | 1.83 | 0.43 |
| 3:D:1087:ARG:HB3 | 3:D:1234:THR:HA | 1.99 | 0.43 |
| 3:D:1087:ARG:HD2 | 3:D:1234:THR:CA | 2.48 | 0.43 |
| 3:N:903:ASP:O | 3:N:904:VAL:HG13 | 2.18 | 0.43 |
| 3:D:1132:LEU:HA | 3:D:1132:LEU:HD12 | 1.74 | 0.43 |
| 2:M:175:GLU:O | 2:M:183:SER:HB2 | 2.19 | 0.43 |
| 2:M:192:PRO:O | 2:M:193:LEU:C | 2.56 | 0.43 |
| 2:M:406:HIS:HA | 2:M:409:ARG:HD2 | 2.00 | 0.43 |
| 2:M:410:ILE:N | 2:M:453:THR:O | 2.51 | 0.43 |
| 3:N:223:LEU:C | 3:N:332:TYR:HA | 2.39 | 0.43 |
| 2:C:265:ARG:HA | 2:C:289:THR:OG1 | 2.18 | 0.43 |
| 2:C:329:GLY:HA3 | 2:C:489:THR:HG23 | 2.00 | 0.43 |
| 3:N:85:VAL:CG2 | 3:N:89:ARG:CZ | 2.91 | 0.43 |
| 3:D:520:LEU:HD21 | 3:D:524:LEU:HB2 | 1.98 | 0.43 |
| 4:E:21:VAL:O | 4:E:24:ALA:HB3 | 2.19 | 0.43 |
| 5:F:100:VAL:O | 5:F:101:GLU:C | 2.55 | 0.43 |
| 3:D:257:GLY:CA | 3:D:274:ARG:CA | 2.93 | 0.43 |
| 3:D:354:VAL:CB | 3:D:367:ILE:O | 2.65 | 0.43 |
| 5:P:352:GLU:CA | 5:P:355:GLU:OE2 | 2.57 | 0.43 |
| 5:P:386:VAL:HG11 | 5:P:394:ARG:N | 2.33 | 0.43 |
| 3:N:1491:THR:HG22 | 3:N:1491:THR:O | 2.17 | 0.43 |
| 1:B:100:LEU:HB3 | 1:B:115:LEU:HD22 | 1.99 | 0.43 |
| 5:F:410:TYR:O | 5:F:413:SER:HB2 | 2.18 | 0.43 |
| 2:M:599:GLU:HB3 | 2:M:615:TYR:CE2 | 2.53 | 0.43 |
| 2:C:368:THR:HB | 2:C:369:PRO:CD | 2.27 | 0.43 |
| 2:C:41:ASN:HD22 | 2:C:42:VAL:N | 2.16 | 0.43 |
| 2:C:55:GLU:HG2 | 2:C:56:GLU:N | 2.33 | 0.43 |
| 5:P:367:MET:HE2 | 5:P:371:LEU:HD21 | 1.99 | 0.43 |
| 2:M:815:LEU:HD13 | 2:M:819:VAL:HG12 | 2.00 | 0.43 |
| 3:D:1011:PHE:CD1 | 3:D:1021:TYR:HB2 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:876:VAL:O | 2:C:879:ARG:N | 2.46 | 0.43 |
| 3:D:788:GLY:O | 3:D:791:TYR:HB3 | 2.18 | 0.43 |
| 2:M:676:ILE:HD13 | 3:N:949:ILE:H | 1.83 | 0.43 |
| 2:M:910:LYS:O | 2:M:911:GLU:C | 2.57 | 0.43 |
| 2:C:693:GLU:HG3 | 2:C:697:ARG:NH1 | 2.32 | 0.43 |
| 2:C:694:LEU:HD23 | 2:C:697:ARG:HH22 | 1.82 | 0.43 |
| 2:C:673:LEU:N | 2:C:868:ASP:OD2 | 2.47 | 0.43 |
| 3:N:1481:VAL:HG12 | 4:O:21:VAL:HG21 | 2.01 | 0.43 |
| 1:K:38:ASN:O | 1:K:39:PRO:C | 2.56 | 0.43 |
| 1:L:42:ARG:HH22 | 2:M:939:ARG:HH21 | 1.66 | 0.43 |
| 2:C:504:GLU:HG3 | 2:C:507:ARG:HD3 | 2.00 | 0.43 |
| 2:C:783:ARG:C | 2:C:785:VAL:H | 2.21 | 0.43 |
| 3:D:887:ALA:CA | 3:D:890:VAL:HG22 | 2.48 | 0.43 |
| 3:D:623:VAL:CG1 | 3:D:624:ASP:N | 2.81 | 0.43 |
| 1:K:1:MET:HA | 1:K:6:LEU:HD22 | 2.00 | 0.43 |
| 3:N:990:ASP:HA | 3:N:993:LEU:HG | 2.00 | 0.43 |
| 3:D:500:ARG:O | 3:D:504:ASP:CB | 2.66 | 0.43 |
| 2:C:685:GLU:C | 2:C:687:ALA:H | 2.20 | 0.43 |
| 4:E:81:PRO:O | 4:E:85:LEU:CD2 | 2.66 | 0.43 |
| 3:D:1145:TYR:CD2 | 3:D:1146:GLY:N | 2.87 | 0.43 |
| 2:M:54:ILE:O | 2:M:54:ILE:HG23 | 2.17 | 0.43 |
| 2:M:204:GLN:CD | 2:M:225:SER:HA | 2.38 | 0.43 |
| 2:M:289:THR:HG22 | 2:M:290:LEU:CD2 | 2.48 | 0.43 |
| 2:M:581:THR:N | 2:M:584:GLU:OE2 | 2.51 | 0.43 |
| 2:C:191:PHE:CD2 | 2:C:195:LEU:CD1 | 3.01 | 0.43 |
| 2:C:517:ARG:O | 2:C:520:GLU:CB | 2.67 | 0.43 |
| 2:C:583:LEU:O | 2:C:586:ARG:N | 2.51 | 0.43 |
| 3:N:130:SER:N | 3:N:568:ARG:HH21 | 2.15 | 0.43 |
| 3:N:573:MET:CE | 5:P:210:LEU:HB2 | 2.48 | 0.43 |
| 3:N:539:ASP:H | 5:P:318:GLU:CD | 2.21 | 0.43 |
| 3:D:106:LYS:HB3 | 3:D:586:ARG:NH1 | 2.32 | 0.43 |
| 3:D:761:ILE:CD1 | 4:E:20:THR:HA | 2.49 | 0.43 |
| 3:N:408:GLU:OE2 | 3:N:444:VAL:HG11 | 2.18 | 0.43 |
| 3:N:1488:ASP:C | 3:N:1490:LYS:N | 2.71 | 0.43 |
| 1:L:78:ILE:O | 1:L:81:ASN:HB2 | 2.18 | 0.43 |
| 3:D:810:GLU:C | 3:D:812:ALA:H | 2.21 | 0.43 |
| 3:D:819:GLY:HA2 | 3:D:822:ALA:HB3 | 1.98 | 0.43 |
| 5:P:276:ARG:C | 5:P:278:LEU:H | 2.22 | 0.43 |
| 5:P:289:GLU:N | 5:P:289:GLU:CD | 2.69 | 0.43 |
| 5:P:373:LYS:HE3 | 5:P:379:ARG:HB3 | 2.00 | 0.43 |
| 3:D:1404:ASN:OD1 | 3:D:1408:ILE:HG22 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:L:114:PHE:O | 1:L:116:PRO:HD3 | 2.18 | 0.43 |
| 3:N:970:LYS:HA | 3:N:973:GLN:NE2 | 2.34 | 0.43 |
| 1:B:188:GLN:CG | 1:B:189:ARG:HG3 | 2.47 | 0.43 |
| 3:D:907:GLU:OE1 | 3:D:909:ASN:N | 2.51 | 0.43 |
| 3:D:553:ARG:HG2 | 3:D:557:LEU:HD11 | 1.99 | 0.43 |
| 2:M:690:ILE:CG2 | 2:M:691:SER:N | 2.81 | 0.43 |
| 3:N:473:LEU:O | 3:N:476:GLU:HB3 | 2.18 | 0.43 |
| 3:D:28:LYS:HE2 | 3:D:42:ASP:HB3 | 2.00 | 0.43 |
| 3:N:1451:ALA:O | 3:N:1454:GLY:N | 2.51 | 0.43 |
| 1:K:124:ASN:CB | 1:K:127:LEU:HB2 | 2.48 | 0.43 |
| 1:K:34:VAL:CB | 1:L:42:ARG:NH1 | 2.79 | 0.43 |
| 2:C:20:GLU:CA | 2:C:23:VAL:HG22 | 2.47 | 0.43 |
| 2:C:18:LEU:O | 2:C:21:ILE:HD13 | 2.18 | 0.43 |
| 3:N:634:GLY:HA3 | 3:N:637:LEU:CG | 2.47 | 0.43 |
| 5:P:328:PHE:CD1 | 5:P:328:PHE:N | 2.87 | 0.43 |
| 3:N:1324:PRO:C | 3:N:1325:LEU:HD23 | 2.39 | 0.43 |
| 3:D:95:LEU:HB3 | 3:D:97:THR:O | 2.19 | 0.43 |
| 2:C:807:ARG:O | 2:C:808:ARG:C | 2.56 | 0.43 |
| 2:C:809:GLY:HA3 | 2:C:813:VAL:CG2 | 2.48 | 0.43 |
| 2:M:559:LEU:HG | 2:M:560:MET:N | 2.31 | 0.43 |
| 2:M:562:SER:O | 2:M:563:ASN:C | 2.56 | 0.43 |
| 5:P:238:TYR:O | 5:P:240:THR:N | 2.51 | 0.43 |
| 3:D:1221:VAL:HG12 | 3:D:1370:ILE:HD13 | 2.01 | 0.43 |
| 5:F:107:GLU:OE2 | 5:F:229:TYR:CD1 | 2.71 | 0.43 |
| 2:M:576:ALA:HB3 | 2:M:900:ARG:NH1 | 2.33 | 0.43 |
| 2:M:768:THR:HB | 2:M:771:GLU:CB | 2.48 | 0.43 |
| 5:F:231:ARG:HB3 | 5:F:233:PHE:HE2 | 1.83 | 0.43 |
| 3:N:1047:LYS:N | 3:N:1051:GLU:O | 2.46 | 0.43 |
| 3:D:1008:PHE:H | 3:D:1008:PHE:HD1 | 1.66 | 0.43 |
| 2:M:185:LYS:HE2 | 2:M:190:LYS:HZ2 | 1.84 | 0.43 |
| 2:M:334:ARG:HH11 | 2:M:418:LEU:CD1 | 2.30 | 0.43 |
| 2:C:195:LEU:O | 2:C:199:VAL:HG23 | 2.18 | 0.43 |
| 2:C:227:PHE:N | 2:C:227:PHE:CD1 | 2.86 | 0.43 |
| 2:C:458:TYR:HB2 | 2:C:538:GLN:HA | 2.00 | 0.43 |
| 3:D:1066:THR:HB | 3:D:1069:GLU:CB | 2.48 | 0.43 |
| 3:N:573:MET:O | 3:N:574:LEU:C | 2.56 | 0.43 |
| 5:P:225:GLU:O | 5:P:227:PHE:N | 2.51 | 0.43 |
| 3:D:1495:ILE:HG13 | 4:E:84:ARG:HH11 | 1.78 | 0.43 |
| 3:D:522:PRO:O | 3:D:524:LEU:N | 2.51 | 0.43 |
| 3:D:408:GLU:HG3 | 3:D:422:ALA:N | 2.34 | 0.43 |
| 4:E:5:GLY:O | 4:E:6:ILE:C | 2.57 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:P:385:GLU:O | 5:P:388:ALA:HB3 | 2.19 | 0.43 |
| 2:C:105:THR:O | 2:C:107:LEU:HG | 2.17 | 0.43 |
| 2:C:110:GLU:CB | 2:C:369:PRO:HB3 | 2.48 | 0.43 |
| 3:D:36:THR:HG22 | 3:D:38:LYS:HE2 | 2.01 | 0.43 |
| 3:D:34:TYR:HE2 | 5:F:261:PRO:HD3 | 1.83 | 0.43 |
| 3:D:801:GLY:HA2 | 3:D:830:ALA:HB3 | 2.01 | 0.43 |
| 3:D:1031:ASN:HB2 | 3:D:1032:PRO:HD2 | 1.99 | 0.43 |
| 3:D:909:ASN:O | 3:D:912:LYS:N | 2.52 | 0.43 |
| 3:N:1434:TRP:NE1 | 3:N:1435:LEU:HD23 | 2.33 | 0.43 |
| 2:M:691:SER:O | 2:M:692:GLU:C | 2.57 | 0.43 |
| 2:M:971:LYS:NZ | 3:N:950:GLY:HA3 | 2.33 | 0.43 |
| 3:N:274:ARG:C | 3:N:275:GLU:HG3 | 2.39 | 0.43 |
| 3:N:1174:LEU:O | 3:N:1177:ALA:HB3 | 2.19 | 0.43 |
| 1:L:211:LEU:O | 1:L:212:ASN:C | 2.56 | 0.43 |
| 1:L:215:VAL:HG23 | 1:L:216:GLU:N | 2.32 | 0.43 |
| 2:M:1087:VAL:O | 2:M:1090:LYS:HB2 | 2.18 | 0.43 |
| 3:N:664:LYS:O | 3:N:666:ILE:N | 2.52 | 0.43 |
| 3:D:629:SER:HB3 | 3:D:726:ILE:CD1 | 2.49 | 0.43 |
| 2:M:961:GLU:OE2 | 2:M:964:LYS:HB3 | 2.19 | 0.43 |
| 2:M:857:ASP:HB2 | 2:M:978:ARG:HG2 | 1.99 | 0.43 |
| 3:D:59:ALA:C | 3:D:61:GLY:H | 2.22 | 0.43 |
| 5:F:157:GLU:O | 5:F:158:GLU:C | 2.56 | 0.43 |
| 3:D:1280:VAL:CG1 | 3:D:1281:VAL:N | 2.81 | 0.43 |
| 1:K:179:PHE:HB2 | 1:K:195:LEU:HD11 | 2.00 | 0.43 |
| 5:P:127:ILE:O | 5:P:130:VAL:N | 2.45 | 0.43 |
| 2:M:1055:LEU:CG | 2:M:1079:PRO:HG3 | 2.48 | 0.43 |
| 3:N:197:SER:OG | 3:N:199:LEU:O | 2.36 | 0.43 |
| 3:N:1260:ILE:O | 3:N:1261:GLU:C | 2.57 | 0.43 |
| 2:M:731:GLU:C | 2:M:733:ALA:H | 2.21 | 0.43 |
| 3:D:754:PHE:O | 3:D:757:ALA:HB3 | 2.18 | 0.43 |
| 2:M:247:PRO:HA | 2:M:248:PRO:HD3 | 1.75 | 0.43 |
| 2:M:205:GLU:N | 2:M:209:ARG:NH1 | 2.66 | 0.43 |
| 2:M:271:GLU:HA | 2:M:274:ARG:HB3 | 2.00 | 0.43 |
| 2:M:439:CYS:CB | 2:M:541:SER:H | 2.31 | 0.43 |
| 2:C:151:ASP:H | 2:C:158:TYR:CB | 2.31 | 0.43 |
| 2:C:285:LEU:HD11 | 2:C:289:THR:HA | 2.01 | 0.43 |
| 3:N:41:ARG:HA | 3:N:46:ASP:OD1 | 2.18 | 0.43 |
| 3:N:45:PHE:O | 3:N:86:ARG:NH2 | 2.52 | 0.43 |
| 3:N:525:ARG:NH1 | 3:N:525:ARG:CG | 2.78 | 0.43 |
| 5:P:188:ILE:HG13 | 5:P:188:ILE:H | 1.61 | 0.43 |
| 3:N:566:ILE:CG2 | 5:P:192:LEU:HD22 | 2.48 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:238:PRO:CG | 3:D:318:ARG:HA | 2.49 | 0.43 |
| 3:D:1439:SER:OG | 3:D:1463:LYS:HE2 | 2.18 | 0.43 |
| 3:D:570:GLU:O | 3:D:571:LYS:C | 2.57 | 0.43 |
| 5:F:114:LYS:O | 5:F:115:LYS:C | 2.55 | 0.43 |
| 3:D:930:LEU:HG | 3:D:934:LEU:CD1 | 2.36 | 0.43 |
| 5:P:347:GLN:O | 5:P:350:LEU:HB3 | 2.18 | 0.43 |
| 3:D:806:PHE:CE1 | 3:D:816:HIS:NE2 | 2.87 | 0.43 |
| 2:M:100:LEU:CD2 | 2:M:368:THR:HA | 2.48 | 0.43 |
| 5:P:288:TYR:O | 5:P:289:GLU:C | 2.56 | 0.43 |
| 3:N:1499:ARG:HD2 | 3:N:1499:ARG:C | 2.39 | 0.43 |
| 3:D:1399:ASP:O | 3:D:1408:ILE:CD1 | 2.66 | 0.43 |
| 2:M:904:PRO:HD2 | 2:M:908:GLY:HA2 | 1.97 | 0.43 |
| 3:N:972:LEU:CD2 | 3:N:972:LEU:N | 2.81 | 0.43 |
| 3:N:1024:ALA:HB2 | 3:N:1035:ILE:HD11 | 1.99 | 0.43 |
| 3:D:206:ARG:HG3 | 3:D:393:ILE:HA | 1.99 | 0.43 |
| 2:C:861:LEU:HG | 2:C:865:THR:OG1 | 2.18 | 0.43 |
| 1:B:80:LEU:HB3 | 3:D:844:ALA:CB | 2.49 | 0.43 |
| 3:D:846:PRO:O | 3:D:849:ALA:N | 2.52 | 0.43 |
| 1:A:191:ASP:O | 2:C:938:LYS:NZ | 2.51 | 0.43 |
| 1:A:5:LYS:C | 1:A:7:LYS:N | 2.72 | 0.43 |
| 3:N:1341:PRO:C | 3:N:1345:GLU:HG3 | 2.39 | 0.43 |
| 2:M:1089:VAL:HG13 | 2:M:1099:VAL:HB | 2.01 | 0.43 |
| 3:N:665:GLY:O | 3:N:667:ALA:N | 2.51 | 0.43 |
| 1:K:214:ALA:O | 1:K:217:ILE:HB | 2.19 | 0.43 |
| 2:M:327:HIS:CE1 | 2:M:433:THR:HG21 | 2.52 | 0.43 |
| 3:D:62:LYS:HE3 | 3:D:75:ARG:CZ | 2.49 | 0.43 |
| 2:M:76:PRO:HA | 2:M:91:GLN:O | 2.19 | 0.43 |
| 2:C:1051:GLU:OE2 | 2:C:1056:LYS:HE3 | 2.18 | 0.43 |
| 3:N:1130:ARG:HH22 | 3:N:1319:VAL:HG12 | 1.84 | 0.43 |
| 2:C:342:ASP:OD1 | 2:C:343:GLN:N | 2.51 | 0.43 |
| 2:C:893:ALA:HB1 | 2:C:897:LEU:CD1 | 2.49 | 0.43 |
| 2:C:353:ARG:CG | 2:C:353:ARG:NH1 | 2.80 | 0.43 |
| 3:N:178:LEU:HG | 3:N:181:ASP:CB | 2.44 | 0.43 |
| 3:N:502:PHE:CZ | 3:N:1452:ILE:HD12 | 2.53 | 0.43 |
| 3:N:606:ILE:HG22 | 3:N:607:LEU:N | 2.33 | 0.43 |
| 3:N:197:SER:C | 3:N:199:LEU:N | 2.71 | 0.43 |
| 3:N:1332:PRO:O | 3:N:1333:HIS:C | 2.56 | 0.43 |
| 2:M:843:HIS:CE1 | 2:M:884:GLN:HA | 2.54 | 0.43 |
| 3:N:891:GLU:HB2 | 3:N:926:LYS:HZ3 | 1.83 | 0.43 |
| 2:C:945:ARG:HB2 | 2:C:945:ARG:HE | 1.63 | 0.43 |
| 2:M:276:LYS:HA | 2:M:280:LYS:HE3 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:D:1069:GLU:HA | 3:D:1072:ILE:HD12 | 2.00 | 0.43 |
| 3:N:434:ARG:NH2 | 3:N:451:ASP:OD1 | 2.51 | 0.43 |
| 3:N:569:ASN:HB2 | 5:P:84:TYR:CD1 | 2.53 | 0.43 |
| 3:D:452:ILE:HG13 | 3:D:452:ILE:O | 2.18 | 0.43 |
| 3:D:93:ILE:HD13 | 3:D:548:ILE:HG12 | 2.01 | 0.43 |
| 5:F:110:MET:O | 5:F:111:GLU:C | 2.57 | 0.43 |
| 5:F:109:GLY:O | 5:F:113:ILE:HG13 | 2.19 | 0.43 |
| 3:N:362:GLU:O | 3:N:363:ALA:C | 2.57 | 0.43 |
| 4:E:6:ILE:HG13 | 4:E:10:PHE:HE1 | 1.76 | 0.43 |
| 1:B:104:GLU:HB2 | 1:B:105:GLY:H | 1.71 | 0.43 |
| 3:D:185:VAL:CG2 | 3:D:203:ALA:N | 2.82 | 0.43 |
| 5:P:373:LYS:NZ | 5:P:373:LYS:CB | 2.72 | 0.43 |
| 3:D:1262:LEU:O | 3:D:1264:GLU:N | 2.52 | 0.43 |
| 3:D:1379:VAL:HA | 3:D:1420:LEU:CG | 2.49 | 0.43 |
| 3:D:491:LYS:O | 3:D:492:ALA:C | 2.57 | 0.43 |
| 5:F:367:MET:CB | 5:F:370:LYS:HE2 | 2.49 | 0.43 |
| 3:D:945:SER:HG | 3:D:947:ILE:HG22 | 1.81 | 0.43 |
| 3:D:414:ARG:HB3 | 3:D:451:ASP:OD1 | 2.18 | 0.43 |
| 5:F:144:ILE:C | 5:F:146:GLY:H | 2.21 | 0.43 |
| 3:N:580:ALA:O | 3:N:584:ASN:HB2 | 2.19 | 0.43 |
| 5:F:85:LEU:C | 5:F:87:GLU:N | 2.71 | 0.43 |
| 2:M:1014:SER:O | 2:M:1018:GLN:HA | 2.19 | 0.43 |
| 2:C:832:LYS:CG | 2:C:833:LEU:N | 2.82 | 0.43 |
| 2:M:1068:GLU:O | 2:M:1071:ILE:HB | 2.18 | 0.43 |
| 3:N:10:ILE:HD13 | 3:N:1450:ALA:HB3 | 2.01 | 0.43 |
| 3:D:631:ILE:HG21 | 3:D:745:MET:CG | 2.35 | 0.43 |
| 2:M:958:THR:O | 2:M:959:PRO:C | 2.57 | 0.43 |
| 3:D:410:SER:OG | 5:F:164:LYS:HE2 | 2.18 | 0.43 |
| 2:C:1052:MET:SD | 3:D:623:VAL:CG2 | 3.07 | 0.43 |
| 2:C:383:ARG:O | 2:C:384:GLU:C | 2.57 | 0.43 |
| 2:C:631:SER:HB2 | 2:C:635:THR:OG1 | 2.19 | 0.43 |
| 5:F:234:LYS:CD | 5:F:236:SER:HB3 | 2.49 | 0.43 |
| 3:D:965:GLU:HA | 3:D:965:GLU:OE1 | 2.19 | 0.43 |
| 2:C:724:ARG:HD2 | 2:C:738:ASP:HA | 2.01 | 0.43 |
| 2:M:734:LEU:O | 2:M:735:ARG:C | 2.57 | 0.43 |
| 2:C:76:PRO:O | 2:C:77:PRO:C | 2.56 | 0.43 |
| 2:M:937:ASP:HB3 | 2:M:940:GLU:HG3 | 1.99 | 0.43 |
| 2:M:185:LYS:NZ | 2:M:190:LYS:HZ3 | 2.17 | 0.43 |
| 2:M:221:LEU:HD23 | 2:M:221:LEU:C | 2.39 | 0.43 |
| 2:C:151:ASP:HA | 2:C:159:ILE:HG12 | 2.00 | 0.43 |
| 2:C:176:VAL:HA | 2:C:183:SER:OG | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:311:PHE:C | 2:C:313:LEU:N | 2.72 | 0.43 |
| 2:C:326:ASP:HB2 | 2:C:431:HIS:HD2 | 1.83 | 0.43 |
| 2:C:517:ARG:O | 2:C:520:GLU:HB2 | 2.18 | 0.43 |
| 2:C:401:LEU:HD21 | 2:C:543:ASN:HB3 | 2.00 | 0.43 |
| 3:N:545:ARG:O | 3:N:546:ARG:C | 2.57 | 0.43 |
| 5:P:189:GLU:HA | 5:P:192:LEU:CD1 | 2.49 | 0.43 |
| 5:P:79:ASP:O | 5:P:80:PRO:C | 2.56 | 0.43 |
| 3:D:109:PRO:HB2 | 3:D:114:THR:CB | 2.48 | 0.43 |
| 5:F:112:ALA:O | 5:F:115:LYS:N | 2.52 | 0.43 |
| 3:D:325:GLU:HG3 | 3:D:325:GLU:O | 2.18 | 0.43 |
| 5:P:355:GLU:CA | 5:P:358:LEU:HB3 | 2.49 | 0.43 |
| 5:P:381:HIS:O | 5:P:384:GLU:N | 2.38 | 0.43 |
| 5:P:385:GLU:HB2 | 5:P:397:ILE:HD13 | 2.00 | 0.43 |
| 3:D:692:GLU:CD | 3:D:692:GLU:C | 2.78 | 0.43 |
| 5:F:295:MET:HB3 | 5:F:299:TRP:CG | 2.53 | 0.43 |
| 5:F:288:TYR:CB | 5:F:301:ALA:HB1 | 2.48 | 0.43 |
| 3:D:1397:LYS:O | 3:D:1401:GLU:OE2 | 2.36 | 0.43 |
| 1:B:5:LYS:CD | 1:B:7:LYS:HD2 | 2.45 | 0.43 |
| 2:C:873:PRO:HB3 | 3:D:949:ILE:HD12 | 2.00 | 0.43 |
| 1:L:19:GLU:O | 1:L:201:THR:N | 2.45 | 0.43 |
| 2:M:692:GLU:HA | 2:M:852:ILE:CG2 | 2.49 | 0.43 |
| 3:N:799:LYS:N | 3:N:829:VAL:CG1 | 2.82 | 0.43 |
| 3:N:256:GLU:HB2 | 3:N:257:GLY:H | 1.59 | 0.43 |
| 3:N:1118:ILE:CG2 | 3:N:1190:SER:HB3 | 2.49 | 0.43 |
| 2:M:1051:GLU:O | 2:M:1052:MET:C | 2.57 | 0.43 |
| 3:N:623:VAL:HG13 | 3:N:624:ASP:H | 1.83 | 0.43 |
| 3:N:698:LYS:HA | 3:N:756:GLN:OE1 | 2.19 | 0.43 |
| 4:O:17:TYR:O | 4:O:18:ARG:C | 2.57 | 0.43 |
| 2:C:594:ALA:HB1 | 2:C:654:LEU:HD13 | 2.00 | 0.43 |
| 2:M:59:LYS:N | 2:M:59:LYS:CD | 2.63 | 0.43 |
| 3:N:1357:ARG:O | 3:N:1360:GLY:N | 2.49 | 0.43 |
| 3:N:15:PRO:HB2 | 3:N:16:GLU:OE1 | 2.17 | 0.43 |
| 1:L:178:ALA:O | 1:L:197:LEU:HD12 | 2.19 | 0.43 |
| 2:M:44:ILE:HG22 | 2:M:48:PHE:CE1 | 2.53 | 0.43 |
| 2:M:1005:MET:CE | 3:N:648:MET:HB2 | 2.49 | 0.43 |
| 2:M:486:MET:SD | 2:M:490:GLU:HB2 | 2.59 | 0.43 |
| 3:D:623:VAL:HG12 | 3:D:624:ASP:N | 2.34 | 0.43 |
| 3:D:1001:GLU:O | 3:D:1002:LYS:C | 2.57 | 0.43 |
| 5:P:163:LEU:N | 5:P:163:LEU:HD23 | 2.32 | 0.43 |
| 1:A:218:LEU:O | 1:A:222:LEU:HG | 2.18 | 0.43 |
| 4:E:46:PRO:O | 4:E:56:ASP:HA | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:958:GLU:C | 3:D:960:LYS:N | 2.72 | 0.43 |
| 1:A:11:PHE:HE2 | 1:B:228:PRO:HA | 1.84 | 0.43 |
| 2:C:494:TYR:N | 2:C:494:TYR:CD1 | 2.87 | 0.43 |
| 3:N:1136:LYS:O | 3:N:1137:ARG:C | 2.57 | 0.43 |
| 5:P:191:ASN:O | 5:P:194:LEU:N | 2.52 | 0.43 |
| 3:D:497:GLU:O | 3:D:498:VAL:C | 2.57 | 0.43 |
| 4:O:66:LYS:HA | 4:O:66:LYS:HD3 | 1.75 | 0.43 |
| 2:M:159:ILE:HG22 | 2:M:175:GLU:HB2 | 2.01 | 0.43 |
| 2:M:208:ALA:HB1 | 2:M:222:MET:CG | 2.49 | 0.43 |
| 2:M:334:ARG:NH2 | 2:M:342:ASP:OD2 | 2.52 | 0.43 |
| 2:C:273:GLY:O | 2:C:277:ALA:N | 2.52 | 0.43 |
| 2:C:334:ARG:O | 2:C:339:LEU:HD11 | 2.19 | 0.43 |
| 3:N:28:LYS:HA | 3:N:29:PRO:HD3 | 1.74 | 0.43 |
| 3:N:138:LYS:CB | 3:N:450:TYR:OH | 2.54 | 0.43 |
| 2:C:1090:LYS:HD2 | 3:D:90:MET:SD | 2.58 | 0.43 |
| 2:C:1114:GLY:C | 2:C:1116:ALA:N | 2.72 | 0.43 |
| 5:F:207:LEU:CB | 5:F:212:LEU:HD21 | 2.40 | 0.43 |
| 2:M:114:PHE:CE2 | 5:P:283:GLY:HA3 | 2.54 | 0.43 |
| 3:D:249:TYR:HD2 | 3:D:288:MET:CE | 2.31 | 0.43 |
| 5:P:380:GLU:C | 5:P:382:THR:H | 2.21 | 0.43 |
| 5:F:379:ARG:C | 5:F:379:ARG:CD | 2.87 | 0.43 |
| 5:F:383:LEU:HD21 | 5:F:394:ARG:HD3 | 2.00 | 0.43 |
| 1:B:185:ARG:HH22 | 3:D:692:GLU:CG | 2.23 | 0.43 |
| 2:C:48:PHE:C | 2:C:50:GLU:H | 2.22 | 0.43 |
| 3:N:671:LYS:HE2 | 3:N:675:ARG:CD | 2.47 | 0.43 |
| 5:P:372:ARG:HA | 5:P:372:ARG:HD2 | 1.77 | 0.43 |
| 3:D:1397:LYS:N | 3:D:1398:TRP:HE3 | 2.17 | 0.43 |
| 3:D:837:GLY:C | 3:D:839:LEU:N | 2.72 | 0.43 |
| 3:N:61:GLY:O | 3:N:62:LYS:C | 2.56 | 0.43 |
| 2:C:882:LEU:O | 2:C:885:ILE:HB | 2.19 | 0.43 |
| 2:M:889:HIS:O | 2:M:892:LEU:HB3 | 2.18 | 0.43 |
| 3:N:826:PRO:HB3 | 3:N:828:LYS:HZ3 | 1.83 | 0.43 |
| 3:N:845:ASN:HB3 | 3:N:847:ASP:OD1 | 2.19 | 0.43 |
| 3:N:845:ASN:N | 3:N:848:GLU:OE1 | 2.40 | 0.43 |
| 3:N:1118:ILE:HG12 | 3:N:1190:SER:HB2 | 2.01 | 0.43 |
| 3:N:1164:ARG:HH21 | 3:N:1170:ASP:CG | 2.22 | 0.43 |
| 3:N:758:GLU:O | 3:N:762:GLN:HG2 | 2.18 | 0.43 |
| 2:C:695:LEU:O | 2:C:696:LYS:C | 2.56 | 0.43 |
| 2:M:495:THR:HB | 2:M:530:GLU:CG | 2.48 | 0.43 |
| 2:M:526:PRO:O | 2:M:527:GLU:C | 2.57 | 0.43 |
| 2:M:1085:PHE:HB2 | 3:N:1468:LEU:O | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:655:PRO:O | 3:N:656:PHE:C | 2.57 | 0.43 |
| 3:D:1353:GLN:C | 3:D:1355:VAL:N | 2.70 | 0.43 |
| 2:M:860:HIS:HA | 2:M:866:PRO:HA | 2.01 | 0.43 |
| 2:M:918:LEU:HD12 | 2:M:968:LEU:C | 2.39 | 0.43 |
| 2:M:472:ARG:NH2 | 2:M:479:VAL:HG12 | 2.34 | 0.43 |
| 5:P:102:LEU:HD11 | 5:P:183:ALA:HB1 | 1.95 | 0.43 |
| 1:A:221:HIS:C | 1:A:223:THR:N | 2.69 | 0.43 |
| 2:M:443:THR:OG1 | 2:M:444:PRO:CD | 2.61 | 0.43 |
| 3:D:817:GLU:O | 3:D:821:VAL:HG23 | 2.19 | 0.43 |
| 3:N:601:ARG:NH1 | 3:N:601:ARG:HG2 | 2.33 | 0.43 |
| 3:D:344:ASP:OD1 | 3:D:345:TYR:N | 2.52 | 0.43 |
| 2:M:185:LYS:HZ3 | 2:M:190:LYS:HZ3 | 1.66 | 0.43 |
| 2:M:196:LEU:HD23 | 2:M:196:LEU:N | 2.33 | 0.43 |
| 2:M:208:ALA:CB | 2:M:221:LEU:HD22 | 2.42 | 0.43 |
| 2:M:276:LYS:O | 2:M:277:ALA:C | 2.56 | 0.43 |
| 2:M:305:PRO:O | 2:M:309:TYR:N | 2.52 | 0.43 |
| 3:N:227:LEU:HB2 | 3:N:329:GLU:O | 2.18 | 0.43 |
| 3:N:287:GLY:CA | 3:N:311:LEU:HD22 | 2.49 | 0.43 |
| 2:C:157:ARG:HD3 | 2:C:158:TYR:CZ | 2.54 | 0.43 |
| 2:C:170:PRO:HD2 | 2:C:263:ASP:O | 2.19 | 0.43 |
| 5:P:84:TYR:C | 5:P:86:HIS:N | 2.69 | 0.43 |
| 2:C:1101:THR:OG1 | 2:C:1109:VAL:O | 2.34 | 0.43 |
| 3:D:128:TYR:O | 3:D:129:PHE:C | 2.55 | 0.43 |
| 3:D:523:ASP:C | 3:D:526:PRO:HG3 | 2.38 | 0.43 |
| 3:D:550:ARG:NH1 | 3:D:573:MET:O | 2.52 | 0.43 |
| 5:F:104:ARG:HG3 | 5:F:105:LYS:H | 1.82 | 0.43 |
| 5:P:348:SER:O | 5:P:352:GLU:OE2 | 2.36 | 0.43 |
| 1:B:211:LEU:O | 1:B:215:VAL:HG13 | 2.18 | 0.43 |
| 5:F:394:ARG:O | 5:F:397:ILE:HB | 2.19 | 0.43 |
| 3:N:1424:VAL:CG2 | 3:N:1425:THR:H | 2.26 | 0.43 |
| 2:C:111:ASP:O | 2:C:112:GLU:HG2 | 2.19 | 0.43 |
| 5:P:278:LEU:O | 5:P:282:LEU:N | 2.31 | 0.43 |
| 5:F:256:ARG:NH2 | 5:F:310:ILE:O | 2.52 | 0.43 |
| 5:P:373:LYS:C | 5:P:373:LYS:HD2 | 2.38 | 0.43 |
| 3:N:1462:LEU:HD22 | 3:N:1472:ILE:HD12 | 2.01 | 0.43 |
| 3:D:168:THR:HB | 3:D:206:ARG:HH12 | 1.84 | 0.43 |
| 3:N:1111:ASP:OD2 | 3:N:1203:LYS:HG3 | 2.19 | 0.43 |
| 2:C:640:ARG:O | 2:C:656:ALA:HA | 2.19 | 0.43 |
| 3:N:191:LEU:HD11 | 3:N:393:ILE:HD12 | 2.01 | 0.43 |
| 3:D:64:LYS:CD | 5:F:377:ASP:OD2 | 2.67 | 0.43 |
| 2:C:1012:PRO:HD3 | 2:C:1026:GLN:CG | 2.41 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:346:VAL:HB | 2:C:350:ARG:CZ | 2.49 | 0.43 |
| 2:M:737:LEU:HD21 | 2:M:741:GLY:O | 2.18 | 0.43 |
| 2:M:522:VAL:HG12 | 2:M:523:ILE:H | 1.83 | 0.43 |
| 5:F:239:ALA:O | 5:F:240:THR:C | 2.56 | 0.43 |
| 3:N:406:ASP:HB2 | 3:N:423:ASP:CA | 2.44 | 0.43 |
| 3:D:469:ASP:O | 3:D:472:ALA:HB3 | 2.19 | 0.43 |
| 5:F:170:HIS:HA | 5:F:173:TYR:HD1 | 1.84 | 0.43 |
| 1:K:48:ILE:HA | 1:K:49:PRO:HD3 | 1.85 | 0.43 |
| 3:D:780:LYS:HB2 | 3:D:781:PRO:HD2 | 2.01 | 0.43 |
| 1:K:33:GLY:HA3 | 1:K:181:VAL:CG2 | 2.46 | 0.43 |
| 3:N:894:LYS:HB3 | 3:N:898:GLU:OE1 | 2.18 | 0.43 |
| 2:C:128:ILE:C | 2:C:129:ILE:HD13 | 2.39 | 0.43 |
| 2:C:247:PRO:HA | 2:C:248:PRO:HD3 | 1.87 | 0.43 |
| 1:K:106:PRO:HD3 | 1:K:134:GLU:HA | 2.00 | 0.43 |
| 2:M:240:THR:C | 2:M:242:LEU:H | 2.22 | 0.42 |
| 3:N:241:ILE:HG22 | 3:N:242:LEU:N | 2.34 | 0.42 |
| 3:N:217:LYS:HE3 | 3:N:341:GLU:CD | 2.39 | 0.42 |
| 2:C:157:ARG:CD | 2:C:314:THR:HG22 | 2.38 | 0.42 |
| 3:N:119:SER:N | 3:N:123:LEU:CG | 2.65 | 0.42 |
| 5:P:207:LEU:HG | 5:P:211:ASP:HB2 | 2.00 | 0.42 |
| 3:D:22:SER:HB2 | 3:D:24:GLY:O | 2.18 | 0.42 |
| 3:D:566:ILE:HA | 3:D:569:ASN:HD22 | 1.83 | 0.42 |
| 4:E:25:LYS:CA | 4:E:28:GLN:NE2 | 2.78 | 0.42 |
| 3:D:639:LEU:HG | 3:D:766:ALA:HB2 | 1.99 | 0.42 |
| 2:M:773:LEU:O | 2:M:774:LEU:C | 2.56 | 0.42 |
| 5:P:356:LYS:HB3 | 5:P:417:LYS:NZ | 2.33 | 0.42 |
| 5:P:418:LEU:O | 5:P:419:ARG:C | 2.57 | 0.42 |
| 5:F:394:ARG:HA | 5:F:397:ILE:HD12 | 2.00 | 0.42 |
| 3:D:661:MET:HB3 | 3:D:667:ALA:CB | 2.49 | 0.42 |
| 2:C:352:ALA:C | 2:C:355:VAL:HG12 | 2.38 | 0.42 |
| 5:F:264:MET:O | 5:F:267:THR:OG1 | 2.31 | 0.42 |
| 3:D:1159:ARG:HG2 | 3:D:1159:ARG:H | 1.63 | 0.42 |
| 3:D:1395:LEU:O | 3:D:1398:TRP:CE3 | 2.72 | 0.42 |
| 3:D:796:ARG:HG3 | 3:D:861:GLN:HB3 | 2.00 | 0.42 |
| 3:D:1126:ASP:OD1 | 3:D:1126:ASP:O | 2.37 | 0.42 |
| 3:N:784:ASP:O | 3:N:785:ILE:C | 2.57 | 0.42 |
| 3:D:394:LEU:HD12 | 3:D:395:VAL:H | 1.83 | 0.42 |
| 3:N:759:ALA:HA | 3:N:763:MET:CG | 2.49 | 0.42 |
| 3:D:867:ARG:HA | 3:D:871:LYS:O | 2.19 | 0.42 |
| 2:C:615:TYR:O | 2:C:616:GLU:C | 2.57 | 0.42 |
| 1:L:209:GLU:HG3 | 1:L:209:GLU:H | 1.58 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:N:729:HIS:O | 3:N:732:VAL:HG22 | 2.19 | 0.42 |
| 5:P:321:ILE:C | 5:P:323:ASP:N | 2.73 | 0.42 |
| 3:N:1401:GLU:N | 3:N:1401:GLU:CD | 2.72 | 0.42 |
| 3:N:702:LEU:O | 3:N:736:PHE:CZ | 2.71 | 0.42 |
| 2:M:737:LEU:HD21 | 2:M:741:GLY:C | 2.39 | 0.42 |
| 5:P:248:ASN:O | 5:P:249:ARG:C | 2.57 | 0.42 |
| 2:M:380:ALA:HB1 | 2:M:384:GLU:CG | 2.49 | 0.42 |
| 2:C:716:LYS:C | 2:C:718:GLY:H | 2.21 | 0.42 |
| 4:O:85:LEU:O | 4:O:86:GLN:C | 2.57 | 0.42 |
| 2:M:27:ARG:C | 2:M:29:ALA:N | 2.72 | 0.42 |
| 1:K:219:ARG:NH1 | 1:K:219:ARG:HG2 | 2.33 | 0.42 |
| 2:M:182:VAL:HG21 | 2:M:194:VAL:CG2 | 2.49 | 0.42 |
| 2:M:198:ARG:CG | 2:M:228:ALA:HA | 2.49 | 0.42 |
| 2:M:289:THR:HG22 | 2:M:290:LEU:HD21 | 2.00 | 0.42 |
| 2:M:537:LYS:HG3 | 2:M:537:LYS:H | 1.36 | 0.42 |
| 2:M:583:LEU:O | 2:M:584:GLU:C | 2.56 | 0.42 |
| 3:N:262:LYS:HG2 | 3:N:263:GLU:N | 2.34 | 0.42 |
| 2:C:202:TYR:HB2 | 2:C:207:LEU:CD1 | 2.47 | 0.42 |
| 2:C:260:LEU:HB2 | 2:C:291:ALA:CB | 2.49 | 0.42 |
| 2:C:432:ARG:HG3 | 2:C:433:THR:N | 2.34 | 0.42 |
| 3:D:1071:PHE:O | 3:D:1072:ILE:C | 2.58 | 0.42 |
| 3:N:119:SER:CA | 3:N:123:LEU:HG | 2.48 | 0.42 |
| 3:D:1232:PRO:HB2 | 3:D:1356:TYR:CE2 | 2.54 | 0.42 |
| 3:D:119:SER:H | 3:D:123:LEU:HB2 | 1.83 | 0.42 |
| 3:D:125:GLN:O | 3:D:126:VAL:C | 2.57 | 0.42 |
| 3:D:608:SER:O | 3:D:609:GLY:C | 2.57 | 0.42 |
| 3:D:87:ARG:HG3 | 3:D:88:TYR:CE2 | 2.54 | 0.42 |
| 4:E:26:ARG:O | 4:E:29:GLN:HG2 | 2.20 | 0.42 |
| 5:F:183:ALA:O | 5:F:184:ARG:C | 2.58 | 0.42 |
| 5:F:99:GLU:O | 5:F:100:VAL:C | 2.58 | 0.42 |
| 3:D:269:PHE:HD1 | 3:D:283:PHE:CB | 2.28 | 0.42 |
| 1:B:61:VAL:CG2 | 1:B:62:LEU:N | 2.82 | 0.42 |
| 2:M:151:ASP:CB | 2:M:157:ARG:O | 2.64 | 0.42 |
| 2:C:1071:ILE:C | 2:C:1073:GLY:N | 2.71 | 0.42 |
| 5:P:287:THR:HG23 | 5:P:290:GLU:CD | 2.38 | 0.42 |
| 5:P:300:ASP:HB3 | 5:P:302:LYS:NZ | 2.34 | 0.42 |
| 3:D:31:THR:OG1 | 5:F:258:ILE:HD13 | 2.19 | 0.42 |
| 3:N:1496:GLU:OE1 | 3:N:1499:ARG:NE | 2.52 | 0.42 |
| 3:N:1489:GLN:NE2 | 4:O:71:GLY:O | 2.39 | 0.42 |
| 3:D:1380:GLU:HB2 | 3:D:1420:LEU:HD11 | 2.01 | 0.42 |
| 3:D:1012:GLU:O | 3:D:1016:PRO:HG3 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:829:VAL:HB | 3:D:830:ALA:H | 1.69 | 0.42 |
| 3:D:915:VAL:O | 3:D:916:TYR:C | 2.57 | 0.42 |
| 3:N:1417:TRP:CD1 | 3:N:1418:LYS:N | 2.88 | 0.42 |
| 2:C:910:LYS:N | 2:C:913:GLU:OE1 | 2.52 | 0.42 |
| 3:N:826:PRO:CD | 3:N:829:VAL:HG11 | 2.37 | 0.42 |
| 3:D:206:ARG:HB3 | 3:D:207:PHE:HD1 | 1.83 | 0.42 |
| 5:F:79:ASP:HB2 | 5:F:81:VAL:HG22 | 2.01 | 0.42 |
| 3:N:749:VAL:HA | 3:N:750:PRO:HD2 | 1.93 | 0.42 |
| 2:C:589:ARG:NH2 | 2:C:652:GLY:O | 2.52 | 0.42 |
| 2:M:1060:ILE:O | 2:M:1061:GLU:C | 2.57 | 0.42 |
| 3:D:632:VAL:N | 3:D:726:ILE:O | 2.46 | 0.42 |
| 1:K:40:LEU:O | 1:K:43:ILE:N | 2.52 | 0.42 |
| 2:C:23:VAL:CG2 | 2:C:24:GLU:N | 2.82 | 0.42 |
| 5:P:330:GLY:C | 5:P:332:PHE:N | 2.70 | 0.42 |
| 2:M:341:THR:O | 2:M:344:PHE:N | 2.51 | 0.42 |
| 3:N:591:VAL:HB | 3:N:598:ARG:O | 2.20 | 0.42 |
| 2:C:605:LYS:HB3 | 2:C:610:ARG:HH22 | 1.80 | 0.42 |
| 3:D:60:CYS:SG | 3:D:76:CYS:CB | 3.04 | 0.42 |
| 3:D:886:VAL:O | 3:D:890:VAL:HG22 | 2.19 | 0.42 |
| 5:F:321:ILE:O | 5:F:323:ASP:N | 2.52 | 0.42 |
| 2:M:20:GLU:O | 2:M:23:VAL:HG23 | 2.18 | 0.42 |
| 1:L:112:ARG:HH11 | 1:L:112:ARG:CB | 2.31 | 0.42 |
| 5:F:300:ASP:OD2 | 5:F:302:LYS:HE3 | 2.20 | 0.42 |
| 2:M:562:SER:O | 2:M:564:MET:N | 2.51 | 0.42 |
| 3:N:1003:VAL:O | 3:N:1004:THR:C | 2.57 | 0.42 |
| 5:P:236:SER:C | 5:P:238:TYR:N | 2.72 | 0.42 |
| 3:D:710:ARG:C | 3:D:712:GLY:N | 2.73 | 0.42 |
| 3:D:1143:GLY:HA2 | 3:D:1365:ASP:OD1 | 2.20 | 0.42 |
| 1:B:118:ALA:C | 1:B:120:VAL:H | 2.22 | 0.42 |
| 2:M:731:GLU:C | 2:M:733:ALA:N | 2.73 | 0.42 |
| 2:M:731:GLU:HA | 2:M:734:LEU:CD1 | 2.49 | 0.42 |
| 2:M:1107:ASN:HA | 2:M:1108:PRO:HD3 | 1.91 | 0.42 |
| 3:D:117:ASP:HB2 | 3:D:495:ARG:NH1 | 2.34 | 0.42 |
| 2:M:193:LEU:HD12 | 2:M:196:LEU:HD12 | 2.01 | 0.42 |
| 2:M:227:PHE:HD1 | 2:M:227:PHE:N | 2.16 | 0.42 |
| 2:M:267:TYR:CD1 | 2:M:272:ALA:HB2 | 2.55 | 0.42 |
| 2:M:409:ARG:HA | 2:M:454:SER:HA | 2.01 | 0.42 |
| 3:N:259:VAL:C | 3:N:260:GLU:HG3 | 2.40 | 0.42 |
| 3:N:331:VAL:HG12 | 3:N:333:LEU:HD23 | 2.00 | 0.42 |
| 3:N:337:LEU:HD23 | 3:N:337:LEU:N | 2.34 | 0.42 |
| 3:N:211:VAL:HA | 3:N:387:LEU:HA | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:198:ARG:HD2 | 2:C:198:ARG:HA | 1.90 | 0.42 |
| 2:C:204:GLN:HG2 | 2:C:222:MET:HG2 | 2.00 | 0.42 |
| 2:C:335:THR:O | 2:C:336:VAL:C | 2.57 | 0.42 |
| 2:C:460:ARG:O | 2:C:467:ILE:HA | 2.19 | 0.42 |
| 3:N:117:ASP:HB2 | 3:N:150:ARG:NH2 | 2.34 | 0.42 |
| 3:N:411:THR:H | 3:N:437:VAL:HG23 | 1.84 | 0.42 |
| 3:N:553:ARG:O | 3:N:554:LEU:C | 2.58 | 0.42 |
| 5:P:208:SER:O | 5:P:209:PHE:C | 2.58 | 0.42 |
| 3:D:610:LYS:O | 3:D:612:GLY:N | 2.46 | 0.42 |
| 3:D:761:ILE:HD13 | 4:E:20:THR:HA | 2.01 | 0.42 |
| 3:D:210:ARG:HD2 | 3:D:389:GLU:HG3 | 2.00 | 0.42 |
| 3:D:227:LEU:HD11 | 3:D:326:GLU:CA | 2.33 | 0.42 |
| 5:P:382:THR:HG21 | 5:P:394:ARG:HB2 | 2.01 | 0.42 |
| 5:F:350:LEU:C | 5:F:352:GLU:N | 2.72 | 0.42 |
| 3:N:1378:TYR:CZ | 3:N:1430:SER:HB2 | 2.54 | 0.42 |
| 2:C:368:THR:CB | 2:C:369:PRO:CD | 2.94 | 0.42 |
| 5:P:371:LEU:O | 5:P:375:LEU:HB3 | 2.19 | 0.42 |
| 3:D:800:LYS:NZ | 3:D:825:ALA:HA | 2.34 | 0.42 |
| 3:D:828:LYS:CE | 3:D:828:LYS:H | 2.32 | 0.42 |
| 3:N:970:LYS:O | 3:N:973:GLN:N | 2.52 | 0.42 |
| 3:N:912:LYS:O | 3:N:915:VAL:HB | 2.19 | 0.42 |
| 3:N:1114:THR:HG23 | 3:N:1114:THR:O | 2.19 | 0.42 |
| 3:N:1118:ILE:HD13 | 3:N:1190:SER:CB | 2.48 | 0.42 |
| 3:D:862:ASP:O | 3:D:877:PRO:HD3 | 2.19 | 0.42 |
| 2:C:701:THR:HA | 2:C:832:LYS:HA | 2.01 | 0.42 |
| 1:A:184:THR:O | 1:A:192:LEU:HB2 | 2.19 | 0.42 |
| 2:M:58:ASP:C | 2:M:59:LYS:HD2 | 2.36 | 0.42 |
| 1:K:221:HIS:C | 1:K:223:THR:N | 2.71 | 0.42 |
| 2:M:928:LYS:HE2 | 2:M:932:GLU:CG | 2.49 | 0.42 |
| 2:M:963:LEU:HD23 | 2:M:963:LEU:N | 2.33 | 0.42 |
| 2:C:472:ARG:CZ | 2:C:479:VAL:HG12 | 2.50 | 0.42 |
| 3:N:1213:ARG:HG2 | 3:N:1213:ARG:NH1 | 2.18 | 0.42 |
| 5:P:102:LEU:O | 5:P:105:LYS:HB2 | 2.18 | 0.42 |
| 3:D:409:VAL:HB | 5:F:164:LYS:HZ3 | 1.84 | 0.42 |
| 1:L:94:LEU:O | 1:L:146:ARG:CZ | 2.68 | 0.42 |
| 3:D:25:GLU:OE2 | 3:D:94:GLU:HB2 | 2.19 | 0.42 |
| 3:D:17:LYS:O | 3:D:18:ILE:C | 2.56 | 0.42 |
| 1:B:55:SER:O | 1:B:143:ARG:HB3 | 2.19 | 0.42 |
| 2:M:563:ASN:O | 2:M:567:GLN:HG3 | 2.19 | 0.42 |
| 3:D:1496:GLU:CA | 3:D:1499:ARG:HB3 | 2.47 | 0.42 |
| 3:N:505:SER:HB3 | 3:N:1453:ALA:O | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:895:VAL:HA | 3:N:898:GLU:CD | 2.40 | 0.42 |
| 2:M:182:VAL:CG2 | 2:M:221:LEU:HA | 2.49 | 0.42 |
| 2:M:182:VAL:HB | 2:M:193:LEU:N | 2.29 | 0.42 |
| 2:M:270:GLY:O | 2:M:271:GLU:C | 2.57 | 0.42 |
| 2:M:267:TYR:CB | 2:M:272:ALA:H | 2.32 | 0.42 |
| 4:E:41:GLU:HB2 | 4:E:42:PRO:CD | 2.37 | 0.42 |
| 2:C:234:ALA:O | 2:C:238:LEU:HG | 2.20 | 0.42 |
| 2:C:260:LEU:C | 2:C:288:ARG:NH2 | 2.73 | 0.42 |
| 2:C:276:LYS:O | 2:C:277:ALA:C | 2.57 | 0.42 |
| 2:C:276:LYS:O | 2:C:280:LYS:HG3 | 2.19 | 0.42 |
| 3:N:455:ARG:HB2 | 3:N:460:ALA:CB | 2.47 | 0.42 |
| 3:N:544:TYR:O | 3:N:547:LEU:N | 2.52 | 0.42 |
| 5:P:209:PHE:HA | 5:P:212:LEU:HG | 2.01 | 0.42 |
| 3:D:1094:LEU:CD1 | 3:D:1098:LEU:HD11 | 2.49 | 0.42 |
| 3:D:1103:HIS:CD2 | 3:D:1462:LEU:N | 2.87 | 0.42 |
| 3:D:462:GLN:HG2 | 3:D:466:LYS:HE3 | 2.00 | 0.42 |
| 3:D:528:VAL:C | 3:D:535:PHE:HB3 | 2.39 | 0.42 |
| 3:D:596:SER:C | 3:D:598:ARG:N | 2.73 | 0.42 |
| 2:C:1015:LEU:HD12 | 5:F:335:ASP:HA | 2.00 | 0.42 |
| 5:P:354:LEU:O | 5:P:355:GLU:C | 2.58 | 0.42 |
| 3:N:1491:THR:HG23 | 3:N:1494:ALA:HB2 | 1.99 | 0.42 |
| 3:D:807:ALA:CB | 3:D:833:GLU:CD | 2.87 | 0.42 |
| 5:F:414:ARG:HE | 5:F:414:ARG:N | 2.17 | 0.42 |
| 2:M:612:VAL:HA | 2:M:622:GLU:HA | 2.01 | 0.42 |
| 2:M:588:VAL:HG21 | 2:M:664:GLY:O | 2.20 | 0.42 |
| 2:C:56:GLU:O | 2:C:359:MET:SD | 2.77 | 0.42 |
| 5:P:276:ARG:C | 5:P:278:LEU:N | 2.73 | 0.42 |
| 5:P:305:GLU:HA | 5:P:308:LEU:CD1 | 2.48 | 0.42 |
| 3:D:37:LEU:HD23 | 3:D:37:LEU:N | 2.33 | 0.42 |
| 5:F:262:VAL:C | 5:F:264:MET:N | 2.69 | 0.42 |
| 3:N:670:VAL:O | 3:N:671:LYS:C | 2.56 | 0.42 |
| 3:D:1197:ARG:HG3 | 3:D:1396:GLU:OE1 | 2.20 | 0.42 |
| 2:M:874:LEU:HD23 | 3:N:1023:MET:SD | 2.59 | 0.42 |
| 3:N:909:ASN:HA | 3:N:912:LYS:HZ2 | 1.85 | 0.42 |
| 3:N:1175:ILE:O | 3:N:1179:GLU:N | 2.48 | 0.42 |
| 3:D:860:LEU:HG | 3:D:860:LEU:H | 1.55 | 0.42 |
| 2:C:575:GLN:HE21 | 2:C:670:GLN:CG | 2.32 | 0.42 |
| 3:D:28:LYS:HA | 3:D:29:PRO:HD3 | 1.77 | 0.42 |
| 2:M:1059:ASP:OD1 | 2:M:1080:SER:OG | 2.37 | 0.42 |
| 2:M:1084:SER:OG | 2:M:1085:PHE:N | 2.52 | 0.42 |
| 2:M:1098:ASP:CB | 3:N:17:LYS:NZ | 2.83 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:N:658:LEU:N | 3:N:661:MET:HE3 | 2.34 | 0.42 |
| 3:N:673:ALA:O | 3:N:677:LEU:HG | 2.19 | 0.42 |
| 3:D:704:ARG:NE | 3:D:738:ALA:HB2 | 2.33 | 0.42 |
| 1:K:110:LYS:HA | 1:K:127:LEU:O | 2.19 | 0.42 |
| 2:C:503:LEU:HD12 | 2:C:508:ILE:CA | 2.36 | 0.42 |
| 3:N:642:CYS:SG | 3:N:716:PHE:CB | 3.00 | 0.42 |
| 1:K:55:SER:HB2 | 1:K:165:ILE:O | 2.19 | 0.42 |
| 3:N:1399:ASP:O | 3:N:1400:VAL:C | 2.56 | 0.42 |
| 2:C:644:VAL:O | 2:C:647:GLN:HB3 | 2.19 | 0.42 |
| 3:N:1207:TYR:HA | 3:N:1214:PRO:HA | 2.02 | 0.42 |
| 2:C:1012:PRO:HD2 | 2:C:1021:LEU:O | 2.19 | 0.42 |
| 2:C:1052:MET:HA | 2:C:1056:LYS:HD2 | 2.01 | 0.42 |
| 1:A:63:HIS:CE1 | 1:A:65:PHE:C | 2.93 | 0.42 |
| 1:A:65:PHE:HA | 2:C:628:PHE:HE2 | 1.85 | 0.42 |
| 4:O:5:GLY:O | 4:O:9:LEU:HG | 2.19 | 0.42 |
| 3:D:18:ILE:HD13 | 3:D:516:ALA:O | 2.19 | 0.42 |
| 3:D:698:LYS:HA | 3:D:756:GLN:HE22 | 1.83 | 0.42 |
| 3:D:1269:LYS:N | 3:D:1269:LYS:HD3 | 2.34 | 0.42 |
| 3:N:602:SER:O | 3:N:605:ASP:HB2 | 2.20 | 0.42 |
| 5:F:107:GLU:OE2 | 5:F:229:TYR:HD1 | 2.02 | 0.42 |
| 3:N:1005:GLN:O | 3:N:1006:ALA:C | 2.57 | 0.42 |
| 2:C:474:VAL:HG12 | 2:C:530:GLU:CA | 2.49 | 0.42 |
| 5:P:361:LEU:HG | 5:P:362:SER:H | 1.83 | 0.42 |
| 3:N:446:VAL:O | 3:N:446:VAL:HG12 | 2.18 | 0.42 |
| 2:M:144:PRO:O | 2:M:276:LYS:NZ | 2.44 | 0.42 |
| 2:M:205:GLU:CA | 2:M:209:ARG:HD3 | 2.49 | 0.42 |
| 1:A:14:ARG:HH11 | 1:A:14:ARG:HG2 | 1.85 | 0.42 |
| 3:N:82:LYS:HB2 | 3:N:84:ILE:CG2 | 2.34 | 0.42 |
| 5:P:135:ILE:C | 5:P:137:GLY:N | 2.72 | 0.42 |
| 5:P:215:GLU:OE1 | 5:P:215:GLU:HA | 2.20 | 0.42 |
| 3:D:102:ILE:O | 3:D:105:VAL:N | 2.51 | 0.42 |
| 3:D:119:SER:HB3 | 3:D:123:LEU:CG | 2.43 | 0.42 |
| 3:D:128:TYR:CD1 | 3:D:457:GLY:CA | 2.98 | 0.42 |
| 3:D:542:ASP:CA | 3:D:545:ARG:HG3 | 2.50 | 0.42 |
| 3:D:545:ARG:HB2 | 3:D:546:ARG:H | 1.64 | 0.42 |
| 4:E:33:HIS:O | 4:E:34:GLY:C | 2.57 | 0.42 |
| 4:E:88:GLU:HA | 4:E:91:ARG:HD2 | 2.02 | 0.42 |
| 3:D:384:VAL:CG1 | 3:D:385:VAL:N | 2.82 | 0.42 |
| 3:D:421:LEU:HB3 | 3:D:427:VAL:C | 2.40 | 0.42 |
| 3:D:288:MET:CG | 3:D:305:ALA:HB1 | 2.50 | 0.42 |
| 3:D:307:ALA:O | 3:D:308:LYS:HD3 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:M:777:ILE:O | 2:M:777:ILE:HG22 | 2.19 | 0.42 |
| 5:P:382:THR:HA | 5:P:385:GLU:HB2 | 2.01 | 0.42 |
| 1:B:217:ILE:O | 1:B:220:GLU:HB3 | 2.19 | 0.42 |
| 3:D:807:ALA:H | 3:D:809:PRO:HD2 | 1.84 | 0.42 |
| 3:D:808:THR:N | 3:D:809:PRO:CD | 2.72 | 0.42 |
| 2:M:602:GLU:CD | 2:M:646:GLY:HA2 | 2.39 | 0.42 |
| 2:M:602:GLU:HG2 | 2:M:603:VAL:N | 2.33 | 0.42 |
| 2:C:1066:ALA:O | 2:C:1069:ALA:HB3 | 2.20 | 0.42 |
| 3:D:673:ALA:C | 3:D:676:MET:HB3 | 2.40 | 0.42 |
| 2:C:58:ASP:C | 2:C:60:GLY:N | 2.73 | 0.42 |
| 5:P:279:GLN:HA | 5:P:286:PRO:CD | 2.49 | 0.42 |
| 5:F:307:THR:O | 5:F:310:ILE:N | 2.52 | 0.42 |
| 4:O:40:LEU:HD13 | 4:O:72:ARG:NH2 | 2.34 | 0.42 |
| 3:D:1169:ASP:O | 3:D:1170:ASP:C | 2.57 | 0.42 |
| 3:D:85:VAL:HG22 | 3:D:89:ARG:HG3 | 1.99 | 0.42 |
| 3:D:85:VAL:CG2 | 3:D:89:ARG:HG3 | 2.49 | 0.42 |
| 3:D:957:PRO:CG | 3:D:1007:VAL:HA | 2.37 | 0.42 |
| 3:D:433:GLY:HA3 | 3:D:447:VAL:O | 2.19 | 0.42 |
| 3:D:1128:VAL:HG23 | 3:D:1131:SER:HB3 | 1.91 | 0.42 |
| 2:M:749:VAL:HG23 | 2:M:750:LYS:N | 2.35 | 0.42 |
| 1:K:185:ARG:HB2 | 1:K:190:THR:HG22 | 2.02 | 0.42 |
| 3:N:1155:VAL:HG11 | 3:N:1177:ALA:HB1 | 2.02 | 0.42 |
| 3:N:1194:CYS:SG | 3:N:1195:GLN:N | 2.92 | 0.42 |
| 1:A:196:THR:HG21 | 2:C:934:PHE:CE2 | 2.55 | 0.42 |
| 1:K:202:ASP:OD1 | 1:K:204:SER:N | 2.53 | 0.42 |
| 2:C:24:GLU:OE2 | 2:C:27:ARG:HD3 | 2.19 | 0.42 |
| 3:N:819:GLY:CA | 3:N:824:ASN:ND2 | 2.70 | 0.42 |
| 1:K:167:VAL:HG12 | 1:K:168:ASP:O | 2.19 | 0.42 |
| 3:N:169:TYR:HB3 | 3:N:195:VAL:CG1 | 2.50 | 0.42 |
| 5:P:96:LEU:O | 5:P:100:VAL:HG23 | 2.19 | 0.42 |
| 3:N:1071:PHE:O | 3:N:1072:ILE:C | 2.58 | 0.42 |
| 2:C:347:GLY:HA2 | 2:C:350:ARG:HB2 | 2.01 | 0.42 |
| 1:A:20:TYR:CG | 1:A:21:GLY:N | 2.87 | 0.42 |
| 2:M:833:LEU:CD1 | 2:M:837:ASP:CB | 2.98 | 0.42 |
| 1:L:10:VAL:O | 1:L:10:VAL:CG2 | 2.68 | 0.42 |
| 2:M:558:ALA:O | 2:M:559:LEU:C | 2.57 | 0.42 |
| 3:N:887:ALA:HA | 3:N:890:VAL:CG2 | 2.47 | 0.42 |
| 3:N:998:GLU:OE2 | 3:N:1002:LYS:HE3 | 2.19 | 0.42 |
| 2:C:569:VAL:HA | 2:C:570:PRO:HD3 | 1.79 | 0.42 |
| 2:M:614:ARG:HG3 | 2:M:620:LEU:HD21 | 2.01 | 0.42 |
| 2:C:13:ILE:N | 2:C:13:ILE:HD13 | 2.33 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:900:ILE:HG22 | 3:D:901:GLN:N | 2.34 | 0.42 |
| 2:M:25:SER:O | 2:M:29:ALA:HB2 | 2.19 | 0.42 |
| 1:K:151:VAL:HG12 | 1:K:156:HIS:ND1 | 2.34 | 0.42 |
| 2:M:191:PHE:HE2 | 2:M:196:LEU:HD21 | 1.81 | 0.42 |
| 2:M:415:PRO:HG2 | 2:M:418:LEU:HD12 | 2.00 | 0.42 |
| 2:C:141:HIS:HE1 | 2:C:144:PRO:HD3 | 1.85 | 0.42 |
| 2:C:177:GLU:HA | 2:C:178:PRO:HD2 | 1.86 | 0.42 |
| 3:D:1078:ARG:C | 3:D:1080:GLY:N | 2.72 | 0.42 |
| 3:N:133:ILE:HG13 | 3:N:158:TYR:CG | 2.54 | 0.42 |
| 5:P:214:GLN:OE1 | 5:P:214:GLN:HA | 2.19 | 0.42 |
| 3:D:154:THR:CG2 | 3:D:156:GLU:OE2 | 2.67 | 0.42 |
| 3:N:407:VAL:CG2 | 3:N:408:GLU:N | 2.63 | 0.42 |
| 3:D:924:MET:CG | 3:D:925:GLU:N | 2.83 | 0.42 |
| 3:D:185:VAL:HA | 3:D:189:GLN:HE22 | 1.83 | 0.42 |
| 2:M:657:ASP:O | 2:M:658:GLY:O | 2.37 | 0.42 |
| 2:C:62:GLY:HA3 | 2:C:103:LYS:HB2 | 2.01 | 0.42 |
| 5:P:302:LYS:O | 5:P:306:GLU:HG2 | 2.20 | 0.42 |
| 2:M:712:ALA:O | 2:M:820:ARG:N | 2.37 | 0.42 |
| 2:M:762:LYS:HB2 | 2:M:786:LYS:HD2 | 2.02 | 0.42 |
| 2:C:967:PHE:O | 2:C:970:GLY:N | 2.50 | 0.42 |
| 2:M:573:ARG:HB2 | 2:M:670:GLN:HE22 | 1.84 | 0.42 |
| 2:M:1040:LEU:HD13 | 2:M:1049:LEU:CA | 2.49 | 0.42 |
| 3:N:13:ALA:HA | 3:N:17:LYS:HD3 | 2.02 | 0.42 |
| 1:A:83:LYS:HE3 | 1:A:167:VAL:HG12 | 2.02 | 0.42 |
| 1:K:100:LEU:CD2 | 1:K:101:LEU:N | 2.81 | 0.42 |
| 2:C:121:MET:HG3 | 2:C:127:PHE:CE1 | 2.54 | 0.42 |
| 2:M:479:VAL:N | 2:M:506:ASN:HB3 | 2.25 | 0.42 |
| 5:P:321:ILE:HG13 | 5:P:332:PHE:CZ | 2.51 | 0.42 |
| 5:F:365:GLU:O | 5:F:368:VAL:CG2 | 2.66 | 0.42 |
| 3:N:106:LYS:HB3 | 3:N:586:ARG:CZ | 2.49 | 0.42 |
| 2:M:430:VAL:HG23 | 2:M:434:HIS:HD2 | 1.83 | 0.42 |
| 5:F:156:VAL:HG23 | 5:F:157:GLU:OE1 | 2.20 | 0.42 |
| 2:C:346:VAL:CG2 | 2:C:347:GLY:N | 2.74 | 0.42 |
| 2:M:121:MET:SD | 2:M:125:GLY:HA2 | 2.60 | 0.42 |
| 3:D:15:PRO:HB2 | 3:D:16:GLU:OE1 | 2.20 | 0.42 |
| 2:M:494:TYR:O | 2:M:517:ARG:HA | 2.20 | 0.42 |
| 3:N:1186:VAL:HA | 3:N:1187:PRO:HD3 | 1.83 | 0.42 |
| 3:D:470:LEU:O | 3:D:472:ALA:N | 2.52 | 0.42 |
| 3:D:739:ASP:OD1 | 3:D:741:ASP:OD1 | 2.37 | 0.42 |
| 2:C:930:LYS:O | 2:C:932:GLU:N | 2.53 | 0.42 |
| 2:M:78:PHE:HD2 | 2:M:82:GLU:OE2 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:O:29:GLN:C | 4:O:31:LEU:N | 2.73 | 0.42 |
| 3:N:1025:GLN:C | 3:N:1027:GLY:N | 2.73 | 0.42 |
| 2:M:1076:VAL:HA | 2:M:1077:PRO:HD3 | 1.80 | 0.42 |
| 2:M:9:ILE:O | 2:M:10:ARG:C | 2.57 | 0.42 |
| 3:N:1385:GLY:HA2 | 3:N:1413:THR:HG21 | 2.00 | 0.42 |
| 2:M:164:PRO:HB2 | 2:M:263:ASP:O | 2.17 | 0.42 |
| 2:M:401:LEU:O | 2:M:404:LEU:N | 2.52 | 0.42 |
| 3:N:268:ALA:CB | 3:N:290:PRO:HG3 | 2.44 | 0.42 |
| 2:C:546:LEU:HD23 | 2:C:583:LEU:HD12 | 2.00 | 0.42 |
| 3:N:47:GLU:C | 3:N:49:ILE:N | 2.72 | 0.42 |
| 2:C:1114:GLY:O | 2:C:1116:ALA:N | 2.52 | 0.42 |
| 3:D:148:GLU:O | 3:D:149:LYS:C | 2.58 | 0.42 |
| 3:D:511:TRP:CA | 3:D:511:TRP:CE3 | 3.02 | 0.42 |
| 2:C:1102:LEU:N | 3:D:7:LYS:O | 2.43 | 0.42 |
| 5:F:140:ARG:HG3 | 5:F:140:ARG:HH11 | 1.83 | 0.42 |
| 3:D:231:VAL:O | 3:D:231:VAL:HG12 | 2.19 | 0.42 |
| 1:L:82:LEU:C | 1:L:84:GLU:N | 2.73 | 0.42 |
| 3:D:654:LYS:CB | 3:D:655:PRO:CD | 2.97 | 0.42 |
| 3:N:1424:VAL:CG2 | 3:N:1425:THR:N | 2.79 | 0.42 |
| 5:P:287:THR:O | 5:P:288:TYR:C | 2.58 | 0.42 |
| 5:F:421:PHE:HD2 | 5:F:422:LEU:N | 2.17 | 0.42 |
| 3:D:56:TYR:CE2 | 3:D:66:GLN:HG3 | 2.55 | 0.42 |
| 3:N:965:GLU:OE2 | 3:N:969:ARG:NE | 2.42 | 0.42 |
| 3:N:783:ARG:O | 3:N:784:ASP:C | 2.58 | 0.42 |
| 3:D:168:THR:OG1 | 3:D:206:ARG:NH1 | 2.53 | 0.42 |
| 2:C:737:LEU:HD11 | 2:C:741:GLY:O | 2.20 | 0.42 |
| 2:C:742:VAL:HG12 | 2:C:743:VAL:H | 1.83 | 0.42 |
| 3:D:854:ALA:C | 3:D:856:GLY:H | 2.22 | 0.42 |
| 2:C:649:VAL:CA | 2:C:650:ARG:HH21 | 2.24 | 0.42 |
| 1:A:31:GLY:O | 1:A:32:PHE:C | 2.58 | 0.42 |
| 1:A:5:LYS:C | 1:A:7:LYS:H | 2.21 | 0.42 |
| 1:L:210:ALA:O | 1:L:213:GLN:HB2 | 2.18 | 0.42 |
| 3:N:1342:GLU:N | 3:N:1342:GLU:OE1 | 2.51 | 0.42 |
| 3:N:1344:VAL:O | 3:N:1348:LEU:HG | 2.19 | 0.42 |
| 1:A:79:ILE:HG13 | 1:A:79:ILE:H | 1.46 | 0.42 |
| 2:M:944:LEU:O | 2:M:945:ARG:C | 2.58 | 0.42 |
| 5:F:282:LEU:CG | 5:F:284:ARG:HG2 | 2.36 | 0.42 |
| 3:N:729:HIS:HE1 | 3:N:935:LYS:HZ3 | 1.67 | 0.42 |
| 2:M:425:PHE:HZ | 3:N:1083:ASP:HB2 | 1.85 | 0.42 |
| 2:C:402:SER:HA | 2:C:566:THR:HG22 | 2.00 | 0.42 |
| 2:M:18:LEU:HG | 2:M:590:ASP:CG | 2.40 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:M:494:TYR:CD1 | 2:M:494:TYR:N | 2.88 | 0.42 |
| 5:P:312:GLN:CA | 5:P:312:GLN:OE1 | 2.66 | 0.42 |
| 3:N:187:LYS:HE3 | 3:N:198:ARG:HG3 | 2.02 | 0.42 |
| 3:D:1042:ARG:HG2 | 3:D:1042:ARG:NH1 | 2.32 | 0.42 |
| 2:M:799:ILE:O | 2:M:827:VAL:HG13 | 2.20 | 0.42 |
| 1:B:91:ASN:ND2 | 1:B:91:ASN:C | 2.72 | 0.42 |
| 3:D:1191:PRO:O | 3:D:1192:LEU:C | 2.58 | 0.42 |
| 5:F:196:VAL:C | 5:F:198:ILE:N | 2.73 | 0.42 |
| 3:N:1272:ALA:HB2 | 3:N:1328:GLY:CA | 2.50 | 0.42 |
| 2:M:455:LEU:HD11 | 2:M:459:ALA:HB3 | 2.02 | 0.42 |
| 2:M:397:GLU:OE2 | 2:M:631:SER:HA | 2.19 | 0.42 |
| 3:N:217:LYS:HD2 | 3:N:262:LYS:HZ1 | 1.84 | 0.42 |
| 3:N:127:LEU:O | 3:N:130:SER:O | 2.37 | 0.42 |
| 3:N:133:ILE:HG22 | 3:N:454:ALA:C | 2.40 | 0.42 |
| 2:C:1084:SER:OG | 2:C:1085:PHE:N | 2.53 | 0.42 |
| 3:D:530:VAL:HG22 | 3:D:534:ARG:C | 2.40 | 0.42 |
| 3:D:258:VAL:O | 3:D:258:VAL:HG12 | 2.20 | 0.42 |
| 3:D:209:ARG:HB2 | 3:D:389:GLU:HB3 | 2.00 | 0.42 |
| 5:F:383:LEU:HG | 5:F:394:ARG:HD3 | 2.00 | 0.42 |
| 2:C:369:PRO:HB2 | 2:C:370:ALA:H | 1.66 | 0.42 |
| 3:D:34:TYR:CG | 3:D:35:ARG:N | 2.88 | 0.42 |
| 3:N:1489:GLN:CG | 3:N:1492:LEU:HD12 | 2.50 | 0.42 |
| 3:D:493:ARG:O | 3:D:1388:ARG:NH1 | 2.53 | 0.42 |
| 1:L:99:LEU:N | 1:L:142:VAL:O | 2.53 | 0.42 |
| 5:F:367:MET:HA | 5:F:370:LYS:HE2 | 2.01 | 0.42 |
| 3:N:1433:SER:HA | 3:N:1457:ASP:CG | 2.39 | 0.42 |
| 3:N:1465:ASN:CG | 3:N:1473:PRO:HD3 | 2.40 | 0.42 |
| 3:N:880:ILE:O | 3:N:881:LEU:C | 2.58 | 0.42 |
| 2:C:857:ASP:HB2 | 2:C:978:ARG:HG2 | 2.00 | 0.42 |
| 1:A:32:PHE:HZ | 1:B:47:SER:HG | 1.68 | 0.42 |
| 2:M:1092:LEU:HG | 2:M:1092:LEU:H | 1.55 | 0.42 |
| 1:K:221:HIS:C | 1:K:223:THR:H | 2.23 | 0.42 |
| 1:L:22:GLU:HA | 1:L:197:LEU:O | 2.19 | 0.42 |
| 1:B:10:VAL:O | 1:B:10:VAL:HG23 | 2.20 | 0.42 |
| 5:F:160:ASP:O | 5:F:164:LYS:HG3 | 2.20 | 0.42 |
| 3:D:1496:GLU:OE1 | 3:D:1499:ARG:HD2 | 2.20 | 0.42 |
| 5:P:130:VAL:O | 5:P:131:VAL:C | 2.56 | 0.42 |
| 1:A:91:ASN:HA | 1:A:92:PRO:HD3 | 1.93 | 0.42 |
| 2:M:480:THR:CG2 | 2:M:482:GLU:HB2 | 2.49 | 0.42 |
| 1:A:96:THR:OG1 | 1:A:97:VAL:N | 2.52 | 0.42 |
| 2:C:137:VAL:HG21 | 2:C:393:GLN:NE2 | 2.35 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:L:117:VAL:HG12 | 1:L:118:ALA:N | 2.35 | 0.42 |
| 3:D:3:LYS:HB3 | 3:D:3:LYS:HE2 | 1.84 | 0.42 |
| 3:D:618:LEU:HD23 | 3:D:618:LEU:N | 2.34 | 0.42 |
| 2:M:252:LYS:C | 2:M:255:ALA:HB3 | 2.39 | 0.42 |
| 2:M:631:SER:O | 2:M:634:GLY:N | 2.43 | 0.42 |
| 3:N:272:LEU:CD1 | 3:N:282:TYR:HE1 | 2.32 | 0.42 |
| 3:N:244:GLU:CG | 3:N:245:LEU:N | 2.80 | 0.42 |
| 2:C:517:ARG:CA | 2:C:520:GLU:HB2 | 2.50 | 0.42 |
| 3:D:217:LYS:HB2 | 3:D:339:TRP:HE1 | 1.80 | 0.42 |
| 3:D:1465:ASN:O | 3:D:1468:LEU:HB3 | 2.20 | 0.42 |
| 3:D:1479:ASP:N | 3:D:1482:ARG:HG3 | 2.34 | 0.42 |
| 3:D:1483:PHE:HD1 | 3:D:1483:PHE:H | 1.65 | 0.42 |
| 3:D:571:LYS:O | 3:D:572:ARG:C | 2.58 | 0.42 |
| 3:D:539:ASP:HB3 | 3:D:600:LEU:HD13 | 2.02 | 0.42 |
| 4:E:22:VAL:O | 4:E:23:VAL:C | 2.58 | 0.42 |
| 5:F:110:MET:CE | 5:F:111:GLU:N | 2.83 | 0.42 |
| 5:F:123:ASP:HA | 5:F:124:PRO:HD3 | 1.90 | 0.42 |
| 3:N:356:PRO:HD3 | 3:N:440:VAL:HB | 2.01 | 0.42 |
| 3:D:347:VAL:HG13 | 3:D:351:MET:CB | 2.50 | 0.42 |
| 3:D:266:GLU:O | 3:D:314:PRO:HG3 | 2.19 | 0.42 |
| 3:D:325:GLU:CD | 3:D:332:TYR:HB3 | 2.40 | 0.42 |
| 3:D:764:LEU:HG | 3:D:766:ALA:H | 1.85 | 0.42 |
| 3:D:764:LEU:HD23 | 3:D:767:HIS:NE2 | 2.35 | 0.42 |
| 5:F:398:ARG:CD | 5:F:399:GLN:N | 2.83 | 0.42 |
| 1:A:36:LEU:HD12 | 1:A:36:LEU:N | 2.33 | 0.42 |
| 1:B:36:LEU:O | 1:B:37:GLY:C | 2.58 | 0.42 |
| 2:M:610:ARG:HD2 | 2:M:622:GLU:HG2 | 2.01 | 0.42 |
| 3:N:1376:MET:O | 3:N:1377:LYS:C | 2.58 | 0.42 |
| 2:M:373:VAL:CG1 | 2:M:374:ASN:N | 2.77 | 0.42 |
| 5:P:287:THR:O | 5:P:291:ILE:HG22 | 2.19 | 0.42 |
| 5:F:262:VAL:O | 5:F:265:VAL:N | 2.53 | 0.42 |
| 2:M:86:LYS:NZ | 2:M:811:PRO:O | 2.53 | 0.42 |
| 3:N:62:LYS:HE3 | 3:N:75:ARG:NH1 | 2.35 | 0.42 |
| 3:N:294:HIS:O | 3:N:303:PRO:HA | 2.20 | 0.42 |
| 3:N:1223:ILE:HG22 | 3:N:1227:GLN:OE1 | 2.19 | 0.42 |
| 3:N:1465:ASN:ND2 | 3:N:1473:PRO:HD3 | 2.35 | 0.42 |
| 2:M:874:LEU:HD12 | 3:N:784:ASP:OD1 | 2.20 | 0.42 |
| 3:N:846:PRO:O | 3:N:849:ALA:N | 2.53 | 0.42 |
| 3:N:857:ILE:C | 3:N:858:VAL:HG23 | 2.39 | 0.42 |
| 3:N:868:TYR:HB3 | 3:N:873:LEU:HD11 | 2.01 | 0.42 |
| 3:N:868:TYR:HB3 | 3:N:873:LEU:CD1 | 2.49 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:847:ASP:O | 3:D:848:GLU:C | 2.58 | 0.42 |
| 2:C:611:ILE:HD11 | 2:C:641:PRO:HB3 | 2.01 | 0.42 |
| 2:C:572:ILE:HA | 2:C:640:ARG:HH22 | 1.84 | 0.42 |
| 1:K:79:ILE:HG13 | 1:K:79:ILE:H | 1.63 | 0.42 |
| 5:P:330:GLY:C | 5:P:332:PHE:H | 2.23 | 0.42 |
| 1:A:104:GLU:CG | 1:A:105:GLY:N | 2.83 | 0.42 |
| 1:A:110:LYS:O | 1:A:129:ILE:HD12 | 2.20 | 0.42 |
| 2:M:317:VAL:H | 2:M:318:PRO:HD3 | 1.75 | 0.42 |
| 3:D:1258:ARG:NH2 | 3:D:1351:GLU:HG3 | 2.35 | 0.42 |
| 5:F:161:GLN:O | 5:F:165:SER:N | 2.52 | 0.42 |
| 5:F:323:ASP:OD1 | 5:F:325:LYS:HD2 | 2.19 | 0.42 |
| 2:C:705:ILE:HD12 | 2:C:705:ILE:H | 1.85 | 0.42 |
| 3:D:14:SER:O | 3:D:17:LYS:N | 2.53 | 0.42 |
| 2:M:560:MET:O | 2:M:564:MET:HB2 | 2.20 | 0.42 |
| 1:K:179:PHE:HB3 | 1:K:197:LEU:CD2 | 2.50 | 0.42 |
| 3:D:1336:LEU:O | 3:D:1340:GLY:CA | 2.67 | 0.42 |
| 3:N:1047:LYS:HD2 | 3:N:1051:GLU:CG | 2.49 | 0.42 |
| 3:N:1330:ILE:HG22 | 3:N:1331:ASP:N | 2.33 | 0.42 |
| 2:M:141:HIS:CE1 | 2:M:332:ARG:HB3 | 2.55 | 0.42 |
| 2:M:227:PHE:HD1 | 2:M:227:PHE:H | 1.67 | 0.42 |
| 2:M:258:TYR:O | 2:M:290:LEU:CD1 | 2.67 | 0.42 |
| 2:M:540:PHE:HB3 | 2:M:544:THR:CG2 | 2.49 | 0.42 |
| 3:D:432:TYR:H | 3:D:432:TYR:HD1 | 1.67 | 0.42 |
| 2:C:267:TYR:HB2 | 2:C:272:ALA:H | 1.83 | 0.42 |
| 2:C:332:ARG:NH2 | 2:C:338:GLU:OE1 | 2.53 | 0.42 |
| 3:N:123:LEU:HD23 | 3:N:123:LEU:N | 2.35 | 0.42 |
| 3:N:134:VAL:O | 3:N:134:VAL:HG12 | 2.19 | 0.42 |
| 3:D:102:ILE:HG23 | 3:D:103:TRP:N | 2.34 | 0.42 |
| 5:F:115:LYS:C | 5:F:119:ILE:HG13 | 2.40 | 0.42 |
| 5:F:119:ILE:HG22 | 5:F:119:ILE:O | 2.20 | 0.42 |
| 5:F:117:SER:HA | 5:F:127:ILE:HD11 | 2.01 | 0.42 |
| 3:D:933:ALA:O | 3:D:936:TYR:HB3 | 2.19 | 0.42 |
| 5:P:382:THR:HG23 | 5:P:397:ILE:CB | 2.50 | 0.42 |
| 5:P:409:LYS:O | 5:P:412:GLU:N | 2.53 | 0.42 |
| 1:B:104:GLU:CA | 1:B:132:LEU:HD13 | 2.43 | 0.42 |
| 1:L:66:SER:C | 1:L:75:VAL:HG23 | 2.39 | 0.42 |
| 5:F:403:LYS:O | 5:F:404:ALA:C | 2.59 | 0.42 |
| 2:C:58:ASP:C | 2:C:60:GLY:H | 2.23 | 0.42 |
| 3:D:1259:VAL:O | 3:D:1262:LEU:HB2 | 2.20 | 0.42 |
| 3:D:67:ARG:HD3 | 3:D:67:ARG:HA | 1.80 | 0.42 |
| 3:N:61:GLY:O | 3:N:63:TYR:N | 2.53 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:N:1226:ALA:O | 3:N:1229:ILE:N | 2.53 | 0.42 |
| 3:N:1464:GLU:O | 3:N:1465:ASN:C | 2.57 | 0.42 |
| 2:M:414:GLY:N | 2:M:419:THR:HG21 | 2.34 | 0.42 |
| 3:N:792:ILE:HG13 | 3:N:793:THR:N | 2.31 | 0.42 |
| 2:C:572:ILE:CG1 | 2:C:573:ARG:N | 2.83 | 0.42 |
| 3:N:1347:TYR:O | 3:N:1348:LEU:C | 2.59 | 0.42 |
| 3:N:371:ILE:HG13 | 3:N:372:ASP:N | 2.30 | 0.42 |
| 1:K:109:VAL:HG13 | 1:K:113:ASP:OD2 | 2.20 | 0.42 |
| 2:M:976:ASP:O | 2:M:978:ARG:N | 2.53 | 0.42 |
| 2:M:857:ASP:HB3 | 2:M:978:ARG:HG2 | 2.01 | 0.42 |
| 3:N:944:THR:O | 3:N:946:GLY:N | 2.52 | 0.42 |
| 2:M:34:VAL:N | 2:M:35:PRO:HD3 | 2.35 | 0.42 |
| 2:C:504:GLU:HG3 | 2:C:507:ARG:HB2 | 2.02 | 0.42 |
| 3:N:730:PRO:O | 3:N:732:VAL:N | 2.53 | 0.42 |
| 3:N:930:LEU:O | 3:N:934:LEU:HD12 | 2.20 | 0.42 |
| 1:K:56:VAL:CG1 | 1:K:57:TYR:N | 2.83 | 0.42 |
| 3:D:1346:ARG:NH1 | 3:D:1346:ARG:CG | 2.83 | 0.42 |
| 2:M:431:HIS:HE1 | 2:M:432:ARG:HG2 | 1.82 | 0.42 |
| 2:M:468:ARG:NE | 2:M:487:THR:HG22 | 2.35 | 0.42 |
| 3:D:64:LYS:HD3 | 5:F:377:ASP:OD2 | 2.20 | 0.42 |
| 2:C:1040:LEU:HD23 | 2:C:1040:LEU:HA | 1.91 | 0.42 |
| 2:C:135:VAL:HG12 | 2:C:136:ILE:N | 2.34 | 0.42 |
| 2:C:630:ARG:NE | 2:C:634:GLY:HA2 | 2.35 | 0.42 |
| 1:A:216:GLU:O | 1:A:219:ARG:HB3 | 2.20 | 0.42 |
| 1:A:221:HIS:C | 1:A:223:THR:H | 2.24 | 0.42 |
| 3:D:1035:ILE:O | 3:D:1036:ARG:C | 2.59 | 0.42 |
| 3:D:470:LEU:O | 3:D:471:GLU:C | 2.57 | 0.42 |
| 3:N:956:ILE:HG12 | 3:N:1039:CYS:O | 2.20 | 0.42 |
| 3:N:1333:HIS:O | 3:N:1334:GLN:C | 2.58 | 0.42 |
| 2:M:354:GLY:HA2 | 2:M:357:GLU:OE2 | 2.19 | 0.42 |
| 2:M:1113:GLU:O | 2:M:1113:GLU:CG | 2.63 | 0.42 |
| 4:O:80:VAL:HB | 4:O:81:PRO:CD | 2.49 | 0.42 |
| 3:D:686:GLU:CD | 3:D:686:GLU:H | 2.23 | 0.42 |
| 1:L:24:VAL:HG12 | 1:L:25:LEU:N | 2.35 | 0.42 |
| 3:N:1429:LEU:HG | 3:N:1429:LEU:O | 2.20 | 0.42 |
| 2:M:360:LEU:C | 2:M:362:GLY:H | 2.22 | 0.42 |
| 1:K:175:ARG:HH11 | 1:K:175:ARG:HG2 | 1.84 | 0.42 |
| 3:D:1150:ALA:HB3 | 3:D:1187:PRO:CB | 2.49 | 0.42 |
| 2:M:193:LEU:O | 2:M:194:VAL:C | 2.58 | 0.41 |
| 2:M:194:VAL:HA | 2:M:197:LEU:HD12 | 1.98 | 0.41 |
| 2:M:218:VAL:HG13 | 2:M:222:MET:CE | 2.49 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:139:GLN:O | 2:M:334:ARG:N | 2.52 | 0.41 |
| 2:M:402:SER:O | 2:M:406:HIS:N | 2.50 | 0.41 |
| 3:N:240:GLU:O | 3:N:313:MET:N | 2.40 | 0.41 |
| 3:N:259:VAL:HG11 | 3:N:293:VAL:CG1 | 2.50 | 0.41 |
| 3:N:262:LYS:NZ | 3:N:339:TRP:HZ2 | 2.18 | 0.41 |
| 2:C:140:ILE:HD12 | 2:C:331:ARG:CZ | 2.50 | 0.41 |
| 2:C:182:VAL:CG1 | 2:C:193:LEU:HB3 | 2.50 | 0.41 |
| 2:C:238:LEU:O | 2:C:239:PHE:C | 2.56 | 0.41 |
| 2:C:270:GLY:O | 2:C:272:ALA:N | 2.53 | 0.41 |
| 2:C:310:LEU:O | 2:C:314:THR:HG23 | 2.20 | 0.41 |
| 2:C:461:VAL:CG2 | 2:C:467:ILE:HG12 | 2.50 | 0.41 |
| 3:D:1076:GLY:O | 3:D:1080:GLY:N | 2.48 | 0.41 |
| 3:N:434:ARG:HH21 | 3:N:451:ASP:CG | 2.23 | 0.41 |
| 3:N:569:ASN:ND2 | 5:P:214:GLN:CD | 2.73 | 0.41 |
| 5:P:210:LEU:O | 5:P:213:ILE:HB | 2.19 | 0.41 |
| 3:D:317:VAL:HB | 3:D:339:TRP:HB3 | 2.01 | 0.41 |
| 3:D:1231:GLU:HB3 | 3:D:1232:PRO:CD | 2.42 | 0.41 |
| 3:D:546:ARG:HH21 | 3:D:577:ALA:CB | 2.33 | 0.41 |
| 3:D:550:ARG:NH1 | 3:D:573:MET:CB | 2.82 | 0.41 |
| 3:D:591:VAL:O | 3:D:593:ASN:N | 2.53 | 0.41 |
| 3:N:362:GLU:O | 3:N:365:ASP:CB | 2.67 | 0.41 |
| 1:B:214:ALA:O | 1:B:215:VAL:C | 2.58 | 0.41 |
| 1:L:81:ASN:O | 1:L:84:GLU:HB2 | 2.20 | 0.41 |
| 1:A:43:ILE:O | 1:A:47:SER:N | 2.53 | 0.41 |
| 2:M:639:GLN:HG2 | 2:M:658:GLY:HA2 | 2.00 | 0.41 |
| 2:C:351:LEU:HD13 | 2:C:374:ASN:O | 2.20 | 0.41 |
| 2:C:50:GLU:C | 2:C:52:PHE:H | 2.20 | 0.41 |
| 2:C:52:PHE:HD1 | 2:C:54:ILE:H | 1.67 | 0.41 |
| 5:P:289:GLU:O | 5:P:290:GLU:C | 2.57 | 0.41 |
| 5:F:291:ILE:CD1 | 5:F:295:MET:HB2 | 2.50 | 0.41 |
| 1:L:138:LEU:HD12 | 1:L:139:ASN:H | 1.85 | 0.41 |
| 1:L:58:ILE:O | 1:L:60:ASP:N | 2.53 | 0.41 |
| 3:D:800:LYS:CE | 3:D:826:PRO:CD | 2.94 | 0.41 |
| 3:N:1031:ASN:HB2 | 3:N:1032:PRO:HD2 | 2.02 | 0.41 |
| 2:C:673:LEU:HB3 | 2:C:867:VAL:HB | 2.01 | 0.41 |
| 3:N:256:GLU:O | 3:N:274:ARG:HB2 | 2.20 | 0.41 |
| 3:N:1118:ILE:HG13 | 3:N:1188:VAL:HG13 | 2.02 | 0.41 |
| 2:M:1049:LEU:O | 2:M:1052:MET:HB3 | 2.20 | 0.41 |
| 3:N:15:PRO:O | 3:N:19:ARG:HG3 | 2.19 | 0.41 |
| 3:N:661:MET:O | 3:N:662:GLU:C | 2.59 | 0.41 |
| 3:N:687:VAL:O | 3:N:690:ALA:HB3 | 2.18 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:K:215:VAL:O | 1:K:216:GLU:C | 2.58 | 0.41 |
| 2:M:503:LEU:HD12 | 2:M:508:ILE:CA | 2.36 | 0.41 |
| 2:M:504:GLU:HG3 | 2:M:504:GLU:O | 2.20 | 0.41 |
| 2:M:38:LYS:CG | 2:M:39:ARG:N | 2.80 | 0.41 |
| 3:N:1397:LYS:C | 3:N:1398:TRP:HD1 | 2.23 | 0.41 |
| 3:D:1344:VAL:HG13 | 3:D:1345:GLU:H | 1.79 | 0.41 |
| 3:N:1082:ALA:O | 3:N:1083:ASP:C | 2.58 | 0.41 |
| 3:D:884:ARG:O | 3:D:885:ILE:C | 2.58 | 0.41 |
| 2:C:843:HIS:O | 2:C:845:ASN:N | 2.53 | 0.41 |
| 2:C:894:GLY:CA | 2:C:901:TYR:OH | 2.68 | 0.41 |
| 5:P:128:ARG:HG3 | 5:P:128:ARG:HH11 | 1.85 | 0.41 |
| 3:N:983:LEU:HD22 | 3:N:987:GLU:CB | 2.49 | 0.41 |
| 1:K:182:GLU:O | 1:K:194:LYS:HB3 | 2.20 | 0.41 |
| 4:O:33:HIS:CE1 | 4:O:89:MET:HG2 | 2.54 | 0.41 |
| 3:D:895:VAL:HA | 3:D:898:GLU:CD | 2.40 | 0.41 |
| 2:C:1047:HIS:NE2 | 3:D:754:PHE:CE1 | 2.88 | 0.41 |
| 1:A:172:SER:HA | 1:A:173:PRO:HD2 | 1.89 | 0.41 |
| 5:P:161:GLN:CD | 5:P:161:GLN:H | 2.23 | 0.41 |
| 2:M:303:PHE:H | 2:M:303:PHE:HD1 | 1.67 | 0.41 |
| 3:N:225:LEU:N | 3:N:331:VAL:O | 2.53 | 0.41 |
| 2:C:270:GLY:O | 2:C:271:GLU:C | 2.59 | 0.41 |
| 2:C:280:LYS:O | 2:C:281:LEU:HD23 | 2.20 | 0.41 |
| 2:C:285:LEU:HD11 | 2:C:289:THR:CA | 2.50 | 0.41 |
| 2:C:333:ILE:HG22 | 2:C:465:GLY:O | 2.19 | 0.41 |
| 2:C:462:ASP:HB2 | 2:C:463:GLU:OE1 | 2.20 | 0.41 |
| 3:N:156:GLU:N | 3:N:156:GLU:OE2 | 2.47 | 0.41 |
| 3:N:434:ARG:NH1 | 3:N:449:SER:OG | 2.52 | 0.41 |
| 3:N:84:ILE:C | 3:N:86:ARG:H | 2.23 | 0.41 |
| 2:C:1088:LEU:HA | 2:C:1091:GLU:OE1 | 2.19 | 0.41 |
| 2:C:1112:PHE:CD1 | 2:C:1116:ALA:HB2 | 2.55 | 0.41 |
| 3:D:127:LEU:CD2 | 3:D:128:TYR:H | 2.27 | 0.41 |
| 3:D:1472:ILE:HG22 | 3:D:1474:ALA:O | 2.19 | 0.41 |
| 2:C:1088:LEU:HD22 | 9:D:1529:NE6:H17 | 2.00 | 0.41 |
| 3:D:466:LYS:O | 3:D:468:LEU:N | 2.54 | 0.41 |
| 3:D:519:VAL:HG13 | 3:D:544:TYR:CZ | 2.55 | 0.41 |
| 3:D:563:PRO:C | 3:D:565:ILE:H | 2.23 | 0.41 |
| 3:D:353:VAL:HG12 | 3:D:368:VAL:HG21 | 2.01 | 0.41 |
| 2:M:95:TYR:CD1 | 2:M:114:PHE:HB3 | 2.55 | 0.41 |
| 3:D:925:GLU:HG2 | 4:E:7:ASP:OD2 | 2.19 | 0.41 |
| 4:E:10:PHE:C | 4:E:12:MET:N | 2.73 | 0.41 |
| 4:E:4:PRO:C | 4:E:6:ILE:H | 2.23 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:F:380:GLU:C | 5:F:382:THR:H | 2.22 | 0.41 |
| 2:C:1068:GLU:OE1 | 5:F:345:ALA:HA | 2.21 | 0.41 |
| 2:C:15:LEU:CD1 | 2:C:15:LEU:N | 2.70 | 0.41 |
| 2:C:676:ILE:O | 2:C:677:MET:HB3 | 2.19 | 0.41 |
| 2:M:676:ILE:O | 2:M:677:MET:HB3 | 2.20 | 0.41 |
| 3:N:851:LEU:HD23 | 3:N:851:LEU:N | 2.35 | 0.41 |
| 3:N:855:HIS:O | 3:N:856:GLY:C | 2.59 | 0.41 |
| 2:M:914:ILE:O | 2:M:915:LYS:C | 2.58 | 0.41 |
| 2:M:1017:THR:HB | 2:M:1019:GLN:HE21 | 1.84 | 0.41 |
| 3:N:1262:LEU:HD22 | 3:N:1352:ILE:CG1 | 2.50 | 0.41 |
| 3:N:481:MET:O | 3:N:489:ARG:HG3 | 2.19 | 0.41 |
| 3:N:9:ARG:HG2 | 3:N:10:ILE:N | 2.35 | 0.41 |
| 1:K:36:LEU:HD12 | 1:K:36:LEU:N | 2.35 | 0.41 |
| 1:L:28:LEU:CD1 | 1:L:33:GLY:N | 2.83 | 0.41 |
| 5:F:274:THR:HG22 | 5:F:278:LEU:HD21 | 2.02 | 0.41 |
| 2:C:317:VAL:HG12 | 2:C:317:VAL:O | 2.21 | 0.41 |
| 2:M:118:ILE:HA | 2:M:119:PRO:HD3 | 1.87 | 0.41 |
| 5:P:245:GLN:CD | 5:P:245:GLN:N | 2.72 | 0.41 |
| 4:E:66:LYS:O | 4:E:69:LEU:HB2 | 2.20 | 0.41 |
| 2:M:217:LEU:C | 2:M:219:GLN:N | 2.70 | 0.41 |
| 3:N:960:LYS:HE2 | 3:N:1063:GLU:OE1 | 2.19 | 0.41 |
| 4:E:50:THR:O | 4:E:55:PHE:HE1 | 1.99 | 0.41 |
| 1:L:149:GLY:H | 1:L:172:SER:HB2 | 1.85 | 0.41 |
| 3:N:277:GLU:HG3 | 3:N:278:PRO:HD2 | 2.03 | 0.41 |
| 3:D:1139:ASP:N | 3:D:1139:ASP:OD1 | 2.51 | 0.41 |
| 2:M:252:LYS:CA | 2:M:255:ALA:HB3 | 2.51 | 0.41 |
| 2:M:461:VAL:CG2 | 2:M:467:ILE:HG12 | 2.51 | 0.41 |
| 2:C:192:PRO:HB2 | 2:C:195:LEU:CD2 | 2.28 | 0.41 |
| 2:C:266:ARG:CG | 2:C:266:ARG:HH11 | 2.24 | 0.41 |
| 2:C:311:PHE:N | 2:C:311:PHE:CD2 | 2.88 | 0.41 |
| 3:N:131:LYS:HA | 3:N:456:MET:CE | 2.51 | 0.41 |
| 3:N:32:ILE:CG2 | 3:N:37:LEU:HA | 2.50 | 0.41 |
| 5:P:184:ARG:O | 5:P:185:GLN:C | 2.58 | 0.41 |
| 2:C:1095:LEU:O | 3:D:101:HIS:NE2 | 2.54 | 0.41 |
| 3:D:569:ASN:HD21 | 5:F:214:GLN:CD | 2.23 | 0.41 |
| 3:D:573:MET:HG3 | 3:D:573:MET:H | 1.58 | 0.41 |
| 4:E:26:ARG:HE | 4:E:30:LEU:HD22 | 1.85 | 0.41 |
| 3:D:767:HIS:HA | 3:D:924:MET:CE | 2.50 | 0.41 |
| 2:C:681:GLY:HA3 | 3:D:939:PHE:CE1 | 2.55 | 0.41 |
| 5:P:393:THR:CG2 | 5:P:394:ARG:N | 2.83 | 0.41 |
| 5:P:406:ARG:O | 5:P:407:LYS:C | 2.59 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:F:287:THR:H | 5:F:290:GLU:CD | 2.24 | 0.41 |
| 3:D:1404:ASN:CA | 3:D:1408:ILE:HB | 2.46 | 0.41 |
| 3:D:71:LYS:N | 3:D:80:VAL:CG2 | 2.83 | 0.41 |
| 3:D:1031:ASN:CG | 3:D:1034:GLN:HE21 | 2.24 | 0.41 |
| 3:D:794:GLN:O | 3:D:861:GLN:HA | 2.20 | 0.41 |
| 3:N:1436:SER:O | 3:N:1439:SER:N | 2.52 | 0.41 |
| 3:N:1379:VAL:O | 3:N:1392:GLY:HA2 | 2.19 | 0.41 |
| 2:C:549:PHE:HE1 | 2:C:909:ALA:HB3 | 1.84 | 0.41 |
| 3:N:711:LEU:CD2 | 3:N:778:LEU:HD23 | 2.43 | 0.41 |
| 2:M:679:PHE:HA | 3:N:943:THR:CG2 | 2.37 | 0.41 |
| 2:M:1014:SER:HB3 | 2:M:1019:GLN:H | 1.85 | 0.41 |
| 2:C:572:ILE:HG13 | 2:C:573:ARG:H | 1.84 | 0.41 |
| 2:M:1066:ALA:O | 2:M:1067:TYR:C | 2.57 | 0.41 |
| 3:N:692:GLU:O | 3:N:695:ILE:HB | 2.21 | 0.41 |
| 2:M:1098:ASP:O | 3:N:9:ARG:O | 2.38 | 0.41 |
| 3:D:630:VAL:N | 3:D:744:GLN:HG2 | 2.34 | 0.41 |
| 1:K:73:GLU:CG | 1:K:130:ALA:HA | 2.50 | 0.41 |
| 1:K:5:LYS:C | 1:K:7:LYS:N | 2.72 | 0.41 |
| 2:M:37:GLU:CB | 2:M:71:TYR:HE2 | 2.34 | 0.41 |
| 2:M:432:ARG:NH1 | 2:M:518:LYS:O | 2.52 | 0.41 |
| 3:N:1070:TYR:O | 3:N:1071:PHE:C | 2.57 | 0.41 |
| 5:P:151:LEU:O | 5:P:156:VAL:HG22 | 2.20 | 0.41 |
| 2:C:631:SER:O | 2:C:632:ASN:C | 2.59 | 0.41 |
| 5:P:251:ILE:O | 5:P:255:ALA:HB2 | 2.21 | 0.41 |
| 3:N:265:GLU:HB2 | 3:N:316:GLN:OE1 | 2.20 | 0.41 |
| 3:D:1041:LEU:HD12 | 3:D:1057:VAL:O | 2.21 | 0.41 |
| 5:F:170:HIS:O | 5:F:173:TYR:N | 2.53 | 0.41 |
| 3:D:710:ARG:O | 3:D:712:GLY:N | 2.52 | 0.41 |
| 3:D:1333:HIS:O | 3:D:1334:GLN:C | 2.59 | 0.41 |
| 5:F:205:ARG:HD2 | 5:F:251:ILE:HD13 | 2.01 | 0.41 |
| 3:D:901:GLN:O | 3:D:904:VAL:HG22 | 2.20 | 0.41 |
| 3:D:821:VAL:C | 3:D:823:LEU:N | 2.73 | 0.41 |
| 1:B:6:LEU:C | 1:B:8:ALA:N | 2.74 | 0.41 |
| 3:D:1189:ARG:NH1 | 3:D:1203:LYS:HG3 | 2.36 | 0.41 |
| 3:N:794:GLN:HG3 | 3:N:1017:PHE:CZ | 2.55 | 0.41 |
| 2:M:148:PHE:H | 2:M:323:ASP:CG | 2.20 | 0.41 |
| 3:N:217:LYS:HE3 | 3:N:341:GLU:OE1 | 2.19 | 0.41 |
| 2:C:267:TYR:HD2 | 2:C:268:ASP:H | 1.68 | 0.41 |
| 2:C:437:ARG:NH2 | 2:C:487:THR:C | 2.74 | 0.41 |
| 2:C:486:MET:HE1 | 2:C:491:GLU:HA | 2.01 | 0.41 |
| 3:N:139:GLY:CA | 3:N:147:VAL:HB | 2.49 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:N:436:GLU:HB2 | 3:N:445:ARG:O | 2.20 | 0.41 |
| 3:N:547:LEU:O | 3:N:548:ILE:C | 2.59 | 0.41 |
| 3:N:572:ARG:HD3 | 5:P:83:GLN:OE1 | 2.20 | 0.41 |
| 3:D:1217:ILE:HD13 | 3:D:1480:PHE:CE2 | 2.55 | 0.41 |
| 3:D:1106:VAL:HG11 | 3:D:1474:ALA:CB | 2.50 | 0.41 |
| 3:D:612:GLY:O | 3:D:616:GLN:HG2 | 2.20 | 0.41 |
| 5:F:220:LEU:O | 5:F:224:VAL:HG23 | 2.20 | 0.41 |
| 3:D:403:PHE:CD1 | 3:D:404:GLU:N | 2.88 | 0.41 |
| 3:D:403:PHE:CE2 | 3:D:442:ASN:HB3 | 2.54 | 0.41 |
| 5:P:382:THR:O | 5:P:385:GLU:N | 2.54 | 0.41 |
| 1:B:58:ILE:O | 1:B:59:GLU:C | 2.58 | 0.41 |
| 3:D:822:ALA:HB3 | 3:D:824:ASN:ND2 | 2.35 | 0.41 |
| 2:M:588:VAL:HG23 | 2:M:596:TYR:OH | 2.19 | 0.41 |
| 3:D:660:LYS:O | 3:D:661:MET:C | 2.58 | 0.41 |
| 2:C:41:ASN:O | 2:C:46:ALA:N | 2.53 | 0.41 |
| 5:F:260:ILE:HD11 | 5:F:264:MET:HB3 | 2.01 | 0.41 |
| 5:F:271:LEU:HB2 | 5:F:272:SER:H | 1.71 | 0.41 |
| 5:P:373:LYS:C | 5:P:375:LEU:N | 2.74 | 0.41 |
| 2:M:713:ARG:HA | 2:M:818:GLY:O | 2.19 | 0.41 |
| 3:N:1489:GLN:NE2 | 4:O:72:ARG:C | 2.74 | 0.41 |
| 3:N:1489:GLN:HE22 | 4:O:73:LEU:N | 2.16 | 0.41 |
| 3:D:1197:ARG:O | 3:D:1198:TYR:CD1 | 2.74 | 0.41 |
| 1:L:55:SER:CB | 1:L:166:PRO:HA | 2.51 | 0.41 |
| 5:F:367:MET:HG2 | 5:F:370:LYS:HE2 | 2.01 | 0.41 |
| 3:N:1226:ALA:O | 3:N:1227:GLN:C | 2.57 | 0.41 |
| 2:M:987:ILE:HG22 | 2:M:988:VAL:O | 2.21 | 0.41 |
| 3:N:827:ILE:CG2 | 3:N:837:GLY:HA3 | 2.50 | 0.41 |
| 2:C:694:LEU:CD2 | 2:C:697:ARG:HH22 | 2.34 | 0.41 |
| 3:N:1117:TYR:HD1 | 3:N:1118:ILE:N | 2.17 | 0.41 |
| 3:N:15:PRO:HD2 | 3:N:16:GLU:OE2 | 2.20 | 0.41 |
| 1:K:206:THR:HG22 | 1:K:208:LEU:N | 2.35 | 0.41 |
| 2:M:45:GLN:HA | 2:M:48:PHE:HD1 | 1.85 | 0.41 |
| 3:D:95:LEU:CB | 3:D:515:GLU:HA | 2.41 | 0.41 |
| 3:N:1021:TYR:O | 3:N:1022:VAL:C | 2.59 | 0.41 |
| 3:N:1078:ARG:O | 3:N:1079:LYS:C | 2.58 | 0.41 |
| 3:N:191:LEU:HB3 | 3:N:195:VAL:HB | 2.03 | 0.41 |
| 2:C:897:LEU:HD21 | 2:C:921:ALA:N | 2.35 | 0.41 |
| 3:D:192:ALA:H | 3:D:195:VAL:HB | 1.84 | 0.41 |
| 3:N:531:ASP:O | 3:N:532:GLY:C | 2.59 | 0.41 |
| 3:D:472:ALA:O | 3:D:473:LEU:C | 2.57 | 0.41 |
| 2:C:726:ILE:O | 2:C:728:HIS:N | 2.54 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:O:81:PRO:O | 4:O:85:LEU:HD21 | 2.20 | 0.41 |
| 3:N:69:GLU:HG3 | 3:N:70:GLY:N | 2.36 | 0.41 |
| 2:M:185:LYS:NZ | 2:M:190:LYS:HZ2 | 2.17 | 0.41 |
| 2:M:202:TYR:CB | 2:M:207:LEU:HD21 | 2.51 | 0.41 |
| 2:M:141:HIS:CB | 2:M:418:LEU:HD22 | 2.50 | 0.41 |
| 3:N:272:LEU:HD12 | 3:N:282:TYR:HE1 | 1.86 | 0.41 |
| 3:N:217:LYS:HD2 | 3:N:339:TRP:CZ2 | 2.56 | 0.41 |
| 3:N:309:GLY:O | 3:N:311:LEU:HG | 2.20 | 0.41 |
| 2:C:333:ILE:HG21 | 2:C:461:VAL:HG21 | 2.02 | 0.41 |
| 2:C:583:LEU:O | 2:C:584:GLU:C | 2.59 | 0.41 |
| 3:N:39:PRO:HB3 | 3:N:45:PHE:C | 2.41 | 0.41 |
| 3:N:521:PRO:HD2 | 3:N:524:LEU:HD12 | 2.02 | 0.41 |
| 3:N:560:GLN:HA | 5:P:132:ARG:HH12 | 1.85 | 0.41 |
| 2:C:1041:GLU:O | 2:C:1044:GLY:N | 2.54 | 0.41 |
| 3:D:1466:VAL:C | 3:D:1468:LEU:H | 2.22 | 0.41 |
| 3:D:1494:ALA:HB2 | 4:E:92:ILE:HD11 | 2.01 | 0.41 |
| 5:F:135:ILE:C | 5:F:137:GLY:H | 2.23 | 0.41 |
| 5:F:209:PHE:HA | 5:F:212:LEU:HG | 2.02 | 0.41 |
| 3:D:361:VAL:HG13 | 3:D:379:ALA:CB | 2.32 | 0.41 |
| 3:D:443:VAL:CG1 | 3:D:444:VAL:N | 2.84 | 0.41 |
| 3:D:262:LYS:O | 3:D:268:ALA:HA | 2.20 | 0.41 |
| 3:D:241:ILE:CG1 | 3:D:312:ARG:CZ | 2.97 | 0.41 |
| 3:D:932:ASP:HA | 3:D:935:LYS:HB3 | 2.03 | 0.41 |
| 1:B:112:ARG:HG3 | 1:B:113:ASP:N | 2.35 | 0.41 |
| 2:M:150:PRO:HA | 2:M:158:TYR:CB | 2.20 | 0.41 |
| 2:C:375:SER:O | 2:C:376:ARG:C | 2.59 | 0.41 |
| 2:M:780:GLU:OE1 | 2:M:780:GLU:HA | 2.20 | 0.41 |
| 3:D:1374:GLN:OE1 | 3:D:1374:GLN:HA | 2.20 | 0.41 |
| 1:L:165:ILE:HG23 | 1:L:166:PRO:HD2 | 2.01 | 0.41 |
| 2:M:691:SER:HB3 | 2:M:868:ASP:HA | 2.02 | 0.41 |
| 2:C:754:ILE:HG12 | 2:C:791:ARG:HD2 | 2.02 | 0.41 |
| 3:N:1147:ARG:HB3 | 3:N:1188:VAL:HG23 | 2.01 | 0.41 |
| 2:M:1045:ALA:HA | 3:N:758:GLU:HB3 | 2.02 | 0.41 |
| 1:A:33:GLY:HA2 | 1:A:195:LEU:HB2 | 2.03 | 0.41 |
| 3:N:1346:ARG:O | 3:N:1347:TYR:C | 2.58 | 0.41 |
| 2:C:1001:VAL:O | 2:C:1004:LYS:HB3 | 2.20 | 0.41 |
| 3:D:735:ALA:C | 3:D:737:ASN:H | 2.23 | 0.41 |
| 1:K:110:LYS:O | 1:K:113:ASP:OD2 | 2.39 | 0.41 |
| 1:L:28:LEU:CD2 | 1:L:29:GLU:N | 2.82 | 0.41 |
| 2:M:922:PHE:CE2 | 2:M:964:LYS:HB2 | 2.56 | 0.41 |
| 1:K:9:PRO:HA | 1:K:27:PRO:HD2 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:N:1399:ASP:HB3 | 3:N:1400:VAL:H | 1.76 | 0.41 |
| 3:N:631:ILE:CG2 | 3:N:745:MET:HB2 | 2.49 | 0.41 |
| 3:D:1315:ASP:O | 3:D:1316:GLY:C | 2.59 | 0.41 |
| 3:D:986:ARG:O | 3:D:987:GLU:C | 2.59 | 0.41 |
| 1:A:222:LEU:O | 1:A:225:PHE:HD1 | 2.02 | 0.41 |
| 3:D:1074:SER:O | 3:D:1077:ALA:N | 2.53 | 0.41 |
| 3:D:219:GLU:O | 3:D:337:LEU:HG | 2.21 | 0.41 |
| 1:K:89:PHE:CD2 | 1:K:94:LEU:HB3 | 2.55 | 0.41 |
| 2:C:1078:GLU:HA | 2:C:1079:PRO:HD3 | 1.77 | 0.41 |
| 3:N:250:LEU:CD1 | 3:N:306:GLU:HG2 | 2.51 | 0.41 |
| 5:P:117:SER:OG | 5:P:124:PRO:HG3 | 2.20 | 0.41 |
| 2:C:662:GLU:C | 2:C:664:GLY:N | 2.74 | 0.41 |
| 2:M:83:CYS:SG | 2:M:90:TYR:HA | 2.61 | 0.41 |
| 2:M:795:GLY:O | 2:M:796:GLU:HG2 | 2.21 | 0.41 |
| 2:M:180:GLY:HA2 | 2:M:223:ASP:OD2 | 2.21 | 0.41 |
| 1:K:222:LEU:HA | 1:K:225:PHE:CD1 | 2.54 | 0.41 |
| 2:M:135:VAL:HG23 | 2:M:395:LYS:HA | 2.02 | 0.41 |
| 2:M:194:VAL:C | 2:M:197:LEU:HG | 2.41 | 0.41 |
| 2:M:461:VAL:HG23 | 2:M:467:ILE:HG12 | 2.02 | 0.41 |
| 3:N:217:LYS:CB | 3:N:339:TRP:HE1 | 2.15 | 0.41 |
| 2:C:196:LEU:O | 2:C:200:LEU:HG | 2.21 | 0.41 |
| 2:C:449:ILE:O | 2:C:451:LEU:HG | 2.20 | 0.41 |
| 2:C:444:PRO:CG | 2:C:452:ILE:HB | 2.51 | 0.41 |
| 2:C:459:ALA:HB1 | 2:C:467:ILE:CG2 | 2.50 | 0.41 |
| 3:N:133:ILE:HG13 | 3:N:153:LEU:HD23 | 2.02 | 0.41 |
| 3:N:22:SER:C | 3:N:24:GLY:N | 2.74 | 0.41 |
| 3:N:573:MET:HE1 | 5:P:211:ASP:OD1 | 2.21 | 0.41 |
| 5:P:224:VAL:O | 5:P:227:PHE:HB3 | 2.20 | 0.41 |
| 3:D:1447:LEU:O | 3:D:1450:ALA:N | 2.54 | 0.41 |
| 3:D:546:ARG:HG3 | 3:D:547:LEU:H | 1.85 | 0.41 |
| 3:D:547:LEU:O | 3:D:548:ILE:C | 2.58 | 0.41 |
| 4:E:26:ARG:NE | 4:E:30:LEU:HD22 | 2.34 | 0.41 |
| 4:E:26:ARG:NH2 | 4:E:38:THR:HA | 2.34 | 0.41 |
| 5:F:135:ILE:CD1 | 5:F:181:GLU:HB3 | 2.50 | 0.41 |
| 4:E:7:ASP:CA | 4:E:10:PHE:HD1 | 2.28 | 0.41 |
| 5:F:346:THR:O | 5:F:349:LEU:HB3 | 2.21 | 0.41 |
| 3:N:1424:VAL:O | 3:N:1425:THR:C | 2.58 | 0.41 |
| 5:P:300:ASP:OD1 | 5:P:301:ALA:N | 2.54 | 0.41 |
| 4:O:42:PRO:O | 4:O:43:GLU:C | 2.59 | 0.41 |
| 2:C:677:MET:N | 2:C:871:LEU:O | 2.53 | 0.41 |
| 2:C:876:VAL:O | 2:C:877:PRO:C | 2.59 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:N:1442:ASN:C | 3:N:1442:ASN:ND2 | 2.74 | 0.41 |
| 1:L:176:ARG:HD3 | 3:N:884:ARG:HH22 | 1.83 | 0.41 |
| 2:M:874:LEU:O | 2:M:876:VAL:N | 2.54 | 0.41 |
| 3:N:472:ALA:O | 3:N:473:LEU:C | 2.58 | 0.41 |
| 3:N:348:GLN:H | 3:N:351:MET:CE | 2.15 | 0.41 |
| 1:K:36:LEU:O | 1:K:37:GLY:C | 2.58 | 0.41 |
| 1:K:86:VAL:HG13 | 1:K:123:MET:CB | 2.43 | 0.41 |
| 2:M:854:PRO:O | 2:M:857:ASP:OD2 | 2.38 | 0.41 |
| 3:N:637:LEU:O | 3:N:935:LYS:NZ | 2.53 | 0.41 |
| 1:A:123:MET:O | 1:A:125:PRO:HD2 | 2.21 | 0.41 |
| 2:C:343:GLN:HG2 | 2:C:385:PHE:CB | 2.50 | 0.41 |
| 2:C:396:ASP:CB | 2:C:406:HIS:HD2 | 2.34 | 0.41 |
| 3:N:230:TRP:CE2 | 3:N:233:LYS:HE3 | 2.55 | 0.41 |
| 2:M:293:PHE:CD1 | 2:M:293:PHE:C | 2.94 | 0.41 |
| 3:D:470:LEU:HG | 3:D:470:LEU:H | 1.62 | 0.41 |
| 5:F:170:HIS:HA | 5:F:173:TYR:CD1 | 2.56 | 0.41 |
| 3:N:179:VAL:HG13 | 3:N:180:LYS:N | 2.36 | 0.41 |
| 3:D:342:PRO:O | 3:D:343:LYS:CG | 2.67 | 0.41 |
| 3:D:1304:LYS:O | 3:D:1305:LEU:HB3 | 2.21 | 0.41 |
| 1:K:143:ARG:NH1 | 1:K:158:ILE:HD12 | 2.35 | 0.41 |
| 2:M:770:GLU:OE1 | 3:N:65:ARG:NH2 | 2.53 | 0.41 |
| 5:F:231:ARG:HB2 | 5:F:233:PHE:CE2 | 2.55 | 0.41 |
| 2:M:27:ARG:C | 2:M:29:ALA:H | 2.23 | 0.41 |
| 3:N:213:VAL:CG1 | 3:N:215:TYR:CE2 | 3.04 | 0.41 |
| 2:M:360:LEU:HB2 | 2:M:361:MET:SD | 2.61 | 0.41 |
| 1:L:109:VAL:HG12 | 1:L:129:ILE:HD12 | 2.01 | 0.41 |
| 3:N:322:VAL:HG22 | 3:N:323:GLU:N | 2.36 | 0.41 |
| 2:C:424:GLY:O | 2:C:425:PHE:C | 2.58 | 0.41 |
| 2:C:512:ARG:HD2 | 2:C:523:ILE:HG12 | 2.02 | 0.41 |
| 3:N:133:ILE:O | 3:N:153:LEU:HB3 | 2.21 | 0.41 |
| 3:N:536:ALA:HB1 | 5:P:317:LEU:HD23 | 2.01 | 0.41 |
| 3:N:564:GLU:HA | 3:N:567:ILE:HB | 2.03 | 0.41 |
| 3:D:121:THR:O | 3:D:125:GLN:HB3 | 2.21 | 0.41 |
| 3:D:1491:THR:O | 3:D:1491:THR:HG22 | 2.20 | 0.41 |
| 3:D:156:GLU:HG2 | 3:D:157:GLU:N | 2.35 | 0.41 |
| 3:D:508:ARG:HB2 | 3:D:511:TRP:CE2 | 2.56 | 0.41 |
| 3:D:536:ALA:C | 5:F:317:LEU:HD21 | 2.41 | 0.41 |
| 3:D:550:ARG:NH1 | 3:D:573:MET:C | 2.74 | 0.41 |
| 5:F:116:LEU:O | 5:F:119:ILE:N | 2.53 | 0.41 |
| 3:D:353:VAL:O | 3:D:353:VAL:HG23 | 2.21 | 0.41 |
| 5:P:353:GLU:CA | 5:P:356:LYS:HB2 | 2.51 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:112:ARG:C | 1:B:114:PHE:N | 2.71 | 0.41 |
| 1:B:206:THR:HG22 | 1:B:208:LEU:N | 2.36 | 0.41 |
| 1:A:38:ASN:N | 1:A:179:PHE:CE2 | 2.88 | 0.41 |
| 1:A:179:PHE:HB3 | 1:A:197:LEU:CD2 | 2.50 | 0.41 |
| 5:F:417:LYS:O | 5:F:419:ARG:N | 2.53 | 0.41 |
| 2:M:63:GLY:H | 2:M:103:LYS:HB2 | 1.85 | 0.41 |
| 5:P:308:LEU:N | 5:P:308:LEU:HD23 | 2.33 | 0.41 |
| 5:P:364:ARG:O | 5:P:367:MET:HG3 | 2.21 | 0.41 |
| 3:D:1400:VAL:HA | 3:D:1408:ILE:HD12 | 2.02 | 0.41 |
| 3:D:1418:LYS:HA | 3:D:1419:PRO:HD3 | 1.95 | 0.41 |
| 1:L:56:VAL:CG1 | 1:L:57:TYR:N | 2.83 | 0.41 |
| 3:D:1006:ALA:O | 3:D:1009:LYS:HB3 | 2.21 | 0.41 |
| 3:D:162:ARG:O | 3:D:449:SER:HB2 | 2.20 | 0.41 |
| 3:N:1388:ARG:HG2 | 3:N:1391:GLU:HG3 | 2.02 | 0.41 |
| 3:N:1031:ASN:O | 3:N:1034:GLN:HB2 | 2.21 | 0.41 |
| 3:N:1224:VAL:HA | 3:N:1227:GLN:OE1 | 2.21 | 0.41 |
| 3:N:792:ILE:O | 3:N:878:GLY:HA3 | 2.20 | 0.41 |
| 3:D:205:TYR:OH | 3:D:445:ARG:NH2 | 2.53 | 0.41 |
| 2:M:186:VAL:HG22 | 2:M:187:ASN:N | 2.35 | 0.41 |
| 3:N:1118:ILE:CG1 | 3:N:1190:SER:HB2 | 2.49 | 0.41 |
| 2:M:1050:GLN:O | 2:M:1051:GLU:C | 2.59 | 0.41 |
| 2:M:1015:LEU:HD12 | 5:P:335:ASP:HB2 | 2.02 | 0.41 |
| 3:D:1299:PHE:N | 3:D:1299:PHE:CD1 | 2.86 | 0.41 |
| 3:N:14:SER:O | 3:N:18:ILE:HG13 | 2.21 | 0.41 |
| 3:N:664:LYS:HB2 | 3:N:666:ILE:HG12 | 2.01 | 0.41 |
| 3:N:350:HIS:O | 3:N:370:ALA:HA | 2.21 | 0.41 |
| 1:K:213:GLN:O | 1:K:216:GLU:HB3 | 2.20 | 0.41 |
| 5:F:278:LEU:O | 5:F:279:GLN:C | 2.57 | 0.41 |
| 3:D:1307:LYS:N | 3:D:1307:LYS:CE | 2.76 | 0.41 |
| 2:M:437:ARG:HG3 | 2:M:437:ARG:NH1 | 2.36 | 0.41 |
| 5:P:97:GLU:HG3 | 5:P:97:GLU:H | 1.71 | 0.41 |
| 3:N:1066:THR:HB | 3:N:1069:GLU:HG3 | 2.03 | 0.41 |
| 3:N:210:ARG:HD2 | 3:N:389:GLU:OE2 | 2.21 | 0.41 |
| 3:D:1114:THR:HA | 3:D:1195:GLN:CD | 2.41 | 0.41 |
| 3:D:1114:THR:HA | 3:D:1195:GLN:NE2 | 2.35 | 0.41 |
| 4:O:76:GLY:HA3 | 4:O:79:LEU:CD2 | 2.42 | 0.41 |
| 3:D:965:GLU:C | 3:D:967:ALA:N | 2.73 | 0.41 |
| 3:D:214:GLU:HG2 | 3:D:342:PRO:CA | 2.50 | 0.41 |
| 1:L:188:GLN:HG3 | 1:L:189:ARG:N | 2.35 | 0.41 |
| 3:N:650:LEU:O | 3:N:651:GLU:C | 2.57 | 0.41 |
| 2:M:754:ILE:HG12 | 2:M:791:ARG:CD | 2.50 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:72:VAL:CG1 | 3:D:73:CYS:N | 2.83 | 0.41 |
| 3:N:101:HIS:C | 3:N:101:HIS:ND1 | 2.73 | 0.41 |
| 2:M:198:ARG:HG3 | 2:M:231:PRO:HA | 2.03 | 0.41 |
| 2:M:255:ALA:O | 2:M:257:VAL:N | 2.53 | 0.41 |
| 2:M:408:ARG:CD | 2:M:542:VAL:HG13 | 2.51 | 0.41 |
| 3:N:325:GLU:H | 3:N:331:VAL:HG13 | 1.86 | 0.41 |
| 2:C:334:ARG:HD2 | 2:C:418:LEU:HD13 | 2.02 | 0.41 |
| 2:C:446:GLY:O | 2:C:449:ILE:N | 2.45 | 0.41 |
| 3:D:318:ARG:CG | 3:D:319:ALA:H | 2.33 | 0.41 |
| 3:D:119:SER:H | 3:D:123:LEU:HG | 1.80 | 0.41 |
| 3:D:536:ALA:HA | 5:F:315:VAL:O | 2.21 | 0.41 |
| 3:D:541:ASN:O | 3:D:545:ARG:CG | 2.69 | 0.41 |
| 3:D:592:THR:HG23 | 3:D:600:LEU:HD21 | 2.02 | 0.41 |
| 3:D:403:PHE:C | 3:D:403:PHE:CD1 | 2.93 | 0.41 |
| 3:D:247:GLU:HA | 3:D:248:PRO:HA | 1.94 | 0.41 |
| 3:D:221:ALA:O | 3:D:334:THR:HG22 | 2.20 | 0.41 |
| 5:P:403:LYS:HZ3 | 5:P:407:LYS:HE2 | 1.86 | 0.41 |
| 1:B:20:TYR:C | 1:B:207:PRO:HG2 | 2.41 | 0.41 |
| 1:B:20:TYR:CG | 1:B:21:GLY:N | 2.88 | 0.41 |
| 5:F:372:ARG:HG3 | 5:F:378:GLY:C | 2.39 | 0.41 |
| 5:F:382:THR:C | 5:F:384:GLU:N | 2.74 | 0.41 |
| 5:F:385:GLU:CA | 5:F:388:ALA:HB3 | 2.30 | 0.41 |
| 2:C:62:GLY:HA3 | 2:C:103:LYS:CG | 2.50 | 0.41 |
| 2:C:60:GLY:C | 2:C:62:GLY:H | 2.24 | 0.41 |
| 5:P:268:ILE:CA | 5:P:271:LEU:HG | 2.51 | 0.41 |
| 3:D:1384:PRO:CB | 3:D:1387:SER:O | 2.68 | 0.41 |
| 5:F:367:MET:HB3 | 5:F:371:LEU:CG | 2.50 | 0.41 |
| 3:D:1019:PRO:O | 3:D:1022:VAL:HB | 2.21 | 0.41 |
| 3:N:1174:LEU:H | 3:N:1174:LEU:HG | 1.55 | 0.41 |
| 2:C:573:ARG:HB2 | 2:C:670:GLN:HE22 | 1.83 | 0.41 |
| 2:C:611:ILE:HG22 | 2:C:612:VAL:N | 2.36 | 0.41 |
| 3:D:46:ASP:C | 3:D:48:ARG:H | 2.24 | 0.41 |
| 3:D:46:ASP:OD2 | 3:D:48:ARG:HB2 | 2.21 | 0.41 |
| 1:A:151:VAL:O | 1:A:156:HIS:HE1 | 2.04 | 0.41 |
| 3:D:630:VAL:HA | 3:D:744:GLN:HG2 | 2.01 | 0.41 |
| 2:M:928:LYS:HG2 | 2:M:932:GLU:HG3 | 2.03 | 0.41 |
| 3:N:806:PHE:CE1 | 3:N:816:HIS:CE1 | 3.09 | 0.41 |
| 3:N:812:ALA:HA | 3:N:816:HIS:N | 2.35 | 0.41 |
| 1:L:143:ARG:C | 1:L:143:ARG:CD | 2.88 | 0.41 |
| 3:D:1347:TYR:O | 3:D:1348:LEU:C | 2.58 | 0.41 |
| 3:N:1078:ARG:C | 3:N:1080:GLY:N | 2.74 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:N:204:LEU:HD12 | 3:N:205:TYR:N | 2.35 | 0.41 |
| 5:P:102:LEU:HD21 | 5:P:187:LEU:H | 1.86 | 0.41 |
| 3:N:1129:THR:CG2 | 3:N:1130:ARG:N | 2.84 | 0.41 |
| 2:C:382:ILE:O | 2:C:383:ARG:C | 2.58 | 0.41 |
| 4:O:6:ILE:HD11 | 4:O:10:PHE:CZ | 2.56 | 0.41 |
| 1:L:111:ALA:HB2 | 1:L:127:LEU:HB3 | 2.02 | 0.41 |
| 2:C:167:LYS:O | 2:C:167:LYS:HG2 | 2.20 | 0.41 |
| 3:D:700:VAL:O | 3:D:701:LEU:HD23 | 2.21 | 0.41 |
| 2:C:680:ASP:H | 3:D:943:THR:HG1 | 1.63 | 0.41 |
| 3:D:1269:LYS:N | 3:D:1269:LYS:CD | 2.84 | 0.41 |
| 5:P:239:ALA:C | 5:P:241:TRP:N | 2.72 | 0.41 |
| 3:N:581:LEU:O | 3:N:582:LEU:C | 2.59 | 0.41 |
| 3:N:583:ASP:HA | 3:N:602:SER:OG | 2.20 | 0.41 |
| 3:N:187:LYS:HG3 | 3:N:198:ARG:HG3 | 2.03 | 0.41 |
| 2:C:724:ARG:CD | 2:C:738:ASP:HA | 2.50 | 0.41 |
| 2:C:1118:LYS:O | 2:C:1119:ARG:HB2 | 2.20 | 0.41 |
| 2:C:1086:ARG:O | 2:C:1087:VAL:C | 2.59 | 0.41 |
| 2:M:138:SER:O | 2:M:410:ILE:HG23 | 2.20 | 0.41 |
| 2:M:396:ASP:HA | 2:M:633:GLN:HE22 | 1.86 | 0.41 |
| 2:M:218:VAL:HG13 | 2:M:222:MET:HE2 | 2.03 | 0.41 |
| 2:M:398:THR:HA | 2:M:633:GLN:CG | 2.44 | 0.41 |
| 2:M:457:ALA:HB2 | 2:M:545:ASN:ND2 | 2.36 | 0.41 |
| 3:N:261:LEU:HD23 | 3:N:270:LEU:CA | 2.51 | 0.41 |
| 2:C:172:ILE:HG23 | 2:C:184:MET:HE3 | 2.02 | 0.41 |
| 2:C:468:ARG:HG2 | 2:C:487:THR:HG22 | 2.03 | 0.41 |
| 2:C:139:GLN:HG2 | 2:C:391:LEU:CD2 | 2.51 | 0.41 |
| 2:C:300:ASP:OD1 | 2:C:303:PHE:N | 2.53 | 0.41 |
| 2:C:410:ILE:N | 2:C:453:THR:O | 2.50 | 0.41 |
| 3:N:128:TYR:CZ | 3:N:461:ILE:HG13 | 2.55 | 0.41 |
| 3:N:92:HIS:C | 3:N:93:ILE:HG13 | 2.41 | 0.41 |
| 3:D:217:LYS:HB2 | 3:D:339:TRP:CD1 | 2.56 | 0.41 |
| 2:C:1016:ILE:O | 2:C:1018:GLN:HG2 | 2.21 | 0.41 |
| 3:D:1464:GLU:HG3 | 3:D:1465:ASN:H | 1.85 | 0.41 |
| 3:D:1096:ARG:HG2 | 6:D:1528:PO4:O2 | 2.21 | 0.41 |
| 3:D:552:ASN:HA | 3:D:555:LYS:CD | 2.38 | 0.41 |
| 3:D:564:GLU:CA | 3:D:567:ILE:HB | 2.50 | 0.41 |
| 3:D:1495:ILE:HA | 4:E:84:ARG:HD3 | 2.03 | 0.41 |
| 3:D:567:ILE:HG13 | 5:F:140:ARG:NH2 | 2.36 | 0.41 |
| 3:D:550:ARG:HD2 | 3:D:577:ALA:HB2 | 2.02 | 0.41 |
| 3:D:564:GLU:HA | 3:D:567:ILE:CB | 2.51 | 0.41 |
| 5:F:222:ARG:CG | 5:F:242:TRP:CZ3 | 3.04 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:378:ILE:HG12 | 3:N:379:ALA:N | 2.35 | 0.41 |
| 2:M:69:LEU:O | 2:M:70:GLU:HG3 | 2.21 | 0.41 |
| 3:D:939:PHE:O | 3:D:940:THR:C | 2.58 | 0.41 |
| 5:P:409:LYS:CG | 5:P:410:TYR:H | 2.33 | 0.41 |
| 1:B:58:ILE:HA | 1:B:140:MET:HA | 2.03 | 0.41 |
| 1:A:43:ILE:HG23 | 1:A:47:SER:CB | 2.51 | 0.41 |
| 2:C:101:ILE:HG12 | 2:C:107:LEU:HA | 2.01 | 0.41 |
| 2:M:66:LEU:HA | 2:M:66:LEU:HD12 | 1.82 | 0.41 |
| 5:P:261:PRO:HB2 | 5:P:264:MET:HB2 | 2.03 | 0.41 |
| 5:P:267:THR:O | 5:P:268:ILE:C | 2.59 | 0.41 |
| 2:M:370:ALA:C | 2:M:372:LEU:N | 2.75 | 0.41 |
| 5:F:257:THR:O | 5:F:258:ILE:HD13 | 2.20 | 0.41 |
| 5:F:269:ASN:C | 5:F:271:LEU:N | 2.74 | 0.41 |
| 2:C:773:LEU:O | 2:C:774:LEU:C | 2.59 | 0.41 |
| 3:D:1149:LEU:HD23 | 3:D:1160:LEU:O | 2.21 | 0.41 |
| 5:F:370:LYS:O | 5:F:374:GLY:N | 2.53 | 0.41 |
| 3:N:62:LYS:HE3 | 3:N:75:ARG:HD3 | 2.02 | 0.41 |
| 3:N:1380:GLU:N | 3:N:1420:LEU:HD22 | 2.35 | 0.41 |
| 3:N:497:GLU:O | 3:N:498:VAL:C | 2.59 | 0.41 |
| 3:N:1379:VAL:HG22 | 3:N:1393:GLN:O | 2.21 | 0.41 |
| 3:N:1229:ILE:HA | 3:N:1363:LEU:HD11 | 2.03 | 0.41 |
| 2:M:674:VAL:HG22 | 2:M:675:ALA:N | 2.36 | 0.41 |
| 2:M:985:GLY:HA2 | 2:M:986:PRO:HD3 | 1.72 | 0.41 |
| 2:C:854:PRO:O | 2:C:855:VAL:C | 2.58 | 0.41 |
| 3:N:1476:THR:CB | 4:O:21:VAL:HG23 | 2.44 | 0.41 |
| 3:D:1278:ASP:HB3 | 3:D:1318:TYR:OH | 2.21 | 0.41 |
| 3:D:1296:SER:C | 3:D:1298:GLY:N | 2.74 | 0.41 |
| 2:C:589:ARG:HG2 | 2:C:596:TYR:CE2 | 2.56 | 0.41 |
| 2:C:575:GLN:C | 2:C:667:ALA:HB1 | 2.40 | 0.41 |
| 3:N:690:ALA:O | 3:N:694:VAL:HG23 | 2.21 | 0.41 |
| 1:A:77:GLU:O | 1:A:81:ASN:ND2 | 2.54 | 0.41 |
| 1:L:28:LEU:HD23 | 1:L:29:GLU:H | 1.84 | 0.41 |
| 1:K:73:GLU:HB3 | 1:K:78:ILE:HG12 | 2.03 | 0.41 |
| 2:C:316:GLY:C | 2:C:318:PRO:HD3 | 2.40 | 0.41 |
| 3:N:1400:VAL:O | 3:N:1404:ASN:ND2 | 2.54 | 0.41 |
| 3:D:1253:THR:CG2 | 3:D:1257:PRO:HB2 | 2.50 | 0.41 |
| 3:D:1258:ARG:HH21 | 3:D:1351:GLU:CG | 2.33 | 0.41 |
| 3:N:1311:LEU:HD12 | 3:N:1312:LEU:N | 2.32 | 0.41 |
| 1:B:19:GLU:HG2 | 1:B:203:GLY:HA2 | 2.02 | 0.41 |
| 5:F:151:LEU:C | 5:F:153:PRO:HD2 | 2.41 | 0.41 |
| 5:F:152:ASP:O | 5:F:156:VAL:HG21 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:F:161:GLN:O | 5:F:165:SER:CB | 2.68 | 0.41 |
| 3:D:142:LEU:HD22 | 3:D:144:GLY:O | 2.20 | 0.41 |
| 2:C:841:ASN:C | 2:C:843:HIS:N | 2.74 | 0.41 |
| 3:D:264:LEU:HB2 | 3:D:267:GLY:CA | 2.50 | 0.41 |
| 3:D:989:TYR:O | 3:D:990:ASP:C | 2.58 | 0.41 |
| 2:C:631:SER:HB3 | 2:C:635:THR:H | 1.82 | 0.41 |
| 4:O:46:PRO:HG2 | 4:O:63:TRP:CG | 2.55 | 0.41 |
| 2:M:558:ALA:O | 2:M:561:GLY:N | 2.53 | 0.41 |
| 3:N:1001:GLU:O | 3:N:1002:LYS:C | 2.58 | 0.41 |
| 3:N:963:TYR:O | 3:N:967:ALA:CB | 2.69 | 0.41 |
| 5:F:245:GLN:O | 5:F:246:ALA:C | 2.59 | 0.41 |
| 3:D:499:VAL:O | 3:D:500:ARG:C | 2.60 | 0.41 |
| 3:N:583:ASP:OD1 | 3:N:604:THR:HB | 2.21 | 0.41 |
| 3:N:606:ILE:O | 3:N:607:LEU:C | 2.59 | 0.41 |
| 3:N:1333:HIS:C | 3:N:1337:GLU:OE2 | 2.59 | 0.41 |
| 2:M:577:PRO:HG3 | 2:M:993:PHE:CG | 2.56 | 0.41 |
| 4:E:85:LEU:CD2 | 4:E:85:LEU:H | 2.27 | 0.41 |
| 1:B:95:GLN:NE2 | 1:B:146:ARG:NH1 | 2.69 | 0.41 |
| 3:D:1046:GLN:HB2 | 3:D:1052:THR:HA | 2.01 | 0.41 |
| 2:M:890:LEU:O | 2:M:893:ALA:N | 2.54 | 0.41 |
| 5:P:194:LEU:HD13 | 5:P:194:LEU:C | 2.41 | 0.41 |
| 3:D:1194:CYS:HB2 | 3:D:1204:CYS:HB3 | 2.03 | 0.41 |
| 3:N:794:GLN:OE1 | 3:N:794:GLN:HA | 2.21 | 0.41 |
| 1:A:87:VAL:HG21 | 1:A:144:VAL:HG11 | 2.03 | 0.41 |
| 3:D:922:LEU:O | 3:D:923:GLY:O | 2.38 | 0.41 |
| 2:M:711:GLU:OE1 | 2:M:711:GLU:N | 2.54 | 0.41 |
| 3:N:464:LEU:HD23 | 3:N:464:LEU:N | 2.36 | 0.41 |
| 3:N:325:GLU:CD | 3:N:332:TYR:HB3 | 2.41 | 0.41 |
| 2:C:151:ASP:H | 2:C:158:TYR:HB3 | 1.86 | 0.41 |
| 2:C:227:PHE:O | 2:C:233:GLU:OE1 | 2.38 | 0.41 |
| 2:C:517:ARG:O | 2:C:518:LYS:C | 2.59 | 0.41 |
| 2:C:435:TYR:HD1 | 3:D:1071:PHE:CD2 | 2.39 | 0.41 |
| 3:N:102:ILE:C | 3:N:104:PHE:N | 2.75 | 0.41 |
| 3:N:124:GLU:O | 3:N:128:TYR:HD2 | 2.04 | 0.41 |
| 2:C:1088:LEU:O | 2:C:1089:VAL:C | 2.58 | 0.41 |
| 3:D:126:VAL:HG12 | 3:D:127:LEU:N | 2.36 | 0.41 |
| 3:D:528:VAL:CG1 | 3:D:529:GLN:N | 2.84 | 0.41 |
| 3:D:539:ASP:CB | 3:D:600:LEU:HB3 | 2.50 | 0.41 |
| 3:D:612:GLY:O | 3:D:615:ARG:HG2 | 2.21 | 0.41 |
| 5:F:102:LEU:HD21 | 5:F:187:LEU:H | 1.85 | 0.41 |
| 5:F:208:SER:O | 5:F:209:PHE:C | 2.59 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:D:273:ARG:O | 3:D:274:ARG:C | 2.59 | 0.41 |
| 3:D:297:ILE:CG2 | 3:D:298:VAL:N | 2.83 | 0.41 |
| 3:D:245:LEU:HG | 3:D:309:GLY:CA | 2.50 | 0.41 |
| 5:P:381:HIS:O | 5:P:384:GLU:HG3 | 2.20 | 0.41 |
| 5:P:356:LYS:HB3 | 5:P:417:LYS:HZ3 | 1.85 | 0.41 |
| 1:B:58:ILE:O | 1:B:58:ILE:HG23 | 2.21 | 0.41 |
| 5:F:408:LEU:O | 5:F:411:HIS:HB3 | 2.20 | 0.41 |
| 1:A:179:PHE:C | 1:A:179:PHE:CD1 | 2.94 | 0.41 |
| 2:M:640:ARG:HD2 | 2:M:642:ARG:NH2 | 2.36 | 0.41 |
| 3:D:662:GLU:C | 3:D:664:LYS:H | 2.23 | 0.41 |
| 2:C:30:LEU:HA | 2:C:44:ILE:HD12 | 2.03 | 0.41 |
| 5:P:280:GLN:CG | 5:P:281:GLU:N | 2.80 | 0.41 |
| 5:F:291:ILE:O | 5:F:294:ALA:N | 2.54 | 0.41 |
| 3:D:1405:GLU:CG | 3:D:1406:ARG:N | 2.83 | 0.41 |
| 1:L:58:ILE:CG1 | 1:L:140:MET:HB3 | 2.45 | 0.41 |
| 3:D:950:GLY:C | 3:D:952:ASP:N | 2.74 | 0.41 |
| 3:N:73:CYS:HB3 | 3:N:76:CYS:SG | 2.61 | 0.41 |
| 3:N:493:ARG:O | 3:N:496:LEU:HB3 | 2.20 | 0.41 |
| 3:N:298:VAL:CB | 3:N:300:LYS:HE3 | 2.49 | 0.41 |
| 3:N:1103:HIS:N | 3:N:1104:GLU:OE1 | 2.54 | 0.41 |
| 3:N:879:ARG:O | 3:N:882:PHE:HB3 | 2.20 | 0.41 |
| 2:C:673:LEU:HB3 | 2:C:867:VAL:HA | 2.02 | 0.41 |
| 2:C:790:LEU:HD12 | 2:C:791:ARG:H | 1.83 | 0.41 |
| 1:A:48:ILE:HA | 1:A:49:PRO:HD3 | 1.72 | 0.41 |
| 1:B:48:ILE:HA | 1:B:49:PRO:HD2 | 1.81 | 0.41 |
| 2:M:944:LEU:O | 2:M:947:ALA:HB3 | 2.21 | 0.41 |
| 2:C:503:LEU:CD1 | 2:C:508:ILE:HA | 2.37 | 0.41 |
| 3:D:1345:GLU:OE2 | 3:D:1376:MET:HG3 | 2.20 | 0.41 |
| 1:B:176:ARG:C | 1:B:200:TRP:HD1 | 2.24 | 0.41 |
| 2:C:958:THR:O | 2:C:962:GLN:HG3 | 2.20 | 0.41 |
| 5:P:156:VAL:HG22 | 5:P:156:VAL:H | 1.67 | 0.41 |
| 2:C:807:ARG:CB | 2:C:807:ARG:CZ | 2.99 | 0.41 |
| 2:C:839:LEU:HA | 2:C:995:MET:O | 2.21 | 0.41 |
| 3:D:1147:ARG:HB2 | 3:D:1166:LEU:CD1 | 2.48 | 0.41 |
| 2:C:683:ASN:HD22 | 2:C:683:ASN:C | 2.24 | 0.41 |
| 3:D:1117:TYR:CA | 3:D:1193:THR:HG21 | 2.51 | 0.41 |
| 3:D:896:ALA:O | 3:D:900:ILE:HG13 | 2.20 | 0.41 |
| 3:N:640:HIS:ND1 | 3:N:641:GLN:HG3 | 2.36 | 0.41 |
| 4:O:29:GLN:HB3 | 4:O:29:GLN:HE21 | 1.69 | 0.41 |
| 5:P:146:GLY:HA3 | 5:P:149:GLU:CD | 2.42 | 0.41 |
| 5:P:202:TYR:CD1 | 5:P:202:TYR:N | 2.89 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1190:SER:OG | 3:D:1191:PRO:HD2 | 2.20 | 0.41 |
| 3:D:740:PHE:CD1 | 3:D:740:PHE:N | 2.89 | 0.41 |
| 2:C:1072:LYS:HG2 | 2:C:1072:LYS:H | 1.65 | 0.41 |
| 2:M:631:SER:O | 2:M:632:ASN:C | 2.60 | 0.40 |
| 2:C:455:LEU:HD11 | 2:C:459:ALA:HB3 | 2.03 | 0.40 |
| 3:N:149:LYS:CE | 3:N:151:GLN:HG3 | 2.47 | 0.40 |
| 3:N:32:ILE:HD12 | 3:N:527:MET:HG2 | 2.03 | 0.40 |
| 3:N:574:LEU:O | 3:N:578:VAL:HG23 | 2.21 | 0.40 |
| 5:P:215:GLU:O | 5:P:218:GLN:HG3 | 2.20 | 0.40 |
| 2:C:1093:GLN:O | 2:C:1096:ALA:N | 2.52 | 0.40 |
| 3:D:1107:VAL:HG12 | 3:D:1217:ILE:HG23 | 2.03 | 0.40 |
| 3:D:123:LEU:O | 3:D:124:GLU:C | 2.59 | 0.40 |
| 3:D:1438:ALA:HA | 3:D:1446:VAL:HG21 | 2.03 | 0.40 |
| 3:D:1439:SER:OG | 3:D:1463:LYS:NZ | 2.53 | 0.40 |
| 3:D:152:LEU:CD1 | 3:D:153:LEU:H | 2.33 | 0.40 |
| 3:D:159:ARG:C | 3:D:161:LEU:N | 2.74 | 0.40 |
| 3:D:608:SER:HB2 | 3:D:614:PHE:CE1 | 2.56 | 0.40 |
| 2:M:73:LEU:HB3 | 2:M:93:PRO:O | 2.21 | 0.40 |
| 3:D:268:ALA:CB | 3:D:290:PRO:HG3 | 2.51 | 0.40 |
| 5:P:343:ASP:O | 5:P:344:ALA:C | 2.60 | 0.40 |
| 1:A:179:PHE:HB3 | 1:A:197:LEU:HD21 | 2.03 | 0.40 |
| 1:A:40:LEU:HA | 1:A:43:ILE:HD12 | 2.03 | 0.40 |
| 3:D:661:MET:O | 3:D:664:LYS:O | 2.40 | 0.40 |
| 2:C:96:ALA:O | 2:C:113:VAL:HG22 | 2.21 | 0.40 |
| 2:M:807:ARG:HA | 2:M:821:GLU:CB | 2.50 | 0.40 |
| 1:L:99:LEU:HA | 1:L:99:LEU:HD23 | 1.90 | 0.40 |
| 3:D:826:PRO:HB3 | 3:D:828:LYS:HZ1 | 1.86 | 0.40 |
| 3:N:496:LEU:O | 3:N:497:GLU:C | 2.59 | 0.40 |
| 1:K:183:ASP:CG | 2:M:938:LYS:HE3 | 2.42 | 0.40 |
| 3:N:1445:HIS:O | 3:N:1448:THR:HB | 2.20 | 0.40 |
| 2:M:869:VAL:HG22 | 2:M:870:ILE:N | 2.35 | 0.40 |
| 2:M:874:LEU:C | 2:M:876:VAL:H | 2.25 | 0.40 |
| 3:N:860:LEU:HA | 3:N:877:PRO:CB | 2.46 | 0.40 |
| 3:D:851:LEU:H | 3:D:851:LEU:CD2 | 2.32 | 0.40 |
| 3:D:875:THR:HG22 | 3:D:876:SER:N | 2.25 | 0.40 |
| 2:C:666:LEU:CD1 | 2:C:668:LEU:HG | 2.42 | 0.40 |
| 1:A:31:GLY:N | 1:A:193:ASP:OD2 | 2.54 | 0.40 |
| 1:A:5:LYS:HZ2 | 1:A:29:GLU:N | 2.18 | 0.40 |
| 3:N:661:MET:HA | 3:N:666:ILE:HD11 | 2.02 | 0.40 |
| 3:N:686:GLU:O | 3:N:687:VAL:C | 2.59 | 0.40 |
| 1:K:206:THR:CB | 1:K:209:GLU:HG3 | 2.36 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:K:42:ARG:O | 1:K:43:ILE:C | 2.59 | 0.40 |
| 3:N:106:LYS:NZ | 3:N:106:LYS:HB3 | 2.36 | 0.40 |
| 3:N:391:ALA:HB2 | 5:P:97:GLU:OE2 | 2.20 | 0.40 |
| 3:D:882:PHE:O | 3:D:885:ILE:HB | 2.21 | 0.40 |
| 2:C:961:GLU:O | 2:C:962:GLN:C | 2.58 | 0.40 |
| 3:D:1281:VAL:HG21 | 3:D:1313:VAL:CG2 | 2.51 | 0.40 |
| 5:P:154:LYS:O | 5:P:155:THR:C | 2.59 | 0.40 |
| 2:C:631:SER:CB | 2:C:635:THR:OG1 | 2.69 | 0.40 |
| 2:M:567:GLN:CB | 2:M:997:LEU:HD22 | 2.51 | 0.40 |
| 2:C:707:ARG:HG2 | 2:C:708:TYR:N | 2.35 | 0.40 |
| 2:C:915:LYS:O | 2:C:968:LEU:HD22 | 2.20 | 0.40 |
| 3:N:996:TRP:HA | 3:N:999:THR:OG1 | 2.19 | 0.40 |
| 5:F:172:ARG:O | 5:F:176:ILE:HG13 | 2.21 | 0.40 |
| 3:N:186:VAL:CG1 | 3:N:187:LYS:N | 2.83 | 0.40 |
| 3:N:957:PRO:HG2 | 3:N:1007:VAL:CA | 2.48 | 0.40 |
| 2:C:726:ILE:CD1 | 2:C:728:HIS:HB2 | 2.51 | 0.40 |
| 2:C:685:GLU:HG3 | 3:D:739:ASP:HB3 | 2.03 | 0.40 |
| 3:D:1274:ILE:HD11 | 3:D:1334:GLN:HB3 | 2.02 | 0.40 |
| 2:C:1076:VAL:HA | 2:C:1077:PRO:HD3 | 1.85 | 0.40 |
| 3:D:1190:SER:OG | 3:D:1191:PRO:CD | 2.69 | 0.40 |
| 3:D:1023:MET:O | 3:D:1024:ALA:C | 2.59 | 0.40 |
| 5:F:193:ARG:O | 5:F:194:LEU:C | 2.59 | 0.40 |
| 3:D:1415:VAL:O | 3:D:1415:VAL:HG23 | 2.21 | 0.40 |
| 2:C:165:LEU:HA | 2:C:165:LEU:HD23 | 1.78 | 0.40 |
| 3:N:832:ARG:HG3 | 3:N:832:ARG:O | 2.20 | 0.40 |
| 2:M:233:GLU:HB2 | 2:M:237:ARG:NH2 | 2.37 | 0.40 |
| 2:M:461:VAL:HA | 2:M:466:PHE:O | 2.20 | 0.40 |
| 3:N:246:PRO:HD2 | 3:N:307:ALA:O | 2.21 | 0.40 |
| 3:N:223:LEU:O | 3:N:332:TYR:CD1 | 2.74 | 0.40 |
| 2:C:267:TYR:HB2 | 2:C:272:ALA:N | 2.36 | 0.40 |
| 2:C:328:LEU:HD12 | 2:C:437:ARG:HD2 | 2.03 | 0.40 |
| 2:C:514:VAL:HG23 | 2:C:514:VAL:O | 2.20 | 0.40 |
| 3:N:112:ILE:HG23 | 3:N:512:MET:CE | 2.51 | 0.40 |
| 3:N:141:ILE:HB | 3:N:450:TYR:HB3 | 2.04 | 0.40 |
| 3:D:1199:GLY:O | 3:D:1373:ARG:NH1 | 2.54 | 0.40 |
| 3:D:244:GLU:OE2 | 3:D:310:LEU:CD2 | 2.69 | 0.40 |
| 3:D:731:LEU:O | 3:D:734:GLU:HG2 | 2.22 | 0.40 |
| 3:D:936:TYR:CE2 | 3:D:940:THR:HG21 | 2.57 | 0.40 |
| 1:B:221:HIS:C | 1:B:223:THR:H | 2.24 | 0.40 |
| 2:M:157:ARG:HG3 | 2:M:158:TYR:N | 2.37 | 0.40 |
| 2:M:603:VAL:HG21 | 2:M:644:VAL:O | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:1064:ASN:ND2 | 2:C:1064:ASN:H | 2.19 | 0.40 |
| 2:C:1066:ALA:O | 2:C:1067:TYR:C | 2.60 | 0.40 |
| 1:A:209:GLU:CA | 1:A:212:ASN:HD22 | 2.34 | 0.40 |
| 2:C:41:ASN:O | 2:C:46:ALA:CB | 2.69 | 0.40 |
| 3:D:481:MET:O | 3:D:489:ARG:CD | 2.69 | 0.40 |
| 3:N:972:LEU:O | 3:N:973:GLN:C | 2.60 | 0.40 |
| 2:M:1102:LEU:O | 3:N:5:VAL:CA | 2.67 | 0.40 |
| 3:N:1436:SER:O | 3:N:1437:ALA:C | 2.59 | 0.40 |
| 3:N:792:ILE:HD13 | 3:N:941:PHE:HE1 | 1.84 | 0.40 |
| 3:N:854:ALA:C | 3:N:856:GLY:N | 2.74 | 0.40 |
| 3:N:950:GLY:O | 3:N:953:ASP:HB2 | 2.22 | 0.40 |
| 2:M:469:THR:HA | 2:M:470:PRO:HD3 | 1.96 | 0.40 |
| 2:M:1036:GLU:CD | 2:M:1036:GLU:N | 2.74 | 0.40 |
| 2:C:640:ARG:O | 2:C:657:ASP:N | 2.50 | 0.40 |
| 2:C:668:LEU:HD23 | 2:C:668:LEU:HA | 1.93 | 0.40 |
| 1:B:48:ILE:HG22 | 1:B:173:PRO:CD | 2.51 | 0.40 |
| 2:M:921:ALA:O | 2:M:922:PHE:C | 2.60 | 0.40 |
| 3:N:934:LEU:O | 3:N:935:LYS:C | 2.60 | 0.40 |
| 2:M:504:GLU:HG3 | 2:M:507:ARG:HD3 | 2.02 | 0.40 |
| 2:C:998:TYR:HE2 | 2:C:1000:MET:HA | 1.86 | 0.40 |
| 3:D:387:LEU:H | 3:D:387:LEU:CD1 | 2.16 | 0.40 |
| 3:N:1165:TYR:CZ | 3:N:1214:PRO:HB3 | 2.56 | 0.40 |
| 1:B:106:PRO:CA | 1:B:133:GLU:HA | 2.40 | 0.40 |
| 3:N:1068:LEU:HD12 | 3:N:1068:LEU:HA | 1.78 | 0.40 |
| 3:D:142:LEU:C | 3:D:142:LEU:HD12 | 2.41 | 0.40 |
| 2:C:806:LEU:HB2 | 2:C:822:VAL:HG22 | 2.03 | 0.40 |
| 2:C:813:VAL:HG11 | 2:C:815:LEU:HG | 2.01 | 0.40 |
| 5:P:235:PHE:O | 5:P:238:TYR:N | 2.54 | 0.40 |
| 3:D:1041:LEU:HG | 3:D:1043:GLY:CA | 2.51 | 0.40 |
| 3:D:504:ASP:O | 3:D:506:GLY:N | 2.54 | 0.40 |
| 3:D:341:GLU:HA | 3:D:342:PRO:HD2 | 1.87 | 0.40 |
| 3:N:1123:PHE:CA | 3:N:1133:ARG:O | 2.69 | 0.40 |
| 2:M:738:ASP:OD1 | 2:M:738:ASP:N | 2.54 | 0.40 |
| 2:C:728:HIS:CD2 | 2:C:730:SER:O | 2.74 | 0.40 |
| 5:F:247:ILE:O | 5:F:248:ASN:C | 2.58 | 0.40 |
| 3:D:73:CYS:O | 3:D:77:GLY:HA2 | 2.21 | 0.40 |
| 2:M:879:ARG:HH11 | 2:M:879:ARG:HG2 | 1.86 | 0.40 |
| 2:C:944:LEU:O | 2:C:945:ARG:C | 2.60 | 0.40 |
| 2:M:937:ASP:O | 2:M:940:GLU:N | 2.54 | 0.40 |
| 3:N:110:SER:O | 3:N:111:LYS:C | 2.58 | 0.40 |
| 2:M:212:GLY:O | 2:M:215:GLY:C | 2.59 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:397:GLU:CD | 2:M:632:ASN:H | 2.23 | 0.40 |
| 3:N:259:VAL:HG11 | 3:N:293:VAL:HG12 | 2.02 | 0.40 |
| 2:C:172:ILE:H | 2:C:172:ILE:HG13 | 1.70 | 0.40 |
| 2:C:328:LEU:HD12 | 2:C:433:THR:C | 2.42 | 0.40 |
| 2:C:906:PHE:HZ | 3:D:1070:TYR:CD2 | 2.39 | 0.40 |
| 3:N:116:LEU:HB2 | 3:N:118:LEU:HG | 2.03 | 0.40 |
| 3:N:119:SER:CB | 3:N:123:LEU:H | 2.25 | 0.40 |
| 3:N:149:LYS:CG | 3:N:150:ARG:H | 2.30 | 0.40 |
| 3:N:416:ALA:CB | 3:N:432:TYR:CA | 2.84 | 0.40 |
| 5:P:215:GLU:O | 5:P:218:GLN:CG | 2.68 | 0.40 |
| 3:D:1440:PHE:CD2 | 3:D:1440:PHE:N | 2.86 | 0.40 |
| 3:D:1447:LEU:O | 3:D:1449:GLU:N | 2.54 | 0.40 |
| 3:D:138:LYS:CB | 3:D:450:TYR:OH | 2.66 | 0.40 |
| 3:D:508:ARG:HA | 3:D:509:PRO:HD2 | 1.80 | 0.40 |
| 3:D:508:ARG:HB2 | 3:D:511:TRP:NE1 | 2.36 | 0.40 |
| 3:D:87:ARG:O | 3:D:524:LEU:HD11 | 2.22 | 0.40 |
| 3:D:564:GLU:HA | 3:D:567:ILE:CG1 | 2.51 | 0.40 |
| 5:F:181:GLU:OE2 | 5:F:184:ARG:HD3 | 2.21 | 0.40 |
| 3:D:226:PRO:HB2 | 3:D:231:VAL:CG2 | 2.50 | 0.40 |
| 3:D:934:LEU:O | 3:D:935:LYS:C | 2.59 | 0.40 |
| 5:P:405:LEU:O | 5:P:408:LEU:HB3 | 2.21 | 0.40 |
| 5:F:381:HIS:HB3 | 5:F:384:GLU:CG | 2.51 | 0.40 |
| 3:D:654:LYS:HD3 | 3:D:655:PRO:HD3 | 2.03 | 0.40 |
| 5:F:260:ILE:CG1 | 5:F:261:PRO:HD2 | 2.51 | 0.40 |
| 3:D:1149:LEU:HB3 | 3:D:1163:GLY:H | 1.86 | 0.40 |
| 3:D:1403:LEU:HB3 | 3:D:1408:ILE:CD1 | 2.51 | 0.40 |
| 1:L:137:ARG:HH22 | 1:L:139:ASN:HD22 | 1.69 | 0.40 |
| 2:C:974:LEU:O | 2:C:983:ILE:HG13 | 2.20 | 0.40 |
| 2:C:987:ILE:CG2 | 3:D:948:THR:HG21 | 2.52 | 0.40 |
| 3:N:1462:LEU:HB3 | 3:N:1472:ILE:CD1 | 2.52 | 0.40 |
| 3:N:784:ASP:OD1 | 3:N:784:ASP:N | 2.50 | 0.40 |
| 2:M:909:ALA:C | 2:M:910:LYS:HD2 | 2.41 | 0.40 |
| 5:F:189:GLU:O | 5:F:191:ASN:N | 2.55 | 0.40 |
| 1:L:208:LEU:HD11 | 1:L:212:ASN:HD21 | 1.85 | 0.40 |
| 2:C:1004:LYS:HG2 | 2:C:1005:MET:N | 2.36 | 0.40 |
| 1:K:111:ALA:C | 1:K:113:ASP:H | 2.23 | 0.40 |
| 3:N:933:ALA:O | 3:N:936:TYR:HB3 | 2.20 | 0.40 |
| 3:N:806:PHE:CE2 | 3:N:809:PRO:C | 2.95 | 0.40 |
| 5:P:321:ILE:HG22 | 5:P:322:GLY:N | 2.37 | 0.40 |
| 5:P:329:TYR:O | 5:P:330:GLY:C | 2.60 | 0.40 |
| 3:D:1339:LYS:CB | 3:D:1343:ALA:CB | 2.99 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:70:GLY:H | 2:C:607:ASP:CG | 2.25 | 0.40 |
| 2:M:446:GLY:O | 2:M:449:ILE:HG22 | 2.22 | 0.40 |
| 2:C:90:TYR:O | 2:C:119:PRO:HA | 2.21 | 0.40 |
| 3:N:645:PRO:O | 3:N:646:LYS:C | 2.60 | 0.40 |
| 3:N:1292:VAL:CG1 | 3:N:1293:PHE:N | 2.82 | 0.40 |
| 2:M:728:HIS:HD2 | 2:M:734:LEU:HD21 | 1.87 | 0.40 |
| 3:D:1179:GLU:C | 3:D:1181:GLY:N | 2.75 | 0.40 |
| 2:M:890:LEU:O | 2:M:891:GLY:C | 2.59 | 0.40 |
| 5:P:320:PRO:HA | 5:P:327:SER:O | 2.20 | 0.40 |
| 2:C:1019:GLN:O | 2:C:1020:PRO:C | 2.60 | 0.40 |
| 1:A:175:ARG:O | 1:A:176:ARG:HB2 | 2.20 | 0.40 |
| 3:D:681:ARG:HG3 | 3:D:682:ASP:OD1 | 2.21 | 0.40 |
| 3:N:34:TYR:CG | 3:N:35:ARG:N | 2.89 | 0.40 |
| 3:N:1283:ILE:HD12 | 3:N:1315:ASP:OD2 | 2.22 | 0.40 |
| 2:C:173:ASP:O | 2:C:174:LEU:HD23 | 2.21 | 0.40 |
| 2:C:300:ASP:OD2 | 2:C:303:PHE:CD1 | 2.74 | 0.40 |
| 3:N:133:ILE:HG22 | 3:N:455:ARG:CA | 2.51 | 0.40 |
| 3:N:32:ILE:HG23 | 3:N:38:LYS:N | 2.36 | 0.40 |
| 3:N:409:VAL:HG12 | 3:N:410:SER:H | 1.85 | 0.40 |
| 3:N:416:ALA:HB1 | 3:N:432:TYR:CD1 | 2.56 | 0.40 |
| 3:N:543:LEU:HA | 3:N:546:ARG:HD3 | 2.03 | 0.40 |
| 3:N:564:GLU:O | 3:N:565:ILE:C | 2.59 | 0.40 |
| 3:D:1453:ALA:O | 3:D:1454:GLY:C | 2.59 | 0.40 |
| 3:D:139:GLY:HA3 | 3:D:147:VAL:HG23 | 2.02 | 0.40 |
| 3:D:209:ARG:HB2 | 3:D:389:GLU:CB | 2.51 | 0.40 |
| 3:D:283:PHE:CE2 | 3:D:313:MET:SD | 3.14 | 0.40 |
| 5:P:402:ASN:ND2 | 5:P:402:ASN:N | 2.70 | 0.40 |
| 1:B:112:ARG:CG | 1:B:113:ASP:H | 2.35 | 0.40 |
| 1:B:211:LEU:HD12 | 1:B:211:LEU:C | 2.42 | 0.40 |
| 2:C:110:GLU:CG | 2:C:369:PRO:HB3 | 2.50 | 0.40 |
| 3:D:1262:LEU:HD13 | 3:D:1352:ILE:HG13 | 2.04 | 0.40 |
| 2:C:965:GLU:O | 2:C:969:GLN:HG3 | 2.22 | 0.40 |
| 3:D:1032:PRO:O | 3:D:1033:GLN:C | 2.60 | 0.40 |
| 3:N:827:ILE:HA | 3:N:836:VAL:CB | 2.34 | 0.40 |
| 2:C:694:LEU:HD23 | 2:C:697:ARG:NH2 | 2.36 | 0.40 |
| 2:C:571:LEU:HD12 | 2:C:670:GLN:HG3 | 2.04 | 0.40 |
| 3:N:1351:GLU:OE2 | 3:N:1354:LYS:HD2 | 2.20 | 0.40 |
| 2:M:1064:ASN:O | 2:M:1065:ALA:C | 2.59 | 0.40 |
| 3:N:657:LEU:HG | 3:N:661:MET:HE3 | 2.04 | 0.40 |
| 3:N:662:GLU:N | 3:N:667:ALA:HB3 | 2.36 | 0.40 |
| 2:M:953:VAL:HG11 | 2:M:962:GLN:HB3 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:P:328:PHE:O | 5:P:332:PHE:CE1 | 2.74 | 0.40 |
| 3:D:517:VAL:HA | 3:D:518:PRO:HD3 | 1.83 | 0.40 |
| 3:N:1067:VAL:HG13 | 3:N:1068:LEU:N | 2.33 | 0.40 |
| 2:C:841:ASN:C | 2:C:843:HIS:H | 2.23 | 0.40 |
| 3:D:1280:VAL:CG1 | 3:D:1316:GLY:HA2 | 2.52 | 0.40 |
| 2:C:806:LEU:O | 2:C:821:GLU:HB2 | 2.21 | 0.40 |
| 2:C:630:ARG:HH11 | 2:C:630:ARG:HG2 | 1.86 | 0.40 |
| 2:M:19:THR:O | 2:M:23:VAL:HG22 | 2.20 | 0.40 |
| 2:M:18:LEU:HD12 | 2:M:590:ASP:CB | 2.52 | 0.40 |
| 3:N:989:TYR:CD1 | 3:N:993:LEU:HD21 | 2.57 | 0.40 |
| 3:N:956:ILE:HA | 3:N:957:PRO:HD3 | 1.90 | 0.40 |
| 2:C:726:ILE:C | 2:C:728:HIS:N | 2.73 | 0.40 |
| 3:D:1047:LYS:HD2 | 3:D:1051:GLU:HG3 | 2.03 | 0.40 |
| 3:D:627:GLY:O | 3:D:747:VAL:HG12 | 2.21 | 0.40 |
| 3:N:66:GLN:O | 3:N:66:GLN:HG2 | 2.21 | 0.40 |
| 3:D:1008:PHE:CD1 | 3:D:1008:PHE:N | 2.89 | 0.40 |
| 2:C:860:HIS:NE2 | 2:C:975:TYR:HB2 | 2.36 | 0.40 |
| 3:N:247:GLU:HA | 3:N:248:PRO:HA | 1.80 | 0.40 |
| 2:C:723:THR:OG1 | 2:C:725:ASP:HB3 | 2.21 | 0.40 |
| 2:C:598:GLU:H | 2:C:598:GLU:HG2 | 1.66 | 0.40 |
| 2:M:280:LYS:O | 2:M:281:LEU:HD23 | 2.20 | 0.40 |
| 3:N:221:ALA:O | 3:N:334:THR:HA | 2.20 | 0.40 |
| 2:C:217:LEU:C | 2:C:219:GLN:H | 2.24 | 0.40 |
| 3:D:1066:THR:HB | 3:D:1069:GLU:CG | 2.51 | 0.40 |
| 3:N:134:VAL:HG12 | 3:N:136:ASP:OD1 | 2.22 | 0.40 |
| 3:N:541:ASN:O | 3:N:544:TYR:HB2 | 2.22 | 0.40 |
| 5:P:315:VAL:HG12 | 5:P:316:SER:N | 2.36 | 0.40 |
| 3:D:1092:GLY:O | 3:D:1095:THR:N | 2.55 | 0.40 |
| 3:D:1103:HIS:HD2 | 3:D:1462:LEU:CB | 2.35 | 0.40 |
| 3:D:148:GLU:C | 3:D:150:ARG:N | 2.74 | 0.40 |
| 3:D:148:GLU:O | 3:D:150:ARG:N | 2.55 | 0.40 |
| 3:D:462:GLN:O | 3:D:463:GLN:C | 2.59 | 0.40 |
| 3:D:520:LEU:HD11 | 3:D:524:LEU:CD1 | 2.51 | 0.40 |
| 2:C:1018:GLN:HG2 | 3:D:87:ARG:NH2 | 2.37 | 0.40 |
| 4:E:29:GLN:C | 4:E:31:LEU:N | 2.75 | 0.40 |
| 5:F:102:LEU:HD12 | 5:F:183:ALA:HB1 | 2.04 | 0.40 |
| 5:F:125:ASP:CG | 5:F:126:LEU:H | 2.25 | 0.40 |
| 5:F:102:LEU:HD11 | 5:F:183:ALA:HA | 2.04 | 0.40 |
| 5:F:314:PRO:CG | 5:F:315:VAL:N | 2.79 | 0.40 |
| 3:N:358:GLY:HA2 | 3:N:385:VAL:O | 2.22 | 0.40 |
| 3:D:245:LEU:CA | 3:D:309:GLY:H | 2.32 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:764:LEU:HD23 | 3:D:767:HIS:CD2 | 2.56 | 0.40 |
| 3:D:932:ASP:O | 3:D:933:ALA:C | 2.60 | 0.40 |
| 5:P:353:GLU:HA | 5:P:356:LYS:CB | 2.51 | 0.40 |
| 3:D:806:PHE:CE2 | 3:D:812:ALA:HB2 | 2.57 | 0.40 |
| 5:F:381:HIS:HB3 | 5:F:384:GLU:CD | 2.42 | 0.40 |
| 2:M:649:VAL:CG1 | 2:M:650:ARG:HH21 | 2.33 | 0.40 |
| 3:D:670:VAL:O | 3:D:671:LYS:C | 2.60 | 0.40 |
| 2:C:359:MET:HG2 | 2:C:359:MET:O | 2.22 | 0.40 |
| 5:F:289:GLU:O | 5:F:290:GLU:C | 2.59 | 0.40 |
| 2:M:129:ILE:N | 2:M:129:ILE:HD13 | 2.37 | 0.40 |
| 2:M:809:GLY:O | 2:M:813:VAL:HB | 2.21 | 0.40 |
| 2:M:86:LYS:O | 2:M:87:ASP:C | 2.60 | 0.40 |
| 3:N:60:CYS:SG | 3:N:62:LYS:HE2 | 2.61 | 0.40 |
| 3:N:73:CYS:C | 3:N:75:ARG:N | 2.75 | 0.40 |
| 3:N:5:VAL:CG1 | 3:N:6:ARG:N | 2.84 | 0.40 |
| 2:C:910:LYS:O | 2:C:911:GLU:C | 2.60 | 0.40 |
| 3:N:871:LYS:NZ | 3:N:897:TRP:CH2 | 2.89 | 0.40 |
| 2:M:1048:THR:HA | 3:N:755:ALA:CB | 2.51 | 0.40 |
| 2:C:612:VAL:HG13 | 2:C:622:GLU:CA | 2.51 | 0.40 |
| 1:A:155:LYS:HB3 | 1:A:156:HIS:H | 1.73 | 0.40 |
| 1:K:22:GLU:C | 1:K:23:PHE:CD1 | 2.95 | 0.40 |
| 2:M:941:VAL:O | 2:M:944:LEU:HB2 | 2.22 | 0.40 |
| 2:M:958:THR:O | 2:M:962:GLN:HG3 | 2.21 | 0.40 |
| 2:C:185:LYS:HE2 | 2:C:190:LYS:HD3 | 2.03 | 0.40 |
| 3:D:95:LEU:HB2 | 3:D:515:GLU:CA | 2.41 | 0.40 |
| 3:D:95:LEU:HD21 | 3:D:517:VAL:CG2 | 2.52 | 0.40 |
| 3:N:206:ARG:NE | 3:N:392:SER:CB | 2.82 | 0.40 |
| 5:P:102:LEU:HD21 | 5:P:187:LEU:HB2 | 2.03 | 0.40 |
| 5:F:148:LYS:O | 5:F:149:GLU:C | 2.60 | 0.40 |
| 2:C:343:GLN:CG | 2:C:385:PHE:HB2 | 2.50 | 0.40 |
| 2:C:385:PHE:O | 2:C:389:SER:N | 2.54 | 0.40 |
| 1:L:86:VAL:HG12 | 1:L:124:ASN:ND2 | 2.36 | 0.40 |
| 3:D:15:PRO:O | 3:D:18:ILE:HB | 2.20 | 0.40 |
| 2:M:512:ARG:HH11 | 2:M:524:VAL:HA | 1.86 | 0.40 |
| 1:A:220:GLU:O | 1:A:224:TYR:CE2 | 2.73 | 0.40 |
| 3:N:984:THR:O | 3:N:987:GLU:HB2 | 2.21 | 0.40 |
| 5:P:239:ALA:O | 5:P:241:TRP:N | 2.54 | 0.40 |
| 3:N:680:GLN:O | 3:N:683:ILE:HB | 2.22 | 0.40 |
| 3:D:1042:ARG:HH11 | 3:D:1042:ARG:CG | 2.31 | 0.40 |
| 1:A:133:GLU:CG | 1:A:134:GLU:N | 2.85 | 0.40 |
| 3:D:686:GLU:O | 3:D:687:VAL:C | 2.59 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:1025:GLN:C | 3:D:1027:GLY:H | 2.24 | 0.40 |
| 1:B:184:THR:HG23 | 1:B:192:LEU:HB2 | 2.04 | 0.40 |
| 2:C:860:HIS:HA | 2:C:866:PRO:HA | 2.03 | 0.40 |
| 3:D:1055:VAL:HA | 3:D:1056:PRO:HD3 | 1.90 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|------------------|------------|------------|-----------|-------------|----|
| 1 | A | 229/315 (73%) | 160 (70%) | 54 (24%) | 15 (7%) | 1 | 8 |
| 1 | B | 241/315 (76%) | 159 (66%) | 64 (27%) | 18 (8%) | 1 | 6 |
| 1 | K | 229/315 (73%) | 168 (73%) | 50 (22%) | 11 (5%) | 3 | 17 |
| 1 | L | 241/315 (76%) | 171 (71%) | 55 (23%) | 15 (6%) | 2 | 10 |
| 2 | C | 1117/1119 (100%) | 774 (69%) | 251 (22%) | 92 (8%) | 1 | 5 |
| 2 | M | 1117/1119 (100%) | 767 (69%) | 246 (22%) | 104 (9%) | 1 | 4 |
| 3 | D | 1502/1524 (99%) | 931 (62%) | 422 (28%) | 149 (10%) | 1 | 3 |
| 3 | N | 1502/1524 (99%) | 907 (60%) | 445 (30%) | 150 (10%) | 1 | 3 |
| 4 | E | 93/99 (94%) | 54 (58%) | 25 (27%) | 14 (15%) | 0 | 1 |
| 4 | O | 93/99 (94%) | 56 (60%) | 27 (29%) | 10 (11%) | 0 | 2 |
| 5 | F | 347/423 (82%) | 167 (48%) | 130 (38%) | 50 (14%) | 0 | 1 |
| 5 | P | 347/423 (82%) | 171 (49%) | 117 (34%) | 59 (17%) | 0 | 1 |
| All | All | 7058/7590 (93%) | 4485 (64%) | 1886 (27%) | 687 (10%) | 1 | 3 |

All (687) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 59 | GLU |
| 1 | A | 112 | ARG |
| 1 | A | 155 | LYS |
| 1 | B | 75 | VAL |
| 1 | B | 118 | ALA |
| 2 | C | 33 | ASP |
| 2 | C | 42 | VAL |
| 2 | C | 113 | VAL |
| 2 | C | 272 | ALA |
| 2 | C | 276 | LYS |
| 2 | C | 294 | GLU |
| 2 | C | 368 | THR |
| 2 | C | 385 | PHE |
| 2 | C | 399 | ASN |
| 2 | C | 909 | ALA |
| 2 | C | 984 | GLU |
| 2 | C | 1060 | ILE |
| 3 | D | 111 | LYS |
| 3 | D | 137 | PRO |
| 3 | D | 248 | PRO |
| 3 | D | 292 | VAL |
| 3 | D | 485 | SER |
| 3 | D | 487 | ALA |
| 3 | D | 545 | ARG |
| 3 | D | 607 | LEU |
| 3 | D | 751 | LEU |
| 3 | D | 836 | VAL |
| 3 | D | 908 | LYS |
| 3 | D | 945 | SER |
| 3 | D | 1074 | SER |
| 3 | D | 1342 | GLU |
| 3 | D | 1366 | LYS |
| 3 | D | 1405 | GLU |
| 3 | D | 1426 | LYS |
| 3 | D | 1427 | SER |
| 3 | D | 1446 | VAL |
| 4 | E | 22 | VAL |
| 4 | E | 38 | THR |
| 4 | E | 87 | LYS |
| 5 | F | 75 | ILE |
| 5 | F | 100 | VAL |
| 5 | F | 116 | LEU |
| 5 | F | 188 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 5 | F | 314 | PRO |
| 5 | F | 363 | GLU |
| 5 | F | 402 | ASN |
| 1 | K | 73 | GLU |
| 1 | L | 59 | GLU |
| 1 | L | 240 | LYS |
| 2 | M | 21 | ILE |
| 2 | M | 33 | ASP |
| 2 | M | 42 | VAL |
| 2 | M | 178 | PRO |
| 2 | M | 183 | SER |
| 2 | M | 194 | VAL |
| 2 | M | 255 | ALA |
| 2 | M | 276 | LYS |
| 2 | M | 542 | VAL |
| 2 | M | 562 | SER |
| 2 | M | 604 | ALA |
| 2 | M | 684 | PHE |
| 2 | M | 730 | SER |
| 2 | M | 782 | ALA |
| 2 | M | 855 | VAL |
| 2 | M | 909 | ALA |
| 2 | M | 1046 | ALA |
| 2 | M | 1060 | ILE |
| 3 | N | 46 | ASP |
| 3 | N | 137 | PRO |
| 3 | N | 149 | LYS |
| 3 | N | 227 | LEU |
| 3 | N | 245 | LEU |
| 3 | N | 248 | PRO |
| 3 | N | 292 | VAL |
| 3 | N | 481 | MET |
| 3 | N | 487 | ALA |
| 3 | N | 492 | ALA |
| 3 | N | 607 | LEU |
| 3 | N | 639 | LEU |
| 3 | N | 650 | LEU |
| 3 | N | 734 | GLU |
| 3 | N | 766 | ALA |
| 3 | N | 808 | THR |
| 3 | N | 836 | VAL |
| 3 | N | 908 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | N | 936 | TYR |
| 3 | N | 962 | GLN |
| 3 | N | 989 | TYR |
| 3 | N | 1007 | VAL |
| 3 | N | 1094 | LEU |
| 3 | N | 1125 | PRO |
| 3 | N | 1405 | GLU |
| 3 | N | 1446 | VAL |
| 3 | N | 1467 | ILE |
| 4 | O | 16 | LYS |
| 5 | P | 75 | ILE |
| 5 | P | 78 | SER |
| 5 | P | 93 | LEU |
| 5 | P | 100 | VAL |
| 5 | P | 159 | ILE |
| 5 | P | 236 | SER |
| 5 | P | 331 | ASP |
| 5 | P | 356 | LYS |
| 5 | P | 363 | GLU |
| 5 | P | 368 | VAL |
| 5 | P | 376 | ILE |
| 5 | P | 400 | ILE |
| 5 | P | 402 | ASN |
| 1 | A | 32 | PHE |
| 1 | A | 35 | THR |
| 1 | A | 47 | SER |
| 1 | A | 217 | ILE |
| 1 | B | 113 | ASP |
| 2 | C | 21 | ILE |
| 2 | C | 80 | GLN |
| 2 | C | 179 | ASN |
| 2 | C | 212 | GLY |
| 2 | C | 241 | LEU |
| 2 | C | 251 | ASP |
| 2 | C | 271 | GLU |
| 2 | C | 284 | ARG |
| 2 | C | 297 | GLU |
| 2 | C | 336 | VAL |
| 2 | C | 369 | PRO |
| 2 | C | 381 | ALA |
| 2 | C | 386 | PHE |
| 2 | C | 447 | ALA |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | C | 500 | ASN |
| 2 | C | 715 | THR |
| 2 | C | 809 | GLY |
| 2 | C | 855 | VAL |
| 2 | C | 856 | GLU |
| 2 | C | 883 | GLY |
| 2 | C | 927 | GLY |
| 2 | C | 929 | ARG |
| 2 | C | 1004 | LYS |
| 2 | C | 1115 | LEU |
| 3 | D | 46 | ASP |
| 3 | D | 65 | ARG |
| 3 | D | 103 | TRP |
| 3 | D | 120 | ALA |
| 3 | D | 124 | GLU |
| 3 | D | 126 | VAL |
| 3 | D | 227 | LEU |
| 3 | D | 246 | PRO |
| 3 | D | 457 | GLY |
| 3 | D | 564 | GLU |
| 3 | D | 565 | ILE |
| 3 | D | 666 | ILE |
| 3 | D | 676 | MET |
| 3 | D | 686 | GLU |
| 3 | D | 737 | ASN |
| 3 | D | 752 | SER |
| 3 | D | 759 | ALA |
| 3 | D | 808 | THR |
| 3 | D | 809 | PRO |
| 3 | D | 811 | GLU |
| 3 | D | 813 | LEU |
| 3 | D | 885 | ILE |
| 3 | D | 894 | LYS |
| 3 | D | 923 | GLY |
| 3 | D | 962 | GLN |
| 3 | D | 966 | GLU |
| 3 | D | 1007 | VAL |
| 3 | D | 1071 | PHE |
| 3 | D | 1072 | ILE |
| 3 | D | 1263 | PHE |
| 3 | D | 1316 | GLY |
| 3 | D | 1338 | ALA |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | D | 1341 | PRO |
| 3 | D | 1347 | TYR |
| 3 | D | 1354 | LYS |
| 3 | D | 1367 | HIS |
| 3 | D | 1384 | PRO |
| 3 | D | 1467 | ILE |
| 3 | D | 1482 | ARG |
| 4 | E | 21 | VAL |
| 4 | E | 71 | GLY |
| 4 | E | 85 | LEU |
| 5 | F | 77 | THR |
| 5 | F | 78 | SER |
| 5 | F | 81 | VAL |
| 5 | F | 93 | LEU |
| 5 | F | 119 | ILE |
| 5 | F | 127 | ILE |
| 5 | F | 131 | VAL |
| 5 | F | 132 | ARG |
| 5 | F | 195 | VAL |
| 5 | F | 205 | ARG |
| 5 | F | 236 | SER |
| 5 | F | 238 | TYR |
| 5 | F | 266 | GLU |
| 5 | F | 288 | TYR |
| 5 | F | 304 | VAL |
| 5 | F | 351 | SER |
| 5 | F | 404 | ALA |
| 1 | K | 5 | LYS |
| 1 | K | 59 | GLU |
| 1 | L | 37 | GLY |
| 1 | L | 118 | ALA |
| 2 | M | 20 | GLU |
| 2 | M | 38 | LYS |
| 2 | M | 49 | ARG |
| 2 | M | 80 | GLN |
| 2 | M | 81 | ASP |
| 2 | M | 111 | ASP |
| 2 | M | 113 | VAL |
| 2 | M | 152 | PRO |
| 2 | M | 218 | VAL |
| 2 | M | 314 | THR |
| 2 | M | 322 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | M | 381 | ALA |
| 2 | M | 423 | ALA |
| 2 | M | 425 | PHE |
| 2 | M | 463 | GLU |
| 2 | M | 583 | LEU |
| 2 | M | 584 | GLU |
| 2 | M | 616 | GLU |
| 2 | M | 658 | GLY |
| 2 | M | 692 | GLU |
| 2 | M | 728 | HIS |
| 2 | M | 735 | ARG |
| 2 | M | 809 | GLY |
| 2 | M | 923 | GLU |
| 2 | M | 927 | GLY |
| 2 | M | 943 | VAL |
| 2 | M | 1050 | GLN |
| 3 | N | 69 | GLU |
| 3 | N | 111 | LYS |
| 3 | N | 122 | GLU |
| 3 | N | 124 | GLU |
| 3 | N | 126 | VAL |
| 3 | N | 146 | PRO |
| 3 | N | 162 | ARG |
| 3 | N | 358 | GLY |
| 3 | N | 407 | VAL |
| 3 | N | 442 | ASN |
| 3 | N | 485 | SER |
| 3 | N | 526 | PRO |
| 3 | N | 532 | GLY |
| 3 | N | 545 | ARG |
| 3 | N | 565 | ILE |
| 3 | N | 654 | LYS |
| 3 | N | 666 | ILE |
| 3 | N | 686 | GLU |
| 3 | N | 731 | LEU |
| 3 | N | 761 | ILE |
| 3 | N | 787 | LEU |
| 3 | N | 846 | PRO |
| 3 | N | 939 | PHE |
| 3 | N | 940 | THR |
| 3 | N | 945 | SER |
| 3 | N | 988 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | N | 1072 | ILE |
| 3 | N | 1082 | ALA |
| 3 | N | 1171 | VAL |
| 3 | N | 1234 | THR |
| 3 | N | 1341 | PRO |
| 3 | N | 1348 | LEU |
| 3 | N | 1349 | VAL |
| 3 | N | 1355 | VAL |
| 3 | N | 1366 | LYS |
| 3 | N | 1377 | LYS |
| 3 | N | 1397 | LYS |
| 3 | N | 1399 | ASP |
| 3 | N | 1424 | VAL |
| 3 | N | 1435 | LEU |
| 3 | N | 1482 | ARG |
| 3 | N | 1503 | VAL |
| 3 | N | 1504 | GLU |
| 4 | O | 30 | LEU |
| 4 | O | 71 | GLY |
| 4 | O | 72 | ARG |
| 4 | O | 82 | GLU |
| 4 | O | 85 | LEU |
| 4 | O | 87 | LYS |
| 5 | P | 85 | LEU |
| 5 | P | 155 | THR |
| 5 | P | 226 | LYS |
| 5 | P | 230 | LYS |
| 5 | P | 232 | ARG |
| 5 | P | 237 | THR |
| 5 | P | 238 | TYR |
| 5 | P | 241 | TRP |
| 5 | P | 247 | ILE |
| 5 | P | 266 | GLU |
| 5 | P | 271 | LEU |
| 5 | P | 277 | GLN |
| 5 | P | 288 | TYR |
| 5 | P | 297 | PRO |
| 5 | P | 307 | THR |
| 5 | P | 322 | GLY |
| 5 | P | 351 | SER |
| 5 | P | 352 | GLU |
| 5 | P | 354 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 5 | P | 360 | LYS |
| 5 | P | 382 | THR |
| 1 | A | 97 | VAL |
| 1 | A | 105 | GLY |
| 1 | B | 59 | GLU |
| 1 | B | 119 | ASP |
| 1 | B | 208 | LEU |
| 2 | C | 7 | GLY |
| 2 | C | 20 | GLU |
| 2 | C | 49 | ARG |
| 2 | C | 152 | PRO |
| 2 | C | 183 | SER |
| 2 | C | 222 | MET |
| 2 | C | 291 | ALA |
| 2 | C | 306 | THR |
| 2 | C | 400 | PRO |
| 2 | C | 423 | ALA |
| 2 | C | 463 | GLU |
| 2 | C | 551 | GLU |
| 2 | C | 772 | ARG |
| 2 | C | 1050 | GLN |
| 3 | D | 128 | TYR |
| 3 | D | 200 | ASP |
| 3 | D | 235 | ALA |
| 3 | D | 237 | LYS |
| 3 | D | 310 | LEU |
| 3 | D | 405 | ASP |
| 3 | D | 467 | GLU |
| 3 | D | 474 | GLU |
| 3 | D | 492 | ALA |
| 3 | D | 504 | ASP |
| 3 | D | 505 | SER |
| 3 | D | 506 | GLY |
| 3 | D | 523 | ASP |
| 3 | D | 612 | GLY |
| 3 | D | 617 | ASN |
| 3 | D | 639 | LEU |
| 3 | D | 684 | LYS |
| 3 | D | 734 | GLU |
| 3 | D | 760 | ARG |
| 3 | D | 791 | TYR |
| 3 | D | 846 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | D | 902 | LEU |
| 3 | D | 989 | TYR |
| 3 | D | 1019 | PRO |
| 3 | D | 1125 | PRO |
| 3 | D | 1245 | GLY |
| 3 | D | 1315 | ASP |
| 3 | D | 1332 | PRO |
| 3 | D | 1397 | LYS |
| 3 | D | 1408 | ILE |
| 3 | D | 1447 | LEU |
| 3 | D | 1480 | PHE |
| 4 | E | 11 | GLY |
| 4 | E | 28 | GLN |
| 4 | E | 72 | ARG |
| 5 | F | 133 | ALA |
| 5 | F | 190 | ALA |
| 5 | F | 225 | GLU |
| 5 | F | 280 | GLN |
| 5 | F | 352 | GLU |
| 5 | F | 354 | LEU |
| 5 | F | 362 | SER |
| 5 | F | 382 | THR |
| 5 | F | 385 | GLU |
| 5 | F | 408 | LEU |
| 1 | K | 9 | PRO |
| 1 | K | 47 | SER |
| 1 | L | 241 | GLU |
| 1 | L | 242 | PRO |
| 2 | M | 19 | THR |
| 2 | M | 66 | LEU |
| 2 | M | 205 | GLU |
| 2 | M | 241 | LEU |
| 2 | M | 251 | ASP |
| 2 | M | 253 | ALA |
| 2 | M | 271 | GLU |
| 2 | M | 360 | LEU |
| 2 | M | 368 | THR |
| 2 | M | 380 | ALA |
| 2 | M | 386 | PHE |
| 2 | M | 400 | PRO |
| 2 | M | 447 | ALA |
| 2 | M | 551 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | M | 563 | ASN |
| 2 | M | 606 | VAL |
| 2 | M | 897 | LEU |
| 2 | M | 944 | LEU |
| 2 | M | 977 | GLY |
| 2 | M | 1061 | GLU |
| 3 | N | 127 | LEU |
| 3 | N | 173 | PRO |
| 3 | N | 237 | LYS |
| 3 | N | 411 | THR |
| 3 | N | 480 | GLU |
| 3 | N | 549 | ASN |
| 3 | N | 606 | ILE |
| 3 | N | 655 | PRO |
| 3 | N | 687 | VAL |
| 3 | N | 737 | ASN |
| 3 | N | 809 | PRO |
| 3 | N | 1032 | PRO |
| 3 | N | 1224 | VAL |
| 3 | N | 1297 | GLU |
| 3 | N | 1338 | ALA |
| 4 | O | 59 | ASN |
| 5 | P | 77 | THR |
| 5 | P | 169 | GLU |
| 5 | P | 190 | ALA |
| 5 | P | 225 | GLU |
| 5 | P | 353 | GLU |
| 1 | B | 44 | LEU |
| 1 | B | 171 | PHE |
| 1 | B | 217 | ILE |
| 1 | B | 236 | PRO |
| 2 | C | 74 | GLY |
| 2 | C | 178 | PRO |
| 2 | C | 231 | PRO |
| 2 | C | 244 | PRO |
| 2 | C | 537 | LYS |
| 2 | C | 584 | GLU |
| 2 | C | 604 | ALA |
| 2 | C | 684 | PHE |
| 2 | C | 730 | SER |
| 2 | C | 876 | VAL |
| 2 | C | 915 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | C | 955 | PRO |
| 2 | C | 1020 | PRO |
| 3 | D | 39 | PRO |
| 3 | D | 69 | GLU |
| 3 | D | 123 | LEU |
| 3 | D | 172 | PRO |
| 3 | D | 199 | LEU |
| 3 | D | 295 | GLY |
| 3 | D | 356 | PRO |
| 3 | D | 377 | VAL |
| 3 | D | 460 | ALA |
| 3 | D | 472 | ALA |
| 3 | D | 546 | ARG |
| 3 | D | 603 | LEU |
| 3 | D | 654 | LYS |
| 3 | D | 668 | PRO |
| 3 | D | 936 | TYR |
| 3 | D | 995 | LEU |
| 3 | D | 1023 | MET |
| 3 | D | 1079 | LYS |
| 3 | D | 1082 | ALA |
| 3 | D | 1093 | TYR |
| 3 | D | 1094 | LEU |
| 3 | D | 1448 | THR |
| 3 | D | 1484 | THR |
| 3 | D | 1497 | GLU |
| 4 | E | 20 | THR |
| 4 | E | 23 | VAL |
| 4 | E | 32 | ARG |
| 5 | F | 83 | GLN |
| 5 | F | 174 | LEU |
| 5 | F | 178 | ARG |
| 5 | F | 233 | PHE |
| 5 | F | 247 | ILE |
| 5 | F | 271 | LEU |
| 1 | L | 9 | PRO |
| 1 | L | 35 | THR |
| 1 | L | 102 | LYS |
| 1 | L | 211 | LEU |
| 1 | L | 217 | ILE |
| 2 | M | 12 | VAL |
| 2 | M | 170 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | M | 171 | TRP |
| 2 | M | 208 | ALA |
| 2 | M | 212 | GLY |
| 2 | M | 213 | ALA |
| 2 | M | 231 | PRO |
| 2 | M | 256 | TYR |
| 2 | M | 305 | PRO |
| 2 | M | 306 | THR |
| 2 | M | 505 | GLY |
| 2 | M | 526 | PRO |
| 2 | M | 608 | GLY |
| 2 | M | 626 | ARG |
| 2 | M | 849 | VAL |
| 2 | M | 876 | VAL |
| 2 | M | 957 | LYS |
| 3 | N | 62 | LYS |
| 3 | N | 125 | GLN |
| 3 | N | 250 | LEU |
| 3 | N | 451 | ASP |
| 3 | N | 474 | GLU |
| 3 | N | 498 | VAL |
| 3 | N | 509 | PRO |
| 3 | N | 603 | LEU |
| 3 | N | 665 | GLY |
| 3 | N | 670 | VAL |
| 3 | N | 676 | MET |
| 3 | N | 757 | ALA |
| 3 | N | 995 | LEU |
| 3 | N | 1083 | ASP |
| 3 | N | 1342 | GLU |
| 3 | N | 1385 | GLY |
| 3 | N | 1391 | GLU |
| 3 | N | 1469 | GLY |
| 4 | O | 41 | GLU |
| 4 | O | 58 | PRO |
| 5 | P | 239 | ALA |
| 5 | P | 306 | GLU |
| 5 | P | 346 | THR |
| 5 | P | 392 | VAL |
| 5 | P | 405 | LEU |
| 5 | P | 420 | ASP |
| 1 | A | 4 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 9 | PRO |
| 1 | A | 30 | ARG |
| 1 | A | 208 | LEU |
| 1 | B | 35 | THR |
| 1 | B | 240 | LYS |
| 2 | C | 153 | ALA |
| 2 | C | 180 | GLY |
| 2 | C | 250 | ARG |
| 2 | C | 794 | PRO |
| 2 | C | 1061 | GLU |
| 2 | C | 1067 | TYR |
| 3 | D | 31 | THR |
| 3 | D | 114 | THR |
| 3 | D | 125 | GLN |
| 3 | D | 127 | LEU |
| 3 | D | 136 | ASP |
| 3 | D | 150 | ARG |
| 3 | D | 459 | GLU |
| 3 | D | 498 | VAL |
| 3 | D | 526 | PRO |
| 3 | D | 578 | VAL |
| 3 | D | 587 | ARG |
| 3 | D | 597 | ASP |
| 3 | D | 655 | PRO |
| 3 | D | 678 | GLU |
| 3 | D | 693 | GLU |
| 3 | D | 920 | LEU |
| 3 | D | 990 | ASP |
| 3 | D | 1029 | ARG |
| 3 | D | 1441 | GLN |
| 3 | D | 1445 | HIS |
| 5 | F | 156 | VAL |
| 5 | F | 213 | ILE |
| 5 | F | 270 | LYS |
| 5 | F | 272 | SER |
| 5 | F | 368 | VAL |
| 1 | K | 30 | ARG |
| 1 | K | 42 | ARG |
| 2 | M | 23 | VAL |
| 2 | M | 188 | LYS |
| 2 | M | 244 | PRO |
| 2 | M | 272 | ALA |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | M | 336 | VAL |
| 2 | M | 510 | ALA |
| 2 | M | 911 | GLU |
| 2 | M | 1063 | ARG |
| 3 | N | 70 | GLY |
| 3 | N | 123 | LEU |
| 3 | N | 180 | LYS |
| 3 | N | 286 | VAL |
| 3 | N | 493 | ARG |
| 3 | N | 494 | LYS |
| 3 | N | 515 | GLU |
| 3 | N | 789 | LEU |
| 3 | N | 896 | ALA |
| 3 | N | 1265 | ALA |
| 3 | N | 1271 | LYS |
| 3 | N | 1332 | PRO |
| 3 | N | 1426 | LYS |
| 3 | N | 1429 | LEU |
| 3 | N | 1444 | THR |
| 3 | N | 1468 | LEU |
| 5 | P | 94 | LEU |
| 5 | P | 133 | ALA |
| 5 | P | 153 | PRO |
| 1 | B | 38 | ASN |
| 1 | B | 112 | ARG |
| 1 | B | 209 | GLU |
| 2 | C | 19 | THR |
| 2 | C | 188 | LYS |
| 2 | C | 248 | PRO |
| 2 | C | 253 | ALA |
| 2 | C | 304 | LEU |
| 2 | C | 376 | ARG |
| 2 | C | 658 | GLY |
| 2 | C | 911 | GLU |
| 3 | D | 412 | GLY |
| 3 | D | 592 | THR |
| 3 | D | 1097 | LYS |
| 3 | D | 1129 | THR |
| 3 | D | 1340 | GLY |
| 5 | F | 241 | TRP |
| 5 | F | 322 | GLY |
| 1 | L | 6 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | L | 38 | ASN |
| 1 | L | 210 | ALA |
| 2 | M | 10 | ARG |
| 2 | M | 166 | PRO |
| 2 | M | 304 | LEU |
| 2 | M | 457 | ALA |
| 2 | M | 545 | ASN |
| 2 | M | 801 | VAL |
| 2 | M | 1062 | GLY |
| 2 | M | 1087 | VAL |
| 3 | N | 226 | PRO |
| 3 | N | 356 | PRO |
| 3 | N | 504 | ASP |
| 3 | N | 530 | VAL |
| 3 | N | 880 | ILE |
| 3 | N | 1040 | GLY |
| 3 | N | 1097 | LYS |
| 3 | N | 1233 | GLY |
| 3 | N | 1245 | GLY |
| 3 | N | 1414 | PRO |
| 3 | N | 1472 | ILE |
| 5 | P | 81 | VAL |
| 5 | P | 289 | GLU |
| 5 | P | 419 | ARG |
| 2 | C | 727 | PRO |
| 3 | D | 225 | LEU |
| 3 | D | 297 | ILE |
| 3 | D | 567 | ILE |
| 3 | D | 594 | PRO |
| 3 | D | 665 | GLY |
| 3 | D | 1003 | VAL |
| 3 | D | 1466 | VAL |
| 2 | M | 727 | PRO |
| 3 | N | 287 | GLY |
| 3 | N | 295 | GLY |
| 3 | N | 548 | ILE |
| 3 | N | 955 | VAL |
| 3 | N | 1003 | VAL |
| 3 | N | 1022 | VAL |
| 3 | N | 1183 | ILE |
| 3 | N | 1413 | THR |
| 1 | A | 37 | GLY |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 215 | VAL |
| 1 | B | 71 | VAL |
| 2 | C | 191 | PHE |
| 2 | C | 812 | GLY |
| 3 | D | 409 | VAL |
| 4 | E | 6 | ILE |
| 5 | F | 400 | ILE |
| 3 | N | 1248 | GLY |
| 5 | P | 146 | GLY |
| 5 | P | 196 | VAL |
| 5 | P | 251 | ILE |
| 1 | B | 13 | VAL |
| 2 | C | 165 | LEU |
| 2 | C | 218 | VAL |
| 2 | C | 542 | VAL |
| 2 | C | 801 | VAL |
| 2 | C | 844 | GLY |
| 2 | C | 924 | VAL |
| 2 | C | 931 | GLY |
| 1 | K | 37 | GLY |
| 1 | K | 43 | ILE |
| 2 | M | 74 | GLY |
| 2 | M | 794 | PRO |
| 3 | N | 39 | PRO |
| 3 | N | 85 | VAL |
| 3 | N | 612 | GLY |
| 3 | N | 788 | GLY |
| 3 | N | 1223 | ILE |
| 3 | N | 1466 | VAL |
| 5 | P | 188 | ILE |
| 5 | P | 261 | PRO |
| 5 | P | 313 | GLU |
| 1 | B | 170 | VAL |
| 2 | C | 505 | GLY |
| 2 | C | 521 | PRO |
| 2 | C | 526 | PRO |
| 2 | C | 606 | VAL |
| 3 | D | 786 | ILE |
| 3 | D | 1349 | VAL |
| 5 | F | 113 | ILE |
| 5 | F | 376 | ILE |
| 1 | K | 97 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | L | 157 | GLY |
| 2 | M | 645 | VAL |
| 2 | M | 659 | PRO |
| 3 | N | 188 | GLY |
| 3 | N | 1019 | PRO |
| 3 | N | 1277 | ILE |
| 5 | P | 304 | VAL |
| 2 | C | 302 | VAL |
| 4 | E | 5 | GLY |
| 1 | K | 75 | VAL |
| 2 | M | 376 | ARG |
| 3 | N | 885 | ILE |
| 3 | N | 1394 | VAL |
| 5 | P | 268 | ILE |

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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 | 202/273 (74%) | 192 (95%) | 10 (5%) | 30 | 70 |
| 1 | B | 210/273 (77%) | 193 (92%) | 17 (8%) | 15 | 47 |
| 1 | K | 202/273 (74%) | 190 (94%) | 12 (6%) | 24 | 63 |
| 1 | L | 210/273 (77%) | 196 (93%) | 14 (7%) | 20 | 57 |
| 2 | C | 941/941 (100%) | 863 (92%) | 78 (8%) | 14 | 46 |
| 2 | M | 941/941 (100%) | 859 (91%) | 82 (9%) | 13 | 43 |
| 3 | D | 1264/1279 (99%) | 1152 (91%) | 112 (9%) | 12 | 42 |
| 3 | N | 1264/1279 (99%) | 1141 (90%) | 123 (10%) | 10 | 37 |
| 4 | E | 83/87 (95%) | 76 (92%) | 7 (8%) | 14 | 45 |
| 4 | O | 83/87 (95%) | 74 (89%) | 9 (11%) | 8 | 30 |
| 5 | F | 304/371 (82%) | 274 (90%) | 30 (10%) | 10 | 35 |
| 5 | P | 304/371 (82%) | 266 (88%) | 38 (12%) | 6 | 24 |
| All | All | 6008/6448 (93%) | 5476 (91%) | 532 (9%) | 12 | 42 |

All (532) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 3 | ASP |
| 1 | A | 23 | PHE |
| 1 | A | 47 | SER |
| 1 | A | 83 | LYS |
| 1 | A | 86 | VAL |
| 1 | A | 94 | LEU |
| 1 | A | 107 | LYS |
| 1 | A | 123 | MET |
| 1 | A | 124 | ASN |
| 1 | A | 224 | TYR |
| 1 | B | 23 | PHE |
| 1 | B | 58 | ILE |
| 1 | B | 82 | LEU |
| 1 | B | 112 | ARG |
| 1 | B | 113 | ASP |
| 1 | B | 114 | PHE |
| 1 | B | 124 | ASN |
| 1 | B | 140 | MET |
| 1 | B | 143 | ARG |
| 1 | B | 175 | ARG |
| 1 | B | 180 | GLN |
| 1 | B | 183 | ASP |
| 1 | B | 188 | GLN |
| 1 | B | 211 | LEU |
| 1 | B | 212 | ASN |
| 1 | B | 224 | TYR |
| 1 | B | 243 | GLU |
| 2 | C | 1 | MET |
| 2 | C | 13 | ILE |
| 2 | C | 15 | LEU |
| 2 | C | 41 | ASN |
| 2 | C | 71 | TYR |
| 2 | C | 73 | LEU |
| 2 | C | 81 | ASP |
| 2 | C | 113 | VAL |
| 2 | C | 115 | LEU |
| 2 | C | 117 | HIS |
| 2 | C | 139 | GLN |
| 2 | C | 158 | TYR |
| 2 | C | 179 | ASN |
| 2 | C | 184 | MET |
| 2 | C | 195 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | C | 221 | LEU |
| 2 | C | 227 | PHE |
| 2 | C | 229 | MET |
| 2 | C | 230 | ARG |
| 2 | C | 233 | GLU |
| 2 | C | 239 | PHE |
| 2 | C | 251 | ASP |
| 2 | C | 263 | ASP |
| 2 | C | 267 | TYR |
| 2 | C | 268 | ASP |
| 2 | C | 285 | LEU |
| 2 | C | 303 | PHE |
| 2 | C | 321 | GLU |
| 2 | C | 361 | MET |
| 2 | C | 367 | LEU |
| 2 | C | 388 | ARG |
| 2 | C | 405 | ARG |
| 2 | C | 408 | ARG |
| 2 | C | 434 | HIS |
| 2 | C | 463 | GLU |
| 2 | C | 507 | ARG |
| 2 | C | 520 | GLU |
| 2 | C | 566 | THR |
| 2 | C | 579 | VAL |
| 2 | C | 584 | GLU |
| 2 | C | 590 | ASP |
| 2 | C | 600 | ASP |
| 2 | C | 607 | ASP |
| 2 | C | 610 | ARG |
| 2 | C | 616 | GLU |
| 2 | C | 622 | GLU |
| 2 | C | 628 | PHE |
| 2 | C | 630 | ARG |
| 2 | C | 632 | ASN |
| 2 | C | 650 | ARG |
| 2 | C | 672 | VAL |
| 2 | C | 674 | VAL |
| 2 | C | 676 | ILE |
| 2 | C | 680 | ASP |
| 2 | C | 683 | ASN |
| 2 | C | 699 | PHE |
| 2 | C | 720 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | C | 723 | THR |
| 2 | C | 731 | GLU |
| 2 | C | 738 | ASP |
| 2 | C | 749 | VAL |
| 2 | C | 761 | PHE |
| 2 | C | 787 | ASP |
| 2 | C | 826 | TYR |
| 2 | C | 857 | ASP |
| 2 | C | 861 | LEU |
| 2 | C | 879 | ARG |
| 2 | C | 881 | ASN |
| 2 | C | 916 | GLU |
| 2 | C | 953 | VAL |
| 2 | C | 958 | THR |
| 2 | C | 1003 | ASP |
| 2 | C | 1020 | PRO |
| 2 | C | 1035 | MET |
| 2 | C | 1048 | THR |
| 2 | C | 1051 | GLU |
| 2 | C | 1099 | VAL |
| 2 | C | 1101 | THR |
| 3 | D | 16 | GLU |
| 3 | D | 33 | ASN |
| 3 | D | 36 | THR |
| 3 | D | 60 | CYS |
| 3 | D | 74 | GLU |
| 3 | D | 81 | THR |
| 3 | D | 87 | ARG |
| 3 | D | 111 | LYS |
| 3 | D | 133 | ILE |
| 3 | D | 135 | LEU |
| 3 | D | 142 | LEU |
| 3 | D | 153 | LEU |
| 3 | D | 156 | GLU |
| 3 | D | 171 | LEU |
| 3 | D | 172 | PRO |
| 3 | D | 178 | LEU |
| 3 | D | 248 | PRO |
| 3 | D | 291 | LEU |
| 3 | D | 297 | ILE |
| 3 | D | 334 | THR |
| 3 | D | 336 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | D | 338 | GLU |
| 3 | D | 351 | MET |
| 3 | D | 361 | VAL |
| 3 | D | 387 | LEU |
| 3 | D | 404 | GLU |
| 3 | D | 413 | ASP |
| 3 | D | 430 | ASP |
| 3 | D | 438 | ASP |
| 3 | D | 442 | ASN |
| 3 | D | 445 | ARG |
| 3 | D | 450 | TYR |
| 3 | D | 451 | ASP |
| 3 | D | 473 | LEU |
| 3 | D | 502 | PHE |
| 3 | D | 511 | TRP |
| 3 | D | 535 | PHE |
| 3 | D | 537 | THR |
| 3 | D | 542 | ASP |
| 3 | D | 546 | ARG |
| 3 | D | 564 | GLU |
| 3 | D | 565 | ILE |
| 3 | D | 569 | ASN |
| 3 | D | 594 | PRO |
| 3 | D | 602 | SER |
| 3 | D | 604 | THR |
| 3 | D | 605 | ASP |
| 3 | D | 614 | PHE |
| 3 | D | 617 | ASN |
| 3 | D | 618 | LEU |
| 3 | D | 624 | ASP |
| 3 | D | 653 | PHE |
| 3 | D | 685 | ASP |
| 3 | D | 724 | GLN |
| 3 | D | 745 | MET |
| 3 | D | 754 | PHE |
| 3 | D | 756 | GLN |
| 3 | D | 776 | GLU |
| 3 | D | 782 | SER |
| 3 | D | 784 | ASP |
| 3 | D | 792 | ILE |
| 3 | D | 797 | LYS |
| 3 | D | 800 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | D | 828 | LYS |
| 3 | D | 829 | VAL |
| 3 | D | 847 | ASP |
| 3 | D | 851 | LEU |
| 3 | D | 907 | GLU |
| 3 | D | 914 | LEU |
| 3 | D | 936 | TYR |
| 3 | D | 937 | TYR |
| 3 | D | 952 | ASP |
| 3 | D | 972 | LEU |
| 3 | D | 991 | GLN |
| 3 | D | 997 | THR |
| 3 | D | 1018 | ASN |
| 3 | D | 1029 | ARG |
| 3 | D | 1067 | VAL |
| 3 | D | 1083 | ASP |
| 3 | D | 1084 | THR |
| 3 | D | 1095 | THR |
| 3 | D | 1104 | GLU |
| 3 | D | 1124 | GLN |
| 3 | D | 1130 | ARG |
| 3 | D | 1139 | ASP |
| 3 | D | 1167 | SER |
| 3 | D | 1190 | SER |
| 3 | D | 1211 | MET |
| 3 | D | 1213 | ARG |
| 3 | D | 1217 | ILE |
| 3 | D | 1239 | ARG |
| 3 | D | 1252 | ILE |
| 3 | D | 1269 | LYS |
| 3 | D | 1285 | GLU |
| 3 | D | 1299 | PHE |
| 3 | D | 1307 | LYS |
| 3 | D | 1337 | GLU |
| 3 | D | 1342 | GLU |
| 3 | D | 1346 | ARG |
| 3 | D | 1350 | GLU |
| 3 | D | 1396 | GLU |
| 3 | D | 1398 | TRP |
| 3 | D | 1401 | GLU |
| 3 | D | 1405 | GLU |
| 3 | D | 1434 | TRP |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | D | 1442 | ASN |
| 3 | D | 1458 | GLU |
| 3 | D | 1472 | ILE |
| 3 | D | 1479 | ASP |
| 3 | D | 1483 | PHE |
| 3 | D | 1495 | ILE |
| 3 | D | 1499 | ARG |
| 4 | E | 23 | VAL |
| 4 | E | 37 | ASN |
| 4 | E | 55 | PHE |
| 4 | E | 57 | ASP |
| 4 | E | 83 | ASP |
| 4 | E | 85 | LEU |
| 4 | E | 93 | TYR |
| 5 | F | 110 | MET |
| 5 | F | 118 | GLU |
| 5 | F | 150 | THR |
| 5 | F | 174 | LEU |
| 5 | F | 218 | GLN |
| 5 | F | 228 | GLU |
| 5 | F | 245 | GLN |
| 5 | F | 257 | THR |
| 5 | F | 287 | THR |
| 5 | F | 291 | ILE |
| 5 | F | 302 | LYS |
| 5 | F | 308 | LEU |
| 5 | F | 312 | GLN |
| 5 | F | 313 | GLU |
| 5 | F | 314 | PRO |
| 5 | F | 329 | TYR |
| 5 | F | 335 | ASP |
| 5 | F | 336 | GLU |
| 5 | F | 343 | ASP |
| 5 | F | 353 | GLU |
| 5 | F | 360 | LYS |
| 5 | F | 377 | ASP |
| 5 | F | 379 | ARG |
| 5 | F | 398 | ARG |
| 5 | F | 405 | LEU |
| 5 | F | 409 | LYS |
| 5 | F | 410 | TYR |
| 5 | F | 411 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | F | 418 | LEU |
| 5 | F | 420 | ASP |
| 1 | K | 3 | ASP |
| 1 | K | 9 | PRO |
| 1 | K | 13 | VAL |
| 1 | K | 64 | GLU |
| 1 | K | 74 | ASP |
| 1 | K | 94 | LEU |
| 1 | K | 100 | LEU |
| 1 | K | 124 | ASN |
| 1 | K | 176 | ARG |
| 1 | K | 182 | GLU |
| 1 | K | 183 | ASP |
| 1 | K | 191 | ASP |
| 1 | L | 9 | PRO |
| 1 | L | 23 | PHE |
| 1 | L | 28 | LEU |
| 1 | L | 40 | LEU |
| 1 | L | 68 | ILE |
| 1 | L | 82 | LEU |
| 1 | L | 113 | ASP |
| 1 | L | 114 | PHE |
| 1 | L | 119 | ASP |
| 1 | L | 140 | MET |
| 1 | L | 143 | ARG |
| 1 | L | 145 | ASP |
| 1 | L | 183 | ASP |
| 1 | L | 193 | ASP |
| 2 | M | 1 | MET |
| 2 | M | 13 | ILE |
| 2 | M | 15 | LEU |
| 2 | M | 26 | TYR |
| 2 | M | 41 | ASN |
| 2 | M | 42 | VAL |
| 2 | M | 71 | TYR |
| 2 | M | 72 | ARG |
| 2 | M | 73 | LEU |
| 2 | M | 81 | ASP |
| 2 | M | 104 | ASP |
| 2 | M | 107 | LEU |
| 2 | M | 113 | VAL |
| 2 | M | 117 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | M | 133 | ASP |
| 2 | M | 158 | TYR |
| 2 | M | 179 | ASN |
| 2 | M | 184 | MET |
| 2 | M | 216 | GLU |
| 2 | M | 226 | VAL |
| 2 | M | 227 | PHE |
| 2 | M | 230 | ARG |
| 2 | M | 233 | GLU |
| 2 | M | 239 | PHE |
| 2 | M | 251 | ASP |
| 2 | M | 269 | LEU |
| 2 | M | 285 | LEU |
| 2 | M | 289 | THR |
| 2 | M | 290 | LEU |
| 2 | M | 320 | HIS |
| 2 | M | 344 | PHE |
| 2 | M | 359 | MET |
| 2 | M | 361 | MET |
| 2 | M | 367 | LEU |
| 2 | M | 371 | LYS |
| 2 | M | 372 | LEU |
| 2 | M | 403 | SER |
| 2 | M | 429 | ASP |
| 2 | M | 441 | VAL |
| 2 | M | 463 | GLU |
| 2 | M | 507 | ARG |
| 2 | M | 516 | ARG |
| 2 | M | 535 | SER |
| 2 | M | 562 | SER |
| 2 | M | 566 | THR |
| 2 | M | 579 | VAL |
| 2 | M | 584 | GLU |
| 2 | M | 600 | ASP |
| 2 | M | 607 | ASP |
| 2 | M | 610 | ARG |
| 2 | M | 616 | GLU |
| 2 | M | 628 | PHE |
| 2 | M | 630 | ARG |
| 2 | M | 632 | ASN |
| 2 | M | 650 | ARG |
| 2 | M | 653 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | M | 657 | ASP |
| 2 | M | 672 | VAL |
| 2 | M | 676 | ILE |
| 2 | M | 699 | PHE |
| 2 | M | 720 | GLU |
| 2 | M | 737 | LEU |
| 2 | M | 739 | GLU |
| 2 | M | 744 | ARG |
| 2 | M | 761 | PHE |
| 2 | M | 787 | ASP |
| 2 | M | 808 | ARG |
| 2 | M | 858 | MET |
| 2 | M | 861 | LEU |
| 2 | M | 876 | VAL |
| 2 | M | 879 | ARG |
| 2 | M | 881 | ASN |
| 2 | M | 916 | GLU |
| 2 | M | 953 | VAL |
| 2 | M | 958 | THR |
| 2 | M | 971 | LYS |
| 2 | M | 975 | TYR |
| 2 | M | 976 | ASP |
| 2 | M | 988 | VAL |
| 2 | M | 1003 | ASP |
| 2 | M | 1058 | ASP |
| 2 | M | 1059 | ASP |
| 3 | N | 16 | GLU |
| 3 | N | 33 | ASN |
| 3 | N | 36 | THR |
| 3 | N | 81 | THR |
| 3 | N | 87 | ARG |
| 3 | N | 111 | LYS |
| 3 | N | 112 | ILE |
| 3 | N | 119 | SER |
| 3 | N | 125 | GLN |
| 3 | N | 131 | LYS |
| 3 | N | 133 | ILE |
| 3 | N | 135 | LEU |
| 3 | N | 149 | LYS |
| 3 | N | 167 | GLU |
| 3 | N | 206 | ARG |
| 3 | N | 213 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | N | 224 | ARG |
| 3 | N | 226 | PRO |
| 3 | N | 315 | ARG |
| 3 | N | 337 | LEU |
| 3 | N | 338 | GLU |
| 3 | N | 350 | HIS |
| 3 | N | 351 | MET |
| 3 | N | 387 | LEU |
| 3 | N | 392 | SER |
| 3 | N | 404 | GLU |
| 3 | N | 430 | ASP |
| 3 | N | 432 | TYR |
| 3 | N | 434 | ARG |
| 3 | N | 441 | ARG |
| 3 | N | 445 | ARG |
| 3 | N | 450 | TYR |
| 3 | N | 451 | ASP |
| 3 | N | 456 | MET |
| 3 | N | 470 | LEU |
| 3 | N | 481 | MET |
| 3 | N | 485 | SER |
| 3 | N | 500 | ARG |
| 3 | N | 502 | PHE |
| 3 | N | 511 | TRP |
| 3 | N | 535 | PHE |
| 3 | N | 564 | GLU |
| 3 | N | 565 | ILE |
| 3 | N | 566 | ILE |
| 3 | N | 602 | SER |
| 3 | N | 605 | ASP |
| 3 | N | 614 | PHE |
| 3 | N | 617 | ASN |
| 3 | N | 618 | LEU |
| 3 | N | 624 | ASP |
| 3 | N | 653 | PHE |
| 3 | N | 669 | ASN |
| 3 | N | 692 | GLU |
| 3 | N | 724 | GLN |
| 3 | N | 725 | SER |
| 3 | N | 734 | GLU |
| 3 | N | 745 | MET |
| 3 | N | 754 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | N | 762 | GLN |
| 3 | N | 769 | LEU |
| 3 | N | 778 | LEU |
| 3 | N | 784 | ASP |
| 3 | N | 798 | GLU |
| 3 | N | 799 | LYS |
| 3 | N | 800 | LYS |
| 3 | N | 809 | PRO |
| 3 | N | 828 | LYS |
| 3 | N | 829 | VAL |
| 3 | N | 832 | ARG |
| 3 | N | 847 | ASP |
| 3 | N | 867 | ARG |
| 3 | N | 875 | THR |
| 3 | N | 907 | GLU |
| 3 | N | 921 | ARG |
| 3 | N | 936 | TYR |
| 3 | N | 941 | PHE |
| 3 | N | 947 | ILE |
| 3 | N | 965 | GLU |
| 3 | N | 972 | LEU |
| 3 | N | 985 | ASP |
| 3 | N | 990 | ASP |
| 3 | N | 991 | GLN |
| 3 | N | 999 | THR |
| 3 | N | 1021 | TYR |
| 3 | N | 1067 | VAL |
| 3 | N | 1084 | THR |
| 3 | N | 1087 | ARG |
| 3 | N | 1095 | THR |
| 3 | N | 1130 | ARG |
| 3 | N | 1139 | ASP |
| 3 | N | 1167 | SER |
| 3 | N | 1188 | VAL |
| 3 | N | 1201 | CYS |
| 3 | N | 1213 | ARG |
| 3 | N | 1215 | VAL |
| 3 | N | 1217 | ILE |
| 3 | N | 1239 | ARG |
| 3 | N | 1251 | ASP |
| 3 | N | 1263 | PHE |
| 3 | N | 1267 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | N | 1285 | GLU |
| 3 | N | 1299 | PHE |
| 3 | N | 1307 | LYS |
| 3 | N | 1308 | GLU |
| 3 | N | 1337 | GLU |
| 3 | N | 1342 | GLU |
| 3 | N | 1346 | ARG |
| 3 | N | 1387 | SER |
| 3 | N | 1401 | GLU |
| 3 | N | 1405 | GLU |
| 3 | N | 1430 | SER |
| 3 | N | 1434 | TRP |
| 3 | N | 1439 | SER |
| 3 | N | 1441 | GLN |
| 3 | N | 1442 | ASN |
| 3 | N | 1449 | GLU |
| 3 | N | 1460 | ILE |
| 3 | N | 1464 | GLU |
| 3 | N | 1472 | ILE |
| 3 | N | 1479 | ASP |
| 3 | N | 1485 | GLN |
| 3 | N | 1495 | ILE |
| 3 | N | 1499 | ARG |
| 4 | O | 23 | VAL |
| 4 | O | 37 | ASN |
| 4 | O | 40 | LEU |
| 4 | O | 57 | ASP |
| 4 | O | 83 | ASP |
| 4 | O | 85 | LEU |
| 4 | O | 86 | GLN |
| 4 | O | 88 | GLU |
| 4 | O | 93 | TYR |
| 5 | P | 94 | LEU |
| 5 | P | 107 | GLU |
| 5 | P | 118 | GLU |
| 5 | P | 138 | SER |
| 5 | P | 143 | HIS |
| 5 | P | 156 | VAL |
| 5 | P | 163 | LEU |
| 5 | P | 212 | LEU |
| 5 | P | 233 | PHE |
| 5 | P | 245 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | P | 257 | THR |
| 5 | P | 264 | MET |
| 5 | P | 287 | THR |
| 5 | P | 291 | ILE |
| 5 | P | 302 | LYS |
| 5 | P | 306 | GLU |
| 5 | P | 308 | LEU |
| 5 | P | 313 | GLU |
| 5 | P | 314 | PRO |
| 5 | P | 327 | SER |
| 5 | P | 328 | PHE |
| 5 | P | 329 | TYR |
| 5 | P | 331 | ASP |
| 5 | P | 334 | PRO |
| 5 | P | 336 | GLU |
| 5 | P | 353 | GLU |
| 5 | P | 355 | GLU |
| 5 | P | 367 | MET |
| 5 | P | 373 | LYS |
| 5 | P | 379 | ARG |
| 5 | P | 382 | THR |
| 5 | P | 409 | LYS |
| 5 | P | 410 | TYR |
| 5 | P | 411 | HIS |
| 5 | P | 414 | ARG |
| 5 | P | 418 | LEU |
| 5 | P | 420 | ASP |
| 5 | P | 422 | LEU |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (140) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 16 | GLN |
| 1 | A | 81 | ASN |
| 1 | A | 91 | ASN |
| 1 | A | 95 | GLN |
| 1 | A | 128 | HIS |
| 1 | A | 163 | ASN |
| 1 | A | 180 | GLN |
| 1 | A | 188 | GLN |
| 1 | A | 212 | ASN |
| 1 | A | 213 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 221 | HIS |
| 1 | B | 91 | ASN |
| 1 | B | 95 | GLN |
| 1 | B | 128 | HIS |
| 1 | B | 139 | ASN |
| 2 | C | 31 | GLN |
| 2 | C | 91 | GLN |
| 2 | C | 99 | GLN |
| 2 | C | 117 | HIS |
| 2 | C | 130 | ASN |
| 2 | C | 141 | HIS |
| 2 | C | 179 | ASN |
| 2 | C | 204 | GLN |
| 2 | C | 374 | ASN |
| 2 | C | 390 | GLN |
| 2 | C | 393 | GLN |
| 2 | C | 575 | GLN |
| 2 | C | 683 | ASN |
| 2 | C | 704 | HIS |
| 2 | C | 829 | GLN |
| 2 | C | 881 | ASN |
| 2 | C | 889 | HIS |
| 2 | C | 969 | GLN |
| 2 | C | 991 | GLN |
| 2 | C | 1006 | HIS |
| 2 | C | 1018 | GLN |
| 2 | C | 1100 | GLN |
| 2 | C | 1107 | ASN |
| 3 | D | 316 | GLN |
| 3 | D | 442 | ASN |
| 3 | D | 549 | ASN |
| 3 | D | 552 | ASN |
| 3 | D | 569 | ASN |
| 3 | D | 680 | GLN |
| 3 | D | 696 | HIS |
| 3 | D | 703 | ASN |
| 3 | D | 727 | GLN |
| 3 | D | 729 | HIS |
| 3 | D | 744 | GLN |
| 3 | D | 748 | HIS |
| 3 | D | 824 | ASN |
| 3 | D | 906 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | D | 962 | GLN |
| 3 | D | 973 | GLN |
| 3 | D | 994 | GLN |
| 3 | D | 1010 | ASN |
| 3 | D | 1014 | ASN |
| 3 | D | 1034 | GLN |
| 3 | D | 1103 | HIS |
| 3 | D | 1124 | GLN |
| 3 | D | 1172 | HIS |
| 3 | D | 1359 | GLN |
| 3 | D | 1442 | ASN |
| 3 | D | 1489 | GLN |
| 4 | E | 28 | GLN |
| 4 | E | 86 | GLN |
| 5 | F | 83 | GLN |
| 5 | F | 170 | HIS |
| 5 | F | 214 | GLN |
| 5 | F | 217 | ASN |
| 5 | F | 245 | GLN |
| 5 | F | 263 | HIS |
| 5 | F | 269 | ASN |
| 5 | F | 347 | GLN |
| 5 | F | 399 | GLN |
| 5 | F | 402 | ASN |
| 5 | F | 411 | HIS |
| 1 | K | 38 | ASN |
| 1 | K | 81 | ASN |
| 1 | K | 128 | HIS |
| 1 | K | 163 | ASN |
| 1 | K | 188 | GLN |
| 1 | K | 212 | ASN |
| 1 | L | 38 | ASN |
| 1 | L | 91 | ASN |
| 1 | L | 95 | GLN |
| 1 | L | 128 | HIS |
| 1 | L | 156 | HIS |
| 1 | L | 188 | GLN |
| 1 | L | 212 | ASN |
| 2 | M | 41 | ASN |
| 2 | M | 91 | GLN |
| 2 | M | 179 | ASN |
| 2 | M | 330 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | M | 374 | ASN |
| 2 | M | 390 | GLN |
| 2 | M | 434 | HIS |
| 2 | M | 567 | GLN |
| 2 | M | 575 | GLN |
| 2 | M | 632 | ASN |
| 2 | M | 633 | GLN |
| 2 | M | 860 | HIS |
| 2 | M | 881 | ASN |
| 2 | M | 899 | GLN |
| 2 | M | 969 | GLN |
| 2 | M | 1047 | HIS |
| 2 | M | 1050 | GLN |
| 2 | M | 1100 | GLN |
| 2 | M | 1107 | ASN |
| 3 | N | 316 | GLN |
| 3 | N | 552 | ASN |
| 3 | N | 569 | ASN |
| 3 | N | 617 | ASN |
| 3 | N | 703 | ASN |
| 3 | N | 714 | GLN |
| 3 | N | 729 | HIS |
| 3 | N | 744 | GLN |
| 3 | N | 824 | ASN |
| 3 | N | 962 | GLN |
| 3 | N | 973 | GLN |
| 3 | N | 994 | GLN |
| 3 | N | 1103 | HIS |
| 3 | N | 1323 | GLN |
| 3 | N | 1442 | ASN |
| 3 | N | 1489 | GLN |
| 4 | O | 28 | GLN |
| 4 | O | 29 | GLN |
| 4 | O | 33 | HIS |
| 4 | O | 86 | GLN |
| 5 | P | 170 | HIS |
| 5 | P | 186 | HIS |
| 5 | P | 214 | GLN |
| 5 | P | 217 | ASN |
| 5 | P | 245 | GLN |
| 5 | P | 254 | GLN |
| 5 | P | 269 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | P | 279 | GLN |
| 5 | P | 347 | GLN |
| 5 | P | 399 | GLN |
| 5 | P | 402 | 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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 7 are monoatomic - leaving 7 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 6 | PO4 | A | 316 | - | 4,4,4 | 1.06 | 0 | 6,6,6 | 0.27 | 0 |
| 10 | MPD | C | 1120 | - | 6,7,7 | 2.12 | 1 (16%) | 7,10,10 | 0.89 | 0 |
| 10 | MPD | C | 1121 | - | 6,7,7 | 2.15 | 1 (16%) | 7,10,10 | 0.88 | 0 |
| 6 | PO4 | D | 1528 | - | 4,4,4 | 1.11 | 0 | 6,6,6 | 0.27 | 0 |
| 9 | NE6 | D | 1529 | - | 26,30,30 | 2.64 | 5 (19%) | 22,39,39 | 1.96 | 5 (22%) |
| 10 | MPD | M | 1120 | - | 6,7,7 | 2.04 | 1 (16%) | 7,10,10 | 0.88 | 0 |
| 9 | NE6 | N | 1528 | - | 26,30,30 | 2.55 | 4 (15%) | 22,39,39 | 2.00 | 5 (22%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|----------|------------|---------|
| 6 | PO4 | A | 316 | - | - | 0/0/0/0 | 0/0/0/0 |
| 10 | MPD | C | 1120 | - | - | 0/5/5/5 | 0/0/0/0 |
| 10 | MPD | C | 1121 | - | - | 0/5/5/5 | 0/0/0/0 |
| 6 | PO4 | D | 1528 | - | - | 0/0/0/0 | 0/0/0/0 |
| 9 | NE6 | D | 1529 | - | 1/1/9/13 | 0/24/46/46 | 0/0/1/1 |
| 10 | MPD | M | 1120 | - | - | 0/5/5/5 | 0/0/0/0 |
| 9 | NE6 | N | 1528 | - | 1/1/9/13 | 0/24/46/46 | 0/0/1/1 |

All (12) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 10 | C | 1121 | MPD | O2-C2 | -5.04 | 1.30 | 1.44 |
| 10 | C | 1120 | MPD | O2-C2 | -5.01 | 1.30 | 1.44 |
| 10 | M | 1120 | MPD | O2-C2 | -4.74 | 1.31 | 1.44 |
| 9 | D | 1529 | NE6 | O14-C13 | 2.10 | 1.38 | 1.33 |
| 9 | N | 1528 | NE6 | C15-C16 | 2.23 | 1.52 | 1.48 |
| 9 | D | 1529 | NE6 | C19-C20 | 2.43 | 1.36 | 1.34 |
| 9 | D | 1529 | NE6 | C15-C16 | 2.84 | 1.53 | 1.48 |
| 9 | N | 1528 | NE6 | C19-C20 | 3.00 | 1.37 | 1.34 |
| 9 | N | 1528 | NE6 | C12-N12 | 4.33 | 1.37 | 1.26 |
| 9 | D | 1529 | NE6 | C12-N12 | 4.94 | 1.39 | 1.26 |
| 9 | N | 1528 | NE6 | O4-C4 | 11.07 | 1.38 | 1.22 |
| 9 | D | 1529 | NE6 | O4-C4 | 11.25 | 1.38 | 1.22 |

All (10) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 9 | D | 1529 | NE6 | O4-C4-C5 | -4.05 | 114.87 | 121.62 |
| 9 | N | 1528 | NE6 | O4-C4-C5 | -4.04 | 114.89 | 121.62 |
| 9 | N | 1528 | NE6 | C9-C10-C11 | -2.01 | 111.19 | 114.53 |
| 9 | D | 1529 | NE6 | C21-C20-C19 | 2.01 | 126.22 | 122.61 |
| 9 | N | 1528 | NE6 | C2-C3-C15 | 2.21 | 119.26 | 111.11 |
| 9 | D | 1529 | NE6 | C2-C3-C15 | 2.42 | 120.02 | 111.11 |
| 9 | N | 1528 | NE6 | O1-C2-O2 | 4.20 | 120.94 | 116.98 |
| 9 | D | 1529 | NE6 | O1-C2-O2 | 4.32 | 121.05 | 116.98 |
| 9 | D | 1529 | NE6 | O14-C13-N12 | 4.70 | 114.46 | 108.75 |
| 9 | N | 1528 | NE6 | O14-C13-N12 | 5.03 | 114.87 | 108.75 |

All (2) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|------|------|------|
| 9 | N | 1528 | NE6 | C3 |
| 9 | D | 1529 | NE6 | C3 |

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 16 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 6 | D | 1528 | PO4 | 1 | 0 |
| 9 | D | 1529 | NE6 | 8 | 0 |
| 9 | N | 1528 | NE6 | 7 | 0 |

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, 95th 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 ²) | Q<0.9 |
|-----|-------|------------------|--------|--------------|-----------------------|-------|
| 1 | A | 231/315 (73%) | -0.65 | 0 100 100 | 43, 72, 100, 115 | 0 |
| 1 | B | 243/315 (77%) | -0.81 | 0 100 100 | 51, 93, 113, 117 | 0 |
| 1 | K | 231/315 (73%) | -0.67 | 0 100 100 | 45, 73, 105, 117 | 0 |
| 1 | L | 243/315 (77%) | -0.80 | 0 100 100 | 56, 89, 112, 117 | 0 |
| 2 | C | 1119/1119 (100%) | -0.72 | 0 100 100 | 36, 77, 115, 117 | 0 |
| 2 | M | 1119/1119 (100%) | -0.71 | 0 100 100 | 31, 79, 115, 117 | 0 |
| 3 | D | 1504/1524 (98%) | -0.69 | 1 (0%) 95 90 | 35, 78, 117, 117 | 0 |
| 3 | N | 1504/1524 (98%) | -0.67 | 4 (0%) 94 84 | 34, 75, 113, 117 | 0 |
| 4 | E | 95/99 (95%) | -0.81 | 0 100 100 | 51, 88, 113, 117 | 0 |
| 4 | O | 95/99 (95%) | -0.77 | 0 100 100 | 52, 85, 109, 116 | 0 |
| 5 | F | 349/423 (82%) | -0.85 | 0 100 100 | 52, 84, 110, 117 | 0 |
| 5 | P | 349/423 (82%) | -0.80 | 0 100 100 | 51, 85, 110, 117 | 0 |
| All | All | 7082/7590 (93%) | -0.71 | 5 (0%) 95 90 | 31, 79, 115, 117 | 0 |

All (5) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3 | N | 243 | ALA | 4.2 |
| 3 | N | 242 | LEU | 3.3 |
| 3 | N | 328 | GLY | 3.1 |
| 3 | D | 329 | GLU | 2.2 |
| 3 | N | 223 | LEU | 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 [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|----------------------------|-------|
| 9 | NE6 | N | 1528 | 30/30 | 0.94 | 0.29 | 3.45 | 72,84,90,91 | 0 |
| 8 | ZN | N | 1525 | 1/1 | 0.99 | 0.19 | 2.79 | 50,50,50,50 | 0 |
| 8 | ZN | D | 1525 | 1/1 | 0.96 | 0.17 | 2.42 | 91,91,91,91 | 0 |
| 8 | ZN | D | 1526 | 1/1 | 1.00 | 0.18 | 2.25 | 77,77,77,77 | 0 |
| 7 | MG | B | 701 | 1/1 | 0.97 | 0.20 | 1.38 | 55,55,55,55 | 0 |
| 9 | NE6 | D | 1529 | 30/30 | 0.96 | 0.22 | 1.28 | 52,70,81,85 | 0 |
| 8 | ZN | N | 1526 | 1/1 | 1.00 | 0.18 | 0.87 | 55,55,55,55 | 0 |
| 6 | PO4 | A | 316 | 5/5 | 0.96 | 0.18 | 0.57 | 71,73,77,77 | 0 |
| 10 | MPD | C | 1120 | 8/8 | 0.97 | 0.17 | 0.57 | 51,56,57,57 | 0 |
| 10 | MPD | M | 1120 | 8/8 | 0.92 | 0.17 | 0.09 | 71,79,84,85 | 0 |
| 6 | PO4 | D | 1528 | 5/5 | 0.96 | 0.14 | -0.61 | 86,86,86,89 | 0 |
| 7 | MG | D | 1527 | 1/1 | 0.96 | 0.07 | - | 79,79,79,79 | 0 |
| 7 | MG | N | 1527 | 1/1 | 0.97 | 0.04 | - | 56,56,56,56 | 0 |
| 10 | MPD | C | 1121 | 8/8 | 0.96 | 0.15 | - | 70,72,73,73 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.