



## Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 01:22 AM UTC

PDB ID : 9D9Z / pdb\_00009d9z  
EMDB ID : EMD-46686  
Title : Structure of human UBR4-KCMF1-CaM E3 ligase complex (Silencing Factor of the Integrated stress response, SiFI)  
Authors : Yang, Z.; Rape, M.  
Deposited on : 2024-08-21  
Resolution : 3.40 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

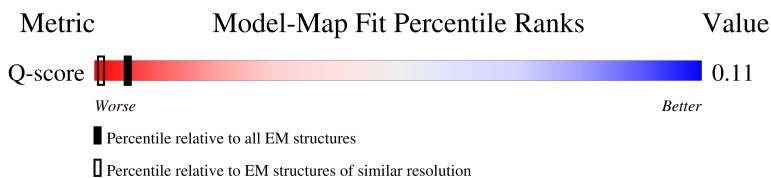
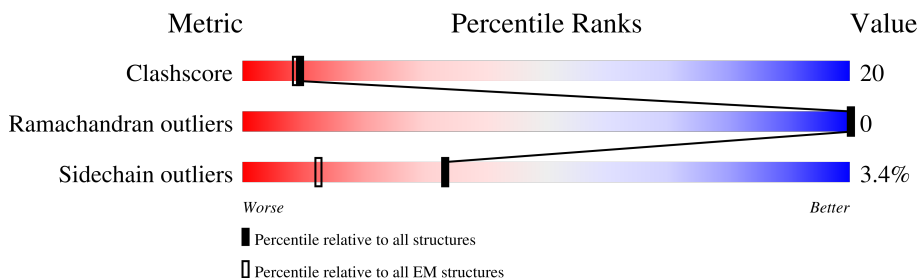
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.40 Å.

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



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 14717 ( 2.90 - 3.90 )                                    |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 5205   |                  |
| 1   | B     | 5205   |                  |
| 2   | C     | 149    |                  |
| 2   | D     | 149    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3   | E     | 381    |                  |
| 3   | F     | 381    |                  |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 4   | ZN   | A     | 5202 | -         | -        | X       | -                |
| 4   | ZN   | B     | 5202 | -         | -        | X       | -                |
| 5   | CA   | D     | 202  | -         | -        | X       | -                |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 66746 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 UBR4 (endogenously FLAG-tagged at the N-terminus),E3 ubiquitin-protein ligase UBR4,E3 ubiquitin-protein ligase UBR4,E3 ubiquitin-protein ligase UBR4.

| Mol | Chain | Residues | Atoms |       |      |      |     | AltConf | Trace |
|-----|-------|----------|-------|-------|------|------|-----|---------|-------|
| 1   | A     | 3917     | Total | C     | N    | O    | S   | 0       | 0     |
|     |       |          | 30658 | 19475 | 5230 | 5749 | 204 |         |       |
| 1   | B     | 3946     | Total | C     | N    | O    | S   | 0       | 0     |
|     |       |          | 30933 | 19647 | 5279 | 5802 | 205 |         |       |

- Molecule 2 is a protein called Calmodulin-1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2   | C     | 144      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1134  | 696 | 182 | 247 | 9 |         |       |
| 2   | D     | 143      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1127  | 692 | 181 | 245 | 9 |         |       |

- Molecule 3 is a protein called E3 ubiquitin-protein ligase KCMF1.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 3   | E     | 182      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1435  | 881 | 250 | 288 | 16 |         |       |
| 3   | F     | 182      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1435  | 881 | 250 | 288 | 16 |         |       |

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 4   | A     | 6        | Total | Zn | 0       |
|     |       |          | 6     | 6  |         |
| 4   | B     | 6        | Total | Zn | 0       |
|     |       |          | 6     | 6  |         |
| 4   | E     | 4        | Total | Zn | 0       |
|     |       |          | 4     | 4  |         |

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| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 4   | F     | 4        | Total | Zn | 0       |
|     |       |          | 4     | 4  |         |

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 5   | C     | 2        | Total | Ca | 0       |
|     |       |          | 2     | 2  |         |
| 5   | D     | 2        | Total | Ca | 0       |
|     |       |          | 2     | 2  |         |



|       |       |       |       |       |       |      |      |      |      |      |      |     |       |       |       |       |       |       |       |      |      |      |      |     |      |
|-------|-------|-------|-------|-------|-------|------|------|------|------|------|------|-----|-------|-------|-------|-------|-------|-------|-------|------|------|------|------|-----|------|
| I1299 | M1239 | Q1179 | Q1119 | I1059 | L999  | E939 | Q879 | H819 | R759 | K699 | ALA  | GLU | I1299 | M1239 | Q1179 | Q1119 | I1059 | L999  | E939  | Q879 | H819 | R759 | K699 | ASP | Q519 |
| E1240 | E1240 | N1180 | S1120 | K1060 | Q1000 | A940 | V880 | N820 | L760 | G700 | S640 | SER | V1300 | E1240 | N1180 | S1120 | K1060 | Q1000 | A940  | V880 | N820 | L760 | G700 | ASP | R520 |
| F1241 | F1241 | F1181 | Y1121 | Q1061 | Y1001 | S941 | Q881 | F821 | L641 | S701 | R641 | SER | W1301 | F1241 | F1181 | Y1121 | Q1061 | Y1001 | S941  | Q881 | F821 | L641 | S701 | SER | I521 |
| P1242 | P1242 | N1182 | Y1122 | G1062 | Y1002 | E942 | H882 | T822 | L762 | S702 | D643 | ASP | S1302 | P1242 | N1182 | Y1122 | G1062 | Y1002 | E942  | H882 | T822 | L762 | S702 | ASP | Q522 |
| M1243 | M1243 | E1183 | T1123 | M1063 | F1003 | S943 | H883 | E823 | I763 | D703 | D644 | ASP | D1304 | M1243 | E1183 | T1123 | M1063 | F1003 | S943  | H883 | E823 | I763 | D703 | ASP | R523 |
| I1244 | I1244 | E1184 | L1124 | K1064 | L1004 | D944 | L884 | T824 | W764 | E704 | P644 | ASP | E1304 | I1244 | E1184 | L1124 | K1064 | L1004 | D944  | L884 | T824 | W764 | E704 | ASP | L524 |
| G1245 | G1245 | GLY   | D1125 | A1065 | T1005 | L945 | L885 | Q825 | Q765 | E705 | E645 | SER | M1305 | G1245 | GLY   | D1125 | A1065 | T1005 | L945  | L885 | Q825 | Q765 | E705 | SER | I525 |
| S1246 | S1246 | THR   | A1126 | E1066 | L1006 | N946 | S886 | Q826 | H766 | F706 | L646 | GLY | N1306 | S1246 | THR   | A1126 | E1066 | L1006 | N946  | S886 | Q826 | H766 | F706 | GLY | D526 |
| M1247 | M1247 | GLU   | A1127 | H1067 | W1007 | R947 | P887 | R827 | K767 | A707 | F647 | PRO | P1307 | M1247 | GLU   | A1127 | H1067 | W1007 | R947  | P887 | R827 | K767 | A707 | PRO | S527 |
| R1248 | R1248 | LYS   | I1128 | A1068 | R1008 | L948 | P888 | A828 | A768 | A708 | L648 | LEU | P1308 | R1248 | LYS   | I1128 | A1068 | R1008 | L948  | P888 | A828 | A768 | A708 | LEU | V528 |
| N1249 | N1249 | P1190 | S1129 | S1069 | I1009 | D949 | PHE  | R829 | S769 | A709 | G649 | GLY | Q1309 | N1249 | P1190 | S1129 | S1069 | I1009 | D949  | PHE  | R829 | S769 | A709 | GLY | P529 |
| A1250 | A1250 | S1191 | K1130 | S1070 | L1010 | S950 | TRP  | L830 | A770 | L710 | L650 | GLN | V1310 | A1250 | S1191 | K1130 | S1070 | L1010 | S950  | TRP  | L830 | A770 | L710 | GLN | L530 |
| F1251 | F1251 | K1192 | Y1131 | L1071 | G1011 | V951 | ALA  | S831 | Q771 | Y711 | A651 | PHE | I1311 | F1251 | K1192 | Y1131 | L1071 | G1011 | V951  | ALA  | S831 | Q771 | Y711 | PHE | M531 |
| A1252 | A1252 | E1193 | Q1132 | E1073 | I1012 | A952 | SER  | L832 | G772 | H712 | S652 | GLY | R1312 | A1252 | E1193 | Q1132 | E1073 | I1012 | A952  | SER  | L832 | G772 | H712 | GLY | N532 |
| T1253 | T1253 | K1194 | V1133 | E1074 | P1014 | C953 | SER  | F833 | D773 | F713 | R653 | GLY | T1313 | T1253 | K1194 | V1133 | E1074 | P1014 | C953  | SER  | F833 | D773 | F713 | GLY | N533 |
| L1314 | L1314 | L1195 | S1134 | L1074 | L1013 | D954 | GLN  | V834 | P774 | N714 | I654 | THR | L1314 | L1314 | L1195 | S1134 | L1074 | L1013 | D954  | GLN  | V834 | P774 | N714 | THR | L534 |
| L1315 | L1255 | Q1196 | L1135 | A1075 | P1015 | V955 | ASP  | Q835 | W775 | H715 | L655 | ILE | L1315 | L1315 | L1255 | Q1196 | L1135 | A1075 | P1015 | V955 | ASP  | W775 | H715 | ILE | L534 |
| P1316 | I1256 | G1197 | D1136 | S1076 | S1016 | L956 | SER  | T836 | V776 | S716 | L656 | PRO | P1316 | P1316 | I1256 | G1197 | D1136 | S1076 | S1016 | L956 | SER  | V776 | S716 | PRO | L535 |
| L1317 | P1257 | F1198 | E1137 | T1077 | S1017 | F957 | ASN  | R837 | P657 | L717 | F657 | SER | L1317 | L1317 | P1257 | F1198 | E1137 | T1077 | S1017 | F957 | ASN  | P657 | L717 | SER | T536 |
| L1318 | S1258 | A1199 | H1138 | T1078 | T1018 | S958 | ARG  | Q838 | E778 | V718 | I658 | LYS | L1318 | L1318 | S1258 | A1199 | H1138 | T1078 | T1018 | S958 | ARG  | Q838 | E778 | LYS | L537 |
| L1319 | E1259 | A1200 | F1139 | K1079 | Y1019 | R959 | ARG  | E839 | C779 | T719 | T659 | GLY | E1320 | L1319 | E1259 | A1200 | F1139 | K1079 | Y1019 | R959 | ARG  | C779 | T719 | GLY | L538 |
| E1320 | S1260 | V1201 | S1140 | C1080 | I1020 | L960 | A903 | L840 | L780 | S720 | S660 | ALA | E1320 | E1320 | S1260 | V1201 | S1140 | C1080 | I1020 | L960 | A903 | L840 | S720 | ALA | T540 |
| S1321 | I1261 | L1202 | K1141 | S1081 | N1021 | V961 | T904 | S841 | K781 | D721 | S661 | PRO | S1321 | S1321 | I1261 | L1202 | K1141 | S1081 | N1021 | V961 | T904 | S841 | D721 | PRO | S541 |
| S1322 | I1262 | A1203 | M1142 | V1082 | Q1022 | K962 | T905 | V842 | W782 | L722 | M662 | PRO | S1322 | S1322 | I1262 | A1203 | M1142 | V1082 | Q1022 | K962 | T905 | W782 | L722 | PRO | Y542 |
| T1323 | S1263 | I1204 | A1143 | S1083 | L1023 | P963 | P906 | H843 | W783 | Q723 | L663 | PRO | T1323 | T1323 | S1263 | I1204 | A1143 | S1083 | L1023 | P963 | P906 | H843 | W783 | PRO | R543 |
| E1324 | A1264 | G1205 | ALA   | K1084 | S1024 | D964 | L907 | H844 | D784 | S724 | N664 | PRO | E1324 | E1324 | A1264 | G1205 | ALA   | K1084 | S1024 | D964 | L907 | H844 | S724 | PRO | K544 |
| S1325 | V1265 | S1206 | GLY   | Y1085 | M1025 | E965 | Y908 | D845 | R785 | P725 | S665 | PRO | S1325 | S1325 | V1265 | S1206 | GLY   | Y1085 | M1025 | E965 | Y908 | D845 | P725 | PRO | A545 |
| Q1266 | Q1266 | R1208 | THR   | D1086 | N1026 | L966 | H909 | A846 | F786 | N726 | R666 | PRO | Q1266 | Q1266 | Q1266 | R1208 | THR   | D1086 | N1026 | L966 | H909 | A846 | N726 | PRO | C546 |
| A1327 | A1267 | C1209 | ASP   | V1087 | S1027 | P967 | G910 | Q847 | L787 | L727 | N657 | PRO | A1327 | A1327 | A1267 | C1209 | ASP   | V1087 | S1027 | P967 | G910 | L787 | L727 | PRO | V547 |
| E1328 | A1268 | HIS   | LYS   | E1088 | P1028 | A968 | F911 | H848 | S788 | Q728 | N668 | PRO | E1328 | E1328 | A1268 | HIS   | LYS   | E1088 | P1028 | A968 | F911 | H848 | Q728 | PRO | L548 |
| H1329 | H1269 | K1210 | S1151 | V1090 | E1029 | A969 | K912 | R849 | T789 | N729 | P689 | GLY | H1329 | H1329 | H1269 | K1210 | S1151 | V1090 | E1029 | A969 | K912 | R849 | T789 | GLY | Q549 |
| S1330 | L1270 | A1211 | S1152 | Y1090 | M1030 | L970 | E913 | F850 | W790 | T730 | L670 | SER | S1330 | S1330 | L1270 | A1211 | S1152 | Y1090 | M1030 | L970 | E913 | F850 | W790 | SER | R550 |
| S1331 | G1271 | M1212 | E1153 | E1091 | S1031 | T971 | V914 | H851 | K791 | L731 | R671 | SER | S1331 | S1331 | G1271 | M1212 | E1153 | E1091 | S1031 | T971 | V914 | H851 | L731 | SER | Q551 |
| M1332 | T1272 | T1213 | I1154 | E1092 | E1032 | A972 | E915 | P852 | Q792 | L732 | N672 | PRO | M1332 | M1332 | T1272 | T1213 | I1154 | E1092 | E1032 | A972 | E915 | P852 | Q792 | PRO | R552 |
| S1333 | L1273 | L1214 | T1155 | Y1093 | C1033 | L973 | E916 | L853 | N793 | Q733 | V673 | VAL | S1333 | S1333 | L1273 | L1214 | T1155 | Y1093 | C1033 | L973 | E916 | L853 | Q733 | VAL | K553 |
| L1334 | C1274 | G1215 | K1156 | F1094 | D1034 | L974 | N917 | T854 | A794 | L734 | L674 | LYS | L1334 | L1334 | C1274 | G1215 | K1156 | F1094 | D1034 | L974 | N917 | T854 | L734 | LYS | G554 |
| E1335 | S1335 | P1216 | N1157 | A1095 | I1035 | A975 | W918 | L855 | L795 | Q734 | S675 | SER | E1335 | E1335 | S1335 | P1216 | N1157 | A1095 | I1035 | A975 | W918 | L855 | Q734 | SER | R554 |
| R1336 | Q1276 | T1217 | L1158 | R1096 | L1036 | A976 | S919 | A856 | Q796 | L735 | V676 | PRO | R1336 | R1336 | Q1276 | T1217 | L1158 | R1096 | L1036 | A976 | S919 | A856 | Q796 | PRO | MET  |
| I1337 | I1337 | L1218 | L1159 | Q1097 | H1037 | G977 | K920 | R857 | G736 | L736 | S677 | SER | I1337 | I1337 | I1337 | L1218 | L1159 | Q1097 | H1037 | G977 | K920 | R857 | G736 | SER | SER  |
| L1338 | L1278 | V1219 | P1160 | I1098 | T1038 | S978 | H921 | L858 | V798 | A738 | L678 | GLN | L1338 | L1338 | L1278 | V1219 | P1160 | I1098 | T1038 | S978 | H921 | L858 | V798 | GLN | ASP  |
| G1339 | P1279 | Q1220 | A1161 | S1099 | L1039 | Q979 | F922 | L859 | W799 | F739 | S679 | ALA | G1339 | G1339 | P1279 | Q1220 | A1161 | S1099 | L1039 | Q979 | F922 | L859 | W799 | ALA | ALA  |
| P1340 | L1280 | N1221 | T1162 | S1100 | R1040 | L980 | S923 | L860 | P800 | F740 | E680 | PRO | P1340 | P1340 | L1280 | N1221 | T1162 | S1100 | R1040 | L980 | S923 | L860 | F740 | PRO | SER  |
| A1341 | A1281 | L1222 | L1163 | F1101 | W1041 | D981 | S924 | L861 | S801 | S741 | H691 | GLY | A1341 | A1341 | A1281 | L1222 | L1163 | F1101 | W1041 | D981 | S924 | L861 | S801 | GLY | ALA  |
| E1342 | A1282 | P1223 | Q1164 | C1102 | S1042 | T982 | D925 | F862 | E802 | E742 | H682 | LYS | E1342 | E1342 | A1282 | P1223 | Q1164 | C1102 | S1042 | T982 | D925 | F862 | E802 | LYS | THR  |
| S1343 | S1283 | S1224 | L1165 | S1103 | S1043 | V983 | A926 | D863 | T803 | G743 | M693 | GLY | S1343 | S1343 | S1283 | S1224 | L1165 | S1103 | S1043 | V983 | A926 | D863 | T803 | GLY | ASP  |
| D1344 | L1284 | S1225 | I1166 | T1104 | R1044 | R984 | V927 | Y864 | E804 | P744 | A684 | ASN | D1344 | D1344 | L1284 | S1225 | I1166 | T1104 | R1044 | R984 | V927 | Y864 | P744 | ASN | ILE  |
| E1345 | K1285 | V1226 | I1166 | D1105 | L1045 | R985 | P928 | L865 | D805 | W745 | T695 | THR | E1345 | E1345 | K1285 | V1226 | I1166 | D1105 | L1045 | R985 | P928 | L865 | D805 | THR | THR  |
| F1346 | H1286 | Q1227 | D1167 | C1106 | R1046 | K986 | H929 | L866 | L806 | P746 | L686 | TYR | F1346 | F1346 | H1286 | Q1227 | D1167 | C1106 | R1046 | K986 | H929 | L866 | P746 | TYR | TYR  |
| L1347 | T1287 | T1168 | Y1169 | T1107 | I1047 | E987 | P930 | H867 | N807 | L747 | A687 | GLY | L1347 | L1347 | T1287 | T1168 | Y1169 | T1107 | I1047 | E987 | P930 | H867 | L747 | GLY | GLY  |
| A1348 | L1288 | A1170 | L1170 | T1108 | S1048 | N988 | R931 | Q868 | V808 | V748 | S688 | ASP | A1348 | A1348 | L1288 | A1170 | L1170 | T1108 | S1048 | N988 | R931 | Q868 | V748 | ASP | ASP  |
| R1349 | L1289 | E1231 | S1171 | I1109 | S1049 | K989 | F932 | Y869 | E809 | I749 | T699 | PHE | R1349 | R1349 | L1289 | E1231 | S1171 | I1109 | S1049 | K989 | F932 | Y869 | E809 | PHE | PHE  |
| V1350 | S1290 | E1231 | F1172 | L1110 | Y1050 | N990 | V933 | S870 | H810 | H750 | T690 | SER | V1350 | V1350 | S1290 | E1231 | F1172 | L1110 | Y1050 | N990 | V933 | S870 | H810 | SER | SER  |
| Y1351 | L1291 | S1232 | T1173 | Q1111 | V1051 | V991 | C934 | R371 | L811 | F751 | K691 | THR | Y1351 | Y1351 | L1291 | S1232 | T1173 | Q1111 | V1051 | V991 | C934 | R371 | L811 | THR | THR  |
| E1352 | V1292 | W1233 | R1174 | L1112 | M1052 | T992 | V935 | A872 | O812 | Q752 | E692 | GLY | E1352 | E1352 | V1292 | W1233 | R1174 | L1112 | M1052 | T992 | V935 | A872 | Q752 | GLY | GLY  |
| R1353 | R1293 | M1234 | A1175 | H1113 | W1053 | A993 | L936 | H873 | H813 | S753 | V693 | ASP | R1353 | R1353 | R1293 | M1234 | A1175 | H1113 | W1053 | A993 | L936 | H873 | S753 | ASP | ASP  |
| L1354 | L1294 | N1235 | Y1176 | E1114 | T1054 | L994 | S937 | V874 | L814 | L754 | D694 | PHE | L1354 | L1354 | L1294 | N1235 | Y1176 | E1114 | T1054 | L994 | S937 | V874 | L754 |     |      |

|       |       |       |       |       |     |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-----|-------|-------|-------|-------|-------|-------|
| P2085 | I2025 | M1960 | C1900 | Q1840 | GLU | E1722 | LYS   | V1539 | S1479 | L1419 | V1359 |
| F2086 | Y2026 | P1961 | V1901 | A1841 | GLU | D1723 | L1663 | V1540 | D1480 | S1420 | M1360 |
| Y2087 | D2027 | C1962 | V1901 | A1841 | PRO | G1724 | C1664 | Y1602 | Q1481 | A1421 | I1361 |
| Z2088 | L2028 | K1963 | S1903 | L1842 | LYS | S1725 | L1602 | A1542 | L1482 | K1422 | L1362 |
| T2089 | C2029 | E1964 | S1904 | E1844 | LYS | C1726 | F1666 | T1543 | D1483 | F1423 | A1363 |
| N2090 |       | D1965 | P1905 | L1845 | SER | L1727 | T1667 | L1544 | V1484 | C1424 | M1364 |
| D2031 | W2030 | H1966 | H1906 | H1846 | SER | A1728 | T1668 | V1606 | T1485 | M1425 | H1365 |
| A2032 | Z2031 | L1967 | G1907 | T1847 | LEU | L1729 | T1669 | T1607 | Q1486 | R1426 | A1366 |
| L2033 | A2032 | A1968 | R1908 | H1848 | CYS | VAL   | GLN   | M1608 | E1487 | V1427 | D1367 |
| S2034 | L2033 | V1969 | ARG   | V1848 | THR | LYS   | LYS   | A1547 | N1488 | L1428 | P1368 |
| N2095 | S2034 | C1970 | THR   | A1849 | VAL | ARG   | GLU   | G1548 | N1488 | L1428 | P1368 |
| H2096 | P2035 | G1971 | VAL   | K1850 | GLY | THR   | PHE   | Q1549 | R1489 | K1429 | N1369 |
| E2097 | T2036 | L1972 | GLY   | A1851 | GLY | PRO   | MET   | G1550 | Q1490 | F1430 | S1370 |
| D2098 | F2037 | K1973 | CYS   | V1852 | CYS | ASN   | ASN   | L1491 | L1491 | F1431 | G1371 |
| F2039 |       |       | ARG   | E1797 | ARG | SER   | Q1676 | L1492 | L1492 | T1432 | L1372 |
| L2040 | Y2039 | H1976 | A1913 | M1854 | GLY | GLY   | H1677 | G1552 | Q1493 | K1433 | D1373 |
| L2041 | L2040 | V1977 | S1915 | T1855 | MET | SER   | M1678 | H1553 | L1494 | L1434 | E1374 |
| P2042 | L2041 | L1978 | H1916 | D1856 | SER | SER   | Y1679 | L1554 | L1494 | S1375 | S1375 |
| S2043 | P2042 | T1979 | E1917 | Q1857 | THR | THR   | H1680 | L1556 | T1496 | Q1436 | I1376 |
| S2044 | S2043 | F1980 | K1918 | Q1858 | MET | MET   | C1681 | H1557 | T1497 | L1437 | L1377 |
| K2045 | S2044 | S1981 | G1919 | M1859 | LYS | GLY   | H1682 | Y1498 | Y1498 | T1438 | E1378 |
| L2046 | K2045 | S1982 | G1919 | V1860 | SER | SER   | T1683 | T1499 | T1499 | E1439 | E1379 |
| R2047 | L2046 | G1983 | K1920 | P1861 | ALA | ALA   | C1684 | V1500 | C1380 | K1440 | C1380 |
| D2048 | R2047 | S1984 | T1922 | F1805 | PHE | PHE   | K1685 | R1501 | R1501 | L1381 | L1381 |
| A2107 | D2048 | S1985 | V1923 | L1862 | GLN | GLN   | H1686 | E1502 | E1502 | P1442 | Q1382 |
| V2049 | G2108 | V1986 | L1924 | G1864 | SER | SER   | V1687 | N1503 | N1503 | N1443 | Y1383 |
| T2060 | T2060 | S1987 | Q1925 | K1865 | PRO | PRO   | ASP   | S1504 | S1504 | P1444 | L1384 |
| F2051 | F2051 | D1988 | L1926 | Q1866 | ILE | ILE   | GLY   | Q1505 | Q1505 | S1446 | K1385 |
| L2118 | L2052 | E1988 | S1927 | E1867 | SER | SER   | G1691 | V1506 | V1506 | L1446 | E1386 |
| L2119 | F2053 | H1989 | L1810 | V1811 | GLU | GLU   | V1692 | G1507 | G1507 | L1447 | Q1387 |
| L2120 | N2054 | L1990 | A1928 | G1868 | LEU | SER   | C1693 | E1508 | E1508 | H1448 | L1388 |
| M2121 | E2055 | V1991 | L1929 | A1869 | VAL | VAL   | T1694 | G1509 | G1509 | L1449 | E1389 |
| L2122 | T2056 | L1992 | D1813 | F1870 | ARG | ARG   | T1694 | V1510 | V1510 | C1450 | S1390 |
| F2123 | G2057 | H1993 | M1814 | L1815 | HIS | HIS   | C1696 | C1511 | C1511 | G1451 | L1391 |
| F2124 | K2058 | P1994 | E1871 | H1872 | ALA | ALA   | A1697 | A1512 | A1512 | S1452 | Q1392 |
| S2125 | N2059 | Q1995 | L1816 | R1873 | THR | THR   | SER   | V1513 | V1513 | L1453 | A1393 |
| Y2126 | L2060 | L1996 | M1875 | R1874 | SER | SER   | C1699 | L1514 | L1514 | A1454 | R1394 |
| C2127 | L2061 | A1997 | N1876 | N1876 | PRO | PRO   | C1700 | Q1455 | Q1455 | Q1455 | K1395 |
| Q2128 | T2062 | T1998 | Y1877 | Y1877 | ALA | ALA   | H1701 | V1576 | G1516 | L1456 | A1396 |
| G2129 | N2064 | N2000 | K1937 | S1878 | ASP | ASP   | K1702 | V1577 | T1517 | A1457 | M1397 |
|       | S2065 | F2001 | R1938 | G1879 | LYS | LYS   | D1703 | E1578 | SER   | C1458 | E1398 |
|       | S2066 | L2002 | K1939 | Q1823 | ALA | ALA   | H1703 | K1579 | T1519 | V1459 | E1399 |
| A2067 | A2067 | L1940 | L1940 | T1880 | LYS | LYS   | E1705 | L1590 | P1520 | E1460 | F1400 |
| Q2068 | Q2068 | K2004 | Q1881 | Q1882 | VAL | VAL   | ASP   | M1581 | P1461 | F1401 | S1402 |
| Y2069 | A2005 | A2005 | Q1882 | Q1882 | THR | THR   | ILE   | ASP   | A1522 | V1462 | D1403 |
| L2136 | L2070 | V2006 | Q1883 | Q1827 | SER | SER   | S1707 | ASN   | T1523 | R1463 | R1463 |
| T2137 | Y2071 | W2007 | T1884 | Q1828 | GLY | GLY   | Y1708 | VAL   | E1524 | L1464 | S1404 |
| S2137 | L2008 | L2008 | L1885 | ALA   | ALA | LYS   | LYS   | MET   | G1405 | Q1465 | E1406 |
| R2138 | T2072 |       | R1886 | SER   | SER | VAL   | VAL   | HIS   | L1526 | A1466 | G1406 |
| T2139 | Q2073 | Q2012 | Q1887 | ALA   | ALA | VAL   | GLY   | GLY   | A1527 | W1467 | L1407 |
| L2140 | L2074 | T2013 | L1888 | VAL   | VAL | ASP   |       |       |       |       |       |
| L2141 | M2075 |       | L1889 | GLY   | GLY |       |       |       |       |       |       |
| E2142 | E2076 | A2016 | P1949 | SER   | SER |       |       |       |       |       |       |
| V2143 | E2077 | L2017 | V1950 | S1835 |     |       | F1714 | V1590 | N1528 | L1468 | V1408 |
| L2144 | A2078 | V2018 | S1836 | F1715 |     |       |       | M1591 | G1529 | Q1469 | Q1409 |
| Q2145 | S2079 |       | A1891 | C1716 |     |       |       | D1530 | T1470 | I1410 | I1410 |
| L2146 | Q2080 | D2021 | H1892 | D1717 |     |       |       | G1531 | M1471 | M1411 | M1411 |
| F2147 | A2081 |       | V1933 | C1718 |     |       |       | T1532 | T1472 | T1472 | M1412 |
| P2148 | Q2082 | F2022 | L1894 | G1719 |     |       |       | E1594 | T1473 | T1473 | A1413 |
| T2149 | Q2083 | K2024 | R1895 | A1720 |     |       |       | C1595 | F1534 | S1474 | T1414 |
| N2150 | Q2084 |       | R1896 | K1721 |     |       |       | C1597 | P1535 | P1475 | A1415 |
|       |       |       | V1897 |       |     |       |       | E1536 | P1476 | P1476 | N1416 |
|       |       |       | A1898 |       |     |       |       | L1537 | E1417 | K1477 | N1417 |
|       |       |       | M1899 |       |     |       |       | M153  |       |       |       |







- Molecule 1: UBR4 (endogenously FLAG-tagged at the N-terminus), E3 ubiquitin-protein ligase UBR4, E3 ubiquitin-protein ligase UBR4, E3 ubiquitin-protein ligase UBR4



|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |      |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|
| L1419 | S1420 | A1421 | K1422 | F1423 | C1424 | N1425 | R1426 | V1427 | L1428 | K1429 | F1430 | F1431 | T1432 | K1433 | L1434 | F1435 | Q1436 | L1437 | T1438 | E1439 | K1440 | S1441 | P1442 | N1443 | P1444 | S1445 | L1446 | L1447 | L1448 | L1449 | C1450 | G1451 | L1452 | L1453 | A1454 | Q1455 | L1456 | A1457 | C1458 | V1459 | E1460 | P1461 | V1462 | R1463 | L1464 | Q1465 | A1466 | W1467 | L1468 | T1469 | R1470 | M1471 | T1472 | T1473 | S1474 | P1475 | PRO   | LYS   | ASP   |      |
| Y1359 | N1360 | I1361 | L1362 | A1363 | N1364 | H1365 | A1366 | D1367 | P1368 | N1369 | S1370 | G1371 | L1372 | D1373 | E1374 | S1375 | L1376 | L1377 | E1378 | E1379 | C1380 | L1381 | Q1382 | Y1383 | L1384 | E1385 | K1386 | Q1387 | L1388 | E1389 | L1390 | S1391 | L1392 | A1393 | R1394 | K1395 | A1396 | M1397 | E1398 | F1399 | F1400 | F1401 | S1402 | D1403 | S1404 | G1405 | E1406 | L1407 | L1408 | Q1409 | I1410 | M1411 | M1412 | A1413 | T1414 | A1415 | P1416 | PRO   | LYS   | ASP  |
| I1299 | V1300 | W1301 | S1302 | D1303 | E1304 | M1305 | N1306 | P1307 | P1308 | Q1309 | V1310 | I1311 | R1312 | T1313 | L1314 | L1315 | P1316 | L1317 | L1318 | L1319 | E1320 | S1321 | S1322 | T1323 | E1324 | S1325 | V1326 | A1327 | E1328 | I1329 | S1330 | M1331 | M1332 | L1333 | L1334 | E1335 | R1336 | I1337 | L1338 | G1339 | P1340 | A1341 | E1342 | S1343 | D1344 | E1345 | F1346 | L1347 | L1348 | R1349 | V1350 | Y1351 | E1352 | K1353 | L1354 | L1355 | T1356 | G1357 | C1358 |      |
| M1239 | E1240 | F1241 | P1242 | N1243 | I1244 | G1245 | S1246 | W1247 | R1248 | N1249 | A1250 | F1251 | A1252 | N1253 | D1254 | T1255 | I1256 | P1257 | S1258 | E1259 | S1260 | Y1261 | I1262 | S1263 | A1264 | V1265 | Q1266 | A1267 | A1268 | H1269 | L1270 | G1271 | L1272 | L1273 | C1274 | S1275 | Q1276 | S1277 | L1278 | V1279 | L1280 | A1281 | A1282 | S1283 | L1284 | K1285 | H1286 | T1287 | L1288 | L1289 | C1290 | S1291 | L1292 | R1293 | L1294 | T1295 | G1296 | D1297 | L1298 |      |
| Q1179 | N1180 | F1181 | N1182 | GLU   | GLU   | GLY   | THR   | THR   | E1188 | K1189 | P1190 | S1191 | K1192 | E1193 | K1194 | L1195 | Q1196 | G1197 | F1198 | A1199 | A1200 | V1201 | L1202 | A1203 | I1204 | G1205 | S1206 | S1207 | R1208 | C1209 | K1210 | A1211 | N1212 | T1213 | L1214 | G1215 | P1216 | T1217 | L1218 | V1219 | Q1220 | N1221 | L1222 | P1223 | S1224 | S1225 | V1226 | Q1227 | T1228 | V1229 | C1230 | E1231 | S1232 | W1233 | M1234 | M1235 | I1236 | N1237 | T1238 |      |
| Q1119 | S1120 | I1121 | Y1122 | T1123 | L1124 | D1125 | A1126 | A1127 | I1128 | S1129 | K1130 | V1131 | Q1132 | V1133 | S1134 | L1135 | D1136 | E1137 | H1138 | F1139 | K1140 | K1141 | M1142 | A1143 | ALA   | GLU   | THR   | ASP   | PRO   | HIS   | LYS   | S1151 | S1152 | E1153 | I1154 | T1155 | K1156 | N1157 | L1158 | P1159 | A1160 | T1161 | L1162 | L1163 | L1164 | L1165 | I1166 | D1167 | T1168 | Y1169 | A1170 | S1171 | F1172 | T1173 | R1174 | A1175 | Y1176 | L1177 | L1178 |      |
| I1069 | K1060 | Q1061 | G1062 | M1063 | K1064 | A1065 | E1066 | H1067 | A1068 | S1069 | S1070 | L1071 | L1072 | E1073 | L1074 | A1075 | S1076 | T1077 | L1078 | K1079 | C1080 | S1081 | S1082 | V1083 | K1084 | Y1085 | D1086 | V1087 | E1088 | I1089 | V1090 | E1091 | E1092 | Y1093 | F1094 | A1095 | R1096 | Q1097 | I1098 | S1099 | F1101 | C1102 | S1103 | I1104 | D1105 | C1106 | T1107 | T1108 | I1109 | L1110 | Q1111 | L1112 | H1113 | E1114 | T1115 | P1116 | S1117 | L1118 |       |      |
| L999  | Q1000 | Y1001 | Y1002 | F1003 | L1004 | I1005 | L1006 | W1007 | R1008 | I1009 | L1010 | G1011 | I1012 | L1013 | P1014 | P1015 | S1016 | K1017 | T1018 | Y1019 | I1020 | N1021 | Q1022 | L1023 | S1024 | M1025 | N1026 | S1027 | P1028 | E1029 | M1030 | S1031 | E1032 | C1033 | D1034 | I1035 | L1036 | H1037 | T1038 | L1039 | R1040 | W1041 | S1042 | S1043 | R1044 | L1045 | R1046 | I1047 | N1048 | S1049 | Y1050 | V1051 | N1052 | W1053 | I1054 | K1055 | D1056 | H1057 | L1058 |      |
| E939  | A940  | S941  | E942  | D943  | D944  | L945  | N946  | R947  | L948  | D949  | S950  | Y951  | A952  | C953  | D954  | V955  | L956  | F957  | S958  | K959  | L960  | V961  | K962  | Y963  | D964  | E965  | L966  | Y967  | A968  | A969  | L970  | T971  | A972  | L973  | L974  | A975  | A976  | G977  | S978  | Q979  | L980  | D981  | T982  | V983  | R984  | R985  | K986  | E987  | N988  | K989  | N990  | V991  | T992  | A993  | L994  | E995  | A996  | C997  | A998  |      |
| H819  | N820  | F821  | T822  | E823  | T824  | G825  | R826  | R827  | A828  | R829  | L830  | S831  | L832  | F833  | V834  | Q835  | I836  | I837  | Q838  | E839  | L840  | S841  | V842  | N843  | M844  | D845  | A846  | R847  | M848  | R849  | F850  | V851  | R852  | L853  | I854  | L855  | A856  | R857  | G977  | K920  | H921  | L858  | L859  | F922  | S923  | SER   | ASP   | ALA   | VAL   | PRO   | HIS   | P930  | R931  | F932  | Y933  | C934  | V935  | L936  | S937  | P938 |
| Q879  | V880  | Q881  | H882  | N883  | L884  | L885  | S886  | P887  | P888  | F889  | G890  | TRP   | ALA   | GLY   | SER   | GLN   | ASP   | SER   | ASN   | SER   | ARG   | ARG   | A903  | T904  | T905  | P906  | L907  | Y908  | H909  | G910  | F911  | K912  | E913  | V914  | E915  | E916  | N917  | W918  | S919  | K920  | H921  | F922  | S923  | SER   | ASP   | ALA   | VAL   | PRO   | HIS   | P930  | R931  | F932  | Y933  | C934  | V935  | L936  | S937  | P938  |       |      |
| R759  | L760  | L761  | L762  | I763  | W764  | Q765  | H766  | K767  | A768  | S769  | A770  | Q771  | G772  | D773  | P774  | D775  | P776  | P777  | E778  | C779  | L780  | K781  | V782  | W783  | D784  | R785  | F786  | L787  | S788  | T789  | M790  | K791  | Q792  | N793  | A794  | L795  | Q796  | G797  | V798  | V799  | P800  | S801  | E802  | T803  | E804  | D805  | L806  | N807  | Y808  | E809  | H810  | L811  | Q812  | M813  | L814  | L815  | L816  | I817  | F818  |      |
| K699  | G700  | S701  | S702  | D703  | E704  | E705  | F706  | A707  | A708  | A709  | L710  | Y711  | H712  | F713  | N714  | H715  | S716  | L717  | V718  | T719  | S720  | D721  | L722  | Q723  | S724  | P725  | N726  | L727  | Q728  | N729  | L730  | L731  | L732  | Q733  | Q734  | L735  | G736  | V737  | A738  | P739  | F740  | S741  | E742  | G743  | P744  | W745  | P746  | L747  | Y748  | I749  | H750  | P751  | Q752  | S753  | L754  | S755  | V756  | L757  | S758  |      |

|       |       |       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| D2213 | P2148 | Q2082 | F2022 | G1959 | M1899 | Q1839 | ASP   | K1721 | ASN   | L1599 | V1539 | SER   |
| M2214 | I2149 | Q2083 | V2023 | M1960 | C1900 | Q1840 | GLU   | E1722 | LYS   | M1600 | V1540 | D1480 |
| V2215 | N2150 | G2084 | F2024 | P1961 | V1901 | A1841 | LYS   | D1723 | L1663 | S1601 | M1541 | Q1481 |
| A2216 | I2151 | P2085 | Y2025 | K1963 | L1902 | L1842 | PRO   | G1724 | C1664 | Y1602 | A1542 | L1482 |
| I2217 | K2152 | F2086 | D2027 | S1904 | S1903 | S1843 | LYS   | S1725 | T1665 | L1603 | T1543 | D1483 |
| R2218 | S2153 | Y2087 | L2028 | P1905 | P1904 | E1844 | SER   | C1726 | F1666 | A1604 | L1544 | V1484 |
| H2219 | S2154 | V2088 | C2029 | H1906 | H1905 | L1845 | SER   | L1727 | T1668 | D1605 | A1545 | I1485 |
| T2220 | N2155 | T2089 | V2030 | L1968 | G1907 | H1846 | LEU   | A1728 | T1669 | V1606 | S1546 | Q1486 |
| A2221 | G2156 | N2090 | D2031 | V1969 | R1908 | T1847 | ARG   | L1729 | Q1670 | T1607 | A1547 | E1487 |
| C2222 | G2157 | C1970 | A2032 | C1971 | L1909 | V1848 | THR   | VAL   | LYS   | N1608 | G1548 | N1488 |
| N2223 | S2158 | E2093 | L2033 | G1971 | Q1910 | K1850 | VAL   | ARG   | K1671 | A1609 | Q1549 | R1489 |
| E2224 | K2159 | L1972 | L2033 | G1972 | H1911 | K1851 | GLU   | THR   | E1672 | Q1550 | G1550 | Q1490 |
| Q2225 | T2160 | K1973 | P2035 | L1974 | L1912 | A1851 | CYS   | PRO   | F1673 | SER   | A1551 | L1491 |
| Q2226 | N2095 | D1975 | T2036 | C1975 | A1913 | E1853 | ARG   | GLY   | M1674 | GLN   | G1552 | L1492 |
| R2227 | H2096 | D1976 | F2037 | H1976 | V1914 | M1854 | GLU   | GLY   | Q1676 | ASN   | H1553 | Q1493 |
| T2228 | E2097 | V1977 | Y2038 | V1977 | S1915 | T1855 | GLY   | MET   | H1677 | GLY   | L1554 | L1494 |
| T2229 | D2098 | L1978 | F2039 | L1978 | H1916 | D1856 | SER   | SER   | V1678 | GLN   | Q1555 | L1495 |
| M2230 | L2099 | L2040 | L2040 | E1917 | E1917 | Q1857 | THR   | MET   | H1679 | PRO   | T1556 | T1496 |
| I2231 | K2100 | P2042 | P2042 | K1918 | K1919 | L1858 | LYS   | GLY   | C1681 | HIS   | H1557 | T1497 |
| L2232 | D2101 | S2043 | S2043 | F1980 | G1919 | M1859 | SER   | GLU   | H1680 | LEU   | N1558 | Y1498 |
| C2233 | S2102 | N2103 | S2044 | S1982 | K1920 | V1860 | ALA   | VAL   | C1682 | SER   | A1560 | V1500 |
| D2235 | N2104 | G2105 | K2045 | S1983 | I1921 | P1861 | ASP   | PHE   | T1683 | ASP   | V1561 | R1501 |
| E2236 | L2106 | Q2105 | T2046 | G1984 | T1922 | L1862 | GLU   | GLN   | T1562 | GLY   | G1562 | E1502 |
| Q2237 | V2106 | A2107 | R2047 | S1985 | L1924 | G1864 | A1808 | SER   | M1686 | GLU   | W1563 | N1503 |
| S2238 | C2179 | D2108 | D2048 | V1986 | Q1925 | G1865 | PRO   | ARG   | VAL   | ARG   | L1564 | S1504 |
| L2239 | V2180 | Q2108 | V2049 | S1987 | L1926 | S1865 | ILE   | ASP   | ASP   | ILE   | S1565 | Q1505 |
| R2240 | Q2181 | G2109 | T2050 | D1988 | L1926 | Q1866 | GLY   | GLY   | R1566 | GLU   | R1566 | V1506 |
| T2241 | T2183 | H2117 | F2051 | H1989 | S1927 | E1867 | SER   | GLU   | V1690 | VAL   | C1567 | G1507 |
| Y2242 | L2184 | V2118 | L2052 | L1990 | A1928 | G1868 | SER   | GLU   | G1691 | ASP   | K1568 | E1508 |
| W2243 | G2185 | F2053 | F2053 | V1991 | L1929 | A1869 | LEU   | VAL   | V1692 | SER   | K1569 | G1509 |
| A2244 | V2186 | M2054 | M2054 | L1992 | L1930 | F1870 | VAL   | VAL   | C1693 | ASP   | Y1570 | V1510 |
| N2245 | P2187 | E2055 | E2055 | H1993 | K1931 | E1871 | ARG   | ARG   | T1694 | VAL   | L1571 | G1511 |
| V2246 | L2188 | M2121 | E2056 | P1994 | Q1932 | N1872 | HIS   | ALA   | V1695 | GLU   | S1572 | A1512 |
| E2247 | V2189 | L2122 | E2057 | Q1995 | A1933 | V1873 | THR   | SER   | F1817 | LEU   | Q1573 | V1513 |
| N2248 | V2190 | F2123 | K2058 | Q1995 | D1934 | R1874 | SER   | SER   | A1697 | ALA   | K1574 | L1514 |
| M2191 | M2191 | F2124 | M2059 | L1996 | S1935 | M1875 | M1819 | SER   | K1698 | VAL   | N1575 | L1515 |
| V2192 | V2192 | S2125 | I2060 | A1997 | S1936 | N1876 | D1820 | PRO   | V1699 | GLU   | V1576 | G1516 |
| P2194 | D2195 | C2127 | I2061 | T1998 | K1937 | Y1877 | A1821 | ASP   | G1700 | GLU   | V1577 | T1517 |
| L2253 | Q2128 | Q2128 | I2063 | G1999 | R1938 | S1878 | LYS   | ASP   | K1702 | ASP   | E1578 | L1518 |
| Q2254 | G2129 | G2129 | M2064 | N2000 | K1939 | G1879 | T1824 | LYS   | D1703 | GLN   | K1579 | P1519 |
| P2255 | K2130 | K2130 | S2065 | I2002 | L1940 | D1880 | VAL   | THR   | H1704 | ALA   | L1580 | P1520 |
| L2198 | S2131 | S2131 | S2066 | T2003 | T1941 | Q1881 | ILE   | THR   | H1705 | GLU   | N1581 | M1521 |
| I2198 | F2132 | F2132 | A2067 | K2004 | L1942 | Q1882 | ASP   | ASP   | S1707 | ASP   | ALA   | T1522 |
| Q2200 | A2133 | A2133 | G2068 | A2005 | T1943 | K1883 | Q1827 | GLY   | Y1708 | ASP   | ASN   | T1523 |
| E2201 | A2134 | A2134 | Y2069 | V2006 | R1944 | T1884 | Q1828 | GLY   | VAL   | GLU   | VAL   | E1524 |
| I2202 | T2135 | T2135 | I2070 | V2007 | L1945 | I1885 | S1830 | LYS   | LYS   | ASP   | HIS   | M1525 |
| K2203 | T2136 | T2136 | Y2071 | L2008 | A1946 | R1886 | A1831 | VAL   | ALA   | LEU   | GLY   | L1526 |
| T2204 | S2137 | S2137 | T2072 | P2009 | S1947 | Q1887 | V1832 | THR   | LYS   | CYS   | HIS   | A1527 |
| L2205 | R2138 | R2138 | Q2073 | L1948 | A1948 | L1888 | G1833 | GLY   | GLY   | GLY   | GLY   | N1528 |
| P2206 | L2074 | L2074 | M2075 | P1949 | P1949 | I1889 | S1834 | SER   | F1714 | M1590 | M1591 | G1529 |
| A2207 | T2139 | T2139 | E2076 | V1950 | P1951 | A1891 | S1836 | THR   | F1715 | L1592 | L1592 | D1530 |
| K2208 | T2141 | T2141 | E2077 | F1952 | P1952 | H1892 | S1890 | ALA   | C1716 | L1593 | L1593 | G1531 |
| A2209 | E2142 | E2142 | E2077 | T2018 | F1952 | H1892 | S1890 | VAL   | D1717 | E1594 | E1594 | T1532 |
| K2210 | V2143 | V2143 | A2078 | T2019 | V1954 | L1894 | R1837 | GLY   | C1718 | C1595 | C1595 | G1533 |
| I2211 | L2144 | L2144 | S2079 | A2020 | V1954 | R1895 | A1838 | VAL   | G1719 | T1596 | T1596 | F1534 |
| Q2212 | Q2145 | Q2145 | S2080 | D2021 | L1955 | L1894 | A1898 | ALA   | A1720 | C1597 | C1597 | P1535 |
|       | L2146 | L2146 | A2081 |       | S1956 | R1896 | A1898 | ALA   |       | Y1598 | Y1598 | E1536 |
|       | F2147 | F2147 |       |       | L1957 | V1897 | A1898 |       |       |       |       | L1537 |
|       |       |       |       |       | T1958 |       |       |       |       |       |       | M1538 |

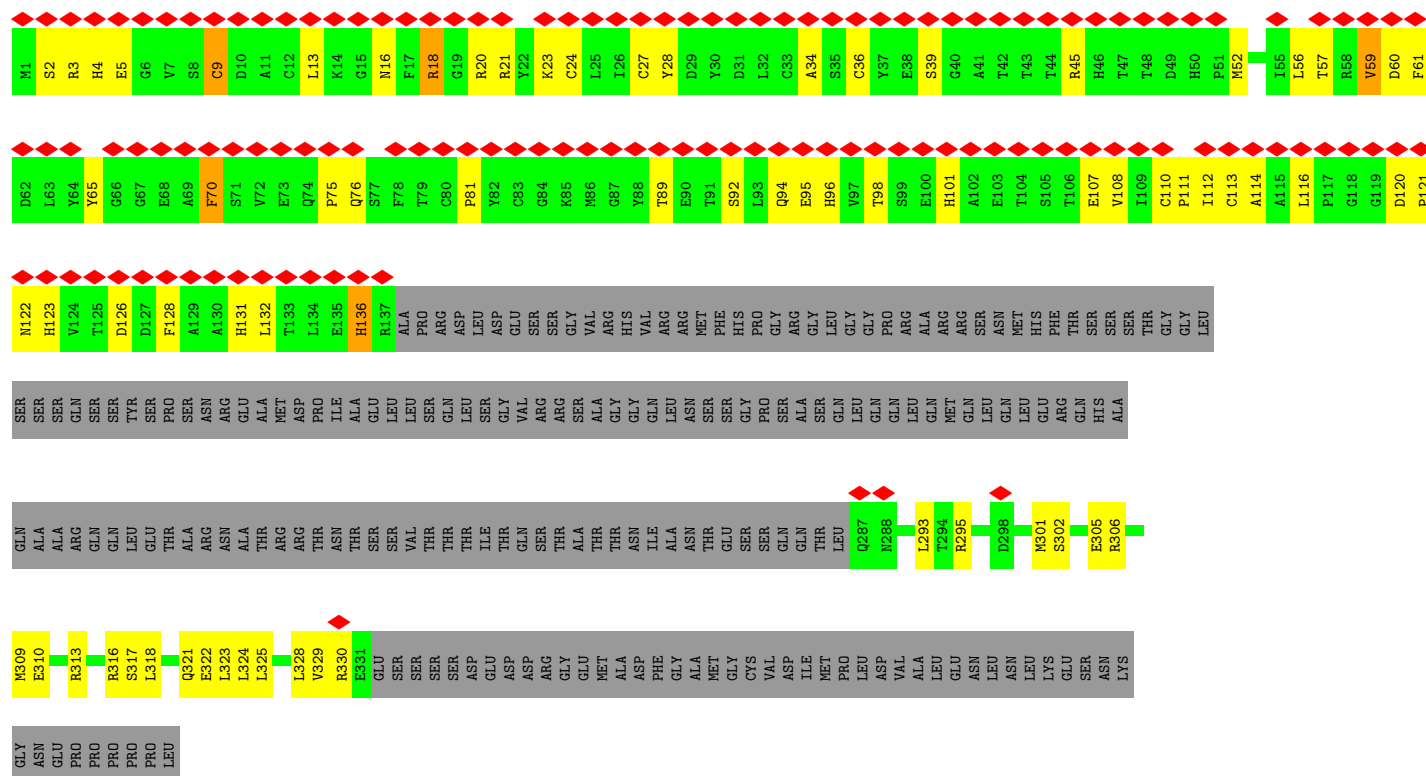
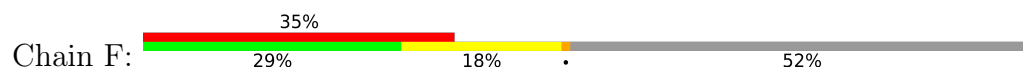


|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| T4230 | D4231 | L4232 | Q4233 | Q4234 | L4238 | K4239 | L4244 | F4248 | R4256 | H4257 | F4258 | K4259 | L4129 | K4260 | R4261 | G4264 | L4267 | L4271 | C4272 | L4273 | R4274 | L4275 | L4276 | V4277 | V4278 | Q4279 | R4280 | T4284 | D4285 | E4286 | T4287 | Q4288 | D4289 | N4290 | D4297 | E4303 | K4307 | F4309 | H4310 | A4311 | V4312 | C4313 | I4314 | E4315 | T4316 | R4319 | T4328 | S4229 |       |       |       |       |       |       |       |       |
| GLU   | ALA   | LEU   | THR   | T4044 | P4047 | C4048 | Q4049 | N4050 | E4051 | H4052 | I4053 | W4059 | F4060 | K4061 | R4062 | W4071 | L4075 | P4076 | L4077 | R4078 | G4079 | I4080 | D4081 | G4082 | N4083 | G4084 | K4085 | A4086 | P4087 | S4088 | K4089 | S4090 | E4091 | L4092 | R4093 | H4094 | L4095 | L4096 | L4097 | T4098 | E4099 | K4100 | Y4101 | V4102 | W4103 | R4104 | W4105 | K4106 | Q4107 | F4108 | L4109 | S4110 | R4111 | R4112 | G4113 |       |
| K4114 | R4115 | T4116 | S4117 | L4118 | L4119 | D4120 | L4123 | G4124 | H4125 | W4126 | N4127 | F4128 | L4129 | R4130 | Q4131 | V4132 | F4134 | T4135 | C4146 | I4155 | R4158 | K4159 | L4165 | Q4169 | L4170 | L4173 | L4186 | Y4187 | I4191 | H4195 | W4196 | V4205 | L4206 | P4207 | L4212 | K4215 | L4216 | L4221 | A4222 | L4223 | E4224 | L4228 | S4229 |       |       |       |       |       |       |       |       |       |       |       |       |       |
| VAL   | LEU   | GLY   | CYS   | H3866 | T3867 | S3868 | C3872 | Y3873 | G3874 | V3879 | T3880 | E3881 | H3882 | C3883 | I3884 | L3887 | R3888 | A3889 | N3893 | P3894 | A3895 | L3896 | R3897 | H3898 | I3899 | L3900 | V3901 | S3902 | Q3903 | G3904 | L3905 | L3909 | F3910 | N3913 | A3918 | A3919 | A3920 | M3921 | R3922 | V3925 | R3926 | Q3927 | L3928 | M3929 | L3932 | N3936 | A3939 |       |       |       |       |       |       |       |       |       |
| T3940 | T3948 | G3949 | K3950 | V3951 | K3956 | D3963 | L3968 | Y3970 | K3971 | H3972 | L3973 | I3979 | C3985 | W3986 | E3987 | L3988 | L3994 | S3995 | L3996 | F3997 | L3998 | W4001 | N4002 | L4003 | K4004 | T4005 | P4006 | V4007 | N4011 | L4012 | C4016 | L4019 | L4020 | Q4021 | L4024 | K4025 | P4026 | P4027 | S4031 | K4035 | D4036 | VAL   | PRO   | VAL   |       |       |       |       |       |       |       |       |       |       |       |       |
| Q3776 | D3777 | D3778 | S3779 | G3780 | T3781 | A3782 | G3783 | G3784 | I3785 | S3786 | T3787 | S3788 | S3789 | A3790 | S3791 | V3792 | N3793 | G3794 | I3795 | L3797 | Q3798 | L3799 | Y3803 | C3807 | E3813 | K3820 | S3824 | R3825 | L3829 | R3836 | K3841 | SER   | SER   | ARG   | THR   | SER   | V3847 | Q3848 | P3849 | T3850 | F3851 | T3852 | A3853 | Q3854 | Q3855 | TYR   | ARG   | ALA   | LEU   | SER   |       |       |       |       |       |       |
| E3694 | K3695 | L3699 | C3703 | G3704 | F3705 | C3706 | R3710 | F3711 | D3712 | F3713 | M3714 | L3715 | Y3716 | A3717 | K3718 | V3723 | E3727 | N3728 | E3729 | E3730 | D3731 | R3732 | K3733 | K3734 | A3735 | I3739 | L3742 | A3746 | D3747 | R3748 | V3749 | Y3750 | H3756 | R3757 | P3758 | Q3759 | L3760 | E3761 | N3762 | L3763 | L3764 | C3765 | K3766 | V3767 | A3770 | E3773 | K3774 | P3775 |       |       |       |       |       |       |       |       |
| K3628 | I3629 | D3630 | L3631 | P3632 | L3633 | L3640 | M3641 | E3643 | F3644 | A3645 | D3646 | F3647 | Y3648 | E3649 | N3650 | V3651 | Q3652 | A3653 | S3654 | T3655 | E3656 | T3657 | L3658 | Q3659 | C3660 | P3661 | R3662 | C3663 | S3664 | A3665 | S3666 | V3667 | P3668 | A3669 | N3670 | P3671 | Q3672 | V3673 | C3674 | Q3675 | N3676 | C3677 | Q3678 | E3679 | N3680 | Y3681 | Q3682 | Q3683 | C3684 | H3685 | K3686 | C3687 | R3688 | N3691 | Y3692 | D3693 |
| L3519 | V3520 | E3521 | Y3525 | Y3526 | L3527 | C3532 | L3533 | Y3534 | V3540 | C3543 | L3547 | R3548 | S3549 | I3550 | K3551 | Y3552 | Y3556 | Q3561 | I3566 | I3571 | G3579 | D3580 | L3581 | K3582 | R3583 | V3587 | R3588 | T3589 | I3590 | N3595 | Q3600 | A3601 | E3604 | L3605 | K3606 | M3607 | K3608 | P3609 | T3621 | P3622 | G3623 | E3626 | V3627 |       |       |       |       |       |       |       |       |       |       |       |       |       |
| K3405 | E3406 | T3407 | L3408 | I3409 | Q3410 | F3411 | L3412 | L3416 | L3417 | E3418 | S3419 | N3420 | V3424 | R3425 | N3438 | S3439 | S3440 | Q3443 | L3447 | L3450 | S3453 | L3454 | W3455 | P3456 | E3457 | L3458 | P3459 | A3460 | Y3461 | A3465 | V3469 | D3470 | S3490 | V3494 | E3495 | I3496 | L3497 | H3507 | P3508 | N3511 | I3512 | Y3513 | H3514 | T3515 | L3516 |       |       |       |       |       |       |       |       |       |       |       |
| ALA   | SER   | SER   | GLY   | SER   | SER   | SER   | ALA   | SER   | SER   | SER   | SER   | PRO   | VAL   | ALA   | ALA   | SER   | GLY   | GLN   | THR   | THR   | GLN   | SER   | LYS   | SER   | THR   | THR   | LYS   | LYS   | GLU   | LYS   | GLU   | LYS   | GLU   | LYS   | GLU   | THR   | SER   | G3385 | G3386 | Q3387 | E3388 | C3392 | L3395 | V3396 | N3397 | Q3398 | D3404 |       |       |       |       |       |       |       |       |       |
| F3250 | L3251 | V3256 | L3269 | I3270 | M3273 | E3274 | H3275 | Q3285 | R3286 | T3287 | F3193 | L3194 | S3195 | E3196 | Y3197 | L3198 | K3199 | I3200 | Q3201 | Q3202 | T3203 | V3206 | R3207 | L3213 | L3214 | L3215 | F3216 | I3217 | S3220 | K3221 | E3222 | K3223 | Y3224 | R3225 | Q3226 | L3227 | L3233 | D3234 | S3235 | H3236 | V3237 | R3238 | G3239 | K3241 | L3244 | E3245 | E3246 | I3249 |       |       |       |       |       |       |       |       |

- Molecule 2: Calmodulin-1



- Molecule 3: E3 ubiquitin-protein ligase KCMF1



## 4 Experimental information

| Property                             | Value                         | Source    |
|--------------------------------------|-------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE               | Depositor |
| Imposed symmetry                     | POINT, Not provided           |           |
| Number of particles used             | 126380                        | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF             | Depositor |
| CTF correction method                | PHASE FLIPPING ONLY           | Depositor |
| Microscope                           | TFS KRIOS                     | Depositor |
| Voltage (kV)                         | 300                           | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 40                            | Depositor |
| Minimum defocus (nm)                 | 800                           | Depositor |
| Maximum defocus (nm)                 | 2600                          | Depositor |
| Magnification                        | Not provided                  |           |
| Image detector                       | GATAN K3 BIOQUANTUM (6k x 4k) | Depositor |
| Maximum map value                    | 1.255                         | Depositor |
| Minimum map value                    | -0.578                        | Depositor |
| Average map value                    | 0.002                         | Depositor |
| Map value standard deviation         | 0.021                         | Depositor |
| Recommended contour level            | 0.13                          | Depositor |
| Map size ( $\text{\AA}$ )            | 440.16, 440.16, 440.16        | wwPDB     |
| Map dimensions                       | 420, 420, 420                 | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0              | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.048, 1.048, 1.048           | Depositor |

## 5 Model quality

### 5.1 Standard geometry

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

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

| Mol | Chain | Bond lengths |                  | Bond angles |                |
|-----|-------|--------------|------------------|-------------|----------------|
|     |       | RMSZ         | $\# Z  > 5$      | RMSZ        | $\# Z  > 5$    |
| 1   | A     | 0.88         | 39/31195 (0.1%)  | 1.04        | 1/42247 (0.0%) |
| 1   | B     | 0.91         | 36/31477 (0.1%)  | 1.10        | 2/42619 (0.0%) |
| 2   | C     | 0.97         | 0/1146           | 1.24        | 0/1539         |
| 2   | D     | 0.98         | 0/1138           | 1.25        | 0/1526         |
| 3   | E     | 1.01         | 12/1463 (0.8%)   | 0.99        | 0/1978         |
| 3   | F     | 1.00         | 13/1463 (0.9%)   | 1.01        | 0/1978         |
| All | All   | 0.91         | 100/67882 (0.1%) | 1.08        | 3/91887 (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 |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 19                  |
| 1   | B     | 0                   | 25                  |
| 2   | D     | 0                   | 1                   |
| 3   | E     | 0                   | 1                   |
| 3   | F     | 0                   | 2                   |
| All | All   | 0                   | 48                  |

All (100) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 1   | A     | 1682 | HIS  | C-N   | -10.20 | 1.20        | 1.33     |
| 1   | B     | 1993 | HIS  | C-N   | 8.77   | 1.43        | 1.34     |
| 1   | A     | 2290 | ASP  | C-N   | -8.62  | 1.22        | 1.33     |
| 1   | B     | 1865 | SER  | C-N   | 8.21   | 1.44        | 1.33     |
| 1   | A     | 1894 | LEU  | C-N   | -8.11  | 1.21        | 1.33     |
| 1   | A     | 1717 | ASP  | C-N   | -8.11  | 1.23        | 1.33     |
| 1   | A     | 1865 | SER  | C-N   | 8.01   | 1.44        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1   | A     | 1681 | CYS  | C-N   | -7.75 | 1.22        | 1.33     |
| 1   | B     | 2318 | LYS  | C-N   | -7.68 | 1.24        | 1.33     |
| 1   | B     | 2327 | TYR  | C-N   | -7.66 | 1.22        | 1.33     |
| 1   | A     | 2038 | TYR  | C-N   | 7.62  | 1.44        | 1.33     |
| 1   | A     | 2318 | LYS  | C-N   | -7.62 | 1.24        | 1.33     |
| 1   | A     | 1860 | VAL  | C-N   | 7.60  | 1.42        | 1.33     |
| 1   | B     | 1860 | VAL  | C-N   | 7.54  | 1.42        | 1.33     |
| 1   | B     | 2038 | TYR  | C-N   | 7.51  | 1.44        | 1.33     |
| 1   | B     | 2076 | GLU  | C-N   | -7.50 | 1.24        | 1.33     |
| 1   | A     | 2146 | LEU  | C-N   | 7.43  | 1.42        | 1.33     |
| 3   | F     | 9    | CYS  | C-N   | -7.42 | 1.22        | 1.33     |
| 1   | A     | 2076 | GLU  | C-N   | -7.38 | 1.24        | 1.33     |
| 3   | E     | 101  | HIS  | C-N   | -7.38 | 1.24        | 1.34     |
| 1   | B     | 2535 | SER  | C-N   | -7.36 | 1.24        | 1.33     |
| 1   | B     | 2146 | LEU  | C-N   | 7.36  | 1.42        | 1.33     |
| 3   | E     | 9    | CYS  | C-N   | -7.32 | 1.22        | 1.33     |
| 3   | F     | 39   | SER  | C-N   | -7.29 | 1.25        | 1.33     |
| 3   | E     | 59   | VAL  | C-N   | -7.18 | 1.24        | 1.34     |
| 3   | E     | 39   | SER  | C-N   | -7.18 | 1.25        | 1.33     |
| 3   | F     | 101  | HIS  | C-N   | -7.12 | 1.24        | 1.34     |
| 3   | E     | 61   | PHE  | C-N   | -7.06 | 1.24        | 1.34     |
| 3   | F     | 59   | VAL  | C-N   | -7.05 | 1.24        | 1.34     |
| 3   | F     | 34   | ALA  | C-N   | -7.03 | 1.24        | 1.33     |
| 3   | F     | 61   | PHE  | C-N   | -6.96 | 1.24        | 1.34     |
| 3   | E     | 34   | ALA  | C-N   | -6.84 | 1.24        | 1.33     |
| 1   | A     | 2251 | TYR  | C-N   | 6.75  | 1.43        | 1.33     |
| 1   | A     | 2294 | HIS  | C-N   | -6.70 | 1.24        | 1.33     |
| 3   | E     | 98   | THR  | C-N   | -6.70 | 1.24        | 1.33     |
| 1   | B     | 2026 | TYR  | C-N   | -6.66 | 1.24        | 1.33     |
| 1   | A     | 2658 | ASN  | C-N   | -6.63 | 1.25        | 1.33     |
| 3   | F     | 98   | THR  | C-N   | -6.59 | 1.24        | 1.33     |
| 1   | A     | 1973 | LYS  | C-N   | 6.58  | 1.43        | 1.33     |
| 1   | B     | 1973 | LYS  | C-N   | 6.54  | 1.42        | 1.33     |
| 1   | A     | 2026 | TYR  | C-N   | -6.54 | 1.24        | 1.33     |
| 1   | B     | 1925 | GLN  | C-N   | 6.44  | 1.43        | 1.33     |
| 1   | A     | 1870 | PHE  | C-N   | -6.26 | 1.24        | 1.33     |
| 1   | B     | 2392 | GLU  | C-N   | -6.21 | 1.25        | 1.33     |
| 1   | A     | 2067 | ALA  | C-N   | 6.11  | 1.42        | 1.33     |
| 1   | B     | 1870 | PHE  | C-N   | -6.08 | 1.25        | 1.33     |
| 1   | A     | 2374 | THR  | C-N   | -6.03 | 1.25        | 1.33     |
| 1   | A     | 1925 | GLN  | C-N   | 6.02  | 1.43        | 1.33     |
| 1   | B     | 2374 | THR  | C-N   | -5.96 | 1.25        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1   | A     | 2242 | TYR  | C-N   | -5.91 | 1.25        | 1.33     |
| 1   | B     | 2315 | GLN  | C-N   | -5.89 | 1.26        | 1.33     |
| 1   | B     | 2067 | ALA  | C-N   | 5.88  | 1.42        | 1.33     |
| 1   | A     | 2315 | GLN  | C-N   | -5.87 | 1.26        | 1.33     |
| 1   | A     | 2366 | SER  | C-N   | -5.87 | 1.26        | 1.33     |
| 1   | B     | 2366 | SER  | C-N   | -5.86 | 1.26        | 1.33     |
| 1   | B     | 2177 | VAL  | C-N   | 5.78  | 1.41        | 1.33     |
| 1   | B     | 2313 | ASN  | C-N   | -5.64 | 1.26        | 1.33     |
| 1   | A     | 1965 | ASP  | C-N   | -5.61 | 1.25        | 1.33     |
| 1   | B     | 2510 | THR  | C-N   | -5.58 | 1.26        | 1.33     |
| 3   | F     | 57   | THR  | C-N   | -5.57 | 1.26        | 1.33     |
| 3   | E     | 57   | THR  | C-N   | -5.55 | 1.26        | 1.33     |
| 1   | A     | 2177 | VAL  | C-N   | 5.49  | 1.41        | 1.33     |
| 1   | B     | 2699 | GLN  | C-N   | -5.49 | 1.26        | 1.33     |
| 3   | F     | 36   | CYS  | C-N   | -5.49 | 1.26        | 1.33     |
| 1   | B     | 1965 | ASP  | C-N   | -5.48 | 1.25        | 1.33     |
| 1   | B     | 2350 | THR  | C-N   | -5.42 | 1.26        | 1.33     |
| 1   | B     | 2084 | GLY  | C-N   | 5.39  | 1.40        | 1.33     |
| 1   | B     | 1825 | ASN  | C-N   | 5.38  | 1.41        | 1.33     |
| 1   | A     | 1895 | ARG  | C-N   | -5.38 | 1.25        | 1.33     |
| 1   | A     | 2350 | THR  | C-N   | -5.38 | 1.26        | 1.33     |
| 1   | A     | 2577 | ALA  | C-N   | -5.35 | 1.27        | 1.33     |
| 3   | E     | 36   | CYS  | C-N   | -5.34 | 1.27        | 1.33     |
| 1   | A     | 2084 | GLY  | C-N   | 5.33  | 1.40        | 1.33     |
| 1   | B     | 1831 | ALA  | C-N   | 5.32  | 1.39        | 1.33     |
| 3   | E     | 95   | GLU  | C-N   | -5.32 | 1.27        | 1.33     |
| 3   | F     | 96   | HIS  | C-N   | -5.29 | 1.27        | 1.33     |
| 1   | A     | 1955 | LEU  | C-N   | 5.29  | 1.40        | 1.33     |
| 1   | B     | 2703 | ARG  | C-N   | -5.27 | 1.27        | 1.33     |
| 1   | A     | 1867 | GLU  | C-N   | 5.24  | 1.40        | 1.33     |
| 3   | E     | 60   | ASP  | C-N   | -5.23 | 1.27        | 1.33     |
| 1   | B     | 2234 | CYS  | C-N   | -5.21 | 1.26        | 1.34     |
| 1   | B     | 2091 | VAL  | C-N   | -5.21 | 1.26        | 1.33     |
| 3   | F     | 60   | ASP  | C-N   | -5.20 | 1.27        | 1.33     |
| 3   | F     | 95   | GLU  | C-N   | -5.20 | 1.27        | 1.33     |
| 3   | E     | 96   | HIS  | C-N   | -5.19 | 1.27        | 1.33     |
| 1   | B     | 2622 | ILE  | C-N   | -5.17 | 1.27        | 1.33     |
| 1   | A     | 2234 | CYS  | C-N   | -5.16 | 1.27        | 1.34     |
| 1   | A     | 1864 | GLY  | C-N   | -5.13 | 1.25        | 1.33     |
| 3   | F     | 110  | CYS  | C-N   | -5.13 | 1.27        | 1.34     |
| 1   | B     | 2216 | ALA  | C-N   | 5.12  | 1.40        | 1.33     |
| 1   | A     | 2579 | SER  | C-N   | -5.11 | 1.27        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1   | B     | 1867 | GLU  | C-N   | 5.09  | 1.40        | 1.33     |
| 1   | A     | 2061 | ILE  | C-N   | -5.09 | 1.27        | 1.33     |
| 1   | B     | 2343 | ASN  | C-N   | -5.09 | 1.25        | 1.33     |
| 1   | B     | 2035 | PRO  | C-N   | -5.07 | 1.27        | 1.33     |
| 1   | A     | 2035 | PRO  | C-N   | -5.05 | 1.27        | 1.33     |
| 1   | A     | 2359 | GLN  | C-N   | -5.03 | 1.27        | 1.33     |
| 1   | A     | 2558 | SER  | C-N   | -5.02 | 1.27        | 1.33     |
| 1   | A     | 2622 | ILE  | C-N   | -5.00 | 1.27        | 1.33     |
| 1   | B     | 2314 | ALA  | C-N   | -5.00 | 1.27        | 1.33     |

All (3) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | A     | 1282 | ALA  | N-CA-C  | -6.39 | 104.32      | 111.28   |
| 1   | B     | 1131 | VAL  | N-CA-CB | 5.70  | 117.22      | 110.55   |
| 1   | B     | 529  | PRO  | N-CA-C  | -5.06 | 102.05      | 112.47   |

There are no chirality outliers.

All (48) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | A     | 1008 | ARG  | Sidechain |
| 1   | A     | 1174 | ARG  | Sidechain |
| 1   | A     | 1293 | ARG  | Sidechain |
| 1   | A     | 1394 | ARG  | Sidechain |
| 1   | A     | 2320 | ARG  | Sidechain |
| 1   | A     | 2703 | ARG  | Sidechain |
| 1   | A     | 3045 | ARG  | Sidechain |
| 1   | A     | 3142 | ARG  | Sidechain |
| 1   | A     | 3166 | ARG  | Sidechain |
| 1   | A     | 325  | ARG  | Sidechain |
| 1   | A     | 3286 | ARG  | Sidechain |
| 1   | A     | 3732 | ARG  | Sidechain |
| 1   | A     | 3825 | ARG  | Sidechain |
| 1   | A     | 3857 | ARG  | Sidechain |
| 1   | A     | 4319 | ARG  | Sidechain |
| 1   | A     | 4491 | ARG  | Sidechain |
| 1   | A     | 849  | ARG  | Sidechain |
| 1   | A     | 94   | ARG  | Sidechain |
| 1   | A     | 985  | ARG  | Sidechain |
| 1   | B     | 1008 | ARG  | Sidechain |
| 1   | B     | 1312 | ARG  | Sidechain |

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| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | B     | 1336 | ARG  | Sidechain |
| 1   | B     | 1470 | ARG  | Sidechain |
| 1   | B     | 185  | ARG  | Sidechain |
| 1   | B     | 1896 | ARG  | Sidechain |
| 1   | B     | 204  | ARG  | Sidechain |
| 1   | B     | 2381 | ARG  | Sidechain |
| 1   | B     | 296  | ARG  | Sidechain |
| 1   | B     | 2974 | ARG  | Sidechain |
| 1   | B     | 2989 | ARG  | Sidechain |
| 1   | B     | 3286 | ARG  | Sidechain |
| 1   | B     | 3732 | ARG  | Sidechain |
| 1   | B     | 3836 | ARG  | Sidechain |
| 1   | B     | 396  | ARG  | Sidechain |
| 1   | B     | 397  | ARG  | Sidechain |
| 1   | B     | 4115 | ARG  | Sidechain |
| 1   | B     | 4256 | ARG  | Sidechain |
| 1   | B     | 4280 | ARG  | Sidechain |
| 1   | B     | 4319 | ARG  | Sidechain |
| 1   | B     | 4607 | ARG  | Sidechain |
| 1   | B     | 520  | ARG  | Sidechain |
| 1   | B     | 759  | ARG  | Sidechain |
| 1   | B     | 849  | ARG  | Sidechain |
| 1   | B     | 985  | ARG  | Sidechain |
| 2   | D     | 75   | ARG  | Sidechain |
| 3   | E     | 3    | ARG  | Sidechain |
| 3   | F     | 18   | ARG  | Sidechain |
| 3   | F     | 330  | ARG  | Sidechain |

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 30658 | 0        | 31020    | 1288    | 0            |
| 1   | B     | 30933 | 0        | 31316    | 1262    | 0            |
| 2   | C     | 1134  | 0        | 1063     | 68      | 0            |
| 2   | D     | 1127  | 0        | 1055     | 61      | 0            |
| 3   | E     | 1435  | 0        | 1344     | 44      | 0            |
| 3   | F     | 1435  | 0        | 1344     | 52      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | A     | 6     | 0        | 0        | 2       | 0            |
| 4   | B     | 6     | 0        | 0        | 3       | 0            |
| 4   | E     | 4     | 0        | 0        | 0       | 0            |
| 4   | F     | 4     | 0        | 0        | 0       | 0            |
| 5   | C     | 2     | 0        | 0        | 0       | 0            |
| 5   | D     | 2     | 0        | 0        | 2       | 0            |
| All | All   | 66746 | 0        | 67142    | 2687    | 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 20.

All (2687) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:3270:ILE:CD1  | 1:B:3632:PRO:HG2  | 1.66                     | 1.25              |
| 1:A:3270:ILE:CD1  | 1:A:3632:PRO:HG2  | 1.66                     | 1.23              |
| 1:B:3087:ALA:CB   | 1:B:3181:ILE:HG21 | 1.73                     | 1.19              |
| 1:A:73:PHE:CD1    | 1:A:159:LYS:HA    | 1.80                     | 1.15              |
| 2:D:98:ASN:HB2    | 5:D:202:CA:CA     | 1.06                     | 1.15              |
| 1:B:3087:ALA:HB2  | 1:B:3181:ILE:HG21 | 1.31                     | 1.11              |
| 1:A:3270:ILE:HD13 | 1:A:3632:PRO:HG2  | 1.25                     | 1.10              |
| 1:A:1450:CYS:HB2  | 1:A:1505:GLN:HB2  | 1.33                     | 1.09              |
| 1:A:1700:CYS:SG   | 1:A:1726:CYS:HA   | 1.92                     | 1.09              |
| 1:A:2212:GLN:NE2  | 1:A:2235:GLU:HA   | 1.65                     | 1.09              |
| 1:B:3087:ALA:HB2  | 1:B:3181:ILE:HD13 | 1.36                     | 1.08              |
| 1:B:910:GLY:HA2   | 1:B:933:TYR:HA    | 1.19                     | 1.08              |
| 1:B:1205:GLY:HA3  | 1:B:1215:GLY:CA   | 1.83                     | 1.08              |
| 1:B:3270:ILE:HD13 | 1:B:3632:PRO:HG2  | 1.25                     | 1.07              |
| 1:A:1500:VAL:HG22 | 1:A:1547:ALA:HB2  | 1.33                     | 1.07              |
| 1:B:2564:ASP:OD1  | 1:B:2631:LYS:HB3  | 1.55                     | 1.06              |
| 1:A:1700:CYS:SG   | 1:A:1727:LEU:N    | 2.29                     | 1.04              |
| 2:C:106:LEU:HD22  | 2:C:126:ILE:HD11  | 1.38                     | 1.04              |
| 1:A:3269:LEU:HB3  | 1:A:3633:LEU:CD1  | 1.89                     | 1.03              |
| 1:B:3269:LEU:HB3  | 1:B:3633:LEU:CD1  | 1.89                     | 1.02              |
| 1:A:2342:ASN:HB3  | 1:A:2399:LYS:HA   | 1.40                     | 1.01              |
| 1:A:1870:PHE:CZ   | 1:A:1924:LEU:HD11 | 1.97                     | 0.99              |
| 1:B:1870:PHE:CZ   | 1:B:1924:LEU:HD11 | 1.97                     | 0.99              |
| 1:B:1205:GLY:HA3  | 1:B:1215:GLY:HA2  | 1.43                     | 0.99              |
| 1:A:1873:VAL:HG11 | 1:A:2233:LEU:HD21 | 1.45                     | 0.99              |
| 1:A:3793:ASN:HA   | 1:B:3521:GLU:HG3  | 1.43                     | 0.99              |
| 1:B:2698:LYS:HD2  | 1:B:2998:PRO:HA   | 1.46                     | 0.98              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2173:HIS:CD2  | 1:A:2253:LEU:HD11 | 1.99                     | 0.98              |
| 1:B:1205:GLY:CA   | 1:B:1215:GLY:HA3  | 1.94                     | 0.97              |
| 1:B:1901:VAL:HG11 | 1:B:2217:ILE:HD12 | 1.45                     | 0.96              |
| 1:B:3410:GLN:HG3  | 1:B:3850:THR:HB   | 1.47                     | 0.96              |
| 1:A:53:VAL:HG11   | 1:A:99:SER:HB3    | 1.47                     | 0.96              |
| 2:D:50:GLN:O      | 2:D:53:ILE:HG22   | 1.65                     | 0.96              |
| 1:A:1901:VAL:HG11 | 1:A:2217:ILE:HD12 | 1.45                     | 0.95              |
| 1:A:2294:HIS:O    | 1:A:2425:LYS:HE2  | 1.68                     | 0.94              |
| 2:D:101:ILE:HB    | 2:D:137:VAL:HB    | 1.48                     | 0.93              |
| 1:B:1870:PHE:HZ   | 1:B:1924:LEU:CD1  | 1.82                     | 0.93              |
| 1:A:1438:THR:HA   | 1:A:1446:LEU:HD13 | 1.47                     | 0.93              |
| 1:A:1870:PHE:HZ   | 1:A:1924:LEU:CD1  | 1.82                     | 0.92              |
| 1:B:3087:ALA:HB1  | 1:B:3181:ILE:HG21 | 1.53                     | 0.91              |
| 1:A:690:ILE:HA    | 1:A:710:LEU:HD21  | 1.51                     | 0.91              |
| 1:B:1438:THR:HA   | 1:B:1446:LEU:HD13 | 1.51                     | 0.91              |
| 1:B:1394:ARG:HA   | 1:B:1397:MET:HE2  | 1.53                     | 0.91              |
| 1:B:2564:ASP:CG   | 1:B:2631:LYS:HB3  | 1.96                     | 0.90              |
| 1:A:1398:GLU:HA   | 1:A:1449:LEU:HD21 | 1.50                     | 0.90              |
| 1:B:1486:GLN:HA   | 1:B:1489:ARG:HD2  | 1.52                     | 0.90              |
| 3:F:94:GLN:HA     | 3:F:132:LEU:HD13  | 1.53                     | 0.90              |
| 1:A:1870:PHE:HE2  | 1:A:2239:LEU:HD11 | 1.37                     | 0.90              |
| 3:E:94:GLN:HA     | 3:E:132:LEU:HD13  | 1.54                     | 0.90              |
| 1:B:3003:ILE:HA   | 1:B:3006:LEU:HD12 | 1.54                     | 0.89              |
| 2:D:98:ASN:CB     | 5:D:202:CA:CA     | 1.79                     | 0.89              |
| 1:A:1105:ASP:H    | 1:A:1110:LEU:HD21 | 1.37                     | 0.89              |
| 1:B:3270:ILE:CD1  | 1:B:3632:PRO:CG   | 2.51                     | 0.89              |
| 1:A:3521:GLU:HG3  | 1:B:3793:ASN:HA   | 1.53                     | 0.89              |
| 1:B:281:SER:HB2   | 1:B:443:ARG:HD2   | 1.56                     | 0.88              |
| 1:B:1166:ILE:HG12 | 1:B:1291:LEU:HB3  | 1.56                     | 0.88              |
| 1:A:3270:ILE:CD1  | 1:A:3632:PRO:CG   | 2.51                     | 0.88              |
| 1:B:1159:LEU:HA   | 1:B:1298:LEU:HD13 | 1.55                     | 0.88              |
| 1:B:134:LYS:HA    | 1:B:315:LEU:HD21  | 1.54                     | 0.87              |
| 1:A:4231:ASP:HB3  | 1:A:4234:GLN:HB2  | 1.56                     | 0.87              |
| 1:B:1600:MET:HA   | 1:B:1603:LEU:HD12 | 1.55                     | 0.87              |
| 1:B:2687:LEU:HD22 | 1:B:2991:VAL:HG21 | 1.56                     | 0.87              |
| 1:A:2027:ASP:OD1  | 1:A:2029:CYS:SG   | 2.33                     | 0.87              |
| 3:E:114:ALA:HA    | 3:E:121:PRO:HA    | 1.56                     | 0.87              |
| 1:A:2040:LEU:HD13 | 1:A:2085:PRO:HB2  | 1.57                     | 0.87              |
| 1:A:3066:THR:HG21 | 1:A:3082:SER:HB3  | 1.57                     | 0.86              |
| 1:B:1493:GLN:HG2  | 1:B:1540:VAL:HG22 | 1.54                     | 0.86              |
| 1:A:1401:PHE:HA   | 1:A:1406:GLU:HG3  | 1.58                     | 0.86              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:4306:THR:HG21 | 1:A:4338:ILE:HG12 | 1.57                     | 0.86              |
| 1:A:3172:LYS:HE3  | 1:A:3217:ILE:HA   | 1.57                     | 0.86              |
| 1:A:4232:LEU:HD13 | 1:B:3750:TYR:HB2  | 1.57                     | 0.86              |
| 1:A:1921:ILE:HB   | 1:A:1948:ALA:HB3  | 1.57                     | 0.86              |
| 2:C:69:PHE:CZ     | 2:C:73:MET:SD     | 2.67                     | 0.86              |
| 1:A:2040:LEU:CD1  | 1:A:2085:PRO:HB2  | 2.06                     | 0.86              |
| 1:A:2173:HIS:HD2  | 1:A:2253:LEU:HD11 | 1.35                     | 0.86              |
| 1:B:2027:ASP:OD1  | 1:B:2029:CYS:SG   | 2.33                     | 0.86              |
| 2:C:106:LEU:CD2   | 2:C:126:ILE:HD11  | 2.05                     | 0.86              |
| 1:A:1338:LEU:HD13 | 1:A:1346:PHE:HA   | 1.56                     | 0.85              |
| 1:A:2375:MET:HG2  | 1:A:2387:PHE:HE1  | 1.40                     | 0.85              |
| 1:B:2040:LEU:CD1  | 1:B:2085:PRO:HB2  | 2.05                     | 0.85              |
| 1:A:1112:LEU:HD13 | 1:A:1179:GLN:HB2  | 1.57                     | 0.85              |
| 1:B:2040:LEU:HD13 | 1:B:2085:PRO:HB2  | 1.57                     | 0.85              |
| 1:B:3419:SER:O    | 1:B:3420:ASN:CG   | 2.19                     | 0.85              |
| 1:A:1453:LEU:HB3  | 1:A:1506:VAL:HG13 | 1.58                     | 0.85              |
| 1:A:687:ALA:HB2   | 1:A:731:LEU:HD12  | 1.58                     | 0.85              |
| 1:B:1278:LEU:HB3  | 1:B:1281:ALA:HB2  | 1.57                     | 0.85              |
| 2:C:106:LEU:HD22  | 2:C:126:ILE:CD1   | 2.07                     | 0.85              |
| 1:A:1960:ASN:HD21 | 1:A:2012:GLN:HA   | 1.41                     | 0.85              |
| 1:B:4444:MET:HE3  | 1:B:4447:LEU:HD13 | 1.58                     | 0.85              |
| 1:B:1870:PHE:HZ   | 1:B:1924:LEU:HD11 | 1.37                     | 0.84              |
| 1:B:910:GLY:CA    | 1:B:933:TYR:HA    | 2.04                     | 0.84              |
| 1:B:2695:PHE:CE1  | 1:B:2699:GLN:NE2  | 2.45                     | 0.84              |
| 1:A:1205:GLY:HA2  | 1:A:1215:GLY:CA   | 2.07                     | 0.84              |
| 1:A:3419:SER:O    | 1:A:3420:ASN:CG   | 2.19                     | 0.84              |
| 1:B:3419:SER:O    | 1:B:3420:ASN:OD1  | 1.96                     | 0.84              |
| 3:F:114:ALA:HA    | 3:F:121:PRO:HA    | 1.57                     | 0.83              |
| 1:A:420:LEU:HD22  | 1:A:442:LEU:HG    | 1.61                     | 0.83              |
| 1:B:2189:VAL:HG22 | 1:B:2230:MET:HE1  | 1.60                     | 0.83              |
| 1:B:4705:LEU:HB3  | 1:B:4754:VAL:HG22 | 1.60                     | 0.83              |
| 1:A:2189:VAL:CG2  | 1:A:2230:MET:HE1  | 2.08                     | 0.83              |
| 2:C:80:THR:O      | 2:C:81:ASP:OD1    | 1.95                     | 0.83              |
| 1:B:2189:VAL:CG2  | 1:B:2230:MET:HE1  | 2.09                     | 0.83              |
| 1:A:73:PHE:HD1    | 1:A:159:LYS:HA    | 1.37                     | 0.83              |
| 1:A:4444:MET:HE3  | 1:A:4447:LEU:HD13 | 1.59                     | 0.83              |
| 1:A:3269:LEU:HB3  | 1:A:3633:LEU:HD11 | 1.61                     | 0.82              |
| 1:A:2189:VAL:HG22 | 1:A:2230:MET:HE1  | 1.60                     | 0.82              |
| 1:B:1407:LEU:HB3  | 1:B:1431:PHE:CE1  | 2.15                     | 0.82              |
| 1:B:1407:LEU:HB3  | 1:B:1431:PHE:HE1  | 1.45                     | 0.82              |
| 1:B:1414:THR:HG23 | 1:B:1423:PHE:HD2  | 1.44                     | 0.82              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:3419:SER:O    | 1:A:3420:ASN:OD1  | 1.96                     | 0.82              |
| 1:A:4328:PRO:HA   | 1:A:4331:ILE:HD12 | 1.61                     | 0.82              |
| 1:A:3940:THR:HG21 | 1:A:3985:CYS:HB3  | 1.60                     | 0.82              |
| 1:B:1475:PRO:HD3  | 1:B:1485:ILE:HD12 | 1.61                     | 0.81              |
| 1:A:349:ILE:HD12  | 1:A:429:LEU:HD11  | 1.62                     | 0.81              |
| 1:B:1499:ILE:HG23 | 1:B:1506:VAL:HB   | 1.61                     | 0.81              |
| 3:E:8:SER:HA      | 3:E:15:GLY:HA2    | 1.62                     | 0.81              |
| 1:A:1417:GLU:HA   | 1:A:1470:ARG:HD2  | 1.62                     | 0.81              |
| 1:B:2122:LEU:HD22 | 1:B:2136:ILE:HD11 | 1.63                     | 0.81              |
| 2:C:49:LEU:C      | 2:C:49:LEU:HD13   | 2.06                     | 0.81              |
| 1:B:1208:ARG:HD2  | 1:B:1327:ALA:HB3  | 1.63                     | 0.81              |
| 1:B:3270:ILE:HD13 | 1:B:3632:PRO:CG   | 2.11                     | 0.81              |
| 1:A:3164:VAL:O    | 1:A:3168:PRO:HD2  | 1.81                     | 0.81              |
| 1:B:2698:LYS:HE3  | 1:B:3001:GLN:HB3  | 1.63                     | 0.81              |
| 1:B:3516:LEU:HD22 | 1:B:3799:LEU:HD21 | 1.63                     | 0.81              |
| 1:A:1700:CYS:SG   | 1:A:1726:CYS:CA   | 2.69                     | 0.80              |
| 1:B:3269:LEU:HB3  | 1:B:3633:LEU:HD11 | 1.61                     | 0.80              |
| 1:A:1904:SER:H    | 1:A:1964:GLU:HB3  | 1.45                     | 0.80              |
| 1:A:2368:ILE:HG23 | 1:A:2377:LEU:HD11 | 1.62                     | 0.80              |
| 1:A:3997:PHE:HB2  | 1:A:4016:CYS:HB3  | 1.63                     | 0.80              |
| 1:A:124:VAL:HG12  | 1:A:129:LEU:HG    | 1.63                     | 0.80              |
| 1:A:352:VAL:HB    | 1:A:426:PRO:HG3   | 1.64                     | 0.80              |
| 1:B:4713:PHE:HE1  | 1:B:4751:LEU:HD21 | 1.46                     | 0.80              |
| 1:B:2368:ILE:HD11 | 1:B:2387:PHE:CZ   | 2.16                     | 0.80              |
| 1:A:659:THR:HA    | 1:A:663:LEU:HD12  | 1.63                     | 0.80              |
| 1:A:712:HIS:HA    | 1:A:715:HIS:CD2   | 2.15                     | 0.79              |
| 1:A:3760:LEU:HD11 | 1:A:3803:TYR:HB2  | 1.63                     | 0.79              |
| 1:B:2122:LEU:CD2  | 1:B:2136:ILE:HD11 | 2.13                     | 0.79              |
| 1:B:1554:LEU:HG   | 1:B:1804:ASN:OD1  | 1.82                     | 0.79              |
| 1:B:2375:MET:HG2  | 1:B:2387:PHE:HE1  | 1.44                     | 0.79              |
| 1:A:1030:MET:HB3  | 1:A:1034:ASP:HB3  | 1.62                     | 0.79              |
| 1:B:263:LEU:HB2   | 1:B:266:PHE:HB2   | 1.65                     | 0.79              |
| 1:A:131:LEU:HD11  | 1:A:142:ARG:HD2   | 1.64                     | 0.79              |
| 1:A:4234:GLN:HE22 | 1:A:4279:GLN:HB3  | 1.48                     | 0.79              |
| 1:A:4335:LEU:HD22 | 1:A:4511:LEU:HD11 | 1.63                     | 0.79              |
| 1:B:3588:ARG:HD2  | 1:B:3646:ASP:OD2  | 1.83                     | 0.79              |
| 1:A:1554:LEU:HG   | 1:A:1802:GLN:HE22 | 1.48                     | 0.79              |
| 1:A:2122:LEU:HD22 | 1:A:2136:ILE:HD11 | 1.63                     | 0.79              |
| 1:B:2122:LEU:HD22 | 1:B:2136:ILE:CD1  | 2.13                     | 0.79              |
| 1:A:3872:CYS:SG   | 1:A:3875:CYS:HB2  | 2.23                     | 0.78              |
| 1:A:1450:CYS:CB   | 1:A:1505:GLN:HB2  | 2.11                     | 0.78              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:3066:THR:HG21 | 1:B:3082:SER:HB2  | 1.65                     | 0.78              |
| 1:A:313:LEU:HD13  | 1:A:388:ILE:HD11  | 1.65                     | 0.78              |
| 1:A:2122:LEU:CD2  | 1:A:2136:ILE:HD11 | 2.13                     | 0.78              |
| 1:A:3588:ARG:HD2  | 1:A:3646:ASP:OD2  | 1.82                     | 0.77              |
| 1:B:1408:VAL:HA   | 1:B:1411:MET:HE2  | 1.66                     | 0.77              |
| 1:A:910:GLY:HA2   | 1:A:933:TYR:HA    | 1.66                     | 0.77              |
| 1:B:3315:VAL:HG22 | 1:B:3633:LEU:HD21 | 1.66                     | 0.77              |
| 1:B:1412:MET:HB3  | 1:B:1463:ARG:NE   | 1.99                     | 0.77              |
| 1:B:3004:LEU:HB2  | 1:B:3058:LEU:HD11 | 1.64                     | 0.77              |
| 1:A:415:LEU:HD11  | 1:A:484:LEU:HD21  | 1.67                     | 0.77              |
| 1:A:2122:LEU:HD22 | 1:A:2136:ILE:CD1  | 2.13                     | 0.77              |
| 1:B:4591:LYS:HB2  | 1:B:4630:LYS:HE3  | 1.65                     | 0.77              |
| 1:A:4635:VAL:HG11 | 1:A:4685:LYS:HG3  | 1.67                     | 0.76              |
| 2:D:50:GLN:O      | 2:D:53:ILE:CG2    | 2.32                     | 0.76              |
| 1:A:3270:ILE:HD13 | 1:A:3632:PRO:CG   | 2.11                     | 0.76              |
| 1:A:793:ASN:HB2   | 1:A:854:ILE:HG21  | 1.66                     | 0.76              |
| 1:A:984:ARG:HH11  | 1:A:984:ARG:HB2   | 1.51                     | 0.76              |
| 1:B:1407:LEU:H    | 1:B:1407:LEU:HD12 | 1.50                     | 0.76              |
| 1:B:352:VAL:HG22  | 1:B:467:GLN:HG2   | 1.67                     | 0.76              |
| 1:B:2070:ILE:HD12 | 1:B:2094:ILE:HD11 | 1.67                     | 0.76              |
| 1:A:656:ASN:HB3   | 1:B:204:ARG:HD3   | 1.67                     | 0.76              |
| 1:B:1218:LEU:HD22 | 1:B:1376:ILE:HG23 | 1.68                     | 0.75              |
| 1:B:2637:PRO:HD3  | 1:B:2648:PRO:HG2  | 1.67                     | 0.75              |
| 1:B:4339:ILE:HG21 | 1:B:4514:TYR:HB3  | 1.67                     | 0.75              |
| 1:A:3167:LEU:HB3  | 1:A:3168:PRO:HD3  | 1.66                     | 0.75              |
| 1:B:1545:ALA:HB1  | 1:B:1553:HIS:HB2  | 1.68                     | 0.75              |
| 1:B:2683:MET:HG3  | 1:B:2999:TYR:HE2  | 1.51                     | 0.75              |
| 1:A:1870:PHE:HZ   | 1:A:1924:LEU:HD11 | 1.37                     | 0.75              |
| 1:A:1814:MET:HA   | 1:A:1817:PHE:CE1  | 2.21                     | 0.75              |
| 1:A:3965:ALA:HA   | 1:A:4011:ASN:HD21 | 1.52                     | 0.75              |
| 1:B:286:PRO:HB3   | 1:B:295:VAL:HG21  | 1.68                     | 0.75              |
| 1:B:1201:VAL:HG13 | 1:B:1218:LEU:HB3  | 1.67                     | 0.75              |
| 1:B:1664:CYS:HB2  | 1:B:1729:LEU:HA   | 1.66                     | 0.75              |
| 1:B:1489:ARG:NH2  | 1:B:1533:GLY:HA2  | 2.01                     | 0.75              |
| 1:B:910:GLY:HA2   | 1:B:933:TYR:CA    | 2.09                     | 0.74              |
| 1:B:1904:SER:H    | 1:B:1964:GLU:HB3  | 1.52                     | 0.74              |
| 1:A:193:PHE:HB2   | 1:B:881:GLN:HE21  | 1.50                     | 0.74              |
| 1:B:860:LEU:HB2   | 1:B:1005:ILE:HD13 | 1.69                     | 0.74              |
| 1:A:1994:PRO:HG3  | 1:A:2002:ILE:HD11 | 1.68                     | 0.74              |
| 1:A:2192:VAL:HG13 | 1:A:2197:PHE:HE1  | 1.52                     | 0.74              |
| 1:A:3459:PRO:HA   | 1:A:3879:VAL:HG21 | 1.69                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:4238:LEU:HG   | 1:B:4287:THR:HG21 | 1.68                     | 0.74              |
| 1:B:112:LEU:HD12  | 1:B:250:LEU:HD12  | 1.68                     | 0.74              |
| 1:B:2682:TYR:HD2  | 1:B:2977:LEU:HD11 | 1.53                     | 0.73              |
| 1:A:1314:LEU:HD13 | 1:A:1317:LEU:HD12 | 1.69                     | 0.73              |
| 1:B:3290:TRP:NE1  | 1:B:3326:ALA:HB2  | 2.03                     | 0.73              |
| 1:A:1518:LEU:HD22 | 1:A:1537:LEU:HD11 | 1.68                     | 0.73              |
| 1:B:3203:THR:HB   | 1:B:3206:VAL:HB   | 1.69                     | 0.73              |
| 1:B:3459:PRO:HA   | 1:B:3879:VAL:HG21 | 1.69                     | 0.73              |
| 1:B:4621:PRO:HB3  | 1:B:4668:GLY:HA3  | 1.69                     | 0.73              |
| 1:B:1205:GLY:HA2  | 1:B:1215:GLY:HA3  | 1.71                     | 0.73              |
| 1:A:4713:PHE:HE1  | 1:A:4751:LEU:HD21 | 1.53                     | 0.73              |
| 1:B:3749:VAL:HG11 | 1:B:3813:GLU:HG2  | 1.70                     | 0.73              |
| 1:B:1204:ILE:HG21 | 1:B:1357:GLY:HA3  | 1.71                     | 0.73              |
| 1:A:200:VAL:HB    | 1:B:715:HIS:CE1   | 2.23                     | 0.73              |
| 1:A:800:PRO:HD2   | 1:A:853:LEU:HD23  | 1.70                     | 0.72              |
| 1:A:1205:GLY:HA2  | 1:A:1215:GLY:HA3  | 1.70                     | 0.72              |
| 1:A:1610:LEU:HD13 | 1:A:1800:GLN:HA   | 1.71                     | 0.72              |
| 1:A:3240:ILE:HD11 | 1:A:3275:HIS:HB2  | 1.70                     | 0.72              |
| 1:B:3057:ARG:HB2  | 1:B:3163:MET:HE1  | 1.68                     | 0.72              |
| 1:B:4105:TRP:HZ2  | 2:D:129:ALA:HB2   | 1.55                     | 0.72              |
| 1:B:3240:ILE:HD11 | 1:B:3275:HIS:HB2  | 1.70                     | 0.72              |
| 1:B:3256:VAL:HG23 | 1:B:3849:PRO:HA   | 1.71                     | 0.72              |
| 1:A:261:LEU:HD21  | 1:A:332:LEU:HB2   | 1.72                     | 0.72              |
| 1:A:3793:ASN:HA   | 1:B:3521:GLU:CG   | 2.20                     | 0.72              |
| 1:B:1515:LEU:HD12 | 1:B:1541:MET:HG3  | 1.71                     | 0.72              |
| 1:B:2305:GLY:HA3  | 1:B:2308:LEU:HB2  | 1.71                     | 0.72              |
| 1:A:1870:PHE:CE1  | 1:A:1924:LEU:HD11 | 2.25                     | 0.72              |
| 1:A:2212:GLN:HE21 | 1:A:2235:GLU:HA   | 1.54                     | 0.72              |
| 1:B:4123:LEU:HD13 | 1:B:4165:LEU:HD22 | 1.71                     | 0.72              |
| 2:C:69:PHE:CE1    | 2:C:73:MET:SD     | 2.82                     | 0.72              |
| 3:E:107:GLU:HA    | 3:E:126:ASP:HA    | 1.71                     | 0.72              |
| 1:A:912:LYS:O     | 1:A:916:GLU:HG3   | 1.89                     | 0.72              |
| 1:B:1561:VAL:HG22 | 1:B:1810:LEU:HD22 | 1.71                     | 0.72              |
| 1:B:3090:LEU:HD11 | 1:B:3184:PRO:HB3  | 1.72                     | 0.72              |
| 1:A:73:PHE:CE1    | 1:A:159:LYS:HA    | 2.24                     | 0.72              |
| 1:A:97:LEU:HD12   | 1:A:235:THR:HG23  | 1.72                     | 0.72              |
| 1:A:420:LEU:HD21  | 1:A:444:VAL:HA    | 1.71                     | 0.72              |
| 1:B:3001:GLN:HB2  | 1:B:3139:PHE:HE2  | 1.54                     | 0.72              |
| 3:F:107:GLU:HA    | 3:F:126:ASP:HA    | 1.71                     | 0.72              |
| 1:A:284:ILE:HD12  | 1:A:442:LEU:HD23  | 1.70                     | 0.72              |
| 1:B:921:HIS:CD2   | 1:B:993:ALA:HB2   | 2.25                     | 0.72              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2622:ILE:HD11 | 1:A:2667:TYR:CG   | 2.25                     | 0.71              |
| 1:A:1863:LEU:HB3  | 1:A:1940:LEU:HD21 | 1.71                     | 0.71              |
| 1:A:3813:GLU:O    | 1:A:3817:ILE:HG13 | 1.90                     | 0.71              |
| 1:A:471:VAL:HG21  | 1:A:641:ARG:H     | 1.55                     | 0.71              |
| 1:A:1854:MET:HE1  | 1:A:2151:ILE:HG23 | 1.71                     | 0.71              |
| 1:A:2151:ILE:HD11 | 1:A:2164:LEU:HD11 | 1.72                     | 0.71              |
| 1:A:2212:GLN:CD   | 1:A:2235:GLU:HA   | 2.14                     | 0.71              |
| 1:A:3955:LEU:HD21 | 1:A:4012:ILE:HD12 | 1.73                     | 0.71              |
| 1:A:3979:ILE:HG21 | 1:A:4019:ILE:HG23 | 1.72                     | 0.71              |
| 1:B:2987:GLN:HA   | 1:B:2990:ASN:HD22 | 1.54                     | 0.71              |
| 1:A:1554:LEU:HD11 | 1:A:1798:GLU:HB2  | 1.73                     | 0.71              |
| 1:B:1870:PHE:CE1  | 1:B:1924:LEU:HD11 | 2.25                     | 0.71              |
| 1:B:3547:LEU:HD13 | 1:B:3715:LEU:HD11 | 1.73                     | 0.71              |
| 1:A:2565:LEU:HD21 | 1:A:2573:LEU:HD12 | 1.72                     | 0.71              |
| 1:B:1117:SER:O    | 1:B:1121:ILE:HG13 | 1.91                     | 0.71              |
| 1:B:3087:ALA:CB   | 1:B:3181:ILE:HD13 | 2.15                     | 0.71              |
| 1:B:2626:VAL:HG21 | 1:B:2681:ILE:HD13 | 1.73                     | 0.70              |
| 1:B:4048:TYR:HE1  | 1:B:4076:PRO:HD3  | 1.54                     | 0.70              |
| 1:A:1576:VAL:HA   | 1:A:1579:LYS:HD2  | 1.73                     | 0.70              |
| 1:A:4314:ILE:HG23 | 1:A:4487:CYS:SG   | 2.31                     | 0.70              |
| 1:A:135:GLY:HA2   | 1:A:140:CYS:O     | 1.90                     | 0.70              |
| 1:B:4127:ASN:HD21 | 1:B:4165:LEU:HD21 | 1.55                     | 0.70              |
| 1:A:4477:GLY:HA3  | 1:A:4518:VAL:HG11 | 1.72                     | 0.70              |
| 1:A:4011:ASN:O    | 1:A:4015:MET:HG2  | 1.90                     | 0.70              |
| 1:A:1963:LYS:HD3  | 1:A:1966:TYR:CE2  | 2.27                     | 0.70              |
| 1:A:3066:THR:HA   | 1:A:3078:SER:HB2  | 1.72                     | 0.70              |
| 1:B:1538:MET:HG2  | 1:B:1598:HIS:HB3  | 1.74                     | 0.70              |
| 1:B:1438:THR:OG1  | 1:B:1446:LEU:HB3  | 1.91                     | 0.70              |
| 1:B:3001:GLN:HB2  | 1:B:3139:PHE:CE2  | 2.26                     | 0.70              |
| 1:A:494:GLU:HB3   | 1:A:498:LYS:HD3   | 1.74                     | 0.69              |
| 1:A:3955:LEU:HD22 | 1:A:4003:ILE:HD12 | 1.74                     | 0.69              |
| 1:A:2308:LEU:HD23 | 1:A:2330:ASN:HD22 | 1.57                     | 0.69              |
| 1:B:1338:LEU:HD13 | 1:B:1346:PHE:HA   | 1.74                     | 0.69              |
| 1:B:3270:ILE:HD12 | 1:B:3632:PRO:HG2  | 1.72                     | 0.69              |
| 1:B:1414:THR:HG23 | 1:B:1423:PHE:CD2  | 2.27                     | 0.69              |
| 1:A:1335:GLU:HA   | 1:A:1339:GLY:O    | 1.93                     | 0.69              |
| 1:A:1961:PRO:HB3  | 1:A:2171:MET:HE1  | 1.75                     | 0.69              |
| 1:A:3518:GLY:HA2  | 1:B:3770:ALA:HB1  | 1.73                     | 0.69              |
| 1:B:4339:ILE:HA   | 1:B:4475:MET:HB2  | 1.75                     | 0.69              |
| 1:A:73:PHE:HD1    | 1:A:158:ALA:O     | 1.75                     | 0.69              |
| 1:B:3556:TYR:O    | 1:B:3606:LYS:HE3  | 1.93                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:200:VAL:HB    | 1:B:715:HIS:ND1   | 2.07                     | 0.69              |
| 1:A:3054:VAL:HA   | 1:A:3057:ARG:HD2  | 1.75                     | 0.69              |
| 1:A:3330:SER:HB3  | 1:A:3333:LEU:HB3  | 1.74                     | 0.69              |
| 1:A:4705:LEU:HB3  | 1:A:4754:VAL:HG22 | 1.73                     | 0.69              |
| 1:B:3095:VAL:HG12 | 1:B:3190:TRP:CZ3  | 2.27                     | 0.69              |
| 1:B:1963:LYS:HD3  | 1:B:1966:TYR:CE2  | 2.27                     | 0.69              |
| 1:B:4597:LEU:HD11 | 1:B:4623:LEU:HD12 | 1.75                     | 0.69              |
| 1:B:130:ILE:HG12  | 1:B:312:THR:HG23  | 1.74                     | 0.69              |
| 1:B:3066:THR:HA   | 1:B:3078:SER:HB2  | 1.75                     | 0.69              |
| 1:A:2632:LEU:O    | 1:A:2649:GLY:HA2  | 1.93                     | 0.68              |
| 1:A:193:PHE:HB2   | 1:B:881:GLN:NE2   | 2.08                     | 0.68              |
| 1:B:1961:PRO:HB3  | 1:B:2171:MET:HE1  | 1.75                     | 0.68              |
| 1:B:2368:ILE:HG23 | 1:B:2377:LEU:HD11 | 1.75                     | 0.68              |
| 1:A:797:GLY:HA3   | 1:A:850:PHE:HB3   | 1.75                     | 0.68              |
| 1:A:3556:TYR:O    | 1:A:3606:LYS:HE3  | 1.93                     | 0.68              |
| 1:A:329:VAL:HG12  | 1:A:388:ILE:HG23  | 1.74                     | 0.68              |
| 1:A:1138:HIS:O    | 1:A:1142:MET:HG2  | 1.94                     | 0.68              |
| 1:A:3812:ASP:O    | 1:A:3816:LYS:HG3  | 1.93                     | 0.68              |
| 1:A:4238:LEU:HG   | 1:A:4287:THR:HG21 | 1.75                     | 0.68              |
| 1:B:1191:SER:HB3  | 1:B:1194:LYS:HG3  | 1.75                     | 0.68              |
| 1:A:845:ASP:HB3   | 1:A:849:ARG:HH12  | 1.57                     | 0.68              |
| 1:A:286:PRO:HB3   | 1:A:295:VAL:HG21  | 1.76                     | 0.68              |
| 1:A:1799:LEU:H    | 1:A:1799:LEU:HD12 | 1.56                     | 0.68              |
| 1:A:2669:THR:HG22 | 1:A:2970:LEU:HD13 | 1.76                     | 0.68              |
| 1:A:3794:ARG:N    | 1:B:3521:GLU:OE2  | 2.20                     | 0.68              |
| 1:A:4105:TRP:HZ2  | 2:C:129:ALA:HB2   | 1.58                     | 0.68              |
| 1:B:1338:LEU:HB3  | 1:B:1345:GLU:HB2  | 1.76                     | 0.68              |
| 1:A:1142:MET:O    | 1:A:1143:ALA:C    | 2.35                     | 0.68              |
| 1:A:4335:LEU:HD13 | 1:A:4511:LEU:HD21 | 1.75                     | 0.68              |
| 1:B:763:ILE:HG22  | 1:B:767:LYS:HE3   | 1.74                     | 0.68              |
| 1:B:852:PRO:HB2   | 1:B:855:LEU:HB3   | 1.76                     | 0.68              |
| 1:A:288:THR:HB    | 1:A:291:ASP:CG    | 2.19                     | 0.67              |
| 1:A:1041:TRP:CZ3  | 1:A:1044:ARG:HD2  | 2.28                     | 0.67              |
| 1:B:3087:ALA:HA   | 1:B:3181:ILE:HD12 | 1.74                     | 0.67              |
| 1:A:1047:ILE:HB   | 1:A:1050:TYR:HD2  | 1.59                     | 0.67              |
| 1:A:1365:HIS:HB3  | 1:A:1372:LEU:HD12 | 1.75                     | 0.67              |
| 1:A:1173:THR:HG22 | 1:A:1233:TRP:HZ2  | 1.60                     | 0.67              |
| 1:A:2292:PHE:HE2  | 1:A:2386:ASP:HB3  | 1.57                     | 0.67              |
| 1:B:4264:GLY:HA2  | 1:B:4312:VAL:HG11 | 1.76                     | 0.67              |
| 1:A:752:GLN:HE21  | 1:A:888:PRO:HG3   | 1.59                     | 0.67              |
| 1:A:3143:GLN:HA   | 1:A:3146:LYS:HE2  | 1.77                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1025:MET:HG2  | 1:B:1026:ASN:N    | 2.10                     | 0.67              |
| 1:B:4522:ARG:HB3  | 1:B:4572:GLU:HG2  | 1.77                     | 0.67              |
| 1:B:2698:LYS:HE3  | 1:B:3001:GLN:CB   | 2.25                     | 0.67              |
| 1:B:39:ALA:HB1    | 1:B:44:PHE:HA     | 1.76                     | 0.67              |
| 1:B:1387:GLN:HG3  | 1:B:1393:ALA:HB1  | 1.74                     | 0.67              |
| 1:B:1555:GLN:HA   | 1:B:1558:ASN:HD22 | 1.59                     | 0.67              |
| 1:B:2702:ILE:HD11 | 1:B:3001:GLN:NE2  | 2.10                     | 0.67              |
| 1:B:3244:LEU:HB3  | 1:B:3249:ILE:HB   | 1.76                     | 0.67              |
| 1:A:1218:LEU:HD13 | 1:A:1376:ILE:HG23 | 1.76                     | 0.67              |
| 1:A:2302:GLU:HB2  | 1:A:2341:SER:HB2  | 1.76                     | 0.67              |
| 1:B:768:ALA:HA    | 1:B:773:ASP:HB2   | 1.75                     | 0.67              |
| 1:A:1682:HIS:CE1  | 1:A:2383:ARG:HB2  | 2.30                     | 0.67              |
| 1:A:3244:LEU:HB3  | 1:A:3249:ILE:HB   | 1.76                     | 0.67              |
| 1:A:3337:ALA:HB1  | 1:A:3423:SER:HB3  | 1.77                     | 0.67              |
| 1:B:1205:GLY:CA   | 1:B:1215:GLY:CA   | 2.56                     | 0.67              |
| 1:B:1679:TYR:CD1  | 1:B:1708:TYR:HA   | 2.30                     | 0.67              |
| 1:A:284:ILE:HG13  | 1:A:442:LEU:HB3   | 1.77                     | 0.66              |
| 1:A:2013:THR:HG21 | 1:A:2029:CYS:HB3  | 1.77                     | 0.66              |
| 1:B:265:TYR:HA    | 1:B:268:ARG:HD3   | 1.77                     | 0.66              |
| 1:B:415:LEU:HD11  | 1:B:484:LEU:HD21  | 1.76                     | 0.66              |
| 1:B:3241:LYS:O    | 1:B:3245:GLU:HG2  | 1.95                     | 0.66              |
| 1:B:4094:HIS:O    | 1:B:4098:THR:HG23 | 1.95                     | 0.66              |
| 1:B:793:ASN:HB2   | 1:B:854:ILE:HG21  | 1.78                     | 0.66              |
| 1:B:1300:VAL:HG13 | 1:B:1336:ARG:HD3  | 1.78                     | 0.66              |
| 1:A:2480:VAL:HA   | 1:A:2524:GLN:CD   | 2.20                     | 0.66              |
| 1:B:1087:VAL:O    | 1:B:1091:GLU:HG3  | 1.96                     | 0.66              |
| 1:A:4271:LEU:HD22 | 1:A:4327:THR:HG23 | 1.77                     | 0.66              |
| 1:B:1247:TRP:HA   | 1:B:1251:PHE:HB2  | 1.76                     | 0.66              |
| 1:B:3994:LEU:HD23 | 1:B:4060:LEU:HD21 | 1.78                     | 0.66              |
| 1:B:4714:LEU:HD11 | 1:B:4754:VAL:HG11 | 1.77                     | 0.66              |
| 1:A:763:ILE:HG22  | 1:A:767:LYS:HE3   | 1.75                     | 0.66              |
| 1:A:1531:GLY:HA3  | 1:A:1591:MET:HB3  | 1.77                     | 0.66              |
| 1:A:1499:ILE:HG23 | 1:A:1506:VAL:HB   | 1.78                     | 0.66              |
| 1:A:2636:LYS:HA   | 1:A:2649:GLY:HA3  | 1.78                     | 0.66              |
| 1:A:3270:ILE:HD12 | 1:A:3632:PRO:HG2  | 1.72                     | 0.66              |
| 1:B:1863:LEU:HB3  | 1:B:1940:LEU:HD21 | 1.76                     | 0.66              |
| 1:B:4027:PRO:HD2  | 3:F:313:ARG:HE    | 1.59                     | 0.66              |
| 1:A:274:GLN:O     | 1:A:277:VAL:HG22  | 1.95                     | 0.66              |
| 1:A:1428:LEU:HB3  | 1:A:1491:LEU:HB3  | 1.78                     | 0.66              |
| 1:B:787:LEU:HD12  | 1:B:832:LEU:HD23  | 1.78                     | 0.66              |
| 1:B:2978:LEU:HD21 | 1:B:3024:LEU:HD22 | 1.77                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2259:PRO:HG3  | 1:A:2647:LEU:HD12 | 1.78                     | 0.65              |
| 1:A:3241:LYS:O    | 1:A:3245:GLU:HG2  | 1.95                     | 0.65              |
| 1:A:1350:VAL:O    | 1:A:1354:LEU:HG   | 1.96                     | 0.65              |
| 1:B:471:VAL:HG21  | 1:B:641:ARG:HA    | 1.76                     | 0.65              |
| 1:B:3175:THR:HG21 | 1:B:3184:PRO:HD3  | 1.79                     | 0.65              |
| 1:A:4094:HIS:O    | 1:A:4098:THR:HG23 | 1.96                     | 0.65              |
| 1:B:33:VAL:O      | 1:B:37:LEU:HG     | 1.95                     | 0.65              |
| 1:B:2683:MET:HG3  | 1:B:2999:TYR:CE2  | 2.31                     | 0.65              |
| 1:A:56:VAL:O      | 1:A:60:GLU:N      | 2.28                     | 0.65              |
| 1:A:1859:MET:HE2  | 1:A:2230:MET:HB2  | 1.78                     | 0.65              |
| 1:B:3087:ALA:HB2  | 1:B:3181:ILE:CD1  | 2.21                     | 0.65              |
| 2:D:93:PHE:CE2    | 2:D:101:ILE:HA    | 2.31                     | 0.65              |
| 1:A:1361:ILE:HA   | 1:A:1365:HIS:HB2  | 1.78                     | 0.65              |
| 1:B:1408:VAL:HG11 | 1:B:1459:VAL:HG11 | 1.78                     | 0.65              |
| 1:A:2054:ASN:HA   | 1:A:2138:ARG:HB3  | 1.78                     | 0.65              |
| 1:A:3536:ASN:O    | 1:A:3538:PRO:HD3  | 1.97                     | 0.65              |
| 2:D:83:GLU:HA     | 2:D:86:ILE:HD12   | 1.79                     | 0.65              |
| 1:A:2345:SER:HA   | 1:A:2399:LYS:HE2  | 1.78                     | 0.65              |
| 1:A:3408:LEU:HD12 | 1:A:3411:PHE:HE2  | 1.62                     | 0.65              |
| 1:B:1519:THR:HB   | 1:B:1520:PRO:HD3  | 1.78                     | 0.65              |
| 3:F:111:PRO:HD2   | 3:F:128:PHE:CE2   | 2.32                     | 0.65              |
| 1:A:3270:ILE:HD12 | 1:A:3632:PRO:CG   | 2.26                     | 0.65              |
| 1:A:3447:LEU:HA   | 1:A:3450:LEU:HD12 | 1.79                     | 0.65              |
| 1:B:1098:ILE:HD11 | 1:B:1161:ALA:HA   | 1.78                     | 0.65              |
| 1:B:1159:LEU:HB3  | 1:B:1160:PRO:HD3  | 1.78                     | 0.65              |
| 1:B:1681:CYS:SG   | 4:B:5202:ZN:ZN    | 1.86                     | 0.65              |
| 1:A:911:PHE:HB3   | 1:A:914:VAL:HB    | 1.77                     | 0.64              |
| 1:A:2978:LEU:O    | 1:A:2982:LEU:HG   | 1.97                     | 0.64              |
| 1:A:4495:ILE:HG21 | 1:A:4505:LEU:HD12 | 1.80                     | 0.64              |
| 3:F:24:CYS:HA     | 3:F:52:MET:SD     | 2.37                     | 0.64              |
| 1:A:507:ALA:O     | 1:A:523:ARG:NE    | 2.30                     | 0.64              |
| 1:B:3516:LEU:HD23 | 1:B:3764:LEU:HD21 | 1.79                     | 0.64              |
| 1:A:1415:ALA:HB2  | 1:A:1467:TRP:HB2  | 1.78                     | 0.64              |
| 1:B:2054:ASN:HA   | 1:B:2138:ARG:HB3  | 1.79                     | 0.64              |
| 1:B:3408:LEU:HD12 | 1:B:3411:PHE:HE2  | 1.61                     | 0.64              |
| 1:A:1104:ILE:HG21 | 1:A:1168:THR:HG23 | 1.79                     | 0.64              |
| 1:A:1500:VAL:CG2  | 1:A:1547:ALA:HB2  | 2.21                     | 0.64              |
| 1:B:3063:MET:HG2  | 1:B:3174:ILE:HD11 | 1.77                     | 0.64              |
| 1:A:1570:TYR:HE2  | 1:A:1576:VAL:HG21 | 1.62                     | 0.64              |
| 1:A:1681:CYS:SG   | 4:A:5202:ZN:ZN    | 1.86                     | 0.64              |
| 1:A:3211:ARG:HH21 | 1:A:3228:ARG:HH22 | 1.45                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1859:MET:HE2  | 1:B:2230:MET:HB2  | 1.78                     | 0.64              |
| 1:A:2040:LEU:CD1  | 1:A:2085:PRO:CB   | 2.76                     | 0.64              |
| 1:A:4487:CYS:HA   | 1:A:4490:ASN:HD22 | 1.62                     | 0.64              |
| 1:B:337:LEU:O     | 1:B:341:VAL:HG13  | 1.97                     | 0.64              |
| 1:A:4522:ARG:HB3  | 1:A:4572:GLU:HG2  | 1.79                     | 0.64              |
| 1:B:3497:LEU:HD11 | 1:B:3913:ASN:HD21 | 1.62                     | 0.64              |
| 1:B:3803:TYR:HA   | 1:B:3807:CYS:HB2  | 1.80                     | 0.64              |
| 1:A:93:PRO:O      | 1:A:97:LEU:N      | 2.30                     | 0.64              |
| 1:A:98:GLN:HG3    | 1:A:201:PHE:CE1   | 2.32                     | 0.64              |
| 1:B:4713:PHE:CE1  | 1:B:4751:LEU:HD21 | 2.30                     | 0.64              |
| 3:F:3:ARG:HG2     | 3:F:18:ARG:HG2    | 1.79                     | 0.64              |
| 1:A:1054:ILE:O    | 1:A:1058:LEU:HG   | 1.98                     | 0.63              |
| 1:A:1679:TYR:CD1  | 1:A:1708:TYR:HA   | 2.33                     | 0.63              |
| 1:B:441:ALA:HB1   | 1:B:443:ARG:HH22  | 1.62                     | 0.63              |
| 1:B:1499:ILE:HG12 | 1:B:1506:VAL:HG21 | 1.80                     | 0.63              |
| 3:E:24:CYS:HA     | 3:E:52:MET:SD     | 2.39                     | 0.63              |
| 1:A:1019:TYR:OH   | 1:A:1038:THR:HA   | 1.99                     | 0.63              |
| 1:A:1474:SER:HA   | 1:A:1485:ILE:HD12 | 1.81                     | 0.63              |
| 1:A:1570:TYR:CE2  | 1:A:1576:VAL:HG21 | 2.32                     | 0.63              |
| 1:A:3463:ARG:HE   | 1:A:3535:CYS:HA   | 1.63                     | 0.63              |
| 1:B:4127:ASN:HD22 | 3:F:328:LEU:HD22  | 1.62                     | 0.63              |
| 3:E:71:SER:HB2    | 3:E:74:GLN:HB2    | 1.80                     | 0.63              |
| 1:A:1708:TYR:HB3  | 1:A:2353:ARG:CZ   | 2.28                     | 0.63              |
| 1:A:1873:VAL:CG1  | 1:A:2233:LEU:HD21 | 2.23                     | 0.63              |
| 1:B:510:SER:HB3   | 1:B:513:ALA:HB2   | 1.80                     | 0.63              |
| 1:B:1214:LEU:HD21 | 1:B:1354:LEU:HD22 | 1.81                     | 0.63              |
| 1:B:1315:LEU:HB3  | 1:B:1316:PRO:HD3  | 1.80                     | 0.63              |
| 1:B:2686:LEU:HD21 | 1:B:3002:VAL:HG21 | 1.79                     | 0.63              |
| 1:B:3447:LEU:HA   | 1:B:3450:LEU:HD12 | 1.80                     | 0.63              |
| 2:C:13:PHE:HB3    | 2:C:69:PHE:HE2    | 1.63                     | 0.63              |
| 1:B:3270:ILE:HD12 | 1:B:3632:PRO:CG   | 2.26                     | 0.63              |
| 1:A:73:PHE:CD1    | 1:A:159:LYS:CA    | 2.70                     | 0.63              |
| 1:A:2692:ALA:HA   | 1:A:2695:PHE:HD1  | 1.63                     | 0.63              |
| 1:B:867:HIS:HE1   | 1:B:1012:ILE:HG21 | 1.63                     | 0.63              |
| 3:E:111:PRO:HD2   | 3:E:128:PHE:CE2   | 2.33                     | 0.63              |
| 1:A:3148:HIS:CE1  | 1:A:3150:ALA:HB3  | 2.33                     | 0.63              |
| 1:A:2192:VAL:HG13 | 1:A:2197:PHE:CE1  | 2.33                     | 0.62              |
| 1:B:1464:LEU:HD23 | 1:B:1517:THR:HG21 | 1.81                     | 0.62              |
| 1:A:104:CYS:HA    | 1:A:107:LEU:HD12  | 1.81                     | 0.62              |
| 1:A:516:THR:HB    | 1:A:519:GLN:HG3   | 1.80                     | 0.62              |
| 1:A:2705:LEU:HG   | 1:A:3005:MET:HB3  | 1.80                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1104:ILE:HG23 | 1:A:1110:LEU:HD11 | 1.82                     | 0.62              |
| 1:A:3497:LEU:HD11 | 1:A:3913:ASN:HD21 | 1.62                     | 0.62              |
| 1:B:46:MET:O      | 1:B:50:PRO:HD3    | 1.99                     | 0.62              |
| 1:A:136:LEU:HD22  | 1:A:239:PHE:HZ    | 1.63                     | 0.62              |
| 1:A:790:MET:HE3   | 1:A:858:LEU:HG    | 1.81                     | 0.62              |
| 1:A:2665:HIS:CD2  | 1:A:2704:VAL:HB   | 2.34                     | 0.62              |
| 1:B:303:VAL:HG22  | 1:B:377:ILE:HG13  | 1.82                     | 0.62              |
| 1:B:1318:LEU:HA   | 1:B:1327:ALA:HB1  | 1.82                     | 0.62              |
| 1:B:4335:LEU:HA   | 1:B:4338:ILE:HD12 | 1.81                     | 0.62              |
| 2:D:29:THR:HG23   | 2:D:31:LYS:HB2    | 1.81                     | 0.62              |
| 2:D:122:VAL:O     | 2:D:126:ILE:HG12  | 1.99                     | 0.62              |
| 1:B:1550:GLY:O    | 1:B:1553:HIS:HB3  | 2.00                     | 0.62              |
| 1:A:2291:PHE:CZ   | 1:A:2350:THR:O    | 2.52                     | 0.62              |
| 1:B:1557:HIS:O    | 1:B:1561:VAL:HG23 | 1.99                     | 0.62              |
| 1:B:1877:TYR:HB2  | 1:B:1886:ARG:HG3  | 1.82                     | 0.62              |
| 1:B:3099:LEU:HD11 | 1:B:3193:PHE:HD1  | 1.65                     | 0.62              |
| 1:B:3273:MET:HE1  | 1:B:3318:VAL:HG21 | 1.81                     | 0.62              |
| 2:D:102:SER:HB2   | 2:D:105:GLU:CD    | 2.25                     | 0.62              |
| 1:A:1047:ILE:HG13 | 1:A:1255:THR:HB   | 1.80                     | 0.62              |
| 1:A:1427:VAL:HG13 | 1:A:1431:PHE:HE2  | 1.64                     | 0.62              |
| 1:B:1178:LEU:HD11 | 1:B:1199:ALA:HB2  | 1.81                     | 0.62              |
| 1:B:1204:ILE:HG12 | 1:B:1357:GLY:HA3  | 1.80                     | 0.62              |
| 1:B:1726:CYS:SG   | 4:B:5206:ZN:ZN    | 1.88                     | 0.62              |
| 1:B:2040:LEU:CD1  | 1:B:2085:PRO:CB   | 2.76                     | 0.62              |
| 1:A:184:LEU:HD22  | 1:A:184:LEU:H     | 1.64                     | 0.61              |
| 1:B:2567:PRO:HG3  | 1:B:2632:LEU:HD22 | 1.82                     | 0.61              |
| 1:A:3007:THR:C    | 1:A:3009:ASP:H    | 2.08                     | 0.61              |
| 1:B:3763:LEU:HD13 | 1:B:3799:LEU:HA   | 1.82                     | 0.61              |
| 1:B:4232:LEU:C    | 1:B:4234:GLN:H    | 2.08                     | 0.61              |
| 1:B:2701:LEU:HD13 | 1:B:3002:VAL:CG1  | 2.29                     | 0.61              |
| 1:B:3327:LEU:O    | 1:B:3392:CYS:SG   | 2.55                     | 0.61              |
| 3:E:112:ILE:HD12  | 3:E:136:HIS:HB3   | 1.80                     | 0.61              |
| 1:A:2626:VAL:HG21 | 1:A:2681:ILE:HG21 | 1.81                     | 0.61              |
| 1:B:2356:ILE:HD13 | 1:B:2377:LEU:HD13 | 1.81                     | 0.61              |
| 2:C:33:LEU:CD2    | 2:C:72:MET:HE1    | 2.30                     | 0.61              |
| 1:A:4591:LYS:HB2  | 1:A:4630:LYS:HD2  | 1.82                     | 0.61              |
| 1:B:2517:ALA:HB3  | 1:B:2522:GLN:HE21 | 1.65                     | 0.61              |
| 2:D:33:LEU:HD13   | 2:D:64:ILE:HG21   | 1.82                     | 0.61              |
| 1:A:1347:LEU:HB3  | 1:A:1351:TYR:CE2  | 2.35                     | 0.61              |
| 1:A:1681:CYS:HG   | 4:A:5202:ZN:ZN    | 1.13                     | 0.61              |
| 1:B:414:LEU:HB3   | 1:B:480:ALA:HB2   | 1.83                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1427:VAL:HG13 | 1:B:1431:PHE:HE2  | 1.65                     | 0.61              |
| 1:B:2698:LYS:HE2  | 1:B:3001:GLN:HE21 | 1.64                     | 0.61              |
| 1:B:3532:CYS:SG   | 1:B:3868:SER:HA   | 2.40                     | 0.61              |
| 1:A:252:GLY:HA2   | 1:A:255:LYS:HD2   | 1.83                     | 0.61              |
| 1:B:1561:VAL:HG22 | 1:B:1810:LEU:CD2  | 2.30                     | 0.61              |
| 1:B:4027:PRO:HB2  | 3:F:313:ARG:HH21  | 1.65                     | 0.61              |
| 1:A:263:LEU:HB2   | 1:A:266:PHE:HB2   | 1.83                     | 0.61              |
| 1:A:497:HIS:O     | 1:A:498:LYS:C     | 2.43                     | 0.61              |
| 1:A:1564:LEU:HB2  | 1:A:1603:LEU:HD11 | 1.82                     | 0.61              |
| 1:A:1682:HIS:HB2  | 1:A:1705:GLU:HB2  | 1.81                     | 0.61              |
| 1:B:4635:VAL:HG11 | 1:B:4685:LYS:HG3  | 1.82                     | 0.61              |
| 1:A:471:VAL:O     | 1:A:475:ILE:HG12  | 1.99                     | 0.61              |
| 1:A:1680:HIS:HB3  | 1:A:1687:VAL:HG12 | 1.82                     | 0.61              |
| 1:A:2698:LYS:HZ3  | 1:A:3001:GLN:HB3  | 1.66                     | 0.61              |
| 1:B:806:LEU:HD21  | 1:B:811:LEU:HB2   | 1.82                     | 0.61              |
| 1:B:3053:LEU:HD13 | 1:B:3160:LEU:HD12 | 1.81                     | 0.61              |
| 1:B:4488:MET:HE3  | 1:B:4511:LEU:HB3  | 1.83                     | 0.61              |
| 2:C:49:LEU:C      | 2:C:49:LEU:CD1    | 2.74                     | 0.61              |
| 1:A:104:CYS:HB3   | 1:A:136:LEU:HD13  | 1.82                     | 0.60              |
| 1:B:740:PHE:HD1   | 1:B:778:GLU:HG3   | 1.66                     | 0.60              |
| 1:A:1052:ASN:O    | 1:A:1053:TRP:C    | 2.45                     | 0.60              |
| 1:A:4594:LEU:O    | 1:A:4598:LEU:HG   | 2.01                     | 0.60              |
| 1:B:1693:CYS:HB3  | 1:B:1716:CYS:HB2  | 1.84                     | 0.60              |
| 2:D:50:GLN:C      | 2:D:53:ILE:HG22   | 2.26                     | 0.60              |
| 2:D:137:VAL:HG13  | 2:D:141:GLU:HB2   | 1.83                     | 0.60              |
| 1:A:1402:SER:HA   | 1:A:1452:SER:HB2  | 1.82                     | 0.60              |
| 1:B:3057:ARG:HB2  | 1:B:3163:MET:CE   | 2.32                     | 0.60              |
| 1:B:1119:GLN:HA   | 1:B:1122:TYR:CE2  | 2.36                     | 0.60              |
| 1:B:1534:PHE:CD2  | 1:B:1595:CYS:HB2  | 2.36                     | 0.60              |
| 1:B:2308:LEU:HD13 | 1:B:2328:VAL:HG11 | 1.84                     | 0.60              |
| 1:A:2483:LEU:HD12 | 1:A:2524:GLN:HB3  | 1.82                     | 0.60              |
| 1:B:851:VAL:HG11  | 1:B:995:GLU:HG2   | 1.84                     | 0.60              |
| 2:C:33:LEU:HD21   | 2:C:72:MET:HE1    | 1.83                     | 0.60              |
| 1:A:1594:GLU:HA   | 1:A:2477:ARG:HH22 | 1.66                     | 0.60              |
| 1:A:2291:PHE:HZ   | 1:A:2350:THR:O    | 1.85                     | 0.60              |
| 1:B:273:PHE:CD2   | 1:B:338:TYR:HB2   | 2.37                     | 0.60              |
| 1:B:1124:LEU:O    | 1:B:1128:ILE:HG12 | 2.01                     | 0.60              |
| 1:B:1290:SER:HA   | 1:B:1293:ARG:HD3  | 1.82                     | 0.60              |
| 1:A:963:TYR:HE1   | 1:A:1013:LEU:HD13 | 1.66                     | 0.60              |
| 1:A:3731:ASP:HA   | 1:A:3734:LYS:HB3  | 1.83                     | 0.60              |
| 1:B:921:HIS:HD2   | 1:B:993:ALA:HB2   | 1.66                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1340:PRO:HD2  | 1:B:1343:SER:HB3  | 1.84                     | 0.60              |
| 1:B:3087:ALA:HB2  | 1:B:3181:ILE:CG2  | 2.19                     | 0.60              |
| 1:A:105:LYS:HG3   | 1:A:246:SER:HB2   | 1.83                     | 0.60              |
| 1:A:202:ASN:HB3   | 1:A:204:ARG:NE    | 2.16                     | 0.60              |
| 1:A:2354:ILE:HG12 | 1:A:2387:PHE:HE2  | 1.67                     | 0.60              |
| 1:A:3187:ASP:H    | 1:A:3190:TRP:CD1  | 2.20                     | 0.60              |
| 1:A:4278:VAL:O    | 1:B:3825:ARG:NH1  | 2.33                     | 0.60              |
| 1:A:4594:LEU:HD11 | 1:A:4620:ILE:HG23 | 1.83                     | 0.60              |
| 1:B:754:LEU:HD22  | 1:B:807:ASN:HD21  | 1.65                     | 0.60              |
| 1:B:1063:MET:HG2  | 1:B:1068:ALA:HB2  | 1.84                     | 0.60              |
| 1:B:2368:ILE:HD11 | 1:B:2387:PHE:CE1  | 2.37                     | 0.60              |
| 1:B:3516:LEU:CD2  | 1:B:3764:LEU:HD21 | 2.31                     | 0.60              |
| 1:B:4621:PRO:HG3  | 1:B:4665:ILE:HA   | 1.82                     | 0.60              |
| 1:A:810:HIS:O     | 1:A:813:MET:HG3   | 2.01                     | 0.60              |
| 1:B:1500:VAL:HG21 | 1:B:1543:THR:O    | 2.02                     | 0.60              |
| 1:B:1996:LEU:HD11 | 1:B:2002:ILE:HG13 | 1.83                     | 0.60              |
| 3:F:75:PRO:HD2    | 3:F:116:LEU:HD23  | 1.84                     | 0.60              |
| 1:A:670:ILE:O     | 1:A:674:LEU:HG    | 2.02                     | 0.59              |
| 1:A:1519:THR:HB   | 1:A:1520:PRO:HD3  | 1.82                     | 0.59              |
| 1:A:3273:MET:HE1  | 1:A:3318:VAL:HG21 | 1.83                     | 0.59              |
| 1:B:1414:THR:HG22 | 1:B:1424:CYS:SG   | 2.41                     | 0.59              |
| 1:B:2581:ALA:HB2  | 1:B:2588:LEU:HD22 | 1.83                     | 0.59              |
| 1:A:1171:SER:HA   | 1:A:1174:ARG:HD2  | 1.83                     | 0.59              |
| 1:B:296:ARG:HH12  | 1:B:347:MET:HE3   | 1.67                     | 0.59              |
| 1:A:4313:CYS:SG   | 1:A:4331:ILE:HG12 | 2.42                     | 0.59              |
| 1:B:3894:PRO:O    | 1:B:3898:HIS:ND1  | 2.35                     | 0.59              |
| 1:A:1607:THR:HB   | 1:A:2488:SER:HB2  | 1.84                     | 0.59              |
| 1:B:1356:THR:HA   | 1:B:1400:PHE:CZ   | 2.36                     | 0.59              |
| 1:B:1398:GLU:HA   | 1:B:1449:LEU:HD21 | 1.85                     | 0.59              |
| 1:B:2682:TYR:CD2  | 1:B:2977:LEU:HD11 | 2.36                     | 0.59              |
| 1:A:1051:VAL:HG22 | 1:A:1072:LEU:HD11 | 1.84                     | 0.59              |
| 1:A:2487:GLU:HB2  | 1:A:2528:LEU:HA   | 1.84                     | 0.59              |
| 1:A:3106:LEU:HG   | 1:A:3110:LYS:HE3  | 1.84                     | 0.59              |
| 1:B:3723:VAL:HG11 | 1:B:3824:SER:OG   | 2.02                     | 0.59              |
| 1:B:4682:ILE:HG23 | 1:B:4687:ILE:HD12 | 1.84                     | 0.59              |
| 2:D:106:LEU:HD11  | 2:D:110:MET:HE2   | 1.83                     | 0.59              |
| 1:A:1045:LEU:HD12 | 1:A:1072:LEU:HD11 | 1.83                     | 0.59              |
| 1:A:1429:LYS:O    | 1:A:1430:PHE:C    | 2.45                     | 0.59              |
| 1:B:4129:LEU:HD23 | 1:B:4165:LEU:HD23 | 1.85                     | 0.59              |
| 1:B:4314:ILE:HG12 | 1:B:4484:GLY:HA2  | 1.85                     | 0.59              |
| 1:A:1514:LEU:O    | 1:A:1518:LEU:HG   | 2.03                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2121:MET:HE2  | 1:A:2133:ALA:HB1  | 1.84                     | 0.59              |
| 1:A:3201:GLN:HA   | 1:A:3207:ARG:HH21 | 1.68                     | 0.59              |
| 1:A:4199:TYR:HA   | 2:C:20:PHE:CZ     | 2.38                     | 0.59              |
| 1:B:151:PHE:HA    | 1:B:154:MET:HE2   | 1.84                     | 0.59              |
| 1:B:1450:CYS:HB2  | 1:B:1505:GLN:HB2  | 1.83                     | 0.59              |
| 1:B:2121:MET:HE2  | 1:B:2133:ALA:HB1  | 1.84                     | 0.59              |
| 1:B:382:LEU:HD12  | 1:B:475:ILE:HG22  | 1.83                     | 0.59              |
| 1:B:1015:PRO:HB2  | 1:B:1020:ILE:HD11 | 1.85                     | 0.59              |
| 1:B:1468:LEU:HA   | 1:B:1471:MET:HE2  | 1.84                     | 0.59              |
| 1:B:2173:HIS:ND1  | 1:B:2176:LEU:HD22 | 2.18                     | 0.59              |
| 1:B:2698:LYS:HE2  | 1:B:3001:GLN:NE2  | 2.17                     | 0.59              |
| 1:B:2702:ILE:HG12 | 1:B:3005:MET:HG2  | 1.85                     | 0.59              |
| 1:B:4271:LEU:HD22 | 1:B:4274:ARG:HH21 | 1.67                     | 0.59              |
| 1:A:1685:LYS:HA   | 1:A:2381:ARG:HH22 | 1.68                     | 0.59              |
| 1:B:1515:LEU:CD1  | 1:B:1541:MET:HG3  | 2.32                     | 0.59              |
| 1:B:1870:PHE:CZ   | 1:B:1924:LEU:CD1  | 2.65                     | 0.59              |
| 1:A:4316:THR:HA   | 1:A:4319:ARG:HE   | 1.67                     | 0.59              |
| 1:A:265:TYR:CZ    | 1:A:301:SER:HB2   | 2.38                     | 0.58              |
| 1:A:2173:HIS:ND1  | 1:A:2176:LEU:HD22 | 2.18                     | 0.58              |
| 1:B:680:GLU:HB3   | 1:B:730:THR:HG21  | 1.84                     | 0.58              |
| 1:B:3270:ILE:O    | 1:B:3274:GLU:HG2  | 2.03                     | 0.58              |
| 1:B:4096:TYR:CE1  | 2:D:48:GLU:HG2    | 2.38                     | 0.58              |
| 1:B:4620:ILE:HB   | 1:B:4621:PRO:HD3  | 1.85                     | 0.58              |
| 1:A:688:SER:O     | 1:A:692:GLU:HG3   | 2.03                     | 0.58              |
| 1:A:2370:ILE:HD11 | 1:A:2401:LEU:HD11 | 1.85                     | 0.58              |
| 1:B:299:PHE:O     | 1:B:303:VAL:HG23  | 2.03                     | 0.58              |
| 1:A:1714:PHE:CZ   | 1:A:1716:CYS:HA   | 2.38                     | 0.58              |
| 1:A:1901:VAL:CG1  | 1:A:2217:ILE:HD12 | 2.28                     | 0.58              |
| 1:B:3683:GLN:OE1  | 1:B:3688:ARG:HD2  | 2.03                     | 0.58              |
| 1:B:4325:TYR:HA   | 1:B:4504:LEU:HD22 | 1.86                     | 0.58              |
| 3:F:302:SER:O     | 3:F:306:ARG:N     | 2.34                     | 0.58              |
| 1:A:967:TYR:HE2   | 1:A:1015:PRO:HA   | 1.66                     | 0.58              |
| 1:A:1119:GLN:HA   | 1:A:1122:TYR:CE2  | 2.38                     | 0.58              |
| 1:A:3240:ILE:HD11 | 1:A:3275:HIS:CB   | 2.33                     | 0.58              |
| 1:A:3679:GLU:CD   | 1:A:3683:GLN:HE22 | 2.11                     | 0.58              |
| 1:B:4355:LYS:HE3  | 1:B:4365:GLY:O    | 2.04                     | 0.58              |
| 1:B:4429:TRP:CE2  | 1:B:4438:MET:HA   | 2.38                     | 0.58              |
| 1:A:1307:PRO:HB2  | 1:A:1308:PRO:HD3  | 1.84                     | 0.58              |
| 1:B:3757:ARG:HB3  | 1:B:3758:PRO:HD3  | 1.86                     | 0.58              |
| 1:A:56:VAL:HA     | 1:A:59:SER:HB2    | 1.85                     | 0.58              |
| 1:A:1808:ALA:HB3  | 1:A:1809:PRO:HD3  | 1.86                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:4089:LYS:HA   | 1:A:4092:LEU:HD12 | 1.86                     | 0.58              |
| 1:A:1191:SER:HB3  | 1:A:1194:LYS:HG3  | 1.85                     | 0.58              |
| 1:A:4429:TRP:CE2  | 1:A:4438:MET:HA   | 2.38                     | 0.58              |
| 1:B:1361:ILE:HA   | 1:B:1365:HIS:HB2  | 1.85                     | 0.58              |
| 1:B:3679:GLU:CD   | 1:B:3683:GLN:HE22 | 2.11                     | 0.58              |
| 1:A:3469:VAL:HG21 | 1:A:3882:HIS:HB3  | 1.86                     | 0.58              |
| 1:B:93:PRO:HB2    | 1:B:96:GLN:HB2    | 1.85                     | 0.58              |
| 1:B:810:HIS:O     | 1:B:813:MET:HG3   | 2.03                     | 0.58              |
| 1:B:2978:LEU:HA   | 1:B:3006:LEU:HD13 | 1.86                     | 0.58              |
| 1:A:53:VAL:O      | 1:A:57:ILE:HG13   | 2.03                     | 0.58              |
| 1:A:787:LEU:HD12  | 1:A:832:LEU:HD23  | 1.85                     | 0.58              |
| 1:A:1428:LEU:HD13 | 1:A:1491:LEU:HB2  | 1.85                     | 0.58              |
| 1:A:2291:PHE:O    | 1:A:2295:ASN:ND2  | 2.35                     | 0.58              |
| 1:B:1118:LEU:HD12 | 1:B:1280:LEU:HD23 | 1.86                     | 0.58              |
| 1:B:4221:LEU:O    | 1:B:4224:GLU:HG3  | 2.04                     | 0.58              |
| 1:A:745:TRP:HE1   | 1:A:810:HIS:CE1   | 2.22                     | 0.57              |
| 1:A:1090:VAL:HG13 | 1:A:1127:ALA:HB1  | 1.85                     | 0.57              |
| 1:B:1515:LEU:HD11 | 1:B:1556:LEU:HD22 | 1.85                     | 0.57              |
| 1:B:2162:PRO:HG2  | 1:B:2181:GLN:HG2  | 1.87                     | 0.57              |
| 1:B:2548:LEU:HD11 | 1:B:2580:ILE:HG21 | 1.85                     | 0.57              |
| 1:A:82:THR:HA     | 1:A:107:LEU:HD13  | 1.86                     | 0.57              |
| 1:A:3683:GLN:OE1  | 1:A:3688:ARG:HD2  | 2.03                     | 0.57              |
| 1:B:908:TYR:CZ    | 1:B:931:ARG:HD3   | 2.39                     | 0.57              |
| 1:B:1600:MET:HB3  | 1:B:2481:SER:HB2  | 1.84                     | 0.57              |
| 1:B:2310:GLN:HG3  | 1:B:2311:VAL:HG23 | 1.84                     | 0.57              |
| 1:B:4223:LEU:O    | 1:B:4279:GLN:NE2  | 2.38                     | 0.57              |
| 1:B:4635:VAL:CG1  | 1:B:4685:LYS:HG3  | 2.34                     | 0.57              |
| 2:C:49:LEU:HD11   | 2:C:53:ILE:HD12   | 1.85                     | 0.57              |
| 1:A:1203:ALA:HA   | 1:A:1320:GLU:HG3  | 1.86                     | 0.57              |
| 1:A:1996:LEU:HD13 | 1:A:2001:PHE:HA   | 1.86                     | 0.57              |
| 1:B:3057:ARG:HD3  | 1:B:3139:PHE:CD1  | 2.39                     | 0.57              |
| 1:A:1870:PHE:HB3  | 1:A:1873:VAL:CG2  | 2.34                     | 0.57              |
| 1:A:2657:VAL:HG11 | 1:A:2693:VAL:O    | 2.05                     | 0.57              |
| 1:A:3547:LEU:HD13 | 1:A:3715:LEU:HD11 | 1.84                     | 0.57              |
| 1:B:1929:LEU:HD11 | 1:B:2241:ILE:HD11 | 1.86                     | 0.57              |
| 1:B:3324:SER:O    | 1:B:3329:GLY:N    | 2.36                     | 0.57              |
| 1:B:39:ALA:CB     | 1:B:44:PHE:HA     | 2.35                     | 0.57              |
| 1:B:1534:PHE:CE2  | 1:B:1595:CYS:HB2  | 2.39                     | 0.57              |
| 1:B:3240:ILE:HD11 | 1:B:3275:HIS:CB   | 2.33                     | 0.57              |
| 1:B:3469:VAL:HG21 | 1:B:3882:HIS:HB3  | 1.86                     | 0.57              |
| 2:C:95:LYS:HG2    | 2:C:105:GLU:HB2   | 1.86                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:800:PRO:HG3   | 1:A:854:ILE:HD11  | 1.85                     | 0.57              |
| 1:A:1037:HIS:CE1  | 1:A:1041:TRP:HE1  | 2.22                     | 0.57              |
| 1:B:1319:LEU:HD21 | 1:B:1350:VAL:HG13 | 1.87                     | 0.57              |
| 1:B:2354:ILE:HG12 | 1:B:2387:PHE:HE2  | 1.68                     | 0.57              |
| 1:B:3087:ALA:CA   | 1:B:3181:ILE:CD1  | 2.83                     | 0.57              |
| 1:A:284:ILE:H     | 1:A:442:LEU:H     | 1.52                     | 0.57              |
| 1:A:3270:ILE:O    | 1:A:3274:GLU:HG2  | 2.03                     | 0.57              |
| 1:A:4307:LYS:HD2  | 1:A:4479:MET:HA   | 1.85                     | 0.57              |
| 1:B:783:TRP:HD1   | 1:B:821:PHE:HE2   | 1.53                     | 0.57              |
| 1:B:1244:ILE:HG13 | 1:B:1248:ARG:HB2  | 1.86                     | 0.57              |
| 1:B:1429:LYS:O    | 1:B:1430:PHE:C    | 2.45                     | 0.57              |
| 1:B:1520:PRO:HA   | 1:B:1523:THR:HB   | 1.87                     | 0.57              |
| 1:B:2340:ILE:HD13 | 1:B:2422:ILE:HD11 | 1.86                     | 0.57              |
| 1:A:3894:PRO:O    | 1:A:3898:HIS:ND1  | 2.35                     | 0.57              |
| 1:B:844:MET:HB3   | 1:B:848:MET:HE3   | 1.85                     | 0.57              |
| 1:B:1554:LEU:HD12 | 1:B:1557:HIS:CD2  | 2.40                     | 0.57              |
| 1:B:1681:CYS:HG   | 4:B:5202:ZN:ZN    | 1.16                     | 0.57              |
| 1:B:3220:SER:HB3  | 1:B:3223:LYS:HE2  | 1.87                     | 0.57              |
| 1:B:4053:HIS:HB2  | 1:B:4071:TRP:CD1  | 2.39                     | 0.57              |
| 1:A:189:VAL:HG21  | 1:B:874:VAL:HG13  | 1.85                     | 0.57              |
| 1:A:1517:THR:O    | 1:A:1520:PRO:HD2  | 2.04                     | 0.57              |
| 1:B:1268:ALA:O    | 1:B:1272:THR:HG23 | 2.05                     | 0.57              |
| 1:B:1495:LEU:HA   | 1:B:1498:TYR:CD2  | 2.40                     | 0.57              |
| 1:B:3087:ALA:CA   | 1:B:3181:ILE:HD12 | 2.35                     | 0.57              |
| 1:B:4617:LEU:O    | 1:B:4621:PRO:HD2  | 2.05                     | 0.57              |
| 1:A:1206:SER:HB2  | 1:A:1319:LEU:HA   | 1.87                     | 0.57              |
| 1:A:1233:TRP:HE3  | 1:A:1278:LEU:HD13 | 1.70                     | 0.57              |
| 1:A:4355:LYS:HE3  | 1:A:4365:GLY:O    | 2.05                     | 0.57              |
| 1:B:1133:VAL:HG22 | 1:B:1246:SER:HB3  | 1.86                     | 0.57              |
| 1:B:1241:PHE:CE1  | 1:B:1272:THR:HG21 | 2.39                     | 0.57              |
| 1:B:4089:LYS:HA   | 1:B:4092:LEU:HD12 | 1.85                     | 0.57              |
| 1:A:2308:LEU:HD13 | 1:A:2328:VAL:HG11 | 1.86                     | 0.56              |
| 1:A:4130:ARG:HB2  | 1:A:4169:TYR:CE1  | 2.40                     | 0.56              |
| 1:A:4714:LEU:HD11 | 1:A:4754:VAL:HG11 | 1.86                     | 0.56              |
| 1:B:479:HIS:HA    | 1:B:482:LYS:HE2   | 1.87                     | 0.56              |
| 1:B:1119:GLN:HA   | 1:B:1122:TYR:CD2  | 2.40                     | 0.56              |
| 1:A:396:ARG:HH21  | 1:B:404:GLN:NE2   | 2.02                     | 0.56              |
| 1:A:1101:PHE:CD2  | 1:A:1168:THR:HG21 | 2.40                     | 0.56              |
| 1:A:1398:GLU:HG3  | 1:A:1445:SER:HA   | 1.86                     | 0.56              |
| 1:A:3463:ARG:NH2  | 1:A:3534:VAL:O    | 2.38                     | 0.56              |
| 1:B:516:THR:HB    | 1:B:519:GLN:HG3   | 1.87                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1415:ALA:HB2  | 1:B:1467:TRP:HB2  | 1.87                     | 0.56              |
| 1:B:2370:ILE:HD11 | 1:B:2401:LEU:HD11 | 1.87                     | 0.56              |
| 2:D:93:PHE:HE2    | 2:D:101:ILE:HA    | 1.69                     | 0.56              |
| 3:E:302:SER:O     | 3:E:306:ARG:N     | 2.34                     | 0.56              |
| 1:A:145:ARG:O     | 1:A:149:ILE:HG13  | 2.06                     | 0.56              |
| 1:B:470:GLY:H     | 1:B:473:SER:HB2   | 1.71                     | 0.56              |
| 1:B:4228:LEU:HD22 | 1:B:4278:VAL:HG11 | 1.88                     | 0.56              |
| 2:C:93:PHE:HB3    | 2:C:101:ILE:HD12  | 1.86                     | 0.56              |
| 1:A:2027:ASP:CG   | 1:A:2029:CYS:HG   | 2.08                     | 0.56              |
| 1:A:4598:LEU:O    | 1:A:4601:ILE:HG23 | 2.05                     | 0.56              |
| 1:B:521:ILE:HG21  | 1:B:670:ILE:HD11  | 1.88                     | 0.56              |
| 1:A:1169:TYR:HA   | 1:A:1172:PHE:HD2  | 1.70                     | 0.56              |
| 1:A:1947:SER:C    | 1:A:3655:THR:HG21 | 2.30                     | 0.56              |
| 1:B:2301:VAL:HG11 | 1:B:2422:ILE:HG13 | 1.86                     | 0.56              |
| 1:A:1173:THR:HG22 | 1:A:1233:TRP:CZ2  | 2.41                     | 0.56              |
| 1:A:1481:GLN:HA   | 1:A:1481:GLN:HE21 | 1.69                     | 0.56              |
| 1:A:1519:THR:HA   | 1:A:1563:TRP:HZ2  | 1.69                     | 0.56              |
| 1:B:1395:LYS:O    | 1:B:1399:GLU:HG2  | 2.06                     | 0.56              |
| 1:B:1560:ALA:HA   | 1:B:1563:TRP:CE3  | 2.40                     | 0.56              |
| 1:B:2977:LEU:HD23 | 1:B:3006:LEU:HD21 | 1.88                     | 0.56              |
| 1:B:3948:ILE:HA   | 1:B:3996:LEU:HD21 | 1.87                     | 0.56              |
| 1:A:273:PHE:O     | 1:A:277:VAL:HG13  | 2.06                     | 0.56              |
| 1:A:2173:HIS:CE1  | 1:A:2176:LEU:HD22 | 2.41                     | 0.56              |
| 1:A:4699:ILE:HD13 | 1:A:4747:ASN:HB3  | 1.87                     | 0.56              |
| 1:B:553:LYS:O     | 1:B:554:GLY:C     | 2.48                     | 0.56              |
| 1:B:3290:TRP:HE1  | 1:B:3326:ALA:HB2  | 1.69                     | 0.56              |
| 1:B:3951:VAL:HG13 | 1:B:4012:ILE:HD13 | 1.87                     | 0.56              |
| 1:A:291:ASP:O     | 1:A:295:VAL:HG23  | 2.06                     | 0.56              |
| 1:A:491:LEU:HD21  | 1:A:518:ILE:HA    | 1.88                     | 0.56              |
| 1:A:1948:ALA:HB1  | 1:A:1978:LEU:HD13 | 1.88                     | 0.56              |
| 1:A:2701:LEU:O    | 1:A:2704:VAL:HG22 | 2.05                     | 0.56              |
| 1:A:1412:MET:HB3  | 1:A:1463:ARG:CZ   | 2.36                     | 0.56              |
| 1:A:3662:ARG:NH2  | 1:A:3679:GLU:OE2  | 2.39                     | 0.56              |
| 1:A:4199:TYR:HA   | 2:C:20:PHE:HZ     | 1.70                     | 0.56              |
| 1:A:4691:ALA:HB1  | 1:A:4722:ILE:HG23 | 1.88                     | 0.56              |
| 1:B:82:THR:HG23   | 1:B:136:LEU:HG    | 1.87                     | 0.56              |
| 1:B:4419:LEU:HD13 | 1:B:4459:LEU:HG   | 1.87                     | 0.56              |
| 2:C:124:GLU:O     | 2:C:128:GLU:HG2   | 2.06                     | 0.56              |
| 1:A:420:LEU:HD21  | 1:A:444:VAL:CA    | 2.35                     | 0.55              |
| 1:A:683:MET:SD    | 1:A:727:LEU:HD23  | 2.46                     | 0.55              |
| 1:A:1159:LEU:HB3  | 1:A:1160:PRO:HD3  | 1.87                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:4682:ILE:HG23 | 1:A:4687:ILE:HD12 | 1.88                     | 0.55              |
| 1:B:2978:LEU:HB2  | 1:B:3006:LEU:HB3  | 1.89                     | 0.55              |
| 3:E:301:MET:O     | 3:E:306:ARG:NH1   | 2.39                     | 0.55              |
| 1:A:404:GLN:HE21  | 1:B:396:ARG:HB2   | 1.72                     | 0.55              |
| 1:A:1058:LEU:HB3  | 1:A:1063:MET:SD   | 2.46                     | 0.55              |
| 1:A:1899:MET:SD   | 1:A:2233:LEU:HB2  | 2.46                     | 0.55              |
| 1:A:4489:LEU:HD21 | 1:A:4532:THR:HG23 | 1.87                     | 0.55              |
| 1:A:4641:TYR:HD1  | 1:A:4655:ASP:HA   | 1.71                     | 0.55              |
| 1:B:663:LEU:HD23  | 1:B:674:LEU:CD1   | 2.36                     | 0.55              |
| 1:B:683:MET:HE3   | 1:B:727:LEU:HD23  | 1.87                     | 0.55              |
| 1:B:827:ARG:HG3   | 1:B:955:VAL:HG13  | 1.88                     | 0.55              |
| 1:B:967:TYR:CE2   | 1:B:1015:PRO:HA   | 2.42                     | 0.55              |
| 1:B:1097:GLN:HA   | 1:B:1097:GLN:HE21 | 1.71                     | 0.55              |
| 1:B:2173:HIS:CE1  | 1:B:2176:LEU:HD22 | 2.41                     | 0.55              |
| 1:B:3072:SER:C    | 1:B:3074:ILE:H    | 2.14                     | 0.55              |
| 1:B:3213:LEU:O    | 1:B:3217:ILE:HG12 | 2.05                     | 0.55              |
| 1:A:183:GLU:H     | 1:A:183:GLU:CD    | 2.13                     | 0.55              |
| 1:A:2358:THR:HA   | 1:A:2382:SER:HB2  | 1.87                     | 0.55              |
| 1:B:1572:SER:O    | 1:B:1573:GLN:C    | 2.49                     | 0.55              |
| 1:B:1603:LEU:HD13 | 1:B:1807:PHE:CZ   | 2.41                     | 0.55              |
| 1:B:1961:PRO:HB3  | 1:B:2171:MET:CE   | 2.37                     | 0.55              |
| 1:B:3662:ARG:NH2  | 1:B:3679:GLU:OE2  | 2.39                     | 0.55              |
| 1:B:3739:ILE:HG12 | 1:B:3824:SER:HB3  | 1.88                     | 0.55              |
| 1:B:4216:GLU:HG2  | 1:B:4238:LEU:HB2  | 1.88                     | 0.55              |
| 1:A:1315:LEU:HB3  | 1:A:1316:PRO:HD3  | 1.87                     | 0.55              |
| 1:A:1556:LEU:HD22 | 1:A:1559:ALA:HB3  | 1.89                     | 0.55              |
| 1:A:2300:ASP:HA   | 1:A:2318:LYS:HZ1  | 1.72                     | 0.55              |
| 1:A:2371:PHE:HZ   | 1:A:2397:ALA:HB2  | 1.71                     | 0.55              |
| 1:B:48:GLU:O      | 1:B:51:GLN:HB3    | 2.07                     | 0.55              |
| 1:B:284:ILE:H     | 1:B:441:ALA:HA    | 1.71                     | 0.55              |
| 1:B:1558:ASN:HD21 | 1:B:1803:ALA:HB1  | 1.70                     | 0.55              |
| 1:B:2263:ILE:HG13 | 1:B:2266:MET:HE2  | 1.87                     | 0.55              |
| 1:B:2312:TYR:CE2  | 1:B:2328:VAL:HG13 | 2.41                     | 0.55              |
| 1:B:3729:GLU:HB3  | 1:B:3733:LYS:HE3  | 1.88                     | 0.55              |
| 1:B:4423:GLU:HB3  | 1:B:4459:LEU:HD13 | 1.87                     | 0.55              |
| 3:F:28:TYR:CE2    | 3:F:122:ASN:HB3   | 2.42                     | 0.55              |
| 1:A:204:ARG:O     | 1:A:205:THR:C     | 2.50                     | 0.55              |
| 1:A:2982:LEU:O    | 1:A:2985:LEU:HB3  | 2.06                     | 0.55              |
| 1:A:4719:LEU:HB3  | 1:A:4720:PRO:HD3  | 1.88                     | 0.55              |
| 1:B:1311:ILE:HA   | 1:B:1334:LEU:HD21 | 1.87                     | 0.55              |
| 1:B:1453:LEU:C    | 1:B:1455:GLN:H    | 2.15                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2181:GLN:HG3  | 1:B:2188:LEU:HD11 | 1.89                     | 0.55              |
| 1:B:4613:LEU:O    | 1:B:4617:LEU:HG   | 2.06                     | 0.55              |
| 1:A:691:LYS:HD3   | 1:A:735:LEU:HA    | 1.88                     | 0.55              |
| 1:A:1269:HIS:CE1  | 1:A:1283:SER:HB3  | 2.42                     | 0.55              |
| 1:B:1088:GLU:HA   | 1:B:1091:GLU:CD   | 2.32                     | 0.55              |
| 1:B:4313:CYS:SG   | 1:B:4335:LEU:HD21 | 2.46                     | 0.55              |
| 1:A:674:LEU:O     | 1:A:678:LEU:HG    | 2.06                     | 0.55              |
| 1:A:1875:MET:SD   | 1:A:1917:GLU:HA   | 2.47                     | 0.55              |
| 1:A:4024:ILE:HD11 | 3:E:324:LEU:HD12  | 1.88                     | 0.55              |
| 1:B:1901:VAL:CG1  | 1:B:2217:ILE:HD12 | 2.28                     | 0.55              |
| 1:B:2212:GLN:N    | 1:B:2233:LEU:O    | 2.40                     | 0.55              |
| 1:B:4239:LYS:HE2  | 1:B:4286:GLU:OE1  | 2.06                     | 0.55              |
| 1:B:4771:LEU:O    | 1:B:4774:HIS:HB3  | 2.07                     | 0.55              |
| 1:A:1118:LEU:HD21 | 1:A:1269:HIS:HB3  | 1.87                     | 0.55              |
| 1:B:973:LEU:HB3   | 1:B:1002:TYR:OH   | 2.06                     | 0.55              |
| 1:B:2040:LEU:HD11 | 1:B:2085:PRO:CB   | 2.37                     | 0.55              |
| 1:B:2966:THR:HA   | 1:B:2969:ARG:HE   | 1.72                     | 0.55              |
| 1:A:261:LEU:CD2   | 1:A:332:LEU:HB2   | 2.36                     | 0.55              |
| 1:B:246:SER:O     | 1:B:250:LEU:HG    | 2.06                     | 0.55              |
| 1:B:3409:ILE:HG12 | 1:B:3450:LEU:HD22 | 1.88                     | 0.55              |
| 2:C:87:ARG:HG3    | 2:C:139:TYR:CE1   | 2.42                     | 0.55              |
| 1:B:313:LEU:HD12  | 1:B:384:ILE:HG23  | 1.89                     | 0.55              |
| 1:A:1529:GLY:HA2  | 1:A:1592:ILE:HD11 | 1.89                     | 0.54              |
| 1:A:1858:LEU:HB2  | 1:A:2200:GLN:OE1  | 2.07                     | 0.54              |
| 1:A:4131:GLN:O    | 1:A:4135:THR:HG23 | 2.07                     | 0.54              |
| 1:B:2360:ALA:HB3  | 1:B:2363:ARG:HB2  | 1.88                     | 0.54              |
| 1:B:3107:GLU:HA   | 1:B:3110:LYS:HD2  | 1.89                     | 0.54              |
| 1:A:1348:ALA:O    | 1:A:1352:GLU:HG3  | 2.07                     | 0.54              |
| 1:A:1961:PRO:HB3  | 1:A:2171:MET:CE   | 2.37                     | 0.54              |
| 1:A:2474:VAL:HA   | 1:A:2477:ARG:HE   | 1.71                     | 0.54              |
| 1:A:2654:GLU:HG2  | 1:A:2692:ALA:HB1  | 1.88                     | 0.54              |
| 1:A:4159:LYS:HZ3  | 1:A:4196:TRP:CD1  | 2.25                     | 0.54              |
| 1:B:1025:MET:HG2  | 1:B:1026:ASN:H    | 1.72                     | 0.54              |
| 1:B:3001:GLN:NE2  | 1:B:3138:PRO:HD3  | 2.22                     | 0.54              |
| 2:D:28:ILE:HD12   | 2:D:33:LEU:HA     | 1.88                     | 0.54              |
| 2:D:76:LYS:HE2    | 2:D:76:LYS:HA     | 1.89                     | 0.54              |
| 3:F:301:MET:O     | 3:F:306:ARG:NH1   | 2.39                     | 0.54              |
| 1:A:35:PRO:HB3    | 1:A:48:GLU:HB3    | 1.90                     | 0.54              |
| 1:A:4107:GLN:O    | 1:A:4111:ARG:HG2  | 2.07                     | 0.54              |
| 1:B:808:VAL:HG21  | 1:B:931:ARG:HD2   | 1.90                     | 0.54              |
| 1:A:183:GLU:O     | 1:A:187:LYS:HD3   | 2.06                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:545:ALA:O     | 1:A:644:PRO:HB3   | 2.07                     | 0.54              |
| 1:A:1700:CYS:SG   | 1:A:1726:CYS:C    | 2.89                     | 0.54              |
| 1:A:3738:ASN:O    | 1:A:3742:LEU:HG   | 2.07                     | 0.54              |
| 1:A:4476:ALA:C    | 1:A:4521:ASN:HD21 | 2.15                     | 0.54              |
| 1:B:1545:ALA:HB2  | 1:B:1556:LEU:HD22 | 1.89                     | 0.54              |
| 1:B:1708:TYR:O    | 1:B:2353:ARG:NH2  | 2.40                     | 0.54              |
| 1:B:1858:LEU:HB2  | 1:B:2200:GLN:OE1  | 2.07                     | 0.54              |
| 1:B:3881:GLU:HG2  | 1:B:3921:MET:HG3  | 1.88                     | 0.54              |
| 2:C:78:LYS:HB2    | 2:C:80:THR:HG23   | 1.88                     | 0.54              |
| 3:E:75:PRO:HD2    | 3:E:116:LEU:HD23  | 1.88                     | 0.54              |
| 1:A:1000:GLN:HA   | 1:A:1270:LEU:HD13 | 1.89                     | 0.54              |
| 1:A:1474:SER:HB2  | 1:A:1485:ILE:HG21 | 1.89                     | 0.54              |
| 1:A:3568:SER:HB3  | 1:A:3721:CYS:HA   | 1.90                     | 0.54              |
| 1:B:3406:GLU:HG3  | 1:B:3850:THR:HG21 | 1.88                     | 0.54              |
| 1:B:4212:LEU:HD23 | 1:B:4215:LYS:HD2  | 1.89                     | 0.54              |
| 1:A:1047:ILE:HB   | 1:A:1050:TYR:CD2  | 2.42                     | 0.54              |
| 1:A:1870:PHE:CZ   | 1:A:1924:LEU:CD1  | 2.66                     | 0.54              |
| 1:A:2040:LEU:HD11 | 1:A:2085:PRO:CB   | 2.37                     | 0.54              |
| 1:A:3095:VAL:HG12 | 1:A:3190:TRP:CZ3  | 2.43                     | 0.54              |
| 1:A:4313:CYS:HB3  | 1:A:4331:ILE:HD13 | 1.88                     | 0.54              |
| 1:B:194:LEU:HD13  | 1:B:197:LEU:HD12  | 1.90                     | 0.54              |
| 1:B:2701:LEU:HD13 | 1:B:3002:VAL:HG11 | 1.90                     | 0.54              |
| 1:B:3706:CYS:O    | 1:B:3710:ARG:NH1  | 2.41                     | 0.54              |
| 1:B:4107:GLN:O    | 1:B:4111:ARG:HG2  | 2.07                     | 0.54              |
| 1:B:4355:LYS:CE   | 1:B:4365:GLY:O    | 2.55                     | 0.54              |
| 1:A:299:PHE:HZ    | 1:A:346:CYS:SG    | 2.31                     | 0.54              |
| 1:A:2266:MET:HE1  | 1:A:2659:ALA:HB2  | 1.90                     | 0.54              |
| 1:A:3409:ILE:HG12 | 1:A:3450:LEU:HD22 | 1.88                     | 0.54              |
| 1:B:336:CYS:O     | 1:B:381:CYS:SG    | 2.65                     | 0.54              |
| 1:B:1306:ASN:HD22 | 1:B:1309:GLN:HB2  | 1.72                     | 0.54              |
| 1:B:2547:LEU:HD12 | 1:B:2580:ILE:HD11 | 1.89                     | 0.54              |
| 1:B:2695:PHE:HE1  | 1:B:2699:GLN:NE2  | 2.02                     | 0.54              |
| 1:B:3172:LYS:HE3  | 1:B:3217:ILE:HA   | 1.89                     | 0.54              |
| 1:B:3198:LEU:HD22 | 1:B:3207:ARG:HG3  | 1.89                     | 0.54              |
| 1:A:85:ILE:HA     | 1:A:88:VAL:HG22   | 1.90                     | 0.54              |
| 1:A:4423:GLU:HB3  | 1:A:4459:LEU:HD13 | 1.89                     | 0.54              |
| 1:B:49:LEU:C      | 1:B:51:GLN:N      | 2.63                     | 0.54              |
| 1:B:261:LEU:HD11  | 1:B:328:ASP:HB3   | 1.90                     | 0.54              |
| 1:B:1394:ARG:NH2  | 1:B:1437:LEU:HD13 | 2.23                     | 0.54              |
| 1:B:2675:ILE:C    | 1:B:2677:THR:H    | 2.15                     | 0.54              |
| 1:B:4537:LEU:HD21 | 1:B:4623:LEU:HD11 | 1.88                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:27:THR:HA     | 2:C:61:ASN:HA     | 1.88                     | 0.54              |
| 1:A:239:PHE:HA    | 1:A:242:GLN:OE1   | 2.08                     | 0.54              |
| 1:A:1022:GLN:O    | 1:A:1026:ASN:N    | 2.40                     | 0.54              |
| 1:A:1435:PHE:CD1  | 1:A:1498:TYR:HB3  | 2.43                     | 0.54              |
| 1:A:2261:SER:HB2  | 1:A:2263:ILE:HG22 | 1.90                     | 0.54              |
| 1:A:2668:CYS:O    | 1:A:2973:VAL:HG21 | 2.08                     | 0.54              |
| 1:A:3881:GLU:HG2  | 1:A:3921:MET:HG3  | 1.89                     | 0.54              |
| 1:A:4540:LEU:HB2  | 1:A:4562:VAL:HG11 | 1.89                     | 0.54              |
| 1:B:1875:MET:SD   | 1:B:1917:GLU:HA   | 2.47                     | 0.54              |
| 1:A:3706:CYS:O    | 1:A:3710:ARG:NH1  | 2.41                     | 0.54              |
| 1:B:2023:VAL:HG23 | 1:B:2046:ILE:HD13 | 1.89                     | 0.54              |
| 1:B:2025:ILE:HD12 | 1:B:2075:MET:HE3  | 1.90                     | 0.54              |
| 1:B:2698:LYS:HD2  | 1:B:2998:PRO:CA   | 2.30                     | 0.54              |
| 1:A:2180:VAL:HG22 | 1:A:2214:MET:HE2  | 1.90                     | 0.53              |
| 1:A:2300:ASP:HA   | 1:A:2318:LYS:NZ   | 2.23                     | 0.53              |
| 1:A:4105:TRP:CZ2  | 2:C:129:ALA:HB2   | 2.42                     | 0.53              |
| 1:B:44:PHE:CD1    | 1:B:84:TYR:HB3    | 2.43                     | 0.53              |
| 1:B:231:SER:HA    | 1:B:234:LYS:HD2   | 1.89                     | 0.53              |
| 1:B:1384:LEU:HD13 | 1:B:1397:MET:SD   | 2.48                     | 0.53              |
| 1:B:3532:CYS:SG   | 1:B:3534:VAL:HB   | 2.48                     | 0.53              |
| 1:B:4423:GLU:CB   | 1:B:4459:LEU:HD13 | 2.38                     | 0.53              |
| 1:A:1407:LEU:HB3  | 1:A:1431:PHE:HE1  | 1.72                     | 0.53              |
| 1:A:2025:ILE:HD12 | 1:A:2075:MET:HE3  | 1.90                     | 0.53              |
| 1:B:30:GLU:O      | 1:B:33:VAL:HG22   | 2.08                     | 0.53              |
| 1:B:63:ILE:HA     | 1:B:74:TYR:HD2    | 1.73                     | 0.53              |
| 1:B:783:TRP:CD1   | 1:B:821:PHE:HE2   | 2.26                     | 0.53              |
| 1:B:1044:ARG:C    | 1:B:1046:ARG:N    | 2.63                     | 0.53              |
| 1:A:1162:THR:O    | 1:A:1166:ILE:HG13 | 2.08                     | 0.53              |
| 1:A:2051:PHE:HB3  | 1:A:2059:ASN:HD21 | 1.73                     | 0.53              |
| 1:A:3512:ILE:O    | 1:A:3516:LEU:HG   | 2.08                     | 0.53              |
| 1:A:3759:GLN:HE21 | 1:A:3763:LEU:HG   | 1.74                     | 0.53              |
| 1:B:286:PRO:HB2   | 1:B:346:CYS:HB2   | 1.89                     | 0.53              |
| 1:B:844:MET:HE2   | 1:B:844:MET:HA    | 1.90                     | 0.53              |
| 1:B:2352:MET:HE1  | 1:B:2403:LEU:HD13 | 1.91                     | 0.53              |
| 1:A:3169:TYR:HD1  | 1:A:3213:LEU:HD13 | 1.74                     | 0.53              |
| 1:B:1805:PHE:HD2  | 1:B:2494:PRO:HD2  | 1.73                     | 0.53              |
| 2:C:87:ARG:HG3    | 2:C:139:TYR:HE1   | 1.73                     | 0.53              |
| 1:A:552:ARG:NH2   | 1:A:643:ASP:HA    | 2.23                     | 0.53              |
| 1:A:2096:HIS:HB3  | 1:A:2099:LEU:HG   | 1.91                     | 0.53              |
| 2:D:138:ASN:CG    | 2:D:139:TYR:H     | 2.17                     | 0.53              |
| 1:A:392:ILE:O     | 1:A:399:GLY:HA2   | 2.09                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1015:PRO:HG3  | 1:A:1041:TRP:CD2  | 2.44                     | 0.53              |
| 1:A:3310:LEU:HA   | 1:A:3859:LEU:HD23 | 1.90                     | 0.53              |
| 1:B:2332:LYS:HA   | 3:F:20:ARG:HH22   | 1.74                     | 0.53              |
| 1:B:2702:ILE:HG23 | 1:B:3005:MET:HG2  | 1.89                     | 0.53              |
| 1:B:4636:GLU:O    | 1:B:4640:PRO:HD3  | 2.08                     | 0.53              |
| 2:C:30:THR:HB     | 2:C:53:ILE:HG12   | 1.90                     | 0.53              |
| 3:F:23:LYS:HD3    | 3:F:114:ALA:HB1   | 1.90                     | 0.53              |
| 1:A:834:VAL:HG13  | 1:A:966:LEU:HD13  | 1.90                     | 0.53              |
| 1:A:1048:SER:HA   | 1:A:1051:VAL:HB   | 1.91                     | 0.53              |
| 1:A:1877:TYR:CE1  | 1:A:1885:ILE:HG21 | 2.43                     | 0.53              |
| 1:A:2187:PRO:HB3  | 1:A:2214:MET:SD   | 2.48                     | 0.53              |
| 1:A:3315:VAL:HG22 | 1:A:3633:LEU:HD21 | 1.90                     | 0.53              |
| 1:A:4123:LEU:HD13 | 1:A:4165:LEU:HD22 | 1.90                     | 0.53              |
| 1:A:4355:LYS:CE   | 1:A:4365:GLY:O    | 2.57                     | 0.53              |
| 1:B:49:LEU:HB3    | 1:B:50:PRO:HD3    | 1.89                     | 0.53              |
| 1:B:443:ARG:HB2   | 1:B:446:ASP:CG    | 2.33                     | 0.53              |
| 1:B:909:HIS:NE2   | 1:B:937:SER:HB2   | 2.24                     | 0.53              |
| 1:B:3106:LEU:HD12 | 1:B:3200:ILE:HD11 | 1.89                     | 0.53              |
| 2:C:33:LEU:CD1    | 2:C:72:MET:HE1    | 2.38                     | 0.53              |
| 3:E:27:CYS:SG     | 3:E:45:ARG:O      | 2.67                     | 0.53              |
| 1:A:103:ALA:O     | 1:A:107:LEU:HG    | 2.09                     | 0.53              |
| 1:B:1191:SER:H    | 1:B:1194:LYS:HD3  | 1.73                     | 0.53              |
| 1:B:1387:GLN:CG   | 1:B:1393:ALA:HB1  | 2.37                     | 0.53              |
| 1:B:1595:CYS:SG   | 1:B:1596:THR:N    | 2.82                     | 0.53              |
| 1:B:3547:LEU:O    | 1:B:3551:LYS:HG3  | 2.09                     | 0.53              |
| 1:A:89:CYS:HB2    | 1:A:239:PHE:CD2   | 2.44                     | 0.53              |
| 1:A:245:ALA:O     | 1:A:249:GLU:HG3   | 2.09                     | 0.53              |
| 1:A:839:GLU:O     | 1:A:842:VAL:HG12  | 2.09                     | 0.53              |
| 1:A:2698:LYS:NZ   | 1:A:3001:GLN:HB3  | 2.24                     | 0.53              |
| 1:A:3547:LEU:O    | 1:A:3551:LYS:HG3  | 2.09                     | 0.53              |
| 1:A:4096:TYR:CE1  | 2:C:48:GLU:HG2    | 2.44                     | 0.53              |
| 1:B:4047:PRO:HA   | 1:B:4075:LEU:CD2  | 2.39                     | 0.53              |
| 1:A:303:VAL:HG22  | 1:A:377:ILE:HG13  | 1.90                     | 0.53              |
| 1:A:3746:ALA:HA   | 1:A:3749:VAL:HG22 | 1.91                     | 0.53              |
| 1:B:136:LEU:O     | 1:B:243:ASN:ND2   | 2.42                     | 0.53              |
| 1:B:1603:LEU:HD13 | 1:B:1807:PHE:HZ   | 1.73                     | 0.53              |
| 1:B:3512:ILE:O    | 1:B:3516:LEU:HG   | 2.08                     | 0.53              |
| 2:C:59:ASP:HB3    | 2:C:63:THR:HB     | 1.89                     | 0.53              |
| 1:A:1306:ASN:HB3  | 1:A:1309:GLN:HB3  | 1.92                     | 0.52              |
| 1:A:1525:MET:HA   | 1:A:1530:ASP:HB2  | 1.91                     | 0.52              |
| 1:A:2352:MET:HE1  | 1:A:2403:LEU:HD13 | 1.91                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1010:LEU:HD22 | 1:B:1037:HIS:CE1  | 2.44                     | 0.52              |
| 1:B:1435:PHE:CD1  | 1:B:1498:TYR:HB3  | 2.43                     | 0.52              |
| 1:B:1600:MET:HB3  | 1:B:2481:SER:CB   | 2.39                     | 0.52              |
| 1:B:2698:LYS:CE   | 1:B:3001:GLN:HE21 | 2.22                     | 0.52              |
| 1:B:3309:PHE:CD2  | 1:B:3850:THR:HA   | 2.44                     | 0.52              |
| 1:B:3419:SER:HB3  | 1:B:3425:ARG:HG3  | 1.92                     | 0.52              |
| 1:A:59:SER:HA     | 1:A:62:GLU:HB2    | 1.91                     | 0.52              |
| 1:A:4665:ILE:O    | 1:A:4669:ILE:HG13 | 2.09                     | 0.52              |
| 1:B:272:ARG:HD2   | 1:B:338:TYR:HE1   | 1.75                     | 0.52              |
| 1:B:420:LEU:HD13  | 1:B:442:LEU:HB2   | 1.91                     | 0.52              |
| 1:B:859:LEU:O     | 1:B:1009:ILE:HD11 | 2.09                     | 0.52              |
| 1:B:1542:ALA:HB1  | 1:B:1602:TYR:CG   | 2.44                     | 0.52              |
| 1:B:1930:LEU:HD13 | 1:B:2219:HIS:HB3  | 1.91                     | 0.52              |
| 1:B:2292:PHE:HA   | 1:B:2295:ASN:HD22 | 1.74                     | 0.52              |
| 1:B:3997:PHE:HB2  | 1:B:4016:CYS:HB3  | 1.90                     | 0.52              |
| 1:A:230:ALA:O     | 1:A:234:LYS:HG3   | 2.09                     | 0.52              |
| 1:A:336:CYS:O     | 1:A:381:CYS:SG    | 2.67                     | 0.52              |
| 1:A:545:ALA:HB2   | 1:A:647:PHE:HB2   | 1.92                     | 0.52              |
| 1:A:2073:GLN:HB2  | 1:A:2088:VAL:HG13 | 1.91                     | 0.52              |
| 1:A:4245:LEU:HD23 | 1:A:4294:MET:HE1  | 1.90                     | 0.52              |
| 1:A:4644:PHE:HB3  | 1:A:4722:ILE:HD11 | 1.90                     | 0.52              |
| 1:B:542:TYR:CE2   | 1:B:689:ILE:HG23  | 2.44                     | 0.52              |
| 1:B:740:PHE:HA    | 1:B:781:LYS:HG2   | 1.91                     | 0.52              |
| 1:B:1097:GLN:HA   | 1:B:1097:GLN:NE2  | 2.24                     | 0.52              |
| 1:B:1162:THR:HG22 | 1:B:1166:ILE:HD11 | 1.90                     | 0.52              |
| 1:B:3042:LYS:HA   | 1:B:3049:ASN:HB3  | 1.92                     | 0.52              |
| 2:C:138:ASN:HB3   | 2:C:140:GLU:HG2   | 1.91                     | 0.52              |
| 1:A:1094:PHE:O    | 1:A:1098:ILE:HG13 | 2.10                     | 0.52              |
| 1:A:1875:MET:HG2  | 1:A:1877:TYR:CE1  | 2.44                     | 0.52              |
| 1:A:2517:ALA:HB2  | 1:A:2521:VAL:HB   | 1.91                     | 0.52              |
| 1:B:943:ASP:O     | 1:B:944:ASP:C     | 2.52                     | 0.52              |
| 1:B:1489:ARG:NH2  | 1:B:1533:GLY:CA   | 2.72                     | 0.52              |
| 1:B:1845:LEU:HD12 | 1:B:1850:LYS:HE3  | 1.92                     | 0.52              |
| 1:B:2052:LEU:HG   | 1:B:2060:ILE:HB   | 1.91                     | 0.52              |
| 1:B:2073:GLN:HB2  | 1:B:2088:VAL:HG13 | 1.91                     | 0.52              |
| 1:B:2701:LEU:HD12 | 1:B:3002:VAL:HG21 | 1.90                     | 0.52              |
| 1:B:4195:HIS:CD2  | 2:D:35:THR:HG21   | 2.45                     | 0.52              |
| 1:A:478:ASN:OD1   | 1:A:650:LEU:HD13  | 2.09                     | 0.52              |
| 1:A:906:PRO:HG2   | 1:A:908:TYR:HE2   | 1.74                     | 0.52              |
| 1:B:1819:MET:CE   | 1:B:2508:LEU:HD12 | 2.39                     | 0.52              |
| 1:B:2291:PHE:HZ   | 1:B:2350:THR:HB   | 1.74                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1169:TYR:HA   | 1:A:1172:PHE:CD2  | 2.44                     | 0.52              |
| 1:A:1571:LEU:C    | 1:A:1573:GLN:N    | 2.65                     | 0.52              |
| 1:A:2292:PHE:CE2  | 1:A:2386:ASP:HB3  | 2.40                     | 0.52              |
| 1:A:4740:ILE:O    | 1:A:4744:SER:HB2  | 2.09                     | 0.52              |
| 1:B:4052:ILE:N    | 1:B:4119:LEU:O    | 2.43                     | 0.52              |
| 2:C:140:GLU:HG3   | 2:C:141:GLU:HG3   | 1.91                     | 0.52              |
| 1:A:491:LEU:HD23  | 1:A:517:SER:OG    | 2.10                     | 0.52              |
| 1:A:661:SER:O     | 1:A:665:SER:HB2   | 2.09                     | 0.52              |
| 1:A:945:LEU:HA    | 1:A:1053:TRP:CD1  | 2.45                     | 0.52              |
| 1:B:144:ASP:HB2   | 1:B:147:GLU:HG3   | 1.91                     | 0.52              |
| 1:B:712:HIS:HA    | 1:B:715:HIS:CD2   | 2.44                     | 0.52              |
| 1:B:3309:PHE:HE1  | 1:B:3411:PHE:HB3  | 1.74                     | 0.52              |
| 1:B:3408:LEU:HD12 | 1:B:3411:PHE:CE2  | 2.44                     | 0.52              |
| 1:B:3968:LEU:CD1  | 1:B:4012:ILE:HD11 | 2.39                     | 0.52              |
| 1:B:4327:THR:HB   | 1:B:4328:PRO:HD3  | 1.90                     | 0.52              |
| 2:C:100:TYR:CE1   | 2:C:138:ASN:HB2   | 2.45                     | 0.52              |
| 3:E:4:HIS:O       | 3:E:16:ASN:HA     | 2.09                     | 0.52              |
| 1:A:844:MET:HA    | 1:A:844:MET:HE2   | 1.90                     | 0.52              |
| 1:A:2997:ILE:HB   | 1:A:2998:PRO:HD3  | 1.90                     | 0.52              |
| 1:B:2375:MET:HG2  | 1:B:2387:PHE:CE1  | 2.35                     | 0.52              |
| 1:B:3513:TYR:CZ   | 1:B:3525:TYR:HB3  | 2.44                     | 0.52              |
| 1:B:4644:PHE:HB3  | 1:B:4722:ILE:HD11 | 1.92                     | 0.52              |
| 1:B:4719:LEU:HB3  | 1:B:4720:PRO:HD3  | 1.92                     | 0.52              |
| 2:C:20:PHE:CD2    | 2:C:36:VAL:HG22   | 2.45                     | 0.52              |
| 1:A:405:ASN:HB2   | 1:A:511:ILE:HA    | 1.92                     | 0.52              |
| 1:A:4560:GLU:HA   | 1:A:4563:LEU:HD12 | 1.90                     | 0.52              |
| 1:A:4723:LEU:HD11 | 1:A:4760:ILE:HG23 | 1.91                     | 0.52              |
| 1:B:90:SER:HA     | 1:B:236:LYS:HB2   | 1.91                     | 0.52              |
| 1:B:313:LEU:HD13  | 1:B:388:ILE:HD11  | 1.92                     | 0.52              |
| 1:B:1542:ALA:HB1  | 1:B:1602:TYR:CD1  | 2.45                     | 0.52              |
| 1:B:1930:LEU:HB3  | 1:B:2219:HIS:CD2  | 2.45                     | 0.52              |
| 1:B:2480:VAL:HG13 | 1:B:2524:GLN:HG3  | 1.91                     | 0.52              |
| 1:B:4077:ILE:HG21 | 2:D:116:LYS:HE3   | 1.92                     | 0.52              |
| 1:A:345:THR:O     | 1:A:349:ILE:HG12  | 2.10                     | 0.52              |
| 1:A:470:GLY:O     | 1:A:474:VAL:HG23  | 2.10                     | 0.52              |
| 1:A:1043:SER:HB3  | 1:A:1256:ILE:HG21 | 1.92                     | 0.52              |
| 1:A:3950:LYS:HG2  | 1:A:3971:GLU:OE1  | 2.10                     | 0.52              |
| 1:A:3954:ALA:HB3  | 1:A:3968:LEU:HD11 | 1.92                     | 0.52              |
| 1:A:4155:ILE:HB   | 1:A:4158:ARG:HD2  | 1.92                     | 0.52              |
| 1:B:1490:GLN:O    | 1:B:1494:LEU:HD13 | 2.09                     | 0.52              |
| 1:B:1558:ASN:HD21 | 1:B:1803:ALA:CB   | 2.23                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:3007:THR:HA   | 1:B:3010:LEU:HG   | 1.91                     | 0.52              |
| 1:B:3793:ASN:OD1  | 1:B:3795:TYR:HB2  | 2.10                     | 0.52              |
| 1:A:254:GLU:HA    | 1:A:257:LEU:HD12  | 1.90                     | 0.51              |
| 1:A:1024:SER:HB3  | 1:A:1074:LEU:HD23 | 1.92                     | 0.51              |
| 1:A:1309:GLN:HA   | 1:A:1312:ARG:HD2  | 1.91                     | 0.51              |
| 1:A:1499:ILE:HG12 | 1:A:1506:VAL:HG21 | 1.92                     | 0.51              |
| 1:A:1845:LEU:HD12 | 1:A:1850:LYS:HE3  | 1.92                     | 0.51              |
| 1:A:3546:LYS:HG2  | 1:A:3714:MET:SD   | 2.51                     | 0.51              |
| 1:B:723:GLN:HG2   | 1:B:728:GLN:HG3   | 1.92                     | 0.51              |
| 1:B:1952:PHE:HE1  | 1:B:1976:HIS:CD2  | 2.28                     | 0.51              |
| 1:B:3936:ASN:HB3  | 1:B:3939:ALA:HB3  | 1.92                     | 0.51              |
| 1:B:4155:ILE:HB   | 1:B:4158:ARG:HD2  | 1.92                     | 0.51              |
| 1:B:4224:GLU:HA   | 1:B:4279:GLN:HE21 | 1.74                     | 0.51              |
| 1:B:4258:PHE:O    | 1:B:4259:LYS:C    | 2.51                     | 0.51              |
| 2:C:49:LEU:HD13   | 2:C:49:LEU:O      | 2.09                     | 0.51              |
| 1:A:73:PHE:HB2    | 1:A:161:PRO:HD3   | 1.92                     | 0.51              |
| 1:A:266:PHE:O     | 1:A:270:ILE:HG13  | 2.10                     | 0.51              |
| 1:A:3419:SER:HB3  | 1:A:3425:ARG:HG3  | 1.92                     | 0.51              |
| 1:A:4195:HIS:CD2  | 2:C:35:THR:HG21   | 2.44                     | 0.51              |
| 1:B:123:ALA:HB1   | 1:B:154:MET:SD    | 2.50                     | 0.51              |
| 1:B:303:VAL:HG21  | 1:B:373:ASP:HB3   | 1.92                     | 0.51              |
| 1:B:1214:LEU:O    | 1:B:1218:LEU:HG   | 2.10                     | 0.51              |
| 1:B:1570:TYR:HA   | 1:B:1573:GLN:HE21 | 1.76                     | 0.51              |
| 1:B:3063:MET:HG3  | 1:B:3170:GLN:HB3  | 1.92                     | 0.51              |
| 1:B:3196:GLU:O    | 1:B:3200:ILE:HG13 | 2.10                     | 0.51              |
| 1:A:80:LEU:HD11   | 1:A:152:THR:HA    | 1.92                     | 0.51              |
| 1:A:1560:ALA:HA   | 1:A:1563:TRP:HE3  | 1.75                     | 0.51              |
| 1:A:83:HIS:O      | 1:A:87:THR:HG23   | 2.10                     | 0.51              |
| 1:A:546:CYS:O     | 1:A:550:ARG:HG3   | 2.11                     | 0.51              |
| 1:A:549:GLN:O     | 1:A:553:LYS:HG2   | 2.09                     | 0.51              |
| 1:B:2072:THR:O    | 1:B:2090:ASN:HB2  | 2.10                     | 0.51              |
| 1:B:3458:LEU:HD11 | 1:B:3465:ALA:HB1  | 1.92                     | 0.51              |
| 1:B:3766:LYS:HB3  | 1:B:3795:TYR:CD2  | 2.45                     | 0.51              |
| 2:C:49:LEU:HD11   | 2:C:53:ILE:CD1    | 2.40                     | 0.51              |
| 3:F:4:HIS:CD2     | 3:F:21:ARG:HB2    | 2.44                     | 0.51              |
| 1:A:202:ASN:HB3   | 1:A:204:ARG:CZ    | 2.41                     | 0.51              |
| 1:A:327:GLN:HA    | 1:A:511:ILE:HD11  | 1.92                     | 0.51              |
| 1:A:539:SER:HB2   | 1:A:543:ARG:NH1   | 2.25                     | 0.51              |
| 1:A:2094:ILE:HG12 | 1:A:2143:VAL:HG21 | 1.93                     | 0.51              |
| 1:A:3071:LYS:HD2  | 1:A:3074:ILE:HB   | 1.91                     | 0.51              |
| 1:A:3404:ASP:OD1  | 1:A:3404:ASP:N    | 2.41                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:112:LEU:HD11  | 1:B:247:LEU:HD12  | 1.92                     | 0.51              |
| 1:A:491:LEU:CD1   | 1:A:670:ILE:HD11  | 2.40                     | 0.51              |
| 1:A:1159:LEU:HA   | 1:A:1298:LEU:HD13 | 1.91                     | 0.51              |
| 1:A:1814:MET:HA   | 1:A:1817:PHE:HE1  | 1.70                     | 0.51              |
| 1:A:3998:LEU:O    | 1:A:4001:VAL:HG12 | 2.10                     | 0.51              |
| 1:B:663:LEU:HD23  | 1:B:674:LEU:HD13  | 1.93                     | 0.51              |
| 1:B:712:HIS:HA    | 1:B:715:HIS:NE2   | 2.25                     | 0.51              |
| 1:B:1169:TYR:HA   | 1:B:1172:PHE:CD2  | 2.46                     | 0.51              |
| 1:B:1401:PHE:HD2  | 1:B:1449:LEU:HD22 | 1.76                     | 0.51              |
| 1:B:1558:ASN:O    | 1:B:1561:VAL:HB   | 2.11                     | 0.51              |
| 1:B:3194:LEU:HB2  | 1:B:3214:LEU:HD13 | 1.93                     | 0.51              |
| 1:B:3940:THR:HG21 | 1:B:3985:CYS:HB3  | 1.90                     | 0.51              |
| 1:B:4130:ARG:HB2  | 1:B:4169:TYR:CE1  | 2.46                     | 0.51              |
| 1:B:4438:MET:HE3  | 1:B:4440:ILE:HD11 | 1.93                     | 0.51              |
| 1:A:1515:LEU:HA   | 1:A:1544:LEU:HD13 | 1.93                     | 0.51              |
| 1:A:4423:GLU:CB   | 1:A:4459:LEU:HD13 | 2.41                     | 0.51              |
| 1:B:31:VAL:O      | 1:B:35:PRO:HD2    | 2.11                     | 0.51              |
| 1:B:1403:ASP:OD2  | 1:B:1404:SER:N    | 2.44                     | 0.51              |
| 1:B:3405:LYS:HB2  | 1:B:3450:LEU:HD21 | 1.93                     | 0.51              |
| 1:B:3519:LEU:HD13 | 1:B:3767:VAL:HG11 | 1.92                     | 0.51              |
| 1:B:4286:GLU:HB3  | 1:B:4290:MET:HE3  | 1.92                     | 0.51              |
| 1:B:4548:GLN:HG3  | 1:B:4605:PHE:HD1  | 1.75                     | 0.51              |
| 2:D:42:GLN:HB2    | 2:D:78:LYS:HG2    | 1.92                     | 0.51              |
| 1:A:918:TRP:O     | 1:A:922:PHE:HB2   | 2.10                     | 0.51              |
| 1:A:1010:LEU:HB3  | 1:A:1037:HIS:CE1  | 2.45                     | 0.51              |
| 1:A:1468:LEU:HD22 | 1:A:1518:LEU:HD21 | 1.92                     | 0.51              |
| 1:A:1995:GLN:HB2  | 1:A:2024:LYS:NZ   | 2.26                     | 0.51              |
| 1:A:3233:LEU:HD13 | 1:A:3290:TRP:HE3  | 1.76                     | 0.51              |
| 1:A:4077:ILE:HG13 | 1:A:4079:GLY:H    | 1.75                     | 0.51              |
| 1:A:4258:PHE:HE1  | 2:C:19:LEU:HD21   | 1.75                     | 0.51              |
| 1:B:1893:VAL:HG12 | 1:B:2001:PHE:HZ   | 1.76                     | 0.51              |
| 1:B:3292:LYS:O    | 1:B:3295:ILE:HG22 | 2.11                     | 0.51              |
| 1:A:967:TYR:CE2   | 1:A:1015:PRO:HA   | 2.44                     | 0.51              |
| 1:A:1010:LEU:HB3  | 1:A:1037:HIS:HE1  | 1.75                     | 0.51              |
| 1:A:3286:ARG:HH21 | 1:A:3286:ARG:HG3  | 1.75                     | 0.51              |
| 1:B:443:ARG:HB2   | 1:B:446:ASP:HB2   | 1.93                     | 0.51              |
| 1:B:1473:THR:O    | 1:B:1485:ILE:HD13 | 2.10                     | 0.51              |
| 1:B:1698:LYS:HG2  | 1:B:2289:ILE:HD12 | 1.92                     | 0.51              |
| 1:B:3001:GLN:HG2  | 1:B:3004:LEU:HD23 | 1.92                     | 0.51              |
| 1:A:44:PHE:HE2    | 1:A:48:GLU:HB2    | 1.75                     | 0.51              |
| 1:A:1019:TYR:CZ   | 1:A:1023:LEU:HD21 | 2.45                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:4679:LYS:NZ   | 1:A:4731:ILE:O    | 2.42                     | 0.51              |
| 1:B:63:ILE:HA     | 1:B:74:TYR:CD2    | 2.46                     | 0.51              |
| 1:B:1417:GLU:HA   | 1:B:1470:ARG:HD2  | 1.93                     | 0.51              |
| 1:B:2359:GLN:HG2  | 1:B:2418:ASP:OD1  | 2.11                     | 0.51              |
| 1:B:4232:LEU:C    | 1:B:4234:GLN:N    | 2.69                     | 0.51              |
| 1:A:4282:LYS:O    | 1:A:4286:GLU:HG2  | 2.11                     | 0.50              |
| 1:B:765:GLN:NE2   | 1:B:817:ILE:HG23  | 2.26                     | 0.50              |
| 1:B:1091:GLU:HG2  | 1:B:1158:LEU:HD13 | 1.92                     | 0.50              |
| 1:B:2296:GLN:HE21 | 1:B:2347:MET:HE1  | 1.76                     | 0.50              |
| 1:A:396:ARG:HH21  | 1:B:404:GLN:CD    | 2.18                     | 0.50              |
| 1:A:816:LEU:HD21  | 1:B:193:PHE:CZ    | 2.46                     | 0.50              |
| 1:A:3007:THR:C    | 1:A:3009:ASP:N    | 2.65                     | 0.50              |
| 1:B:909:HIS:CE1   | 1:B:937:SER:HB2   | 2.46                     | 0.50              |
| 1:B:1428:LEU:CD1  | 1:B:1488:ASN:HA   | 2.42                     | 0.50              |
| 1:B:1960:ASN:HD21 | 1:B:2012:GLN:HA   | 1.76                     | 0.50              |
| 1:B:2023:VAL:HG21 | 1:B:2049:VAL:HG21 | 1.93                     | 0.50              |
| 1:B:3307:VAL:O    | 1:B:3311:VAL:HG13 | 2.12                     | 0.50              |
| 1:B:3330:SER:HA   | 1:B:3333:LEU:HB2  | 1.93                     | 0.50              |
| 2:C:33:LEU:HD11   | 2:C:72:MET:HE1    | 1.91                     | 0.50              |
| 1:A:548:LEU:HD11  | 1:A:647:PHE:CE2   | 2.46                     | 0.50              |
| 1:A:1205:GLY:HA2  | 1:A:1215:GLY:C    | 2.36                     | 0.50              |
| 1:A:1515:LEU:CA   | 1:A:1544:LEU:HD13 | 2.42                     | 0.50              |
| 1:A:1682:HIS:CE1  | 1:A:2383:ARG:HD2  | 2.45                     | 0.50              |
| 1:B:31:VAL:O      | 1:B:34:ARG:HB3    | 2.12                     | 0.50              |
| 1:B:739:PRO:HB3   | 1:B:782:VAL:HG23  | 1.94                     | 0.50              |
| 1:B:2327:TYR:CD1  | 1:B:2359:GLN:HG3  | 2.46                     | 0.50              |
| 1:A:3511:ASN:HB2  | 1:B:4007:VAL:HG22 | 1.94                     | 0.50              |
| 1:B:49:LEU:C      | 1:B:51:GLN:H      | 2.19                     | 0.50              |
| 1:B:71:GLU:OE1    | 1:B:122:CYS:HA    | 2.11                     | 0.50              |
| 1:B:143:LEU:HD13  | 1:B:151:PHE:CE2   | 2.47                     | 0.50              |
| 1:B:808:VAL:HG11  | 1:B:908:TYR:HB3   | 1.94                     | 0.50              |
| 1:B:834:VAL:HG11  | 1:B:961:VAL:HG13  | 1.93                     | 0.50              |
| 1:B:3100:HIS:O    | 1:B:3103:LYS:HG3  | 2.11                     | 0.50              |
| 3:E:324:LEU:O     | 3:E:328:LEU:HG    | 2.10                     | 0.50              |
| 1:A:650:LEU:O     | 1:A:654:ILE:HG13  | 2.11                     | 0.50              |
| 1:A:846:ALA:HB1   | 1:A:850:PHE:CE2   | 2.47                     | 0.50              |
| 1:A:2385:PHE:HB3  | 1:A:2387:PHE:CZ   | 2.46                     | 0.50              |
| 1:A:3458:LEU:HD11 | 1:A:3465:ALA:HB1  | 1.92                     | 0.50              |
| 1:A:4597:LEU:O    | 1:A:4601:ILE:HG22 | 2.11                     | 0.50              |
| 1:B:2009:PRO:HB2  | 1:B:2642:LEU:HD21 | 1.94                     | 0.50              |
| 1:B:2049:VAL:HG22 | 1:B:2063:ILE:HG12 | 1.93                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:E:113:CYS:SG    | 3:E:136:HIS:CE1   | 3.04                     | 0.50              |
| 1:A:3405:LYS:HB2  | 1:A:3450:LEU:HD21 | 1.93                     | 0.50              |
| 1:B:83:HIS:O      | 1:B:87:THR:HG23   | 2.11                     | 0.50              |
| 1:B:864:TYR:HA    | 1:B:936:LEU:HG    | 1.94                     | 0.50              |
| 1:B:3872:CYS:O    | 1:B:3873:TYR:C    | 2.55                     | 0.50              |
| 1:B:4749:HIS:O    | 1:B:4753:GLN:HG3  | 2.11                     | 0.50              |
| 2:C:137:VAL:HG13  | 2:C:141:GLU:HB2   | 1.93                     | 0.50              |
| 1:A:317:VAL:HG12  | 1:A:318:LEU:N     | 2.26                     | 0.50              |
| 1:A:491:LEU:HD22  | 1:A:518:ILE:HG12  | 1.92                     | 0.50              |
| 1:A:723:GLN:HG2   | 1:A:728:GLN:HG3   | 1.92                     | 0.50              |
| 1:A:786:PHE:CE1   | 1:A:806:LEU:HD13  | 2.47                     | 0.50              |
| 1:A:873:PRO:HG2   | 1:A:876:LEU:HB2   | 1.93                     | 0.50              |
| 1:A:1050:TYR:HE2  | 1:A:1255:THR:HG21 | 1.77                     | 0.50              |
| 1:A:1196:GLN:HG2  | 1:A:1365:HIS:HE1  | 1.76                     | 0.50              |
| 1:A:2340:ILE:HD12 | 1:A:2401:LEU:HD23 | 1.93                     | 0.50              |
| 1:A:3000:MET:HE2  | 1:A:3058:LEU:HD13 | 1.93                     | 0.50              |
| 1:A:3200:ILE:HG22 | 1:A:3202:GLN:H    | 1.75                     | 0.50              |
| 1:A:3408:LEU:HD12 | 1:A:3411:PHE:CE2  | 2.44                     | 0.50              |
| 1:A:3937:PRO:HA   | 1:A:3940:THR:HG22 | 1.94                     | 0.50              |
| 1:B:39:ALA:CB     | 1:B:44:PHE:CD1    | 2.95                     | 0.50              |
| 1:B:2189:VAL:HG21 | 1:B:2230:MET:HE1  | 1.93                     | 0.50              |
| 1:B:2667:TYR:O    | 1:B:2668:CYS:SG   | 2.69                     | 0.50              |
| 1:B:2988:LEU:HD21 | 1:B:2999:TYR:CD1  | 2.47                     | 0.50              |
| 1:B:3003:ILE:O    | 1:B:3007:THR:HG23 | 2.12                     | 0.50              |
| 1:B:3404:ASP:OD1  | 1:B:3404:ASP:N    | 2.41                     | 0.50              |
| 1:B:4035:LYS:O    | 1:B:4036:ASP:C    | 2.54                     | 0.50              |
| 1:B:4077:ILE:HG22 | 2:D:114:GLY:O     | 2.11                     | 0.50              |
| 1:B:4768:LEU:HA   | 1:B:4771:LEU:HD12 | 1.94                     | 0.50              |
| 1:A:1058:LEU:HD23 | 1:A:1061:GLN:HE22 | 1.75                     | 0.50              |
| 1:A:1427:VAL:HG13 | 1:A:1431:PHE:CE2  | 2.47                     | 0.50              |
| 1:A:2311:VAL:HG13 | 3:E:56:LEU:HD11   | 1.94                     | 0.50              |
| 1:A:4108:PHE:O    | 1:A:4112:ARG:HG3  | 2.12                     | 0.50              |
| 1:B:1057:HIS:O    | 1:B:1061:GLN:HG3  | 2.12                     | 0.50              |
| 1:B:1450:CYS:CB   | 1:B:1505:GLN:HB2  | 2.41                     | 0.50              |
| 1:B:1453:LEU:C    | 1:B:1455:GLN:N    | 2.69                     | 0.50              |
| 1:B:1553:HIS:HD2  | 1:B:1556:LEU:HD23 | 1.77                     | 0.50              |
| 1:B:3273:MET:O    | 1:B:3273:MET:HE3  | 2.11                     | 0.50              |
| 2:C:44:PRO:HB2    | 2:C:48:GLU:HB2    | 1.94                     | 0.50              |
| 2:D:124:GLU:O     | 2:D:128:GLU:HG2   | 2.12                     | 0.50              |
| 1:A:73:PHE:CD1    | 1:A:158:ALA:O     | 2.60                     | 0.50              |
| 1:A:418:LEU:HD21  | 1:A:476:LEU:HB2   | 1.93                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:683:MET:HE2   | 1:A:683:MET:HA    | 1.93                     | 0.50              |
| 1:A:881:GLN:HA    | 1:A:885:LEU:HD12  | 1.92                     | 0.50              |
| 1:A:1156:LYS:HG2  | 1:A:1304:GLU:HG2  | 1.94                     | 0.50              |
| 1:A:1356:THR:HA   | 1:A:1400:PHE:HE2  | 1.77                     | 0.50              |
| 1:A:3007:THR:HG21 | 1:A:3062:PHE:CZ   | 2.46                     | 0.50              |
| 1:B:341:VAL:HB    | 1:B:417:SER:HB2   | 1.94                     | 0.50              |
| 1:B:834:VAL:HG13  | 1:B:966:LEU:HD13  | 1.93                     | 0.50              |
| 1:B:852:PRO:CB    | 1:B:855:LEU:HB3   | 2.41                     | 0.50              |
| 1:B:1044:ARG:C    | 1:B:1046:ARG:H    | 2.19                     | 0.50              |
| 1:B:1162:THR:O    | 1:B:1166:ILE:HG13 | 2.12                     | 0.50              |
| 1:B:1359:TYR:CD1  | 1:B:1406:GLU:HB3  | 2.47                     | 0.50              |
| 1:B:1485:ILE:O    | 1:B:1489:ARG:HG3  | 2.12                     | 0.50              |
| 1:B:1570:TYR:CE2  | 1:B:1592:ILE:HG13 | 2.47                     | 0.50              |
| 1:B:2246:VAL:HG13 | 1:B:2250:SER:HB3  | 1.94                     | 0.50              |
| 1:B:2474:VAL:HG22 | 1:B:2477:ARG:NH2  | 2.27                     | 0.50              |
| 3:F:27:CYS:SG     | 3:F:45:ARG:O      | 2.69                     | 0.50              |
| 1:A:85:ILE:CG2    | 1:A:100:VAL:HG13  | 2.42                     | 0.49              |
| 1:A:662:MET:HB3   | 1:A:674:LEU:HD11  | 1.94                     | 0.49              |
| 1:A:3273:MET:HE3  | 1:A:3273:MET:O    | 2.11                     | 0.49              |
| 1:A:3307:VAL:C    | 1:A:3309:PHE:H    | 2.19                     | 0.49              |
| 1:B:37:LEU:HD12   | 1:B:38:SER:N      | 2.26                     | 0.49              |
| 1:B:1296:GLY:O    | 1:B:1300:VAL:HG22 | 2.12                     | 0.49              |
| 1:B:1553:HIS:O    | 1:B:1553:HIS:CG   | 2.65                     | 0.49              |
| 1:B:2103:ASN:C    | 1:B:2105:GLN:H    | 2.19                     | 0.49              |
| 1:B:2632:LEU:O    | 1:B:2649:GLY:HA2  | 2.12                     | 0.49              |
| 1:B:2993:GLY:HA3  | 1:B:3050:GLU:OE1  | 2.12                     | 0.49              |
| 1:B:4108:PHE:O    | 1:B:4112:ARG:HG3  | 2.11                     | 0.49              |
| 2:C:24:GLY:HA3    | 2:C:28:ILE:HD12   | 1.92                     | 0.49              |
| 2:D:86:ILE:HD11   | 2:D:146:MET:HG2   | 1.94                     | 0.49              |
| 1:A:1233:TRP:HH2  | 1:A:1281:ALA:HB1  | 1.77                     | 0.49              |
| 1:A:1300:VAL:HA   | 1:A:1336:ARG:NH1  | 2.27                     | 0.49              |
| 1:A:1565:SER:O    | 1:A:1569:LYS:HG2  | 2.11                     | 0.49              |
| 1:A:3100:HIS:O    | 1:A:3103:LYS:HG3  | 2.11                     | 0.49              |
| 1:A:4335:LEU:HD13 | 1:A:4511:LEU:CD2  | 2.41                     | 0.49              |
| 1:B:3000:MET:HE3  | 1:B:3054:VAL:HG12 | 1.92                     | 0.49              |
| 1:A:535:LEU:HD12  | 1:A:682:HIS:CD2   | 2.46                     | 0.49              |
| 1:A:914:VAL:HG11  | 1:A:1001:TYR:HD1  | 1.76                     | 0.49              |
| 1:A:1101:PHE:HA   | 1:A:1104:ILE:HD13 | 1.95                     | 0.49              |
| 1:A:2047:ARG:HE   | 1:A:2066:SER:HB3  | 1.78                     | 0.49              |
| 1:A:2335:GLY:HA3  | 1:A:2405:ILE:O    | 2.12                     | 0.49              |
| 1:A:3951:VAL:HG13 | 1:A:4012:ILE:HD13 | 1.93                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:4310:MET:HE3  | 1:A:4335:LEU:HG   | 1.95                     | 0.49              |
| 1:A:4595:VAL:HA   | 1:A:4598:LEU:HD12 | 1.94                     | 0.49              |
| 1:B:288:THR:HG22  | 1:B:432:LYS:HB3   | 1.93                     | 0.49              |
| 1:B:786:PHE:HZ    | 1:B:806:LEU:HD22  | 1.77                     | 0.49              |
| 1:B:1819:MET:CE   | 1:B:2508:LEU:CD1  | 2.91                     | 0.49              |
| 1:B:1952:PHE:CD1  | 1:B:1974:ASP:HB2  | 2.47                     | 0.49              |
| 1:B:2070:ILE:HD12 | 1:B:2094:ILE:CD1  | 2.40                     | 0.49              |
| 1:A:159:LYS:O     | 1:A:160:LEU:C     | 2.52                     | 0.49              |
| 1:A:244:VAL:O     | 1:A:248:GLN:HG2   | 2.12                     | 0.49              |
| 1:A:547:VAL:O     | 1:A:551:GLN:HG3   | 2.11                     | 0.49              |
| 1:A:1929:LEU:HD21 | 1:A:2241:ILE:HD11 | 1.94                     | 0.49              |
| 1:A:4413:LYS:HD3  | 1:A:4456:ILE:HD11 | 1.94                     | 0.49              |
| 1:B:477:ALA:O     | 1:B:481:ILE:HG12  | 2.11                     | 0.49              |
| 3:F:301:MET:SD    | 3:F:306:ARG:HG3   | 2.53                     | 0.49              |
| 1:A:397:ARG:O     | 1:A:398:ALA:HB3   | 2.12                     | 0.49              |
| 1:A:1460:GLU:HB2  | 1:A:1463:ARG:HB3  | 1.94                     | 0.49              |
| 1:A:1510:VAL:O    | 1:A:1514:LEU:HG   | 2.13                     | 0.49              |
| 1:A:1567:CYS:SG   | 1:A:1596:THR:HG23 | 2.52                     | 0.49              |
| 1:A:1870:PHE:CE2  | 1:A:2239:LEU:HD11 | 2.30                     | 0.49              |
| 1:A:2687:LEU:O    | 1:A:2688:CYS:C    | 2.55                     | 0.49              |
| 1:B:745:TRP:HE1   | 1:B:810:HIS:CE1   | 2.31                     | 0.49              |
| 1:B:808:VAL:HG22  | 1:B:933:TYR:CD2   | 2.48                     | 0.49              |
| 1:B:867:HIS:O     | 1:B:949:ASP:HB2   | 2.13                     | 0.49              |
| 1:B:1451:GLY:O    | 1:B:1454:ALA:HB3  | 2.12                     | 0.49              |
| 1:B:1848:VAL:O    | 1:B:1850:LYS:NZ   | 2.38                     | 0.49              |
| 1:B:3588:ARG:HG3  | 1:B:3648:TYR:CZ   | 2.47                     | 0.49              |
| 1:B:4476:ALA:HB1  | 1:B:4515:CYS:HA   | 1.94                     | 0.49              |
| 3:E:301:MET:SD    | 3:E:306:ARG:HG3   | 2.53                     | 0.49              |
| 1:A:686:LEU:O     | 1:A:690:ILE:HG13  | 2.12                     | 0.49              |
| 1:A:740:PHE:CD1   | 1:A:778:GLU:HG3   | 2.48                     | 0.49              |
| 1:A:1241:PHE:HE2  | 1:A:1269:HIS:CD2  | 2.30                     | 0.49              |
| 1:A:1347:LEU:HD22 | 1:A:1351:TYR:OH   | 2.13                     | 0.49              |
| 1:A:1925:GLN:HB3  | 1:A:1943:THR:HB   | 1.95                     | 0.49              |
| 1:A:2626:VAL:HG21 | 1:A:2681:ILE:HD13 | 1.93                     | 0.49              |
| 1:A:4277:VAL:HG21 | 1:B:3732:ARG:HH22 | 1.78                     | 0.49              |
| 1:B:1300:VAL:CG1  | 1:B:1336:ARG:HD3  | 2.43                     | 0.49              |
| 1:B:1388:LEU:HG   | 1:B:1397:MET:HE1  | 1.95                     | 0.49              |
| 1:B:1486:GLN:HG3  | 1:B:1489:ARG:HH11 | 1.78                     | 0.49              |
| 1:B:3979:ILE:HG21 | 1:B:4019:ILE:HG23 | 1.93                     | 0.49              |
| 1:B:4560:GLU:HA   | 1:B:4563:LEU:HD12 | 1.93                     | 0.49              |
| 1:A:31:VAL:O      | 1:A:35:PRO:HD2    | 2.12                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:909:HIS:CD2   | 1:A:937:SER:HA    | 2.48                     | 0.49              |
| 1:A:1135:LEU:O    | 1:A:1139:PHE:HD2  | 1.96                     | 0.49              |
| 1:A:1453:LEU:HB3  | 1:A:1506:VAL:CG1  | 2.37                     | 0.49              |
| 1:A:2356:ILE:HD13 | 1:A:2377:LEU:HD13 | 1.94                     | 0.49              |
| 1:A:2363:ARG:HH11 | 1:A:2416:MET:HE1  | 1.76                     | 0.49              |
| 1:A:3988:LEU:H    | 1:A:3988:LEU:HD12 | 1.77                     | 0.49              |
| 1:B:2292:PHE:CE2  | 1:B:2386:ASP:HB3  | 2.47                     | 0.49              |
| 1:B:2295:ASN:HB3  | 1:B:2423:TYR:HB3  | 1.94                     | 0.49              |
| 1:B:3063:MET:HE2  | 1:B:3170:GLN:HG2  | 1.95                     | 0.49              |
| 1:B:3221:LYS:HD2  | 1:B:3224:TYR:HD2  | 1.76                     | 0.49              |
| 1:B:4130:ARG:O    | 1:B:4134:PHE:HD2  | 1.96                     | 0.49              |
| 2:D:60:GLY:HA2    | 2:D:64:ILE:HG12   | 1.94                     | 0.49              |
| 3:E:309:MET:O     | 3:E:313:ARG:HG2   | 2.12                     | 0.49              |
| 1:A:129:LEU:HA    | 1:A:132:LEU:HD12  | 1.94                     | 0.49              |
| 1:A:531:MET:HE1   | 1:A:535:LEU:HD11  | 1.94                     | 0.49              |
| 1:A:2405:ILE:HD12 | 1:A:2417:ILE:HD11 | 1.95                     | 0.49              |
| 1:A:2581:ALA:HB2  | 1:A:2588:LEU:HD22 | 1.95                     | 0.49              |
| 1:A:3412:LEU:HD22 | 1:A:3454:ILE:HD12 | 1.95                     | 0.49              |
| 1:A:3872:CYS:SG   | 1:A:3875:CYS:CB   | 2.93                     | 0.49              |
| 1:A:4692:LEU:HD21 | 1:A:4740:ILE:HG12 | 1.94                     | 0.49              |
| 1:B:1159:LEU:HD13 | 1:B:1298:LEU:HB2  | 1.94                     | 0.49              |
| 1:B:2040:LEU:HD11 | 1:B:2085:PRO:HB3  | 1.95                     | 0.49              |
| 1:B:2052:LEU:HD11 | 1:B:2060:ILE:HD12 | 1.95                     | 0.49              |
| 1:B:3309:PHE:HD2  | 1:B:3850:THR:HA   | 1.77                     | 0.49              |
| 1:A:396:ARG:HH21  | 1:B:404:GLN:HE22  | 1.61                     | 0.49              |
| 1:A:1666:PHE:HA   | 1:A:1669:THR:OG1  | 2.13                     | 0.49              |
| 1:A:2474:VAL:HG13 | 1:A:2477:ARG:HH21 | 1.78                     | 0.49              |
| 1:A:2548:LEU:HD11 | 1:A:2588:LEU:HA   | 1.95                     | 0.49              |
| 1:A:2555:LEU:HD23 | 1:A:2565:LEU:HD22 | 1.95                     | 0.49              |
| 1:A:3410:GLN:HE21 | 1:A:3857:ARG:HH11 | 1.60                     | 0.49              |
| 1:A:3548:SER:HA   | 1:A:3551:LYS:HE2  | 1.95                     | 0.49              |
| 1:A:4228:LEU:HD11 | 1:B:3829:LEU:HD22 | 1.95                     | 0.49              |
| 1:B:1151:SER:O    | 1:B:1154:ILE:HG12 | 2.13                     | 0.49              |
| 1:B:1930:LEU:HD13 | 1:B:2219:HIS:CB   | 2.42                     | 0.49              |
| 1:B:2982:LEU:HD11 | 1:B:3027:GLN:CB   | 2.43                     | 0.49              |
| 1:B:3735:ALA:O    | 1:B:3739:ILE:HG13 | 2.13                     | 0.49              |
| 3:F:309:MET:O     | 3:F:313:ARG:HG2   | 2.12                     | 0.49              |
| 1:A:1351:TYR:HA   | 1:A:1354:LEU:HD12 | 1.95                     | 0.49              |
| 1:A:3307:VAL:C    | 1:A:3309:PHE:N    | 2.71                     | 0.49              |
| 1:A:4001:VAL:C    | 1:A:4003:ILE:N    | 2.69                     | 0.49              |
| 1:B:946:ASN:O     | 1:B:947:ARG:C     | 2.56                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1673:PHE:HD1  | 1:B:1714:PHE:HA   | 1.78                     | 0.49              |
| 1:B:3226:GLN:HA   | 1:B:3289:ASN:ND2  | 2.28                     | 0.49              |
| 2:C:10:ILE:HG13   | 2:C:66:PHE:HZ     | 1.76                     | 0.49              |
| 2:D:100:TYR:CD1   | 2:D:136:GLN:HB2   | 2.48                     | 0.49              |
| 1:A:675:SER:HB3   | 1:A:722:LEU:HD12  | 1.95                     | 0.48              |
| 1:A:1515:LEU:HB2  | 1:A:1544:LEU:HB3  | 1.95                     | 0.48              |
| 1:A:1895:ARG:NH2  | 1:A:2180:VAL:HG11 | 2.27                     | 0.48              |
| 1:A:2373:ARG:NH2  | 1:A:2393:GLU:OE2  | 2.45                     | 0.48              |
| 1:A:4480:ALA:HB2  | 1:A:4521:ASN:OD1  | 2.12                     | 0.48              |
| 1:B:1355:ILE:HD13 | 1:B:1397:MET:HG2  | 1.93                     | 0.48              |
| 1:B:2266:MET:HE1  | 1:B:2659:ALA:HB2  | 1.93                     | 0.48              |
| 1:B:3412:LEU:HD22 | 1:B:3454:ILE:HD12 | 1.95                     | 0.48              |
| 1:B:4309:PHE:CE1  | 1:B:4338:ILE:HD11 | 2.48                     | 0.48              |
| 1:B:4314:ILE:HD11 | 1:B:4479:MET:HE1  | 1.95                     | 0.48              |
| 1:B:4485:LEU:HD12 | 1:B:4524:GLN:HG2  | 1.93                     | 0.48              |
| 3:E:3:ARG:HG2     | 3:E:18:ARG:HG2    | 1.93                     | 0.48              |
| 1:A:92:ILE:HD12   | 1:A:97:LEU:HA     | 1.94                     | 0.48              |
| 1:A:874:VAL:HG13  | 1:B:189:VAL:HG11  | 1.94                     | 0.48              |
| 1:A:1383:TYR:O    | 1:A:1387:GLN:HG2  | 2.13                     | 0.48              |
| 1:A:1515:LEU:CD2  | 1:A:1555:GLN:HG3  | 2.43                     | 0.48              |
| 1:A:3521:GLU:N    | 1:B:3791:SER:O    | 2.46                     | 0.48              |
| 1:B:272:ARG:HD2   | 1:B:338:TYR:CE1   | 2.47                     | 0.48              |
| 1:B:313:LEU:HD21  | 1:B:332:LEU:HD21  | 1.95                     | 0.48              |
| 1:B:1118:LEU:HD13 | 1:B:1273:LEU:HB2  | 1.94                     | 0.48              |
| 1:B:1374:GLU:O    | 1:B:1375:SER:C    | 2.56                     | 0.48              |
| 1:B:1536:GLU:O    | 1:B:1540:VAL:HG23 | 2.13                     | 0.48              |
| 1:B:1859:MET:HE2  | 1:B:2230:MET:CB   | 2.44                     | 0.48              |
| 1:B:2676:ASN:C    | 1:B:2678:ALA:N    | 2.70                     | 0.48              |
| 1:B:3410:GLN:NE2  | 1:B:3853:ALA:HB2  | 2.28                     | 0.48              |
| 2:C:106:LEU:CD2   | 2:C:126:ILE:CD1   | 2.80                     | 0.48              |
| 2:D:16:ALA:O      | 2:D:20:PHE:HD2    | 1.95                     | 0.48              |
| 1:A:334:LEU:HD11  | 1:A:409:LEU:HD13  | 1.95                     | 0.48              |
| 1:A:1682:HIS:HE1  | 1:A:2383:ARG:HB2  | 1.76                     | 0.48              |
| 1:A:3108:TYR:O    | 1:A:3112:GLN:HG2  | 2.13                     | 0.48              |
| 1:A:4602:ASN:HA   | 1:A:4607:ARG:HE   | 1.77                     | 0.48              |
| 1:B:711:TYR:CD2   | 1:B:887:PRO:HA    | 2.48                     | 0.48              |
| 1:B:811:LEU:HD23  | 1:B:933:TYR:HE1   | 1.77                     | 0.48              |
| 1:B:857:ARG:O     | 1:B:861:ILE:HG13  | 2.13                     | 0.48              |
| 1:B:1384:LEU:HB3  | 1:B:1430:PHE:CE1  | 2.47                     | 0.48              |
| 1:B:1555:GLN:HA   | 1:B:1558:ASN:ND2  | 2.26                     | 0.48              |
| 1:B:4101:TYR:OH   | 2:D:85:GLU:HB2    | 2.14                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:4238:LEU:CG   | 1:B:4287:THR:HG21 | 2.38                     | 0.48              |
| 1:A:548:LEU:HD13  | 1:A:642:LYS:C     | 2.38                     | 0.48              |
| 1:A:1190:PRO:HG2  | 1:A:1195:LEU:HD21 | 1.95                     | 0.48              |
| 1:A:1459:VAL:HG21 | 1:A:1464:LEU:HD13 | 1.95                     | 0.48              |
| 1:A:1899:MET:CE   | 1:A:2233:LEU:HB2  | 2.43                     | 0.48              |
| 1:A:2118:VAL:HA   | 1:A:2644:PRO:HA   | 1.94                     | 0.48              |
| 1:A:3045:ARG:NH2  | 1:A:3153:PHE:HB2  | 2.28                     | 0.48              |
| 1:A:3226:GLN:HA   | 1:A:3289:ASN:ND2  | 2.27                     | 0.48              |
| 1:A:4252:GLU:O    | 1:A:4256:ARG:HG3  | 2.13                     | 0.48              |
| 1:A:4641:TYR:CD1  | 1:A:4655:ASP:HA   | 2.48                     | 0.48              |
| 1:B:3095:VAL:HG12 | 1:B:3190:TRP:HZ3  | 1.76                     | 0.48              |
| 1:B:4020:LEU:O    | 1:B:4024:ILE:HG13 | 2.13                     | 0.48              |
| 1:B:4258:PHE:O    | 1:B:4261:ARG:N    | 2.44                     | 0.48              |
| 1:B:4696:LYS:O    | 1:B:4699:ILE:HG22 | 2.13                     | 0.48              |
| 1:A:422:LEU:HD11  | 1:A:537:LEU:HD23  | 1.95                     | 0.48              |
| 1:A:1665:THR:O    | 1:A:1669:THR:HG23 | 2.13                     | 0.48              |
| 1:A:2296:GLN:HE21 | 1:A:2347:MET:HE1  | 1.77                     | 0.48              |
| 1:A:2320:ARG:HH21 | 3:E:68:GLU:HB3    | 1.78                     | 0.48              |
| 1:A:3212:LYS:HA   | 1:A:3215:LEU:HG   | 1.94                     | 0.48              |
| 1:A:3922:ARG:NH1  | 1:A:3970:TYR:OH   | 2.46                     | 0.48              |
| 1:B:2025:ILE:CD1  | 1:B:2075:MET:HE3  | 2.44                     | 0.48              |
| 1:B:2301:VAL:HG21 | 1:B:2422:ILE:HG21 | 1.95                     | 0.48              |
| 1:B:2564:ASP:OD1  | 1:B:2631:LYS:CB   | 2.45                     | 0.48              |
| 1:B:3309:PHE:CE1  | 1:B:3411:PHE:HB3  | 2.48                     | 0.48              |
| 1:A:411:ALA:O     | 1:A:412:TRP:C     | 2.56                     | 0.48              |
| 1:A:1030:MET:HE3  | 1:A:1035:ILE:HD13 | 1.96                     | 0.48              |
| 1:A:1118:LEU:HA   | 1:A:1121:ILE:HD12 | 1.95                     | 0.48              |
| 1:A:2189:VAL:HG21 | 1:A:2230:MET:HE1  | 1.92                     | 0.48              |
| 1:A:2480:VAL:HA   | 1:A:2524:GLN:HG3  | 1.95                     | 0.48              |
| 1:A:2578:ARG:HD2  | 1:A:2659:ALA:HA   | 1.96                     | 0.48              |
| 1:A:3161:THR:O    | 1:A:3165:LEU:HG   | 2.14                     | 0.48              |
| 1:A:3418:GLU:HG2  | 1:A:3461:TYR:CE1  | 2.49                     | 0.48              |
| 1:A:3521:GLU:CG   | 1:B:3793:ASN:HA   | 2.37                     | 0.48              |
| 1:B:255:LYS:HG2   | 1:B:258:ARG:NH2   | 2.29                     | 0.48              |
| 1:B:740:PHE:CD1   | 1:B:778:GLU:HG3   | 2.48                     | 0.48              |
| 1:B:1009:ILE:O    | 1:B:1013:LEU:HG   | 2.14                     | 0.48              |
| 1:B:1094:PHE:HB3  | 1:B:1161:ALA:HB1  | 1.93                     | 0.48              |
| 1:B:4311:ALA:O    | 1:B:4315:GLU:HG2  | 2.13                     | 0.48              |
| 2:D:20:PHE:CD2    | 2:D:36:VAL:HG22   | 2.49                     | 0.48              |
| 3:F:112:ILE:HG22  | 3:F:136:HIS:CE1   | 2.48                     | 0.48              |
| 1:A:349:ILE:CD1   | 1:A:424:LEU:HD13  | 2.43                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1404:SER:HB2  | 1:A:1406:GLU:HG2  | 1.95                     | 0.48              |
| 1:A:2300:ASP:HB2  | 1:A:3583:ARG:HH22 | 1.79                     | 0.48              |
| 1:A:3063:MET:HE1  | 1:A:3167:LEU:HD12 | 1.95                     | 0.48              |
| 1:A:4071:TRP:O    | 1:A:4075:LEU:HD12 | 2.13                     | 0.48              |
| 1:B:1427:VAL:HG13 | 1:B:1431:PHE:CE2  | 2.47                     | 0.48              |
| 1:B:1428:LEU:HD13 | 1:B:1491:LEU:HB2  | 1.94                     | 0.48              |
| 1:B:1428:LEU:HB3  | 1:B:1491:LEU:HB3  | 1.95                     | 0.48              |
| 1:B:1457:ALA:H    | 1:B:1510:VAL:HG22 | 1.78                     | 0.48              |
| 1:B:3308:SER:HA   | 1:B:3319:LEU:HD13 | 1.96                     | 0.48              |
| 1:A:284:ILE:HG22  | 1:A:286:PRO:HD2   | 1.96                     | 0.48              |
| 1:A:948:LEU:HG    | 1:A:953:CYS:SG    | 2.54                     | 0.48              |
| 1:A:4325:TYR:CZ   | 1:A:4495:ILE:HA   | 2.48                     | 0.48              |
| 1:B:286:PRO:HB3   | 1:B:295:VAL:CG2   | 2.41                     | 0.48              |
| 1:B:1194:LYS:HA   | 1:B:1370:SER:C    | 2.38                     | 0.48              |
| 1:B:1256:ILE:HG12 | 1:B:1259:GLU:H    | 1.78                     | 0.48              |
| 1:B:1551:ALA:O    | 1:B:1554:LEU:HD22 | 2.14                     | 0.48              |
| 1:B:1924:LEU:HD23 | 1:B:1944:ARG:HA   | 1.95                     | 0.48              |
| 1:B:1925:GLN:HB2  | 1:B:1945:LEU:HD21 | 1.96                     | 0.48              |
| 1:B:4071:TRP:O    | 1:B:4075:LEU:HD12 | 2.13                     | 0.48              |
| 2:C:52:MET:O      | 2:C:56:VAL:HG22   | 2.13                     | 0.48              |
| 1:A:738:ALA:HB3   | 1:A:741:SER:HB3   | 1.96                     | 0.48              |
| 1:A:857:ARG:O     | 1:A:861:ILE:HG13  | 2.14                     | 0.48              |
| 1:A:1027:SER:N    | 1:A:1028:PRO:HD2  | 2.29                     | 0.48              |
| 1:A:1859:MET:HE2  | 1:A:2230:MET:CB   | 2.44                     | 0.48              |
| 1:A:2405:ILE:CD1  | 1:A:2417:ILE:HD11 | 2.44                     | 0.48              |
| 1:A:3930:CYS:HB3  | 1:A:3981:LYS:HG3  | 1.95                     | 0.48              |
| 1:A:4307:LYS:CD   | 1:A:4479:MET:HA   | 2.44                     | 0.48              |
| 1:A:4438:MET:HE3  | 1:A:4440:ILE:HD11 | 1.95                     | 0.48              |
| 1:B:836:ILE:O     | 1:B:840:LEU:HG    | 2.14                     | 0.48              |
| 1:B:1082:SER:HA   | 1:B:1085:TYR:HB3  | 1.96                     | 0.48              |
| 1:B:1237:ASN:HA   | 1:B:1285:LYS:HD2  | 1.96                     | 0.48              |
| 2:C:65:ASP:H      | 2:C:68:GLU:HB3    | 1.78                     | 0.48              |
| 1:A:913:GLU:CD    | 1:A:913:GLU:H     | 2.20                     | 0.48              |
| 1:A:1022:GLN:C    | 1:A:1024:SER:N    | 2.71                     | 0.48              |
| 1:A:1434:LEU:CD1  | 1:A:1449:LEU:HD12 | 2.44                     | 0.48              |
| 1:A:1601:SER:N    | 1:A:2481:SER:HB3  | 2.29                     | 0.48              |
| 1:A:1902:LEU:HD21 | 1:A:1967:LEU:HD13 | 1.96                     | 0.48              |
| 1:A:2517:ALA:HB3  | 1:A:2522:GLN:HG2  | 1.94                     | 0.48              |
| 1:A:2985:LEU:HD12 | 1:A:2988:LEU:HD13 | 1.95                     | 0.48              |
| 1:A:3226:GLN:OE1  | 1:A:3227:LEU:HD22 | 2.14                     | 0.48              |
| 1:A:3532:CYS:O    | 1:A:3536:ASN:HB3  | 2.14                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:97:LEU:HD13   | 1:B:201:PHE:HZ    | 1.79                     | 0.48              |
| 1:B:1278:LEU:HB3  | 1:B:1281:ALA:CB   | 2.38                     | 0.48              |
| 1:B:1895:ARG:HH22 | 1:B:2180:VAL:HG11 | 1.78                     | 0.48              |
| 1:B:2220:THR:CG2  | 1:B:2224:GLU:HA   | 2.44                     | 0.48              |
| 1:B:4021:GLN:HG2  | 1:B:4025:LYS:HE2  | 1.96                     | 0.48              |
| 1:B:4665:ILE:O    | 1:B:4669:ILE:HG13 | 2.14                     | 0.48              |
| 1:A:1177:LEU:HG   | 1:A:1233:TRP:CD2  | 2.48                     | 0.47              |
| 1:A:2040:LEU:HD11 | 1:A:2085:PRO:HB3  | 1.95                     | 0.47              |
| 1:B:296:ARG:HA    | 1:B:299:PHE:CD2   | 2.49                     | 0.47              |
| 1:B:1319:LEU:HD22 | 1:B:1354:LEU:HD21 | 1.96                     | 0.47              |
| 1:B:1921:ILE:HD11 | 1:B:1969:VAL:HG11 | 1.96                     | 0.47              |
| 1:B:2405:ILE:HG13 | 1:B:2417:ILE:HD11 | 1.96                     | 0.47              |
| 1:B:3516:LEU:HD11 | 1:B:3760:LEU:HD21 | 1.95                     | 0.47              |
| 1:A:1693:CYS:HB3  | 1:A:1716:CYS:HB2  | 1.95                     | 0.47              |
| 1:A:4596:MET:O    | 1:A:4600:GLN:HG2  | 2.14                     | 0.47              |
| 1:B:303:VAL:HG22  | 1:B:377:ILE:CG1   | 2.44                     | 0.47              |
| 1:B:347:MET:HE2   | 1:B:351:HIS:HE1   | 1.80                     | 0.47              |
| 1:B:863:ASP:HB2   | 1:B:1009:ILE:HG12 | 1.96                     | 0.47              |
| 1:B:908:TYR:CD2   | 1:B:908:TYR:N     | 2.81                     | 0.47              |
| 1:B:1412:MET:HB3  | 1:B:1463:ARG:HE   | 1.78                     | 0.47              |
| 1:B:3226:GLN:OE1  | 1:B:3227:LEU:HD22 | 2.14                     | 0.47              |
| 1:A:92:ILE:HG21   | 1:A:100:VAL:HG21  | 1.96                     | 0.47              |
| 1:A:273:PHE:HD2   | 1:A:338:TYR:HB2   | 1.79                     | 0.47              |
| 1:A:786:PHE:HE1   | 1:A:806:LEU:HD13  | 1.78                     | 0.47              |
| 1:A:864:TYR:HA    | 1:A:936:LEU:HD21  | 1.97                     | 0.47              |
| 1:A:906:PRO:HG2   | 1:A:908:TYR:CE2   | 2.49                     | 0.47              |
| 1:A:3142:ARG:O    | 1:A:3146:LYS:HG3  | 2.14                     | 0.47              |
| 1:A:4119:LEU:HD23 | 3:E:329:VAL:HG21  | 1.96                     | 0.47              |
| 1:B:1831:ALA:O    | 1:B:2568:GLU:HG2  | 2.14                     | 0.47              |
| 1:B:2405:ILE:CD1  | 1:B:2417:ILE:HD11 | 2.44                     | 0.47              |
| 1:B:3440:SER:OG   | 1:B:3443:GLN:OE1  | 2.20                     | 0.47              |
| 1:B:3747:ASP:O    | 1:B:3750:TYR:HB3  | 2.14                     | 0.47              |
| 1:A:137:CYS:O     | 1:A:240:ILE:HG23  | 2.13                     | 0.47              |
| 1:A:799:VAL:HB    | 1:A:851:VAL:HG11  | 1.96                     | 0.47              |
| 1:A:1023:LEU:HD22 | 1:A:1038:THR:HG23 | 1.96                     | 0.47              |
| 1:A:1176:TYR:CD1  | 1:A:1281:ALA:HB3  | 2.50                     | 0.47              |
| 1:A:1570:TYR:C    | 1:A:1570:TYR:CD2  | 2.93                     | 0.47              |
| 1:A:2025:ILE:CD1  | 1:A:2075:MET:HE3  | 2.44                     | 0.47              |
| 1:A:2704:VAL:O    | 1:A:2974:ARG:NH2  | 2.47                     | 0.47              |
| 1:A:3175:THR:HA   | 1:A:3181:ILE:HG13 | 1.95                     | 0.47              |
| 1:B:1500:VAL:HG13 | 1:B:1547:ALA:HA   | 1.95                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2181:GLN:HG3  | 1:B:2188:LEU:CD1  | 2.44                     | 0.47              |
| 1:B:2688:CYS:O    | 1:B:2689:PRO:C    | 2.56                     | 0.47              |
| 1:B:2982:LEU:HD11 | 1:B:3027:GLN:HG3  | 1.96                     | 0.47              |
| 1:B:3950:LYS:HG2  | 1:B:3971:GLU:OE1  | 2.15                     | 0.47              |
| 1:B:4745:ILE:CD1  | 1:B:4771:LEU:HD13 | 2.45                     | 0.47              |
| 2:C:28:ILE:HG22   | 2:C:32:GLU:HG2    | 1.96                     | 0.47              |
| 3:F:325:LEU:O     | 3:F:329:VAL:HG23  | 2.15                     | 0.47              |
| 1:A:29:TRP:CD1    | 1:A:160:LEU:HD21  | 2.50                     | 0.47              |
| 1:A:984:ARG:HG2   | 1:A:989:LYS:HB2   | 1.97                     | 0.47              |
| 1:A:1825:ASN:HB3  | 1:A:2475:LEU:HD23 | 1.96                     | 0.47              |
| 1:A:4413:LYS:CD   | 1:A:4456:ILE:HD11 | 2.45                     | 0.47              |
| 1:B:239:PHE:O     | 1:B:243:ASN:ND2   | 2.48                     | 0.47              |
| 1:B:345:THR:O     | 1:B:349:ILE:HG12  | 2.14                     | 0.47              |
| 1:B:1576:VAL:HA   | 1:B:1579:LYS:HD2  | 1.96                     | 0.47              |
| 1:B:1909:ARG:HB3  | 1:B:1911:HIS:CD2  | 2.49                     | 0.47              |
| 1:B:3173:LYS:HA   | 1:B:3216:PHE:HZ   | 1.78                     | 0.47              |
| 1:B:3418:GLU:HG2  | 1:B:3461:TYR:CE1  | 2.49                     | 0.47              |
| 1:B:3884:ILE:HD11 | 1:B:3913:ASN:HD22 | 1.80                     | 0.47              |
| 2:C:49:LEU:CD1    | 2:C:53:ILE:HD12   | 2.45                     | 0.47              |
| 1:A:3588:ARG:HG3  | 1:A:3648:TYR:CZ   | 2.49                     | 0.47              |
| 1:A:3772:PRO:HG2  | 1:B:3918:ALA:HA   | 1.95                     | 0.47              |
| 1:A:4424:VAL:HA   | 1:A:4459:LEU:HD21 | 1.96                     | 0.47              |
| 1:A:4547:GLU:HG2  | 1:A:4605:PHE:CE2  | 2.49                     | 0.47              |
| 1:B:694:ASP:CG    | 1:B:750:HIS:HB3   | 2.40                     | 0.47              |
| 1:B:963:TYR:OH    | 1:B:1013:LEU:HB3  | 2.15                     | 0.47              |
| 1:B:2368:ILE:CD1  | 1:B:2387:PHE:CZ   | 2.93                     | 0.47              |
| 1:B:3548:SER:HA   | 1:B:3551:LYS:HE2  | 1.95                     | 0.47              |
| 1:B:4125:HIS:HA   | 1:B:4165:LEU:HD12 | 1.96                     | 0.47              |
| 1:A:270:ILE:O     | 1:A:274:GLN:HG3   | 2.14                     | 0.47              |
| 1:A:327:GLN:NE2   | 1:A:512:MET:SD    | 2.88                     | 0.47              |
| 1:A:710:LEU:HG    | 1:A:714:ASN:HD21  | 1.80                     | 0.47              |
| 1:A:860:LEU:HB2   | 1:A:1005:ILE:HD13 | 1.96                     | 0.47              |
| 1:A:1039:LEU:CD2  | 1:A:1089:ILE:HD13 | 2.44                     | 0.47              |
| 1:A:1159:LEU:CD2  | 1:A:1305:MET:HB3  | 2.45                     | 0.47              |
| 1:A:1388:LEU:O    | 1:A:1394:ARG:NE   | 2.46                     | 0.47              |
| 1:A:1708:TYR:HB3  | 1:A:2353:ARG:NH2  | 2.30                     | 0.47              |
| 1:A:2356:ILE:HG13 | 1:A:2379:LEU:HD13 | 1.95                     | 0.47              |
| 1:A:3455:TRP:CZ3  | 1:A:3458:LEU:HD22 | 2.50                     | 0.47              |
| 1:A:3530:ASP:O    | 1:A:3531:PRO:C    | 2.58                     | 0.47              |
| 1:A:3884:ILE:HD11 | 1:A:3913:ASN:HD22 | 1.79                     | 0.47              |
| 1:A:4071:TRP:CE2  | 1:A:4075:LEU:HD11 | 2.49                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:4307:LYS:NZ   | 1:A:4478:VAL:HB   | 2.30                     | 0.47              |
| 1:A:4533:LEU:HB2  | 1:A:4587:LEU:HB3  | 1.96                     | 0.47              |
| 1:B:49:LEU:O      | 1:B:51:GLN:N      | 2.48                     | 0.47              |
| 1:B:544:LYS:O     | 1:B:548:LEU:HG    | 2.14                     | 0.47              |
| 1:B:549:GLN:O     | 1:B:553:LYS:HG2   | 2.14                     | 0.47              |
| 1:B:755:SER:O     | 1:B:759:ARG:HG3   | 2.14                     | 0.47              |
| 1:B:1094:PHE:CE1  | 1:B:1162:THR:HA   | 2.50                     | 0.47              |
| 1:B:1909:ARG:HB3  | 1:B:1911:HIS:NE2  | 2.30                     | 0.47              |
| 1:B:3034:MET:SD   | 1:B:3034:MET:N    | 2.87                     | 0.47              |
| 1:B:3098:CYS:SG   | 1:B:3167:LEU:HD22 | 2.55                     | 0.47              |
| 1:B:3417:LEU:HD13 | 1:B:3461:TYR:CD2  | 2.50                     | 0.47              |
| 1:B:3515:THR:O    | 1:B:3519:LEU:HG   | 2.15                     | 0.47              |
| 1:B:4109:LEU:CD1  | 1:B:4114:LYS:HB2  | 2.45                     | 0.47              |
| 1:B:4267:LEU:O    | 1:B:4271:LEU:HG   | 2.15                     | 0.47              |
| 1:B:4413:LYS:HD3  | 1:B:4456:ILE:HD11 | 1.97                     | 0.47              |
| 1:B:4615:GLY:HA2  | 1:B:4618:ARG:HD2  | 1.97                     | 0.47              |
| 1:A:310:LEU:HD11  | 1:A:383:GLU:HG2   | 1.97                     | 0.47              |
| 1:A:793:ASN:O     | 1:A:797:GLY:N     | 2.48                     | 0.47              |
| 1:B:45:GLU:O      | 1:B:46:MET:C      | 2.58                     | 0.47              |
| 1:B:283:PHE:HB3   | 1:B:443:ARG:NH2   | 2.30                     | 0.47              |
| 1:B:1126:ALA:HB1  | 1:B:1262:ILE:HG23 | 1.96                     | 0.47              |
| 1:B:1896:ARG:HA   | 1:B:1955:LEU:O    | 2.15                     | 0.47              |
| 1:B:3969:GLN:O    | 1:B:3973:LEU:HG   | 2.15                     | 0.47              |
| 1:B:4525:LEU:HB3  | 1:B:4532:THR:HG21 | 1.97                     | 0.47              |
| 2:C:66:PHE:HB3    | 2:C:67:PRO:HD3    | 1.97                     | 0.47              |
| 3:F:65:TYR:HB3    | 3:F:70:PHE:HE2    | 1.80                     | 0.47              |
| 1:A:191:MET:N     | 1:A:191:MET:SD    | 2.88                     | 0.47              |
| 1:A:271:ASN:N     | 1:A:271:ASN:HD22  | 2.13                     | 0.47              |
| 1:A:292:ALA:HB1   | 1:A:346:CYS:HB2   | 1.95                     | 0.47              |
| 1:A:315:LEU:O     | 1:A:317:VAL:HG23  | 2.15                     | 0.47              |
| 1:A:1048:SER:O    | 1:A:1049:SER:C    | 2.55                     | 0.47              |
| 1:A:1515:LEU:HD11 | 1:A:1556:LEU:HD23 | 1.97                     | 0.47              |
| 1:A:1594:GLU:HG2  | 1:A:1595:CYS:N    | 2.30                     | 0.47              |
| 1:A:1921:ILE:HD11 | 1:A:1969:VAL:HG11 | 1.96                     | 0.47              |
| 1:A:3284:ALA:HA   | 1:A:3331:LYS:HD2  | 1.97                     | 0.47              |
| 1:B:285:MET:N     | 1:B:286:PRO:HD2   | 2.30                     | 0.47              |
| 1:B:733:GLN:HA    | 1:B:738:ALA:HB2   | 1.96                     | 0.47              |
| 1:B:1356:THR:HA   | 1:B:1400:PHE:CE2  | 2.50                     | 0.47              |
| 1:B:3190:TRP:CD1  | 1:B:3190:TRP:H    | 2.33                     | 0.47              |
| 1:B:3848:GLN:HE21 | 1:B:3849:PRO:HD2  | 1.80                     | 0.47              |
| 1:B:4071:TRP:CE2  | 1:B:4075:LEU:HD11 | 2.49                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:F:113:CYS:HB3   | 3:F:120:ASP:O     | 2.15                     | 0.47              |
| 3:F:120:ASP:HB3   | 3:F:123:HIS:HB2   | 1.97                     | 0.47              |
| 1:A:506:PRO:HG3   | 1:A:526:ASP:OD2   | 2.14                     | 0.47              |
| 1:A:530:LEU:O     | 1:A:534:LEU:HG    | 2.14                     | 0.47              |
| 1:A:1570:TYR:CD2  | 1:A:1592:ILE:HG21 | 2.50                     | 0.47              |
| 1:A:1875:MET:HG2  | 1:A:1877:TYR:CZ   | 2.50                     | 0.47              |
| 1:A:2122:LEU:HD23 | 1:A:2136:ILE:HD11 | 1.96                     | 0.47              |
| 1:A:2223:ASN:HB2  | 1:A:2225:GLN:HG3  | 1.97                     | 0.47              |
| 1:A:2479:VAL:HG21 | 1:A:2521:VAL:HG13 | 1.97                     | 0.47              |
| 1:A:3292:LYS:O    | 1:A:3295:ILE:HG22 | 2.15                     | 0.47              |
| 1:A:4006:PRO:HG2  | 1:B:3507:HIS:O    | 2.14                     | 0.47              |
| 1:A:4135:THR:H    | 1:A:4142:ARG:HD3  | 1.79                     | 0.47              |
| 1:B:1431:PHE:O    | 1:B:1435:PHE:HD2  | 1.98                     | 0.47              |
| 1:B:2202:ILE:HG21 | 1:B:2232:LEU:HD11 | 1.97                     | 0.47              |
| 1:B:2405:ILE:HD12 | 1:B:2417:ILE:HD11 | 1.96                     | 0.47              |
| 1:B:2701:LEU:HD13 | 1:B:3002:VAL:HG13 | 1.95                     | 0.47              |
| 1:A:82:THR:HB     | 1:A:132:LEU:HD22  | 1.96                     | 0.46              |
| 1:A:485:THR:O     | 1:A:489:GLN:HG2   | 2.15                     | 0.46              |
| 1:A:1233:TRP:HH2  | 1:A:1281:ALA:CB   | 2.27                     | 0.46              |
| 1:A:1453:LEU:CB   | 1:A:1506:VAL:HG13 | 2.38                     | 0.46              |
| 1:A:3766:LYS:HB3  | 1:A:3795:TYR:CE2  | 2.50                     | 0.46              |
| 1:B:3090:LEU:CD1  | 1:B:3184:PRO:HB3  | 2.43                     | 0.46              |
| 1:B:4112:ARG:NH2  | 2:D:128:GLU:HB3   | 2.30                     | 0.46              |
| 2:D:70:LEU:O      | 2:D:73:MET:HG2    | 2.15                     | 0.46              |
| 1:A:260:CYS:O     | 1:A:263:LEU:HG    | 2.15                     | 0.46              |
| 1:A:317:VAL:O     | 1:A:318:LEU:HG    | 2.15                     | 0.46              |
| 1:A:318:LEU:HD13  | 1:A:329:VAL:HG11  | 1.97                     | 0.46              |
| 1:A:1194:LYS:HA   | 1:A:1370:SER:C    | 2.41                     | 0.46              |
| 1:A:1295:THR:O    | 1:A:1299:ILE:HG13 | 2.15                     | 0.46              |
| 1:A:1571:LEU:C    | 1:A:1573:GLN:H    | 2.23                     | 0.46              |
| 1:A:3417:LEU:HD13 | 1:A:3461:TYR:CD2  | 2.49                     | 0.46              |
| 1:A:3456:PRO:HA   | 1:A:3496:ILE:HD11 | 1.96                     | 0.46              |
| 1:B:986:LYS:HG3   | 1:B:1113:HIS:CE1  | 2.50                     | 0.46              |
| 1:B:1963:LYS:HD3  | 1:B:1966:TYR:CZ   | 2.50                     | 0.46              |
| 1:B:3905:LEU:HD23 | 1:B:3932:LEU:HD11 | 1.96                     | 0.46              |
| 1:B:4128:TRP:O    | 1:B:4129:LEU:C    | 2.57                     | 0.46              |
| 1:B:4710:TRP:O    | 1:B:4714:LEU:HG   | 2.15                     | 0.46              |
| 1:A:1159:LEU:HD23 | 1:A:1305:MET:HB3  | 1.98                     | 0.46              |
| 1:A:1431:PHE:O    | 1:A:1435:PHE:HD2  | 1.98                     | 0.46              |
| 1:A:1525:MET:SD   | 1:A:1534:PHE:HA   | 2.56                     | 0.46              |
| 1:A:2523:GLN:HA   | 1:A:2526:LYS:HD2  | 1.97                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2700:ALA:O    | 1:A:2704:VAL:HG13 | 2.14                     | 0.46              |
| 1:A:3301:LEU:HD23 | 1:A:3301:LEU:HA   | 1.76                     | 0.46              |
| 1:A:3419:SER:HB3  | 1:A:3425:ARG:CG   | 2.46                     | 0.46              |
| 1:A:3749:VAL:HG21 | 1:A:3817:ILE:HD12 | 1.97                     | 0.46              |
| 1:A:3887:LEU:HD13 | 1:A:3905:LEU:HD21 | 1.97                     | 0.46              |
| 1:A:4328:PRO:HB2  | 1:A:4332:PHE:HE2  | 1.79                     | 0.46              |
| 1:B:341:VAL:HB    | 1:B:417:SER:CB    | 2.45                     | 0.46              |
| 1:B:470:GLY:O     | 1:B:474:VAL:HG23  | 2.15                     | 0.46              |
| 1:B:765:GLN:HE22  | 1:B:817:ILE:HG23  | 1.80                     | 0.46              |
| 1:B:1019:TYR:OH   | 1:B:1038:THR:HA   | 2.15                     | 0.46              |
| 1:B:2053:PHE:O    | 1:B:2138:ARG:HD2  | 2.15                     | 0.46              |
| 1:B:3456:PRO:HA   | 1:B:3496:ILE:HD11 | 1.96                     | 0.46              |
| 1:A:273:PHE:CD2   | 1:A:338:TYR:HB2   | 2.51                     | 0.46              |
| 1:A:471:VAL:HG21  | 1:A:641:ARG:HG2   | 1.98                     | 0.46              |
| 1:A:847:GLN:HG3   | 1:A:976:ALA:HB2   | 1.98                     | 0.46              |
| 1:A:1058:LEU:HD23 | 1:A:1061:GLN:NE2  | 2.29                     | 0.46              |
| 1:A:3527:LEU:HD21 | 1:A:3757:ARG:HD3  | 1.97                     | 0.46              |
| 1:A:3536:ASN:HD21 | 1:A:3815:SER:HB2  | 1.80                     | 0.46              |
| 1:A:4101:TYR:HA   | 1:A:4104:ARG:HB2  | 1.97                     | 0.46              |
| 1:A:4195:HIS:NE2  | 2:C:35:THR:HG21   | 2.30                     | 0.46              |
| 1:B:274:GLN:O     | 1:B:277:VAL:HG22  | 2.16                     | 0.46              |
| 1:B:471:VAL:O     | 1:B:475:ILE:HG12  | 2.15                     | 0.46              |
| 1:B:1159:LEU:CA   | 1:B:1298:LEU:HD13 | 2.35                     | 0.46              |
| 1:B:2262:VAL:HG13 | 1:B:2265:ILE:HD12 | 1.97                     | 0.46              |
| 1:B:2509:ALA:HB2  | 1:B:2528:LEU:HD23 | 1.97                     | 0.46              |
| 1:B:2985:LEU:HD23 | 1:B:2988:LEU:HD22 | 1.97                     | 0.46              |
| 1:B:3053:LEU:HD13 | 1:B:3160:LEU:CD1  | 2.45                     | 0.46              |
| 1:B:3419:SER:HB3  | 1:B:3425:ARG:CG   | 2.46                     | 0.46              |
| 1:B:3455:TRP:CZ3  | 1:B:3458:LEU:HD22 | 2.50                     | 0.46              |
| 1:B:4128:TRP:CZ2  | 3:F:328:LEU:HD21  | 2.51                     | 0.46              |
| 1:B:4750:LYS:O    | 1:B:4754:VAL:HG23 | 2.15                     | 0.46              |
| 1:A:71:GLU:HB2    | 1:A:72:PRO:HD3    | 1.97                     | 0.46              |
| 1:A:718:VAL:HG12  | 1:A:763:ILE:HD12  | 1.97                     | 0.46              |
| 1:A:862:PHE:O     | 1:A:866:LEU:HG    | 2.15                     | 0.46              |
| 1:A:984:ARG:HH11  | 1:A:984:ARG:CB    | 2.24                     | 0.46              |
| 1:A:1233:TRP:CE3  | 1:A:1278:LEU:HD13 | 2.51                     | 0.46              |
| 1:A:1963:LYS:HD3  | 1:A:1966:TYR:CZ   | 2.50                     | 0.46              |
| 1:A:2194:PRO:HG2  | 1:A:2251:TYR:OH   | 2.16                     | 0.46              |
| 1:B:89:CYS:SG     | 1:B:239:PHE:CD2   | 2.97                     | 0.46              |
| 1:B:284:ILE:O     | 1:B:441:ALA:N     | 2.48                     | 0.46              |
| 1:B:387:MET:O     | 1:B:390:GLN:HG2   | 2.15                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:658:ILE:O     | 1:B:662:MET:HB2   | 2.16                     | 0.46              |
| 1:B:3001:GLN:NE2  | 1:B:3138:PRO:CD   | 2.78                     | 0.46              |
| 1:B:3021:LEU:HD12 | 1:B:3024:LEU:HD23 | 1.97                     | 0.46              |
| 1:B:4632:GLN:HA   | 1:B:4681:LEU:HD21 | 1.98                     | 0.46              |
| 3:E:302:SER:OG    | 3:E:305:GLU:HB3   | 2.16                     | 0.46              |
| 3:F:324:LEU:O     | 3:F:328:LEU:HG    | 2.16                     | 0.46              |
| 1:A:104:CYS:SG    | 1:A:136:LEU:HD22  | 2.56                     | 0.46              |
| 1:A:349:ILE:HG23  | 1:A:429:LEU:HD11  | 1.96                     | 0.46              |
| 1:A:735:LEU:HD13  | 1:A:753:SER:HA    | 1.96                     | 0.46              |
| 1:A:847:GLN:HG3   | 1:A:976:ALA:CB    | 2.46                     | 0.46              |
| 1:A:1203:ALA:O    | 1:A:1204:ILE:C    | 2.57                     | 0.46              |
| 1:A:1428:LEU:CD1  | 1:A:1488:ASN:HA   | 2.46                     | 0.46              |
| 1:B:1561:VAL:CG2  | 1:B:1810:LEU:HD22 | 2.43                     | 0.46              |
| 1:B:2264:SER:HB3  | 1:B:2652:HIS:CE1  | 2.51                     | 0.46              |
| 1:B:2307:ASP:HB2  | 1:B:2336:PHE:HB2  | 1.97                     | 0.46              |
| 1:B:2368:ILE:CG2  | 1:B:2377:LEU:HD11 | 2.43                     | 0.46              |
| 2:D:6:THR:HG23    | 2:D:9:GLN:H       | 1.79                     | 0.46              |
| 3:E:28:TYR:CE2    | 3:E:122:ASN:HB3   | 2.51                     | 0.46              |
| 1:A:280:ASN:HD22  | 1:A:523:ARG:HH11  | 1.64                     | 0.46              |
| 1:A:283:PHE:HA    | 1:A:442:LEU:O     | 2.16                     | 0.46              |
| 1:A:963:TYR:OH    | 1:A:1013:LEU:HB3  | 2.16                     | 0.46              |
| 1:A:3910:PHE:HB2  | 1:A:3929:MET:HE1  | 1.97                     | 0.46              |
| 1:A:4001:VAL:C    | 1:A:4003:ILE:H    | 2.22                     | 0.46              |
| 1:A:4232:LEU:HD13 | 1:B:3750:TYR:CB   | 2.36                     | 0.46              |
| 1:A:4325:TYR:HB3  | 1:A:4501:GLY:HA2  | 1.98                     | 0.46              |
| 1:B:1105:ASP:HB3  | 1:B:1108:THR:HB   | 1.98                     | 0.46              |
| 1:B:1561:VAL:HG13 | 1:B:1810:LEU:HD22 | 1.97                     | 0.46              |
| 1:B:2117:HIS:CD2  | 1:B:2642:LEU:HD22 | 2.51                     | 0.46              |
| 1:B:2677:THR:HA   | 1:B:2680:LYS:HD2  | 1.98                     | 0.46              |
| 1:B:4206:LEU:HB2  | 1:B:4207:PRO:HD3  | 1.98                     | 0.46              |
| 1:B:4745:ILE:HB   | 1:B:4746:PRO:HD3  | 1.97                     | 0.46              |
| 1:A:664:ASN:HD21  | 1:B:202:ASN:HB3   | 1.81                     | 0.46              |
| 1:A:917:ASN:HA    | 1:A:920:LYS:HD2   | 1.98                     | 0.46              |
| 1:A:1101:PHE:O    | 1:A:1104:ILE:HB   | 2.14                     | 0.46              |
| 1:A:1678:TRP:HB3  | 1:A:1714:PHE:CD1  | 2.51                     | 0.46              |
| 1:A:3313:GLU:O    | 1:A:3317:PRO:HD3  | 2.15                     | 0.46              |
| 1:A:3880:THR:O    | 1:A:3884:ILE:HG12 | 2.16                     | 0.46              |
| 1:A:4281:THR:HG22 | 1:A:4283:LEU:H    | 1.81                     | 0.46              |
| 1:A:4339:ILE:HD13 | 1:A:4476:ALA:HB2  | 1.97                     | 0.46              |
| 1:B:62:GLU:O      | 1:B:66:HIS:HB3    | 2.15                     | 0.46              |
| 1:B:327:GLN:O     | 1:B:331:VAL:HG23  | 2.16                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1596:THR:HG22 | 1:B:2478:LEU:HD13 | 1.98                     | 0.46              |
| 1:B:2291:PHE:CZ   | 1:B:2350:THR:HB   | 2.51                     | 0.46              |
| 1:B:4101:TYR:HA   | 1:B:4104:ARG:HB2  | 1.97                     | 0.46              |
| 2:D:51:ASP:HA     | 2:D:54:ASN:HD22   | 1.81                     | 0.46              |
| 2:D:118:THR:O     | 2:D:119:ASP:C     | 2.58                     | 0.46              |
| 1:A:110:PHE:CZ    | 1:A:114:ARG:HD2   | 2.51                     | 0.46              |
| 1:A:506:PRO:HB2   | 1:A:523:ARG:NH2   | 2.29                     | 0.46              |
| 1:A:1039:LEU:HD22 | 1:A:1130:LYS:HE2  | 1.98                     | 0.46              |
| 1:A:1515:LEU:HD23 | 1:A:1555:GLN:HG3  | 1.98                     | 0.46              |
| 1:B:269:TYR:CD1   | 1:B:339:ALA:HA    | 2.50                     | 0.46              |
| 1:B:484:LEU:O     | 1:B:488:PHE:HD1   | 1.99                     | 0.46              |
| 1:B:668:ASN:HA    | 1:B:671:ARG:HB2   | 1.98                     | 0.46              |
| 1:B:1377:LEU:HD12 | 1:B:1377:LEU:H    | 1.81                     | 0.46              |
| 1:B:2687:LEU:HD13 | 1:B:2991:VAL:HG11 | 1.98                     | 0.46              |
| 1:B:3046:SER:HB2  | 1:B:3049:ASN:HD21 | 1.80                     | 0.46              |
| 1:B:3108:TYR:O    | 1:B:3112:GLN:HG2  | 2.15                     | 0.46              |
| 1:B:4730:ALA:O    | 1:B:4731:ILE:C    | 2.59                     | 0.46              |
| 2:C:26:GLY:O      | 2:C:61:ASN:HA     | 2.16                     | 0.46              |
| 1:A:200:VAL:CB    | 1:B:715:HIS:ND1   | 2.77                     | 0.46              |
| 1:A:511:ILE:HG13  | 1:A:512:MET:N     | 2.31                     | 0.46              |
| 1:A:1015:PRO:HG3  | 1:A:1041:TRP:CE2  | 2.50                     | 0.46              |
| 1:A:1132:GLN:HE22 | 1:A:1293:ARG:HH21 | 1.62                     | 0.46              |
| 1:A:1380:CYS:O    | 1:A:1380:CYS:SG   | 2.74                     | 0.46              |
| 1:A:1568:LYS:HG2  | 1:A:1817:PHE:HZ   | 1.80                     | 0.46              |
| 1:A:1877:TYR:HB2  | 1:A:1886:ARG:HG3  | 1.98                     | 0.46              |
| 1:A:2385:PHE:HB3  | 1:A:2387:PHE:CE2  | 2.50                     | 0.46              |
| 1:A:2405:ILE:HG13 | 1:A:2417:ILE:HD11 | 1.97                     | 0.46              |
| 1:B:1345:GLU:CD   | 1:B:1345:GLU:H    | 2.24                     | 0.46              |
| 1:B:3099:LEU:HB2  | 1:B:3190:TRP:CZ3  | 2.51                     | 0.46              |
| 1:B:3909:LEU:HD22 | 1:B:3925:VAL:HG13 | 1.98                     | 0.46              |
| 1:B:4621:PRO:HB3  | 1:B:4668:GLY:CA   | 2.44                     | 0.46              |
| 1:A:337:LEU:HD11  | 1:A:414:LEU:HD21  | 1.98                     | 0.45              |
| 1:A:2202:ILE:HG21 | 1:A:2232:LEU:HD11 | 1.97                     | 0.45              |
| 1:A:3234:ASP:O    | 1:A:3238:ARG:HG2  | 2.16                     | 0.45              |
| 1:A:3533:LEU:HD12 | 1:A:3819:GLN:HG2  | 1.98                     | 0.45              |
| 1:B:313:LEU:CD1   | 1:B:384:ILE:HG23  | 2.45                     | 0.45              |
| 1:B:747:LEU:HB3   | 1:B:806:LEU:N     | 2.31                     | 0.45              |
| 1:B:858:LEU:HA    | 1:B:858:LEU:HD23  | 1.80                     | 0.45              |
| 1:B:2356:ILE:HG13 | 1:B:2379:LEU:HD13 | 1.98                     | 0.45              |
| 2:C:13:PHE:HB3    | 2:C:69:PHE:CE2    | 2.47                     | 0.45              |
| 2:D:93:PHE:CZ     | 2:D:101:ILE:HA    | 2.51                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:190:GLN:O     | 1:A:193:PHE:HB3   | 2.16                     | 0.45              |
| 1:A:285:MET:N     | 1:A:286:PRO:CD    | 2.79                     | 0.45              |
| 1:A:1081:SER:HA   | 1:A:1084:LYS:HD2  | 1.97                     | 0.45              |
| 1:A:1233:TRP:CH2  | 1:A:1281:ALA:CB   | 2.99                     | 0.45              |
| 1:A:4750:LYS:O    | 1:A:4754:VAL:HG23 | 2.17                     | 0.45              |
| 1:B:761:LEU:HB3   | 1:B:779:CYS:SG    | 2.56                     | 0.45              |
| 1:B:1093:TYR:O    | 1:B:1096:ARG:HG2  | 2.15                     | 0.45              |
| 1:B:1489:ARG:O    | 1:B:1493:GLN:HG3  | 2.16                     | 0.45              |
| 1:B:3005:MET:HA   | 1:B:3008:THR:HG23 | 1.98                     | 0.45              |
| 1:A:135:GLY:CA    | 1:A:140:CYS:O     | 2.63                     | 0.45              |
| 1:A:338:TYR:HA    | 1:A:341:VAL:HG22  | 1.97                     | 0.45              |
| 1:A:477:ALA:O     | 1:A:481:ILE:HG12  | 2.15                     | 0.45              |
| 1:A:1023:LEU:CD2  | 1:A:1038:THR:HG23 | 2.46                     | 0.45              |
| 1:A:1032:GLU:O    | 1:A:1033:CYS:SG   | 2.71                     | 0.45              |
| 1:A:1087:VAL:O    | 1:A:1091:GLU:HG3  | 2.17                     | 0.45              |
| 1:A:2101:ASP:HB3  | 1:A:2106:VAL:HG22 | 1.98                     | 0.45              |
| 1:A:2371:PHE:CZ   | 1:A:2397:ALA:HB2  | 2.51                     | 0.45              |
| 1:A:4031:SER:N    | 3:E:310:GLU:OE2   | 2.50                     | 0.45              |
| 1:B:2295:ASN:CB   | 1:B:2423:TYR:HB3  | 2.45                     | 0.45              |
| 1:B:2626:VAL:HG21 | 1:B:2681:ILE:HG21 | 1.98                     | 0.45              |
| 1:B:4003:ILE:HG22 | 1:B:4005:THR:H    | 1.81                     | 0.45              |
| 2:D:20:PHE:HB3    | 2:D:32:GLU:HB3    | 1.99                     | 0.45              |
| 2:D:39:SER:C      | 2:D:41:GLY:H      | 2.25                     | 0.45              |
| 2:D:121:GLU:O     | 2:D:125:MET:HG2   | 2.16                     | 0.45              |
| 1:A:543:ARG:O     | 1:A:547:VAL:HG23  | 2.16                     | 0.45              |
| 1:A:1959:GLY:O    | 1:A:1961:PRO:HD3  | 2.16                     | 0.45              |
| 1:A:2092:LEU:HD23 | 1:A:2094:ILE:HD11 | 1.97                     | 0.45              |
| 1:A:4135:THR:O    | 1:A:4142:ARG:NH1  | 2.46                     | 0.45              |
| 1:B:827:ARG:NE    | 1:B:955:VAL:HG22  | 2.31                     | 0.45              |
| 1:B:1240:GLU:CD   | 1:B:1240:GLU:H    | 2.24                     | 0.45              |
| 1:B:1408:VAL:O    | 1:B:1412:MET:HG2  | 2.17                     | 0.45              |
| 1:B:1593:LEU:HB3  | 1:B:2474:VAL:HG11 | 1.99                     | 0.45              |
| 1:B:1902:LEU:HD21 | 1:B:1967:LEU:HD13 | 1.98                     | 0.45              |
| 1:B:2255:PRO:C    | 1:B:2257:LEU:N    | 2.74                     | 0.45              |
| 1:B:2636:LYS:HD2  | 1:B:2653:ILE:HD11 | 1.98                     | 0.45              |
| 1:B:2982:LEU:HD13 | 1:B:2982:LEU:C    | 2.41                     | 0.45              |
| 3:F:302:SER:OG    | 3:F:305:GLU:HB3   | 2.16                     | 0.45              |
| 1:A:333:SER:HB2   | 1:A:388:ILE:CG1   | 2.46                     | 0.45              |
| 1:A:485:THR:HG22  | 1:A:657:PHE:HD1   | 1.81                     | 0.45              |
| 1:A:1019:TYR:CE2  | 1:A:1023:LEU:HD11 | 2.52                     | 0.45              |
| 1:A:1039:LEU:HD21 | 1:A:1089:ILE:HD13 | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1105:ASP:N    | 1:A:1110:LEU:HD21 | 2.18                     | 0.45              |
| 1:A:3972:MET:HE3  | 1:A:3972:MET:HB3  | 1.73                     | 0.45              |
| 1:B:34:ARG:HB3    | 1:B:35:PRO:HD3    | 1.99                     | 0.45              |
| 1:B:255:LYS:HG2   | 1:B:258:ARG:HH21  | 1.80                     | 0.45              |
| 1:B:1541:MET:HG2  | 1:B:1556:LEU:HD11 | 1.99                     | 0.45              |
| 1:B:3410:GLN:HG3  | 1:B:3850:THR:CB   | 2.33                     | 0.45              |
| 1:B:3910:PHE:HB2  | 1:B:3929:MET:HE1  | 1.97                     | 0.45              |
| 1:A:144:ASP:O     | 1:A:148:ILE:HG13  | 2.17                     | 0.45              |
| 1:A:1388:LEU:O    | 1:A:1394:ARG:HB2  | 2.17                     | 0.45              |
| 1:A:1509:GLY:O    | 1:A:1513:VAL:HG23 | 2.17                     | 0.45              |
| 1:A:3038:ASP:O    | 1:A:3042:LYS:HG2  | 2.17                     | 0.45              |
| 1:A:3251:LEU:HD12 | 1:A:3303:PHE:CD2  | 2.51                     | 0.45              |
| 1:A:3626:GLU:OE1  | 1:A:3628:LYS:HE3  | 2.17                     | 0.45              |
| 1:A:4745:ILE:HB   | 1:A:4746:PRO:HD3  | 1.99                     | 0.45              |
| 1:B:908:TYR:O     | 1:B:908:TYR:CG    | 2.70                     | 0.45              |
| 1:B:985:ARG:HH11  | 1:B:1280:LEU:HD11 | 1.81                     | 0.45              |
| 1:B:1110:LEU:H    | 1:B:1175:ALA:CB   | 2.29                     | 0.45              |
| 1:B:1174:ARG:O    | 1:B:1178:LEU:HG   | 2.16                     | 0.45              |
| 1:B:2698:LYS:HG3  | 1:B:3002:VAL:HG23 | 1.98                     | 0.45              |
| 1:B:4053:HIS:HB2  | 1:B:4071:TRP:HD1  | 1.81                     | 0.45              |
| 1:B:4711:LYS:HA   | 1:B:4714:LEU:HD12 | 1.99                     | 0.45              |
| 1:A:44:PHE:CE2    | 1:A:48:GLU:HB2    | 2.51                     | 0.45              |
| 1:A:136:LEU:O     | 1:A:243:ASN:ND2   | 2.49                     | 0.45              |
| 1:A:416:ASN:HD22  | 1:A:416:ASN:N     | 2.15                     | 0.45              |
| 1:A:680:GLU:HB3   | 1:A:730:THR:HG21  | 1.99                     | 0.45              |
| 1:A:974:LEU:HD23  | 1:A:1006:LEU:HD23 | 1.99                     | 0.45              |
| 1:A:1163:LEU:HA   | 1:A:1166:ILE:HD12 | 1.98                     | 0.45              |
| 1:A:2122:LEU:HB2  | 1:A:2136:ILE:HD12 | 1.99                     | 0.45              |
| 1:A:4170:LEU:O    | 1:A:4173:LEU:HB3  | 2.17                     | 0.45              |
| 1:A:4313:CYS:HB3  | 1:A:4331:ILE:CD1  | 2.47                     | 0.45              |
| 1:B:478:ASN:OD1   | 1:B:650:LEU:HD13  | 2.17                     | 0.45              |
| 1:B:2122:LEU:HD23 | 1:B:2136:ILE:HD11 | 1.96                     | 0.45              |
| 1:B:2622:ILE:HD11 | 1:B:2667:TYR:CG   | 2.52                     | 0.45              |
| 1:B:2702:ILE:CD1  | 1:B:3001:GLN:NE2  | 2.79                     | 0.45              |
| 1:B:3056:MET:HA   | 1:B:3059:LEU:HD12 | 1.99                     | 0.45              |
| 1:B:3714:MET:HE3  | 1:B:3714:MET:HB3  | 1.78                     | 0.45              |
| 1:A:279:ALA:O     | 1:A:280:ASN:C     | 2.59                     | 0.45              |
| 1:A:284:ILE:O     | 1:A:442:LEU:N     | 2.50                     | 0.45              |
| 1:A:1456:LEU:HD22 | 1:A:1510:VAL:HG13 | 1.98                     | 0.45              |
| 1:A:3337:ALA:HB3  | 1:A:3427:GLN:HE21 | 1.81                     | 0.45              |
| 1:A:3909:LEU:HD22 | 1:A:3925:VAL:HG13 | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:4098:THR:HB   | 2:C:109:VAL:HG13  | 1.99                     | 0.45              |
| 1:A:4310:MET:HG2  | 1:A:4335:LEU:CD1  | 2.47                     | 0.45              |
| 1:A:4419:LEU:HD13 | 1:A:4459:LEU:HG   | 1.97                     | 0.45              |
| 1:A:4710:TRP:O    | 1:A:4714:LEU:HG   | 2.16                     | 0.45              |
| 1:B:678:LEU:HB3   | 1:B:727:LEU:CD2   | 2.46                     | 0.45              |
| 1:B:686:LEU:HA    | 1:B:686:LEU:HD23  | 1.73                     | 0.45              |
| 1:B:1077:THR:HA   | 1:B:1082:SER:HB2  | 1.98                     | 0.45              |
| 1:B:1407:LEU:H    | 1:B:1407:LEU:CD1  | 2.25                     | 0.45              |
| 1:B:3301:LEU:HD23 | 1:B:3301:LEU:HA   | 1.76                     | 0.45              |
| 1:B:3461:TYR:O    | 1:B:3534:VAL:HG11 | 2.17                     | 0.45              |
| 2:D:7:GLU:HA      | 2:D:10:ILE:HG22   | 1.99                     | 0.45              |
| 1:A:55:SER:O      | 1:A:59:SER:N      | 2.36                     | 0.45              |
| 1:A:1090:VAL:HG11 | 1:A:1131:VAL:HG22 | 1.99                     | 0.45              |
| 1:A:1468:LEU:HA   | 1:A:1471:MET:HE2  | 1.99                     | 0.45              |
| 1:A:1515:LEU:CD1  | 1:A:1541:MET:HG3  | 2.47                     | 0.45              |
| 1:A:1570:TYR:CG   | 1:A:1592:ILE:HG21 | 2.52                     | 0.45              |
| 1:A:1807:PHE:O    | 1:A:1810:LEU:HB3  | 2.17                     | 0.45              |
| 1:A:1924:LEU:HD23 | 1:A:1944:ARG:HA   | 1.99                     | 0.45              |
| 1:A:2390:THR:O    | 1:A:2391:ARG:C    | 2.59                     | 0.45              |
| 1:A:2480:VAL:HA   | 1:A:2524:GLN:CG   | 2.46                     | 0.45              |
| 1:A:2978:LEU:HB2  | 1:A:3006:LEU:HD13 | 1.99                     | 0.45              |
| 1:A:3194:LEU:HD13 | 1:A:3214:LEU:HD21 | 1.97                     | 0.45              |
| 1:A:3478:LYS:HD2  | 1:A:3478:LYS:HA   | 1.83                     | 0.45              |
| 1:B:1204:ILE:CG2  | 1:B:1357:GLY:HA3  | 2.43                     | 0.45              |
| 1:B:1831:ALA:HB2  | 1:B:2260:SER:HB3  | 1.97                     | 0.45              |
| 1:B:3887:LEU:HD13 | 1:B:3905:LEU:HD21 | 1.98                     | 0.45              |
| 1:B:4052:ILE:HG23 | 3:F:322:GLU:HB3   | 1.99                     | 0.45              |
| 3:E:317:SER:O     | 3:E:321:GLN:HG3   | 2.17                     | 0.45              |
| 1:A:31:VAL:O      | 1:A:34:ARG:HB3    | 2.17                     | 0.45              |
| 1:A:488:PHE:HE2   | 1:A:670:ILE:HD12  | 1.82                     | 0.45              |
| 1:A:1557:HIS:HB2  | 1:A:1799:LEU:HD23 | 1.97                     | 0.45              |
| 1:A:1610:LEU:HD21 | 1:A:1799:LEU:HB2  | 1.99                     | 0.45              |
| 1:A:1807:PHE:O    | 1:A:1811:VAL:HG23 | 2.17                     | 0.45              |
| 1:A:1950:VAL:HG11 | 1:A:1969:VAL:HG11 | 1.98                     | 0.45              |
| 1:A:2375:MET:HG2  | 1:A:2387:PHE:CE1  | 2.32                     | 0.45              |
| 1:A:2540:HIS:HB3  | 1:A:2584:ARG:NE   | 2.32                     | 0.45              |
| 1:A:3148:HIS:CE1  | 1:A:3152:VAL:H    | 2.34                     | 0.45              |
| 1:A:3229:ASP:HB2  | 1:A:3289:ASN:HD22 | 1.82                     | 0.45              |
| 1:A:3905:LEU:HD23 | 1:A:3932:LEU:HD11 | 1.99                     | 0.45              |
| 1:A:4026:PRO:O    | 1:A:4027:PRO:C    | 2.59                     | 0.45              |
| 1:A:4595:VAL:CG2  | 1:A:4630:LYS:HA   | 2.46                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:283:PHE:HB3   | 1:B:443:ARG:CZ    | 2.47                     | 0.45              |
| 1:B:1047:ILE:O    | 1:B:1051:VAL:HG23 | 2.17                     | 0.45              |
| 1:B:1498:TYR:O    | 1:B:1504:SER:HB2  | 2.17                     | 0.45              |
| 1:B:1959:GLY:O    | 1:B:1961:PRO:HD3  | 2.16                     | 0.45              |
| 1:B:2978:LEU:HD23 | 1:B:3010:LEU:HD11 | 1.98                     | 0.45              |
| 1:B:3012:GLY:H    | 1:B:3077:SER:HB2  | 1.80                     | 0.45              |
| 1:B:3226:GLN:HA   | 1:B:3289:ASN:HD22 | 1.81                     | 0.45              |
| 1:B:3756:HIS:HB2  | 1:B:3807:CYS:SG   | 2.57                     | 0.45              |
| 1:B:4050:ASN:OD1  | 2:D:38:ARG:NH2    | 2.50                     | 0.45              |
| 1:A:97:LEU:HD23   | 1:A:98:GLN:N      | 2.32                     | 0.44              |
| 1:A:3033:GLY:O    | 1:A:3034:MET:C    | 2.61                     | 0.44              |
| 1:A:3642:ILE:HD13 | 1:A:3713:PHE:CE1  | 2.52                     | 0.44              |
| 1:A:4570:LEU:HD13 | 1:A:4622:TYR:CB   | 2.47                     | 0.44              |
| 1:A:4639:LYS:HB3  | 1:A:4640:PRO:HD3  | 1.99                     | 0.44              |
| 1:B:414:LEU:O     | 1:B:418:LEU:HG    | 2.17                     | 0.44              |
| 1:B:722:LEU:H     | 1:B:722:LEU:HD12  | 1.82                     | 0.44              |
| 1:B:1564:LEU:HD13 | 1:B:1596:THR:HG23 | 1.98                     | 0.44              |
| 1:B:1728:ALA:O    | 1:B:1729:LEU:C    | 2.60                     | 0.44              |
| 1:B:2695:PHE:CZ   | 1:B:2699:GLN:NE2  | 2.84                     | 0.44              |
| 1:B:3234:ASP:O    | 1:B:3238:ARG:HG2  | 2.16                     | 0.44              |
| 1:A:94:ARG:H      | 1:A:94:ARG:HD2    | 1.81                     | 0.44              |
| 1:A:252:GLY:O     | 1:A:256:LEU:HG    | 2.18                     | 0.44              |
| 1:A:471:VAL:CG2   | 1:A:641:ARG:H     | 2.26                     | 0.44              |
| 1:A:738:ALA:O     | 1:A:785:ARG:NH1   | 2.50                     | 0.44              |
| 1:A:1346:PHE:O    | 1:A:1350:VAL:HG23 | 2.17                     | 0.44              |
| 1:A:1903:SER:HB2  | 1:A:1910:GLN:HA   | 1.99                     | 0.44              |
| 1:A:2622:ILE:HD11 | 1:A:2667:TYR:CB   | 2.47                     | 0.44              |
| 1:A:4120:ASP:OD1  | 1:A:4120:ASP:N    | 2.46                     | 0.44              |
| 1:A:4332:PHE:HB2  | 1:A:4507:VAL:HG12 | 2.00                     | 0.44              |
| 1:B:418:LEU:HD11  | 1:B:477:ALA:HA    | 1.98                     | 0.44              |
| 1:B:1174:ARG:HG2  | 1:B:1320:GLU:OE2  | 2.16                     | 0.44              |
| 1:B:2122:LEU:HB2  | 1:B:2136:ILE:HD12 | 1.99                     | 0.44              |
| 1:B:3058:LEU:HD12 | 1:B:3058:LEU:HA   | 1.82                     | 0.44              |
| 1:B:3099:LEU:HD11 | 1:B:3193:PHE:CD1  | 2.51                     | 0.44              |
| 1:B:4170:LEU:O    | 1:B:4173:LEU:HB3  | 2.17                     | 0.44              |
| 1:B:4313:CYS:HB3  | 1:B:4331:ILE:HG23 | 1.99                     | 0.44              |
| 3:F:24:CYS:CA     | 3:F:52:MET:SD     | 3.05                     | 0.44              |
| 1:A:202:ASN:CG    | 1:A:204:ARG:HG3   | 2.43                     | 0.44              |
| 1:A:288:THR:HG22  | 1:A:290:ALA:H     | 1.81                     | 0.44              |
| 1:A:1180:ASN:O    | 1:A:1181:PHE:C    | 2.58                     | 0.44              |
| 1:B:115:LEU:HD13  | 1:B:130:ILE:HG13  | 2.00                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:333:SER:OG    | 1:B:385:TYR:HA    | 2.18                     | 0.44              |
| 1:B:674:LEU:O     | 1:B:678:LEU:HG    | 2.18                     | 0.44              |
| 1:B:813:MET:HB2   | 1:B:813:MET:HE3   | 1.68                     | 0.44              |
| 1:B:1295:THR:HG22 | 1:B:1299:ILE:HD13 | 2.00                     | 0.44              |
| 1:B:3058:LEU:HG   | 1:B:3062:PHE:CZ   | 2.52                     | 0.44              |
| 1:B:3642:ILE:HD13 | 1:B:3713:PHE:CE1  | 2.52                     | 0.44              |
| 1:B:3880:THR:O    | 1:B:3884:ILE:HG12 | 2.16                     | 0.44              |
| 1:B:4705:LEU:CD1  | 1:B:4753:GLN:HB2  | 2.47                     | 0.44              |
| 3:E:24:CYS:CA     | 3:E:52:MET:SD     | 3.06                     | 0.44              |
| 1:A:264:PRO:HG2   | 1:A:305:ASP:OD2   | 2.18                     | 0.44              |
| 1:A:1381:LEU:HB3  | 1:A:1426:ARG:NH2  | 2.32                     | 0.44              |
| 1:A:3513:TYR:CD1  | 1:A:3525:TYR:HD1  | 2.35                     | 0.44              |
| 1:A:3525:TYR:CE2  | 1:A:3874:GLY:HA2  | 2.53                     | 0.44              |
| 1:A:4746:PRO:O    | 1:A:4750:LYS:HG3  | 2.16                     | 0.44              |
| 1:B:1664:CYS:HB3  | 1:B:1667:THR:HG23 | 1.99                     | 0.44              |
| 1:B:2300:ASP:OD2  | 1:B:2344:ASN:ND2  | 2.50                     | 0.44              |
| 1:B:4093:ARG:NH2  | 2:D:51:ASP:OD2    | 2.51                     | 0.44              |
| 2:D:60:GLY:H      | 2:D:63:THR:HB     | 1.82                     | 0.44              |
| 2:D:93:PHE:CE2    | 2:D:101:ILE:HG12  | 2.52                     | 0.44              |
| 1:A:59:SER:O      | 1:A:63:ILE:HG13   | 2.17                     | 0.44              |
| 1:A:844:MET:HB3   | 1:A:848:MET:HE3   | 1.98                     | 0.44              |
| 1:A:1534:PHE:N    | 1:A:1535:PRO:HD2  | 2.32                     | 0.44              |
| 1:A:1899:MET:HE2  | 1:A:2233:LEU:HB3  | 2.00                     | 0.44              |
| 1:A:2349:MET:HB2  | 1:A:2397:ALA:O    | 2.18                     | 0.44              |
| 1:A:3004:LEU:HD22 | 1:A:3061:VAL:HG11 | 2.00                     | 0.44              |
| 1:A:3273:MET:HG3  | 1:A:3633:LEU:CD2  | 2.48                     | 0.44              |
| 1:B:382:LEU:HD23  | 1:B:382:LEU:HA    | 1.82                     | 0.44              |
| 1:B:443:ARG:HB2   | 1:B:446:ASP:CB    | 2.47                     | 0.44              |
| 1:B:909:HIS:ND1   | 1:B:934:CYS:O     | 2.49                     | 0.44              |
| 1:B:1859:MET:SD   | 1:B:2244:ALA:HA   | 2.58                     | 0.44              |
| 1:B:1891:ALA:HB3  | 1:B:1893:VAL:HG23 | 1.98                     | 0.44              |
| 1:B:1976:HIS:ND1  | 1:B:1989:HIS:NE2  | 2.57                     | 0.44              |
| 1:B:2129:GLY:HA3  | 1:B:2161:SER:O    | 2.17                     | 0.44              |
| 1:B:3004:LEU:O    | 1:B:3008:THR:HG23 | 2.18                     | 0.44              |
| 2:C:13:PHE:CD1    | 2:C:40:LEU:HD13   | 2.52                     | 0.44              |
| 1:A:284:ILE:HG22  | 1:A:286:PRO:CD    | 2.47                     | 0.44              |
| 1:A:718:VAL:HG13  | 1:A:760:LEU:HD23  | 1.98                     | 0.44              |
| 1:A:911:PHE:HD2   | 1:A:1001:TYR:CD1  | 2.35                     | 0.44              |
| 1:A:1434:LEU:HD11 | 1:A:1449:LEU:HD12 | 2.00                     | 0.44              |
| 1:A:2309:LEU:O    | 3:E:77:SER:OG     | 2.34                     | 0.44              |
| 1:A:2522:GLN:O    | 1:A:2526:LYS:HG3  | 2.16                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2692:ALA:HA   | 1:A:2695:PHE:CD1  | 2.49                     | 0.44              |
| 1:A:3291:GLN:HA   | 1:A:3395:LEU:HD11 | 1.99                     | 0.44              |
| 1:A:3412:LEU:O    | 1:A:3416:LEU:HB2  | 2.18                     | 0.44              |
| 1:A:4047:PRO:HA   | 1:A:4075:LEU:HD23 | 1.99                     | 0.44              |
| 1:B:1414:THR:HG21 | 1:B:1424:CYS:HA   | 1.99                     | 0.44              |
| 1:B:2048:ASP:OD1  | 1:B:2049:VAL:N    | 2.51                     | 0.44              |
| 1:B:2215:VAL:HG23 | 1:B:2231:ILE:HB   | 1.99                     | 0.44              |
| 1:B:2264:SER:HB3  | 1:B:2652:HIS:NE2  | 2.32                     | 0.44              |
| 1:B:2540:HIS:HB3  | 1:B:2584:ARG:CZ   | 2.48                     | 0.44              |
| 1:B:2985:LEU:O    | 1:B:2988:LEU:HB2  | 2.17                     | 0.44              |
| 1:B:3273:MET:HG3  | 1:B:3633:LEU:CD2  | 2.48                     | 0.44              |
| 1:B:4234:GLN:HE22 | 1:B:4279:GLN:HB3  | 1.83                     | 0.44              |
| 1:A:405:ASN:ND2   | 1:A:513:ALA:O     | 2.51                     | 0.44              |
| 1:A:1489:ARG:O    | 1:A:1493:GLN:HG3  | 2.18                     | 0.44              |
| 1:A:1680:HIS:O    | 1:A:1706:ILE:HA   | 2.17                     | 0.44              |
| 1:A:1867:GLU:HG2  | 1:A:2236:ASP:OD2  | 2.18                     | 0.44              |
| 1:A:3087:ALA:HB2  | 1:A:3181:ILE:HG21 | 2.00                     | 0.44              |
| 1:A:3963:ASP:O    | 1:A:3964:LEU:C    | 2.60                     | 0.44              |
| 1:B:115:LEU:HD12  | 1:B:133:ILE:HD12  | 1.99                     | 0.44              |
| 1:B:302:LEU:O     | 1:B:303:VAL:C     | 2.61                     | 0.44              |
| 1:B:1191:SER:O    | 1:B:1192:LYS:C    | 2.61                     | 0.44              |
| 1:B:1952:PHE:CZ   | 1:B:1969:VAL:HG12 | 2.53                     | 0.44              |
| 1:B:2060:ILE:HG12 | 1:B:2074:LEU:HD12 | 2.00                     | 0.44              |
| 1:B:3251:LEU:HD12 | 1:B:3303:PHE:CD2  | 2.52                     | 0.44              |
| 1:B:3626:GLU:OE1  | 1:B:3628:LYS:HE3  | 2.17                     | 0.44              |
| 1:B:3998:LEU:O    | 1:B:4001:VAL:HG12 | 2.18                     | 0.44              |
| 2:D:86:ILE:CD1    | 2:D:146:MET:HG2   | 2.48                     | 0.44              |
| 1:A:867:HIS:CD2   | 1:A:947:ARG:HD2   | 2.52                     | 0.44              |
| 1:A:1098:ILE:O    | 1:A:1101:PHE:HB2  | 2.18                     | 0.44              |
| 1:A:1378:GLU:HG2  | 1:A:1426:ARG:HG3  | 2.00                     | 0.44              |
| 1:A:2973:VAL:O    | 1:A:2976:MET:HG3  | 2.17                     | 0.44              |
| 1:A:3889:ALA:HB2  | 3:E:293:LEU:HD13  | 2.00                     | 0.44              |
| 1:B:185:ARG:HA    | 1:B:185:ARG:HE    | 1.83                     | 0.44              |
| 1:B:648:LEU:HD23  | 1:B:648:LEU:HA    | 1.69                     | 0.44              |
| 1:B:1429:LYS:O    | 1:B:1432:THR:N    | 2.51                     | 0.44              |
| 1:B:1480:ASP:HB3  | 1:B:1483:ASP:HB2  | 2.00                     | 0.44              |
| 1:B:2151:ILE:HD12 | 1:B:2162:PRO:HD2  | 1.99                     | 0.44              |
| 1:B:3087:ALA:CA   | 1:B:3181:ILE:HD13 | 2.47                     | 0.44              |
| 1:B:3269:LEU:HB3  | 1:B:3633:LEU:HD12 | 1.92                     | 0.44              |
| 1:B:3305:LEU:HB2  | 1:B:3323:LEU:HD21 | 1.99                     | 0.44              |
| 1:B:3571:ILE:HG12 | 1:B:3717:ALA:HB2  | 2.00                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:4606:VAL:HG13 | 1:B:4612:VAL:HG12 | 1.99                     | 0.44              |
| 2:D:147:THR:O     | 2:D:148:ALA:C     | 2.60                     | 0.44              |
| 3:E:301:MET:HE1   | 3:E:305:GLU:HG2   | 2.00                     | 0.44              |
| 1:A:1039:LEU:HD22 | 1:A:1130:LYS:CD   | 2.48                     | 0.44              |
| 1:A:1048:SER:O    | 1:A:1051:VAL:HB   | 2.18                     | 0.44              |
| 1:A:1130:LYS:O    | 1:A:1131:VAL:C    | 2.59                     | 0.44              |
| 1:A:1299:ILE:HG22 | 1:A:1336:ARG:HH11 | 1.83                     | 0.44              |
| 1:A:1474:SER:CB   | 1:A:1485:ILE:HG21 | 2.48                     | 0.44              |
| 1:A:1571:LEU:O    | 1:A:1573:GLN:N    | 2.51                     | 0.44              |
| 1:A:4115:ARG:NH2  | 2:C:125:MET:SD    | 2.91                     | 0.44              |
| 1:B:155:MET:C     | 1:B:157:SER:N     | 2.74                     | 0.44              |
| 1:B:1077:THR:C    | 1:B:1078:THR:HG1  | 2.26                     | 0.44              |
| 1:B:1355:ILE:HD13 | 1:B:1397:MET:CG   | 2.47                     | 0.44              |
| 1:B:1468:LEU:O    | 1:B:1472:THR:HG23 | 2.17                     | 0.44              |
| 1:B:2973:VAL:O    | 1:B:2977:LEU:HB2  | 2.18                     | 0.44              |
| 1:B:3899:ILE:O    | 1:B:3903:GLN:HG2  | 2.18                     | 0.44              |
| 1:B:3922:ARG:NH1  | 1:B:3970:TYR:OH   | 2.50                     | 0.44              |
| 2:C:145:MET:HE3   | 2:C:145:MET:HB3   | 1.90                     | 0.44              |
| 3:F:301:MET:HE1   | 3:F:305:GLU:HG2   | 2.00                     | 0.44              |
| 1:A:34:ARG:HB3    | 1:A:35:PRO:HD3    | 2.00                     | 0.43              |
| 1:A:261:LEU:HD23  | 1:A:332:LEU:HD13  | 1.99                     | 0.43              |
| 1:A:321:LEU:HD23  | 1:A:321:LEU:HA    | 1.86                     | 0.43              |
| 1:A:1197:GLY:C    | 1:A:1372:LEU:HD21 | 2.43                     | 0.43              |
| 1:A:2072:THR:O    | 1:A:2090:ASN:HB2  | 2.18                     | 0.43              |
| 1:A:2194:PRO:HD3  | 1:A:2251:TYR:CE1  | 2.52                     | 0.43              |
| 1:A:4101:TYR:CD2  | 2:C:89:ALA:HB2    | 2.53                     | 0.43              |
| 1:A:4159:LYS:HE2  | 1:A:4159:LYS:HB3  | 1.84                     | 0.43              |
| 1:B:1000:GLN:HG3  | 1:B:1270:LEU:HD13 | 2.00                     | 0.43              |
| 1:B:1815:LEU:HD12 | 1:B:2508:LEU:HD21 | 1.99                     | 0.43              |
| 1:B:1854:MET:HE2  | 1:B:2152:LYS:N    | 2.32                     | 0.43              |
| 1:B:4127:ASN:ND2  | 3:F:328:LEU:HD22  | 2.31                     | 0.43              |
| 2:D:37:MET:HG2    | 2:D:69:PHE:HE1    | 1.83                     | 0.43              |
| 2:D:101:ILE:N     | 2:D:137:VAL:O     | 2.48                     | 0.43              |
| 1:A:539:SER:O     | 1:A:543:ARG:HD3   | 2.18                     | 0.43              |
| 1:A:853:LEU:O     | 1:A:857:ARG:HG2   | 2.18                     | 0.43              |
| 1:A:3083:SER:HB3  | 1:A:3178:ASN:HD22 | 1.84                     | 0.43              |
| 1:A:3826:LYS:HE2  | 1:A:3826:LYS:HB3  | 1.84                     | 0.43              |
| 1:A:4419:LEU:HD22 | 1:A:4459:LEU:HD12 | 1.99                     | 0.43              |
| 1:B:1534:PHE:N    | 1:B:1535:PRO:HD2  | 2.33                     | 0.43              |
| 1:B:3412:LEU:O    | 1:B:3416:LEU:HB2  | 2.18                     | 0.43              |
| 1:B:3490:SER:O    | 1:B:3494:VAL:HG23 | 2.18                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:3746:ALA:HA   | 1:B:3749:VAL:HG22 | 1.99                     | 0.43              |
| 1:B:3764:LEU:HD23 | 1:B:3764:LEU:HA   | 1.83                     | 0.43              |
| 1:B:3972:MET:HG3  | 1:B:4011:ASN:O    | 2.18                     | 0.43              |
| 1:B:4125:HIS:HA   | 1:B:4165:LEU:CD1  | 2.48                     | 0.43              |
| 1:A:98:GLN:HG3    | 1:A:201:PHE:CZ    | 2.54                     | 0.43              |
| 1:A:765:GLN:NE2   | 1:A:817:ILE:HG23  | 2.33                     | 0.43              |
| 1:A:1811:VAL:HA   | 1:A:1814:MET:HE2  | 2.00                     | 0.43              |
| 1:A:3308:SER:HA   | 1:A:3319:LEU:HD13 | 2.00                     | 0.43              |
| 1:A:3317:PRO:HG3  | 1:A:3424:VAL:CG2  | 2.48                     | 0.43              |
| 1:A:4146:CYS:HA   | 1:A:4186:LEU:HD22 | 2.00                     | 0.43              |
| 1:A:4310:MET:HE3  | 1:A:4335:LEU:CD2  | 2.49                     | 0.43              |
| 1:A:4360:GLU:CD   | 1:A:4366:ARG:HH21 | 2.26                     | 0.43              |
| 1:B:280:ASN:HB3   | 1:B:283:PHE:HE1   | 1.84                     | 0.43              |
| 1:B:3068:SER:HA   | 1:B:3075:CYS:HB2  | 2.00                     | 0.43              |
| 1:B:4413:LYS:CD   | 1:B:4456:ILE:HD11 | 2.48                     | 0.43              |
| 3:E:9:CYS:O       | 3:E:13:LEU:HA     | 2.18                     | 0.43              |
| 3:E:23:LYS:HD3    | 3:E:114:ALA:HB1   | 2.00                     | 0.43              |
| 1:A:110:PHE:O     | 1:A:114:ARG:HG2   | 2.18                     | 0.43              |
| 1:A:197:LEU:HD23  | 1:A:197:LEU:HA    | 1.84                     | 0.43              |
| 1:A:1178:LEU:HD21 | 1:A:1202:LEU:HD21 | 2.00                     | 0.43              |
| 1:A:1192:LYS:HA   | 1:A:1195:LEU:HB2  | 2.00                     | 0.43              |
| 1:A:2698:LYS:NZ   | 1:A:2998:PRO:O    | 2.52                     | 0.43              |
| 1:A:3505:THR:OG1  | 1:A:3916:ARG:NH1  | 2.37                     | 0.43              |
| 1:A:3595:ASN:HD21 | 1:A:3605:LEU:HD13 | 1.83                     | 0.43              |
| 1:A:4278:VAL:O    | 1:B:3825:ARG:HD3  | 2.18                     | 0.43              |
| 1:B:124:VAL:HG21  | 1:B:129:LEU:HD21  | 1.99                     | 0.43              |
| 1:B:855:LEU:HD23  | 1:B:1002:TYR:HE2  | 1.82                     | 0.43              |
| 1:B:1177:LEU:HD21 | 1:B:1233:TRP:HB2  | 1.99                     | 0.43              |
| 1:B:1209:CYS:SG   | 1:B:1210:LYS:N    | 2.91                     | 0.43              |
| 1:B:1244:ILE:HG12 | 1:B:1249:ASN:HB3  | 2.01                     | 0.43              |
| 1:B:2675:ILE:C    | 1:B:2677:THR:N    | 2.75                     | 0.43              |
| 1:B:2997:ILE:HB   | 1:B:2998:PRO:HD3  | 2.00                     | 0.43              |
| 1:B:3301:LEU:HD21 | 1:B:3326:ALA:HB3  | 1.99                     | 0.43              |
| 1:B:3889:ALA:HB2  | 3:F:293:LEU:HD13  | 1.99                     | 0.43              |
| 1:B:4746:PRO:O    | 1:B:4750:LYS:HG3  | 2.18                     | 0.43              |
| 2:D:130:ASP:OD2   | 2:D:135:GLY:N     | 2.48                     | 0.43              |
| 3:E:21:ARG:HB3    | 3:E:55:ILE:HB     | 2.01                     | 0.43              |
| 1:A:34:ARG:O      | 1:A:35:PRO:C      | 2.61                     | 0.43              |
| 1:A:516:THR:HG22  | 1:A:518:ILE:H     | 1.84                     | 0.43              |
| 1:A:864:TYR:HA    | 1:A:936:LEU:CD2   | 2.48                     | 0.43              |
| 1:A:1021:ASN:OD1  | 1:A:1071:LEU:HD21 | 2.17                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2578:ARG:HD2  | 1:A:2659:ALA:CB   | 2.48                     | 0.43              |
| 1:A:3173:LYS:HB3  | 1:A:3173:LYS:HE2  | 1.76                     | 0.43              |
| 1:A:3773:GLU:HB3  | 1:A:3794:ARG:HE   | 1.83                     | 0.43              |
| 1:A:3899:ILE:O    | 1:A:3903:GLN:HG2  | 2.19                     | 0.43              |
| 1:A:3986:TRP:CZ2  | 3:E:316:ARG:HG2   | 2.54                     | 0.43              |
| 1:A:4007:VAL:HG22 | 1:B:3511:ASN:HB2  | 2.00                     | 0.43              |
| 1:A:4749:HIS:O    | 1:A:4753:GLN:HG3  | 2.18                     | 0.43              |
| 1:B:428:ALA:O     | 1:B:432:LYS:HG2   | 2.18                     | 0.43              |
| 1:B:796:GLN:HB2   | 1:B:798:VAL:HG23  | 2.00                     | 0.43              |
| 1:B:1289:LEU:HD11 | 1:B:1325:SER:HB2  | 2.00                     | 0.43              |
| 1:B:2038:TYR:C    | 1:B:2038:TYR:CD2  | 2.96                     | 0.43              |
| 1:B:2984:THR:O    | 1:B:2987:GLN:N    | 2.51                     | 0.43              |
| 1:B:3033:GLY:C    | 1:B:3035:ASP:N    | 2.76                     | 0.43              |
| 1:B:3727:GLU:H    | 1:B:3731:ASP:HB2  | 1.82                     | 0.43              |
| 1:B:4146:CYS:HA   | 1:B:4186:LEU:HD22 | 2.01                     | 0.43              |
| 1:B:4159:LYS:HZ3  | 1:B:4196:TRP:CD1  | 2.36                     | 0.43              |
| 2:C:54:ASN:C      | 2:C:56:VAL:N      | 2.77                     | 0.43              |
| 1:A:773:ASP:HB3   | 1:A:774:PRO:HD2   | 1.99                     | 0.43              |
| 1:A:872:ALA:O     | 1:B:186:GLN:NE2   | 2.52                     | 0.43              |
| 1:A:1429:LYS:O    | 1:A:1432:THR:N    | 2.51                     | 0.43              |
| 1:A:1707:SER:O    | 1:A:1708:TYR:C    | 2.62                     | 0.43              |
| 1:A:4136:PRO:HB2  | 1:B:3508:PRO:HB3  | 2.00                     | 0.43              |
| 1:A:4273:LEU:HD12 | 1:A:4291:LEU:HD12 | 2.00                     | 0.43              |
| 1:B:793:ASN:O     | 1:B:797:GLY:N     | 2.52                     | 0.43              |
| 1:B:1345:GLU:O    | 1:B:1349:ARG:HG2  | 2.18                     | 0.43              |
| 1:B:1996:LEU:HD22 | 1:B:2019:THR:HG21 | 2.00                     | 0.43              |
| 1:B:2683:MET:HE2  | 1:B:2999:TYR:OH   | 2.19                     | 0.43              |
| 1:B:3001:GLN:HG3  | 1:B:3139:PHE:CZ   | 2.54                     | 0.43              |
| 1:B:3301:LEU:HD21 | 1:B:3326:ALA:CB   | 2.48                     | 0.43              |
| 2:C:100:TYR:CD1   | 2:C:136:GLN:HB3   | 2.54                     | 0.43              |
| 1:A:270:ILE:HG12  | 1:A:335:SER:CB    | 2.48                     | 0.43              |
| 1:A:317:VAL:HG12  | 1:A:318:LEU:H     | 1.82                     | 0.43              |
| 1:A:420:LEU:O     | 1:A:424:LEU:HG    | 2.19                     | 0.43              |
| 1:A:1332:ASN:HA   | 1:A:1335:GLU:CD   | 2.44                     | 0.43              |
| 1:A:1521:MET:HB2  | 1:A:1537:LEU:HD21 | 1.99                     | 0.43              |
| 1:A:1606:VAL:O    | 1:A:1610:LEU:HG   | 2.19                     | 0.43              |
| 1:A:2305:GLY:HA2  | 1:A:2339:GLU:H    | 1.83                     | 0.43              |
| 1:A:2340:ILE:HD13 | 1:A:2422:ILE:HD11 | 2.00                     | 0.43              |
| 1:A:2363:ARG:NH1  | 1:A:2416:MET:HE1  | 2.34                     | 0.43              |
| 1:A:2698:LYS:NZ   | 1:A:3002:VAL:HG23 | 2.33                     | 0.43              |
| 1:A:3057:ARG:HG3  | 1:A:3141:LEU:HG   | 2.01                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:4128:TRP:HA   | 1:A:4131:GLN:HG2  | 2.01                     | 0.43              |
| 1:A:4318:LYS:HA   | 1:A:4491:ARG:HH22 | 1.83                     | 0.43              |
| 1:A:4491:ARG:O    | 1:A:4495:ILE:HG13 | 2.19                     | 0.43              |
| 1:B:66:HIS:NE2    | 1:B:71:GLU:HG2    | 2.33                     | 0.43              |
| 1:B:257:LEU:HD23  | 1:B:257:LEU:HA    | 1.59                     | 0.43              |
| 1:B:1038:THR:O    | 1:B:1039:LEU:C    | 2.61                     | 0.43              |
| 1:B:1077:THR:HG23 | 1:B:1082:SER:H    | 1.84                     | 0.43              |
| 1:B:1191:SER:N    | 1:B:1194:LYS:HD3  | 2.32                     | 0.43              |
| 1:B:1388:LEU:C    | 1:B:1390:SER:H    | 2.26                     | 0.43              |
| 1:B:3540:VAL:HB   | 1:B:3718:LYS:HD2  | 1.99                     | 0.43              |
| 1:B:4024:ILE:HD11 | 3:F:324:LEU:HD12  | 2.00                     | 0.43              |
| 1:B:4414:ILE:HD11 | 1:B:4451:ALA:HB1  | 2.01                     | 0.43              |
| 1:B:4601:ILE:HD11 | 1:B:4620:ILE:CD1  | 2.49                     | 0.43              |
| 1:A:124:VAL:HG11  | 1:A:129:LEU:CD2   | 2.48                     | 0.43              |
| 1:A:296:ARG:HA    | 1:A:299:PHE:CE2   | 2.54                     | 0.43              |
| 1:A:404:GLN:OE1   | 1:A:404:GLN:HA    | 2.17                     | 0.43              |
| 1:A:659:THR:HA    | 1:A:663:LEU:CD1   | 2.40                     | 0.43              |
| 1:A:817:ILE:HG22  | 1:A:821:PHE:CE2   | 2.53                     | 0.43              |
| 1:A:1281:ALA:HA   | 1:A:1284:LEU:CG   | 2.49                     | 0.43              |
| 1:A:1394:ARG:HH11 | 1:A:1443:ASN:HD21 | 1.65                     | 0.43              |
| 1:A:2661:VAL:HG11 | 1:A:2701:LEU:HG   | 2.01                     | 0.43              |
| 1:A:2688:CYS:O    | 1:A:2689:PRO:C    | 2.61                     | 0.43              |
| 1:A:3207:ARG:O    | 1:A:3211:ARG:HG3  | 2.18                     | 0.43              |
| 1:B:321:LEU:HD12  | 1:B:395:SER:CB    | 2.49                     | 0.43              |
| 1:B:862:PHE:CE1   | 1:B:866:LEU:HD11  | 2.53                     | 0.43              |
| 1:B:2493:GLY:O    | 1:B:2498:LYS:HE3  | 2.19                     | 0.43              |
| 1:B:2544:ASP:HA   | 1:B:2580:ILE:HD12 | 2.00                     | 0.43              |
| 1:B:2564:ASP:OD2  | 1:B:2631:LYS:O    | 2.37                     | 0.43              |
| 1:B:3095:VAL:HG11 | 1:B:3186:PHE:HE1  | 1.84                     | 0.43              |
| 2:D:38:ARG:HD2    | 2:D:43:ASN:HA     | 2.00                     | 0.43              |
| 1:A:255:LYS:O     | 1:A:259:VAL:HG23  | 2.19                     | 0.43              |
| 1:A:732:LEU:HD21  | 1:A:760:LEU:HD12  | 2.00                     | 0.43              |
| 1:A:1298:LEU:HA   | 1:A:1301:TRP:NE1  | 2.34                     | 0.43              |
| 1:A:2023:VAL:HG21 | 1:A:2049:VAL:HG21 | 2.01                     | 0.43              |
| 1:A:2368:ILE:HD11 | 1:A:2387:PHE:CZ   | 2.54                     | 0.43              |
| 1:A:3490:SER:O    | 1:A:3494:VAL:HG23 | 2.18                     | 0.43              |
| 1:A:4600:GLN:O    | 1:A:4601:ILE:C    | 2.62                     | 0.43              |
| 1:B:282:PHE:HB3   | 1:B:420:LEU:HD11  | 1.99                     | 0.43              |
| 1:B:1359:TYR:CE1  | 1:B:1406:GLU:HB3  | 2.53                     | 0.43              |
| 1:B:1407:LEU:HB3  | 1:B:1431:PHE:CZ   | 2.51                     | 0.43              |
| 1:B:1560:ALA:HB1  | 1:B:1599:ILE:HG23 | 2.01                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2027:ASP:CG   | 1:B:2029:CYS:SG   | 3.00                     | 0.43              |
| 1:B:2622:ILE:HD11 | 1:B:2667:TYR:CB   | 2.47                     | 0.43              |
| 1:B:3310:LEU:HG   | 1:B:3851:PHE:HB3  | 2.01                     | 0.43              |
| 1:B:3409:ILE:HD13 | 1:B:3454:ILE:HD11 | 2.01                     | 0.43              |
| 1:B:3460:ALA:O    | 1:B:3868:SER:N    | 2.40                     | 0.43              |
| 1:B:3525:TYR:HE2  | 1:B:3874:GLY:HA2  | 1.84                     | 0.43              |
| 3:F:317:SER:O     | 3:F:321:GLN:HG3   | 2.17                     | 0.43              |
| 1:A:329:VAL:CG1   | 1:A:388:ILE:HD12  | 2.49                     | 0.43              |
| 1:A:547:VAL:HA    | 1:A:550:ARG:HH11  | 1.83                     | 0.43              |
| 1:A:811:LEU:HD23  | 1:A:933:TYR:HE1   | 1.84                     | 0.43              |
| 1:A:852:PRO:O     | 1:A:853:LEU:C     | 2.61                     | 0.43              |
| 1:A:1281:ALA:HB2  | 1:A:1284:LEU:HD12 | 2.01                     | 0.43              |
| 1:A:2683:MET:HE3  | 1:A:2683:MET:HB2  | 1.90                     | 0.43              |
| 1:A:2698:LYS:O    | 1:A:2702:ILE:HG13 | 2.19                     | 0.43              |
| 1:A:3007:THR:O    | 1:A:3009:ASP:N    | 2.52                     | 0.43              |
| 1:A:4477:GLY:CA   | 1:A:4518:VAL:HG11 | 2.46                     | 0.43              |
| 1:B:29:TRP:CE3    | 1:B:73:PHE:HZ     | 2.37                     | 0.43              |
| 1:B:194:LEU:HD13  | 1:B:194:LEU:HA    | 1.89                     | 0.43              |
| 1:B:405:ASN:O     | 1:B:409:LEU:HG    | 2.19                     | 0.43              |
| 1:B:801:SER:O     | 1:B:805:ASP:N     | 2.52                     | 0.43              |
| 1:B:1514:LEU:O    | 1:B:1518:LEU:HG   | 2.19                     | 0.43              |
| 1:B:2263:ILE:HG12 | 1:B:2655:ALA:HB1  | 2.00                     | 0.43              |
| 1:B:3294:CYS:HB3  | 1:B:3301:LEU:HG   | 1.99                     | 0.43              |
| 1:B:3295:ILE:HD12 | 1:B:3295:ILE:HA   | 1.93                     | 0.43              |
| 1:B:4598:LEU:HD11 | 1:B:4634:LEU:HB2  | 2.00                     | 0.43              |
| 1:B:4606:VAL:HG11 | 1:B:4616:LEU:HD22 | 2.00                     | 0.43              |
| 1:B:4751:LEU:HD23 | 1:B:4751:LEU:HA   | 1.77                     | 0.43              |
| 1:A:248:GLN:HB3   | 1:B:496:LEU:HD11  | 2.01                     | 0.42              |
| 1:A:280:ASN:HB2   | 1:A:412:TRP:HE1   | 1.84                     | 0.42              |
| 1:A:405:ASN:CB    | 1:A:511:ILE:HA    | 2.49                     | 0.42              |
| 1:A:484:LEU:O     | 1:A:488:PHE:HD1   | 2.02                     | 0.42              |
| 1:A:864:TYR:HD2   | 1:A:865:LEU:HD23  | 1.84                     | 0.42              |
| 1:A:973:LEU:HD23  | 1:A:973:LEU:HA    | 1.85                     | 0.42              |
| 1:A:1345:GLU:H    | 1:A:1345:GLU:CD   | 2.27                     | 0.42              |
| 1:A:1859:MET:N    | 1:A:2200:GLN:OE1  | 2.43                     | 0.42              |
| 1:A:2698:LYS:HG2  | 1:A:2998:PRO:HA   | 2.00                     | 0.42              |
| 1:A:3021:LEU:O    | 1:A:3025:LEU:HG   | 2.18                     | 0.42              |
| 1:A:3699:LEU:HD23 | 1:A:3706:CYS:HB2  | 2.01                     | 0.42              |
| 1:A:4101:TYR:CE2  | 2:C:89:ALA:HB2    | 2.54                     | 0.42              |
| 1:A:4622:TYR:HA   | 1:A:4670:LYS:HE3  | 2.00                     | 0.42              |
| 1:B:256:LEU:HD12  | 1:B:317:VAL:HG22  | 2.01                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:265:TYR:HB3   | 1:B:302:LEU:HD13  | 2.01                     | 0.42              |
| 1:B:654:ILE:O     | 1:B:658:ILE:HG13  | 2.19                     | 0.42              |
| 1:B:881:GLN:HA    | 1:B:885:LEU:HD12  | 2.00                     | 0.42              |
| 1:B:1032:GLU:O    | 1:B:1035:ILE:HB   | 2.19                     | 0.42              |
| 1:B:1405:GLY:O    | 1:B:1409:GLN:HG2  | 2.18                     | 0.42              |
| 1:B:2192:VAL:HG13 | 1:B:2197:PHE:HE1  | 1.82                     | 0.42              |
| 1:B:3396:VAL:HG11 | 1:B:3438:ASN:CB   | 2.49                     | 0.42              |
| 1:B:3986:TRP:CZ2  | 3:F:316:ARG:HG2   | 2.54                     | 0.42              |
| 1:A:666:ARG:HA    | 1:A:671:ARG:HE    | 1.84                     | 0.42              |
| 1:A:1269:HIS:ND1  | 1:A:1283:SER:HB3  | 2.35                     | 0.42              |
| 1:A:1288:LEU:O    | 1:A:1292:VAL:HG23 | 2.18                     | 0.42              |
| 1:A:1324:GLU:HA   | 1:A:1327:ALA:HB2  | 2.01                     | 0.42              |
| 1:A:3440:SER:OG   | 1:A:3443:GLN:OE1  | 2.20                     | 0.42              |
| 1:A:4003:ILE:HB   | 1:A:4008:VAL:HG11 | 2.01                     | 0.42              |
| 1:A:4199:TYR:HE1  | 2:C:39:SER:HA     | 1.84                     | 0.42              |
| 1:A:4727:ARG:O    | 1:A:4731:ILE:HG13 | 2.19                     | 0.42              |
| 1:A:4744:SER:O    | 1:A:4748:LEU:HG   | 2.19                     | 0.42              |
| 1:B:474:VAL:HG11  | 1:B:646:LEU:HG    | 1.99                     | 0.42              |
| 1:B:866:LEU:HD13  | 1:B:1013:LEU:HD21 | 2.01                     | 0.42              |
| 1:B:1177:LEU:HD23 | 1:B:1177:LEU:HA   | 1.84                     | 0.42              |
| 1:B:1387:GLN:HB3  | 1:B:1397:MET:SD   | 2.59                     | 0.42              |
| 1:B:1701:HIS:HB2  | 1:B:1706:ILE:HD11 | 2.01                     | 0.42              |
| 1:B:3021:LEU:O    | 1:B:3025:LEU:HG   | 2.19                     | 0.42              |
| 1:B:3525:TYR:CE2  | 1:B:3874:GLY:HA2  | 2.54                     | 0.42              |
| 1:B:4360:GLU:CD   | 1:B:4366:ARG:HH21 | 2.25                     | 0.42              |
| 2:D:45:THR:OG1    | 2:D:48:GLU:HG3    | 2.19                     | 0.42              |
| 3:F:2:SER:H       | 3:F:59:VAL:HG21   | 1.84                     | 0.42              |
| 1:A:718:VAL:HG13  | 1:A:760:LEU:CD2   | 2.49                     | 0.42              |
| 1:A:1377:LEU:H    | 1:A:1377:LEU:HD12 | 1.84                     | 0.42              |
| 1:A:2023:VAL:HG23 | 1:A:2046:ILE:HD13 | 2.02                     | 0.42              |
| 1:A:3095:VAL:HG12 | 1:A:3190:TRP:CH2  | 2.54                     | 0.42              |
| 1:A:3515:THR:HG21 | 1:A:3764:LEU:HD22 | 2.01                     | 0.42              |
| 1:A:3736:VAL:HG12 | 1:A:3740:ASN:HD21 | 1.85                     | 0.42              |
| 1:A:4570:LEU:HD13 | 1:A:4622:TYR:HB2  | 2.01                     | 0.42              |
| 1:B:1097:GLN:HE21 | 1:B:1097:GLN:CA   | 2.31                     | 0.42              |
| 1:B:1560:ALA:HB1  | 1:B:1599:ILE:CG2  | 2.49                     | 0.42              |
| 1:B:1575:ASN:O    | 1:B:1579:LYS:HG3  | 2.20                     | 0.42              |
| 1:B:2151:ILE:HD11 | 1:B:2164:LEU:HD21 | 2.01                     | 0.42              |
| 1:B:2379:LEU:HD23 | 1:B:2379:LEU:H    | 1.84                     | 0.42              |
| 1:B:3527:LEU:HD11 | 1:B:3757:ARG:HB2  | 2.00                     | 0.42              |
| 1:B:3647:PHE:HB2  | 1:B:3649:GLU:HG3  | 2.00                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:E:318:LEU:O     | 3:E:322:GLU:HG2   | 2.20                     | 0.42              |
| 1:A:240:ILE:O     | 1:A:244:VAL:HG23  | 2.19                     | 0.42              |
| 1:A:296:ARG:HA    | 1:A:299:PHE:CZ    | 2.54                     | 0.42              |
| 1:A:317:VAL:C     | 1:A:318:LEU:HG    | 2.44                     | 0.42              |
| 1:A:699:LYS:O     | 1:A:703:ASP:HB2   | 2.19                     | 0.42              |
| 1:A:1556:LEU:HD21 | 1:A:1563:TRP:CZ3  | 2.54                     | 0.42              |
| 1:A:2071:TYR:CE1  | 1:A:2091:VAL:HG22 | 2.55                     | 0.42              |
| 1:A:2355:GLN:HB2  | 1:A:2384:TRP:CE2  | 2.55                     | 0.42              |
| 1:A:2695:PHE:O    | 1:A:2698:LYS:HB3  | 2.19                     | 0.42              |
| 1:A:3023:ASN:O    | 1:A:3027:GLN:HG2  | 2.19                     | 0.42              |
| 1:A:4281:THR:HB   | 1:A:4284:ILE:HG12 | 2.00                     | 0.42              |
| 1:A:4484:GLY:O    | 1:A:4485:LEU:C    | 2.62                     | 0.42              |
| 1:B:154:MET:O     | 1:B:157:SER:OG    | 2.34                     | 0.42              |
| 1:B:183:GLU:O     | 1:B:187:LYS:HG2   | 2.19                     | 0.42              |
| 1:B:488:PHE:HE2   | 1:B:670:ILE:HD12  | 1.84                     | 0.42              |
| 1:B:881:GLN:HA    | 1:B:885:LEU:HB2   | 2.01                     | 0.42              |
| 1:B:1014:PRO:HB3  | 1:B:1057:HIS:CD2  | 2.55                     | 0.42              |
| 1:B:1110:LEU:O    | 1:B:1175:ALA:HB1  | 2.20                     | 0.42              |
| 1:B:1912:LEU:HB2  | 1:B:1926:LEU:HD11 | 2.02                     | 0.42              |
| 1:B:2192:VAL:HG13 | 1:B:2197:PHE:CE1  | 2.54                     | 0.42              |
| 1:B:3595:ASN:HD21 | 1:B:3605:LEU:HD13 | 1.83                     | 0.42              |
| 1:B:4372:TYR:HD1  | 1:B:4376:GLU:OE2  | 2.02                     | 0.42              |
| 2:D:66:PHE:HB3    | 2:D:67:PRO:HD3    | 2.01                     | 0.42              |
| 1:A:856:ALA:HB1   | 1:A:1001:TYR:HD2  | 1.85                     | 0.42              |
| 1:A:1057:HIS:HA   | 1:A:1060:LYS:HD2  | 2.01                     | 0.42              |
| 1:A:1176:TYR:CZ   | 1:A:1280:LEU:HB2  | 2.55                     | 0.42              |
| 1:A:1817:PHE:CE2  | 1:A:1818:LEU:HG   | 2.55                     | 0.42              |
| 1:A:1854:MET:HE2  | 1:A:2152:LYS:H    | 1.83                     | 0.42              |
| 1:A:3409:ILE:HD13 | 1:A:3454:ILE:HD11 | 2.01                     | 0.42              |
| 1:A:4659:LEU:HG   | 1:A:4721:PHE:HB3  | 2.01                     | 0.42              |
| 1:A:4716:ARG:HA   | 1:A:4717:PRO:HD3  | 1.94                     | 0.42              |
| 1:B:1473:THR:O    | 1:B:1485:ILE:HG21 | 2.19                     | 0.42              |
| 1:B:1867:GLU:HG2  | 1:B:2236:ASP:OD2  | 2.18                     | 0.42              |
| 1:B:2009:PRO:CB   | 1:B:2642:LEU:HD21 | 2.50                     | 0.42              |
| 1:B:4513:SER:O    | 1:B:4517:LYS:HG2  | 2.19                     | 0.42              |
| 3:E:4:HIS:CD2     | 3:E:21:ARG:HB2    | 2.55                     | 0.42              |
| 3:E:113:CYS:SG    | 3:E:131:HIS:CE1   | 3.13                     | 0.42              |
| 1:A:926:ALA:O     | 1:A:928:PRO:HD3   | 2.19                     | 0.42              |
| 1:A:2178:CYS:HB3  | 1:A:2214:MET:HE1  | 2.02                     | 0.42              |
| 1:A:3195:SER:HG   | 1:A:3231:HIS:CE1  | 2.34                     | 0.42              |
| 1:A:3997:PHE:HZ   | 1:A:4128:TRP:CE3  | 2.37                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:136:LEU:HD23  | 1:B:136:LEU:HA    | 1.82                     | 0.42              |
| 1:B:313:LEU:HD21  | 1:B:332:LEU:CD2   | 2.49                     | 0.42              |
| 1:B:352:VAL:HG21  | 1:B:424:LEU:HD13  | 2.02                     | 0.42              |
| 1:B:1545:ALA:HB2  | 1:B:1556:LEU:CD2  | 2.48                     | 0.42              |
| 1:B:1597:CYS:SG   | 1:B:2477:ARG:HB2  | 2.59                     | 0.42              |
| 1:B:2405:ILE:CG1  | 1:B:2417:ILE:HD11 | 2.49                     | 0.42              |
| 1:B:4119:LEU:HD11 | 3:F:329:VAL:HG11  | 2.00                     | 0.42              |
| 1:B:4346:VAL:HG21 | 1:B:4425:TYR:CD1  | 2.55                     | 0.42              |
| 3:E:111:PRO:HD2   | 3:E:128:PHE:CZ    | 2.54                     | 0.42              |
| 3:E:295:ARG:HG2   | 3:E:295:ARG:O     | 2.19                     | 0.42              |
| 3:F:295:ARG:HG2   | 3:F:295:ARG:O     | 2.19                     | 0.42              |
| 3:F:318:LEU:O     | 3:F:322:GLU:HG2   | 2.20                     | 0.42              |
| 1:A:112:LEU:HD13  | 1:A:252:GLY:HA3   | 2.02                     | 0.42              |
| 1:A:273:PHE:CE1   | 1:A:334:LEU:HB3   | 2.54                     | 0.42              |
| 1:A:415:LEU:HD21  | 1:A:484:LEU:HD11  | 2.01                     | 0.42              |
| 1:A:1219:VAL:O    | 1:A:1227:GLN:NE2  | 2.53                     | 0.42              |
| 1:A:1233:TRP:CH2  | 1:A:1281:ALA:HB1  | 2.54                     | 0.42              |
| 1:A:1345:GLU:O    | 1:A:1349:ARG:HG2  | 2.19                     | 0.42              |
| 1:A:2263:ILE:HA   | 1:A:2575:ILE:HD11 | 2.02                     | 0.42              |
| 1:A:2266:MET:SD   | 1:A:2575:ILE:HG12 | 2.60                     | 0.42              |
| 1:A:3295:ILE:HD12 | 1:A:3295:ILE:HA   | 1.84                     | 0.42              |
| 1:A:3550:ILE:HD11 | 1:A:3715:LEU:HD12 | 2.01                     | 0.42              |
| 1:A:3884:ILE:HD11 | 1:A:3913:ASN:ND2  | 2.34                     | 0.42              |
| 1:B:30:GLU:H      | 1:B:30:GLU:HG3    | 1.66                     | 0.42              |
| 1:B:131:LEU:HD11  | 1:B:142:ARG:HG3   | 2.01                     | 0.42              |
| 1:B:2137:SER:O    | 1:B:2141:LEU:N    | 2.51                     | 0.42              |
| 1:B:3269:LEU:HB3  | 1:B:3633:LEU:HD13 | 1.90                     | 0.42              |
| 1:B:4491:ARG:O    | 1:B:4495:ILE:HG13 | 2.20                     | 0.42              |
| 2:C:123:ASP:O     | 2:C:127:ARG:HG2   | 2.20                     | 0.42              |
| 3:F:111:PRO:HD2   | 3:F:128:PHE:CZ    | 2.55                     | 0.42              |
| 1:A:1090:VAL:HG21 | 1:A:1131:VAL:HG13 | 2.02                     | 0.42              |
| 1:A:1138:HIS:HA   | 1:A:1141:LYS:HD3  | 2.02                     | 0.42              |
| 1:A:1912:LEU:HB2  | 1:A:1926:LEU:HD11 | 2.02                     | 0.42              |
| 1:A:2049:VAL:HG22 | 1:A:2063:ILE:HG12 | 2.01                     | 0.42              |
| 1:A:2551:ALA:HA   | 1:A:2573:LEU:HD22 | 2.01                     | 0.42              |
| 1:A:4414:ILE:HD11 | 1:A:4451:ALA:HB1  | 2.02                     | 0.42              |
| 1:B:115:LEU:CD1   | 1:B:130:ILE:HG13  | 2.50                     | 0.42              |
| 1:B:255:LYS:O     | 1:B:259:VAL:HG23  | 2.20                     | 0.42              |
| 1:B:919:SER:HA    | 1:B:922:PHE:CD2   | 2.54                     | 0.42              |
| 1:B:943:ASP:OD2   | 1:B:943:ASP:N     | 2.52                     | 0.42              |
| 1:B:2300:ASP:OD1  | 1:B:2300:ASP:N    | 2.53                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2701:LEU:HD12 | 1:B:3002:VAL:CG2  | 2.50                     | 0.42              |
| 2:C:34:GLY:HA2    | 2:C:37:MET:HE2    | 2.01                     | 0.42              |
| 2:C:95:LYS:HE2    | 2:C:109:VAL:HG23  | 2.02                     | 0.42              |
| 1:A:94:ARG:O      | 1:A:97:LEU:HB3    | 2.19                     | 0.42              |
| 1:A:130:ILE:HD12  | 1:A:308:MET:HG3   | 2.02                     | 0.42              |
| 1:A:150:THR:O     | 1:A:154:MET:HG3   | 2.20                     | 0.42              |
| 1:A:1848:VAL:O    | 1:A:1850:LYS:NZ   | 2.38                     | 0.42              |
| 1:A:2042:PRO:HD3  | 1:A:2088:VAL:O    | 2.20                     | 0.42              |
| 1:A:3749:VAL:HG23 | 1:A:3814:LEU:HD13 | 2.02                     | 0.42              |
| 1:A:3773:GLU:O    | 1:A:3774:LYS:C    | 2.63                     | 0.42              |
| 1:B:414:LEU:HD12  | 1:B:483:LEU:HD12  | 2.01                     | 0.42              |
| 1:B:1591:MET:O    | 1:B:1594:GLU:HG2  | 2.20                     | 0.42              |
| 1:B:1693:CYS:N    | 1:B:1716:CYS:SG   | 2.92                     | 0.42              |
| 1:B:2551:ALA:HA   | 1:B:2573:LEU:HD22 | 2.01                     | 0.42              |
| 1:B:2686:LEU:HD11 | 1:B:3002:VAL:HG11 | 2.02                     | 0.42              |
| 1:B:3050:GLU:O    | 1:B:3054:VAL:HG23 | 2.19                     | 0.42              |
| 1:B:3061:VAL:O    | 1:B:3065:ARG:N    | 2.44                     | 0.42              |
| 1:B:3076:GLU:H    | 1:B:3076:GLU:HG3  | 1.73                     | 0.42              |
| 1:B:3233:LEU:HD13 | 1:B:3290:TRP:HE3  | 1.85                     | 0.42              |
| 1:B:3699:LEU:HD23 | 1:B:3706:CYS:HB2  | 2.01                     | 0.42              |
| 1:B:3922:ARG:O    | 1:B:3926:ARG:HG3  | 2.20                     | 0.42              |
| 1:B:4224:GLU:HA   | 1:B:4279:GLN:NE2  | 2.35                     | 0.42              |
| 1:B:4510:LYS:HE2  | 1:B:4514:TYR:OH   | 2.19                     | 0.42              |
| 2:D:28:ILE:H      | 2:D:28:ILE:HG12   | 1.48                     | 0.42              |
| 3:E:3:ARG:HG2     | 3:E:18:ARG:CG     | 2.50                     | 0.42              |
| 1:A:124:VAL:HG11  | 1:A:129:LEU:HD23  | 2.02                     | 0.42              |
| 1:A:336:CYS:SG    | 1:A:384:ILE:HD12  | 2.59                     | 0.42              |
| 1:A:699:LYS:O     | 1:A:704:GLU:HG3   | 2.20                     | 0.42              |
| 1:A:2405:ILE:CG1  | 1:A:2417:ILE:HD11 | 2.50                     | 0.42              |
| 1:A:3269:LEU:HB3  | 1:A:3633:LEU:HD13 | 1.91                     | 0.42              |
| 1:A:4328:PRO:O    | 1:A:4331:ILE:HB   | 2.19                     | 0.42              |
| 1:A:4372:TYR:HD1  | 1:A:4376:GLU:OE2  | 2.02                     | 0.42              |
| 1:A:4748:LEU:HB2  | 1:A:4768:LEU:HD21 | 2.02                     | 0.42              |
| 1:B:159:LYS:HA    | 1:B:159:LYS:HD2   | 1.85                     | 0.42              |
| 1:B:321:LEU:HD23  | 1:B:321:LEU:HA    | 1.87                     | 0.42              |
| 1:B:1307:PRO:HB2  | 1:B:1308:PRO:HD3  | 2.01                     | 0.42              |
| 1:B:1486:GLN:HG3  | 1:B:1489:ARG:NH1  | 2.35                     | 0.42              |
| 1:B:1554:LEU:HA   | 1:B:1557:HIS:CD2  | 2.54                     | 0.42              |
| 1:B:1563:TRP:HD1  | 1:B:1566:ARG:HH11 | 1.68                     | 0.42              |
| 1:B:2369:GLU:HA   | 1:B:2373:ARG:O    | 2.20                     | 0.42              |
| 1:B:2379:LEU:HB3  | 1:B:2385:PHE:HZ   | 1.85                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:3054:VAL:HG13 | 1:B:3057:ARG:HD2  | 2.02                     | 0.42              |
| 1:B:4273:LEU:HD22 | 1:B:4284:ILE:CG2  | 2.49                     | 0.42              |
| 1:A:184:LEU:HD22  | 1:A:184:LEU:N     | 2.32                     | 0.41              |
| 1:A:1046:ARG:HD2  | 1:A:1046:ARG:HA   | 1.88                     | 0.41              |
| 1:A:3453:SER:O    | 1:A:3456:PRO:HD2  | 2.20                     | 0.41              |
| 1:B:100:VAL:HG12  | 1:B:239:PHE:HE1   | 1.85                     | 0.41              |
| 1:B:3988:LEU:HD12 | 1:B:3988:LEU:H    | 1.85                     | 0.41              |
| 1:B:4309:PHE:CD1  | 1:B:4338:ILE:HD11 | 2.54                     | 0.41              |
| 2:C:73:MET:O      | 2:C:77:MET:N      | 2.46                     | 0.41              |
| 3:F:9:CYS:O       | 3:F:13:LEU:HA     | 2.19                     | 0.41              |
| 3:F:81:PRO:HB2    | 3:F:108:VAL:HB    | 2.02                     | 0.41              |
| 1:A:29:TRP:HA     | 1:A:32:ALA:HB3    | 2.01                     | 0.41              |
| 1:A:292:ALA:O     | 1:A:296:ARG:HG3   | 2.19                     | 0.41              |
| 1:A:643:ASP:HA    | 1:A:644:PRO:HD2   | 1.96                     | 0.41              |
| 1:A:768:ALA:HA    | 1:A:773:ASP:HB2   | 2.01                     | 0.41              |
| 1:A:853:LEU:HD13  | 1:A:998:ALA:HB2   | 2.02                     | 0.41              |
| 1:A:1382:GLN:N    | 1:A:1426:ARG:HH21 | 2.18                     | 0.41              |
| 1:A:1682:HIS:HA   | 1:A:2381:ARG:NH2  | 2.35                     | 0.41              |
| 1:A:2038:TYR:C    | 1:A:2038:TYR:CD2  | 2.96                     | 0.41              |
| 1:A:2118:VAL:HG11 | 1:A:2174:PRO:HB3  | 2.03                     | 0.41              |
| 1:A:3167:LEU:HB3  | 1:A:3168:PRO:CD   | 2.43                     | 0.41              |
| 1:A:3396:VAL:HG11 | 1:A:3438:ASN:CB   | 2.49                     | 0.41              |
| 1:A:3771:ALA:HB1  | 1:B:3919:ALA:HB2  | 2.02                     | 0.41              |
| 1:A:3922:ARG:O    | 1:A:3926:ARG:HG3  | 2.20                     | 0.41              |
| 1:A:4492:LEU:HD23 | 1:A:4492:LEU:HA   | 1.87                     | 0.41              |
| 1:A:4710:TRP:HZ3  | 1:A:4751:LEU:HD23 | 1.86                     | 0.41              |
| 1:B:943:ASP:HB3   | 1:B:1255:THR:HG21 | 2.01                     | 0.41              |
| 1:B:1679:TYR:HB2  | 1:B:1692:VAL:HG22 | 2.02                     | 0.41              |
| 1:B:1805:PHE:CD2  | 1:B:2494:PRO:HD2  | 2.52                     | 0.41              |
| 1:B:2046:ILE:HG23 | 1:B:2063:ILE:HG23 | 2.01                     | 0.41              |
| 1:B:2118:VAL:HG11 | 1:B:2174:PRO:HB3  | 2.02                     | 0.41              |
| 1:B:2259:PRO:HB2  | 1:B:2651:THR:HG21 | 2.00                     | 0.41              |
| 1:B:2593:GLU:HG3  | 1:B:2667:TYR:OH   | 2.20                     | 0.41              |
| 1:B:3729:GLU:HA   | 1:B:3732:ARG:HB3  | 2.02                     | 0.41              |
| 1:B:3884:ILE:HD11 | 1:B:3913:ASN:ND2  | 2.34                     | 0.41              |
| 1:B:4307:LYS:HG2  | 1:B:4478:VAL:CG1  | 2.50                     | 0.41              |
| 1:B:4695:MET:HE1  | 1:B:4748:LEU:HD21 | 2.01                     | 0.41              |
| 1:A:73:PHE:HD2    | 1:A:74:TYR:HD1    | 1.67                     | 0.41              |
| 1:A:366:LYS:HA    | 1:A:369:ASP:CG    | 2.45                     | 0.41              |
| 1:A:694:ASP:CB    | 1:A:750:HIS:HB3   | 2.50                     | 0.41              |
| 1:A:995:GLU:O     | 1:A:999:LEU:HG    | 2.21                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1060:LYS:O    | 1:A:1061:GLN:C    | 2.63                     | 0.41              |
| 1:A:1194:LYS:HA   | 1:A:1370:SER:O    | 2.20                     | 0.41              |
| 1:A:1201:VAL:HG13 | 1:A:1218:LEU:HB3  | 2.02                     | 0.41              |
| 1:A:2639:ASN:HB3  | 1:A:2642:LEU:HG   | 2.01                     | 0.41              |
| 1:A:3053:LEU:HA   | 1:A:3056:MET:HE2  | 2.01                     | 0.41              |
| 1:A:3099:LEU:HD22 | 1:A:3190:TRP:CE2  | 2.55                     | 0.41              |
| 1:A:3470:ASP:OD1  | 3:E:293:LEU:HG    | 2.21                     | 0.41              |
| 1:A:3964:LEU:HA   | 1:A:3967:SER:HB2  | 2.02                     | 0.41              |
| 1:A:3991:ARG:HA   | 1:A:4059:TRP:CZ3  | 2.55                     | 0.41              |
| 1:A:4699:ILE:HA   | 1:A:4700:PRO:HD3  | 1.94                     | 0.41              |
| 1:B:320:PRO:O     | 1:B:325:ARG:NH1   | 2.49                     | 0.41              |
| 1:B:321:LEU:HD12  | 1:B:395:SER:HB2   | 2.03                     | 0.41              |
| 1:B:655:LEU:HD23  | 1:B:655:LEU:HA    | 1.75                     | 0.41              |
| 1:B:1243:ASN:OD1  | 1:B:1243:ASN:N    | 2.53                     | 0.41              |
| 1:B:1678:TRP:CD1  | 1:B:1678:TRP:H    | 2.39                     | 0.41              |
| 1:B:1859:MET:N    | 1:B:2200:GLN:OE1  | 2.43                     | 0.41              |
| 1:B:2187:PRO:HB3  | 1:B:2214:MET:SD   | 2.59                     | 0.41              |
| 1:B:3320:LEU:HD23 | 1:B:3320:LEU:HA   | 1.92                     | 0.41              |
| 1:B:3387:GLN:HG2  | 1:B:3388:GLU:N    | 2.35                     | 0.41              |
| 1:B:4108:PHE:HA   | 1:B:4111:ARG:CG   | 2.50                     | 0.41              |
| 1:B:4363:LEU:HD21 | 1:B:4444:MET:HG3  | 2.00                     | 0.41              |
| 2:C:10:ILE:HG13   | 2:C:66:PHE:CZ     | 2.55                     | 0.41              |
| 3:F:5:GLU:HA      | 3:F:16:ASN:OD1    | 2.21                     | 0.41              |
| 1:A:29:TRP:O      | 1:A:33:VAL:HG13   | 2.19                     | 0.41              |
| 1:A:1204:ILE:HD11 | 1:A:1357:GLY:CA   | 2.50                     | 0.41              |
| 1:A:1232:SER:O    | 1:A:1236:ILE:HG13 | 2.21                     | 0.41              |
| 1:A:1679:TYR:CE1  | 1:A:1708:TYR:HA   | 2.55                     | 0.41              |
| 1:A:2479:VAL:HG21 | 1:A:2521:VAL:HG22 | 2.02                     | 0.41              |
| 1:A:2517:ALA:CB   | 1:A:2521:VAL:HB   | 2.50                     | 0.41              |
| 1:A:3181:ILE:HA   | 1:A:3182:PRO:HD3  | 1.88                     | 0.41              |
| 1:A:3311:VAL:HB   | 1:A:3315:VAL:HB   | 2.03                     | 0.41              |
| 1:A:4132:VAL:CG1  | 1:A:4145:ALA:HB2  | 2.50                     | 0.41              |
| 1:A:4244:LEU:O    | 1:A:4248:PHE:HD1  | 2.03                     | 0.41              |
| 1:B:139:GLY:HA2   | 1:B:240:ILE:HD11  | 2.02                     | 0.41              |
| 1:B:310:LEU:HA    | 1:B:313:LEU:HB2   | 2.03                     | 0.41              |
| 1:B:310:LEU:O     | 1:B:314:SER:N     | 2.50                     | 0.41              |
| 1:B:422:LEU:HD11  | 1:B:537:LEU:HG    | 2.02                     | 0.41              |
| 1:B:1132:GLN:HE22 | 1:B:1293:ARG:HH21 | 1.69                     | 0.41              |
| 1:B:1244:ILE:HG21 | 1:B:1249:ASN:HB3  | 2.01                     | 0.41              |
| 1:B:1428:LEU:HB3  | 1:B:1491:LEU:CB   | 2.51                     | 0.41              |
| 1:B:1600:MET:HG2  | 1:B:2478:LEU:HD12 | 2.01                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2025:ILE:HD13 | 1:B:2075:MET:CE   | 2.50                     | 0.41              |
| 1:B:3102:LEU:O    | 1:B:3197:TYR:OH   | 2.31                     | 0.41              |
| 1:B:4129:LEU:HD12 | 1:B:4129:LEU:HA   | 1.85                     | 0.41              |
| 1:B:4187:TYR:O    | 1:B:4191:ILE:HG12 | 2.21                     | 0.41              |
| 1:B:4331:ILE:O    | 1:B:4335:LEU:HG   | 2.21                     | 0.41              |
| 2:C:131:ILE:HD11  | 2:C:144:GLN:HG2   | 2.03                     | 0.41              |
| 1:A:108:ILE:O     | 1:A:112:LEU:HG    | 2.20                     | 0.41              |
| 1:A:418:LEU:O     | 1:A:422:LEU:HG    | 2.21                     | 0.41              |
| 1:A:1178:LEU:CD2  | 1:A:1202:LEU:HD21 | 2.50                     | 0.41              |
| 1:A:1294:LEU:O    | 1:A:1298:LEU:HG   | 2.20                     | 0.41              |
| 1:A:2025:ILE:HD13 | 1:A:2075:MET:CE   | 2.50                     | 0.41              |
| 1:A:3142:ARG:HA   | 1:A:3142:ARG:HD3  | 1.85                     | 0.41              |
| 1:A:4767:LEU:O    | 1:A:4771:LEU:HG   | 2.21                     | 0.41              |
| 1:B:114:ARG:HD3   | 1:B:114:ARG:HA    | 1.68                     | 0.41              |
| 1:B:694:ASP:OD2   | 1:B:750:HIS:HB3   | 2.20                     | 0.41              |
| 1:B:808:VAL:HG11  | 1:B:908:TYR:CB    | 2.49                     | 0.41              |
| 1:B:936:LEU:HD13  | 1:B:1008:ARG:NH2  | 2.35                     | 0.41              |
| 1:B:1374:GLU:OE1  | 1:B:1423:PHE:HB2  | 2.21                     | 0.41              |
| 1:B:2058:LYS:HB2  | 1:B:2074:LEU:HD11 | 2.01                     | 0.41              |
| 1:B:2564:ASP:OD1  | 1:B:2631:LYS:HD3  | 2.20                     | 0.41              |
| 1:B:2985:LEU:HA   | 1:B:2988:LEU:HD13 | 2.02                     | 0.41              |
| 1:B:3311:VAL:HG23 | 1:B:3312:ASP:O    | 2.20                     | 0.41              |
| 1:B:3396:VAL:HG11 | 1:B:3438:ASN:HB3  | 2.02                     | 0.41              |
| 1:B:3512:ILE:HD11 | 1:B:3761:GLU:HG2  | 2.02                     | 0.41              |
| 1:B:3901:VAL:HG11 | 1:B:3939:ALA:HB2  | 2.02                     | 0.41              |
| 1:B:4244:LEU:O    | 1:B:4248:PHE:HD1  | 2.03                     | 0.41              |
| 1:B:4727:ARG:NE   | 1:B:4766:ASN:HB3  | 2.35                     | 0.41              |
| 1:A:418:LEU:HD11  | 1:A:477:ALA:HA    | 2.01                     | 0.41              |
| 1:A:481:ILE:O     | 1:A:485:THR:HG23  | 2.20                     | 0.41              |
| 1:A:548:LEU:HD22  | 1:A:642:LYS:HA    | 2.02                     | 0.41              |
| 1:A:693:VAL:HG21  | 1:A:710:LEU:HD22  | 2.02                     | 0.41              |
| 1:A:834:VAL:HG11  | 1:A:961:VAL:HG13  | 2.03                     | 0.41              |
| 1:A:921:HIS:HB2   | 1:A:993:ALA:HB2   | 2.03                     | 0.41              |
| 1:A:1178:LEU:HA   | 1:A:1181:PHE:CE2  | 2.55                     | 0.41              |
| 1:A:1255:THR:OG1  | 1:A:1256:ILE:N    | 2.54                     | 0.41              |
| 1:A:1536:GLU:O    | 1:A:1540:VAL:HG23 | 2.20                     | 0.41              |
| 1:A:1556:LEU:HD13 | 1:A:1560:ALA:HB2  | 2.01                     | 0.41              |
| 1:A:2054:ASN:HB3  | 1:A:2060:ILE:HD11 | 2.02                     | 0.41              |
| 1:A:3053:LEU:HD22 | 1:A:3156:TYR:CD1  | 2.55                     | 0.41              |
| 1:A:3463:ARG:NH2  | 1:A:3538:PRO:HA   | 2.35                     | 0.41              |
| 1:A:3519:LEU:CD1  | 1:A:3767:VAL:HG11 | 2.51                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:4108:PHE:HA   | 1:A:4111:ARG:CG   | 2.50                     | 0.41              |
| 1:A:4694:TYR:CD1  | 1:A:4694:TYR:C    | 2.98                     | 0.41              |
| 1:B:229:GLN:O     | 1:B:233:ILE:HG13  | 2.20                     | 0.41              |
| 1:B:916:GLU:O     | 1:B:920:LYS:HG3   | 2.20                     | 0.41              |
| 1:B:1388:LEU:HD23 | 1:B:1394:ARG:HG3  | 2.02                     | 0.41              |
| 1:B:1475:PRO:HG2  | 1:B:1481:GLN:HB2  | 2.01                     | 0.41              |
| 1:B:1590:VAL:HA   | 1:B:1593:LEU:HD13 | 2.01                     | 0.41              |
| 1:B:2414:VAL:HG11 | 1:B:2416:MET:HE3  | 2.02                     | 0.41              |
| 1:B:3087:ALA:CB   | 1:B:3181:ILE:CD1  | 2.89                     | 0.41              |
| 1:A:325:ARG:O     | 1:A:326:LEU:C     | 2.64                     | 0.41              |
| 1:A:414:LEU:HD12  | 1:A:483:LEU:HD12  | 2.01                     | 0.41              |
| 1:A:942:GLU:HB3   | 1:A:947:ARG:NE    | 2.35                     | 0.41              |
| 1:A:1268:ALA:O    | 1:A:1272:THR:HG23 | 2.20                     | 0.41              |
| 1:A:1384:LEU:HD22 | 1:A:1384:LEU:HA   | 1.95                     | 0.41              |
| 1:A:1729:LEU:HD23 | 1:A:1729:LEU:HA   | 1.90                     | 0.41              |
| 1:A:1798:GLU:H    | 1:A:1798:GLU:CD   | 2.28                     | 0.41              |
| 1:A:2311:VAL:HG11 | 3:E:64:TYR:CD1    | 2.56                     | 0.41              |
| 1:A:3049:ASN:HB3  | 1:A:3156:TYR:OH   | 2.19                     | 0.41              |
| 1:A:3283:ALA:HB1  | 1:A:3325:CYS:CB   | 2.50                     | 0.41              |
| 1:A:4303:GLU:HB2  | 1:A:4475:MET:SD   | 2.60                     | 0.41              |
| 1:A:4336:CYS:HB3  | 1:A:4514:TYR:HE2  | 1.85                     | 0.41              |
| 1:A:4713:PHE:CE1  | 1:A:4751:LEU:HD21 | 2.44                     | 0.41              |
| 1:B:1486:GLN:O    | 1:B:1490:GLN:HG3  | 2.20                     | 0.41              |
| 1:B:1859:MET:CE   | 1:B:2230:MET:HB2  | 2.50                     | 0.41              |
| 1:B:2094:ILE:HD13 | 1:B:2124:PHE:CZ   | 2.56                     | 0.41              |
| 1:B:2687:LEU:O    | 1:B:2688:CYS:C    | 2.63                     | 0.41              |
| 1:B:3003:ILE:O    | 1:B:3006:LEU:HB2  | 2.21                     | 0.41              |
| 1:B:3105:LEU:HB2  | 1:B:3197:TYR:OH   | 2.21                     | 0.41              |
| 1:B:3287:THR:OG1  | 1:B:3330:SER:HB3  | 2.20                     | 0.41              |
| 1:B:3306:GLN:O    | 1:B:3309:PHE:HB2  | 2.21                     | 0.41              |
| 1:B:3928:LEU:O    | 1:B:3932:LEU:HG   | 2.21                     | 0.41              |
| 1:B:4562:VAL:O    | 1:B:4566:MET:HG3  | 2.20                     | 0.41              |
| 1:B:4616:LEU:O    | 1:B:4620:ILE:HG13 | 2.21                     | 0.41              |
| 2:C:83:GLU:HA     | 2:C:86:ILE:HB     | 2.03                     | 0.41              |
| 1:A:108:ILE:HD11  | 1:A:243:ASN:HB3   | 2.03                     | 0.41              |
| 1:A:925:ASP:N     | 1:A:925:ASP:OD1   | 2.54                     | 0.41              |
| 1:A:1001:TYR:O    | 1:A:1005:ILE:HG13 | 2.21                     | 0.41              |
| 1:A:1395:LYS:O    | 1:A:1399:GLU:HG2  | 2.21                     | 0.41              |
| 1:A:1976:HIS:ND1  | 1:A:1989:HIS:NE2  | 2.57                     | 0.41              |
| 1:A:2246:VAL:O    | 1:A:2250:SER:OG   | 2.37                     | 0.41              |
| 1:A:2686:LEU:HD13 | 1:A:2999:TYR:HA   | 2.03                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2975:LEU:HD11 | 1:A:3020:ALA:CB   | 2.51                     | 0.41              |
| 1:A:3107:GLU:HA   | 1:A:3110:LYS:HD2  | 2.02                     | 0.41              |
| 1:A:3450:LEU:O    | 1:A:3454:ILE:HG13 | 2.21                     | 0.41              |
| 1:A:3522:PHE:HD1  | 1:A:3522:PHE:H    | 1.67                     | 0.41              |
| 1:A:4759:GLY:O    | 1:A:4763:LEU:HG   | 2.21                     | 0.41              |
| 1:B:132:LEU:HD21  | 1:B:143:LEU:CD1   | 2.50                     | 0.41              |
| 1:B:1001:TYR:CE2  | 1:B:1005:ILE:HD11 | 2.56                     | 0.41              |
| 1:B:1169:TYR:O    | 1:B:1173:THR:HG23 | 2.21                     | 0.41              |
| 1:B:2044:SER:OG   | 1:B:2065:SER:HB2  | 2.20                     | 0.41              |
| 1:B:2298:LEU:N    | 1:B:2422:ILE:O    | 2.43                     | 0.41              |
| 1:B:3236:HIS:O    | 1:B:3240:ILE:HG12 | 2.21                     | 0.41              |
| 1:B:3320:LEU:HD12 | 1:B:3424:VAL:HG13 | 2.03                     | 0.41              |
| 1:B:4570:LEU:HD13 | 1:B:4622:TYR:HB3  | 2.03                     | 0.41              |
| 2:D:121:GLU:O     | 2:D:122:VAL:C     | 2.60                     | 0.41              |
| 3:F:89:THR:N      | 3:F:92:SER:OG     | 2.50                     | 0.41              |
| 1:A:86:THR:CG2    | 1:A:141:SER:HB3   | 2.51                     | 0.41              |
| 1:A:469:PHE:CZ    | 1:A:474:VAL:HG22  | 2.55                     | 0.41              |
| 1:A:884:LEU:C     | 1:A:886:SER:H     | 2.29                     | 0.41              |
| 1:A:1039:LEU:HB3  | 1:A:1130:LYS:HD2  | 2.03                     | 0.41              |
| 1:A:1041:TRP:HA   | 1:A:1044:ARG:HG3  | 2.03                     | 0.41              |
| 1:A:1133:VAL:HG22 | 1:A:1247:TRP:CE2  | 2.56                     | 0.41              |
| 1:A:1210:LYS:HE3  | 1:A:1210:LYS:HB2  | 1.93                     | 0.41              |
| 1:A:1515:LEU:HD11 | 1:A:1556:LEU:CD2  | 2.50                     | 0.41              |
| 1:A:1952:PHE:HE1  | 1:A:1976:HIS:CD2  | 2.39                     | 0.41              |
| 1:A:2229:THR:CG2  | 1:A:2241:ILE:HG23 | 2.51                     | 0.41              |
| 1:A:2250:SER:O    | 1:A:2254:GLN:HG3  | 2.21                     | 0.41              |
| 1:A:2301:VAL:HG13 | 1:A:2340:ILE:HG23 | 2.02                     | 0.41              |
| 1:A:2311:VAL:HG11 | 3:E:64:TYR:CG     | 2.56                     | 0.41              |
| 1:A:2324:THR:C    | 1:A:2326:MET:H    | 2.29                     | 0.41              |
| 1:A:2506:GLN:HG3  | 1:A:2546:ALA:HB1  | 2.02                     | 0.41              |
| 1:A:3053:LEU:HD22 | 1:A:3156:TYR:CE1  | 2.56                     | 0.41              |
| 1:A:3098:CYS:O    | 1:A:3101:VAL:HG12 | 2.21                     | 0.41              |
| 1:A:3105:LEU:HB2  | 1:A:3197:TYR:OH   | 2.21                     | 0.41              |
| 1:A:3236:HIS:O    | 1:A:3240:ILE:HG12 | 2.21                     | 0.41              |
| 1:A:3413:ARG:NH1  | 1:A:3457:GLU:OE1  | 2.41                     | 0.41              |
| 1:A:3951:VAL:HA   | 1:A:3968:LEU:HD22 | 2.03                     | 0.41              |
| 1:A:4077:ILE:HG22 | 2:C:114:GLY:O     | 2.21                     | 0.41              |
| 1:A:4717:PRO:O    | 1:A:4720:PRO:HD2  | 2.21                     | 0.41              |
| 1:B:120:GLU:H     | 1:B:120:GLU:HG3   | 1.59                     | 0.41              |
| 1:B:348:ALA:CB    | 1:B:421:ILE:HG23  | 2.51                     | 0.41              |
| 1:B:945:LEU:HG    | 1:B:946:ASN:OD1   | 2.21                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1213:THR:O    | 1:B:1217:THR:HG23 | 2.20                     | 0.41              |
| 1:B:2173:HIS:HE2  | 1:B:2253:LEU:HD11 | 1.86                     | 0.41              |
| 1:B:2255:PRO:C    | 1:B:2257:LEU:H    | 2.29                     | 0.41              |
| 1:B:2620:SER:C    | 1:B:2622:ILE:N    | 2.78                     | 0.41              |
| 1:B:3031:GLU:O    | 1:B:3052:HIS:NE2  | 2.54                     | 0.41              |
| 1:B:3453:SER:O    | 1:B:3456:PRO:HD2  | 2.20                     | 0.41              |
| 1:B:4205:VAL:HG11 | 1:B:4248:PHE:CE2  | 2.56                     | 0.41              |
| 1:B:4476:ALA:C    | 1:B:4521:ASN:HD21 | 2.25                     | 0.41              |
| 2:D:106:LEU:O     | 2:D:110:MET:HG2   | 2.21                     | 0.41              |
| 3:F:3:ARG:HG2     | 3:F:18:ARG:CG     | 2.49                     | 0.41              |
| 3:F:94:GLN:HG3    | 3:F:132:LEU:HB3   | 2.03                     | 0.41              |
| 1:A:478:ASN:O     | 1:A:482:LYS:HG3   | 2.20                     | 0.41              |
| 1:A:659:THR:O     | 1:A:663:LEU:HB2   | 2.21                     | 0.41              |
| 1:A:740:PHE:CD2   | 1:A:781:LYS:HG2   | 2.56                     | 0.41              |
| 1:A:1051:VAL:HG13 | 1:A:1072:LEU:HG   | 2.02                     | 0.41              |
| 1:A:1218:LEU:HD22 | 1:A:1376:ILE:HA   | 2.02                     | 0.41              |
| 1:A:1240:GLU:H    | 1:A:1240:GLU:CD   | 2.29                     | 0.41              |
| 1:A:1428:LEU:HD12 | 1:A:1488:ASN:HA   | 2.01                     | 0.41              |
| 1:A:1664:CYS:SG   | 1:A:1666:PHE:HB3  | 2.61                     | 0.41              |
| 1:A:1929:LEU:HD11 | 1:A:2241:ILE:HD11 | 2.02                     | 0.41              |
| 1:A:2054:ASN:OD1  | 1:A:2058:LYS:N    | 2.53                     | 0.41              |
| 1:A:4132:VAL:O    | 1:A:4133:LEU:C    | 2.64                     | 0.41              |
| 1:A:4343:GLU:HB3  | 1:A:4426:LYS:NZ   | 2.36                     | 0.41              |
| 1:B:268:ARG:HB3   | 1:B:272:ARG:HH21  | 1.85                     | 0.41              |
| 1:B:1035:ILE:HD13 | 1:B:1035:ILE:HA   | 1.91                     | 0.41              |
| 1:B:1870:PHE:HE2  | 1:B:2239:LEU:HD11 | 1.86                     | 0.41              |
| 1:B:2191:MET:HB3  | 1:B:2198:LEU:HB2  | 2.03                     | 0.41              |
| 1:B:2198:LEU:HD23 | 1:B:2198:LEU:HA   | 1.88                     | 0.41              |
| 1:B:3000:MET:HE2  | 1:B:3000:MET:HB2  | 1.79                     | 0.41              |
| 1:B:3095:VAL:HG11 | 1:B:3186:PHE:CE1  | 2.56                     | 0.41              |
| 1:B:3439:SER:HB3  | 1:B:3443:GLN:HB2  | 2.03                     | 0.41              |
| 1:B:3450:LEU:O    | 1:B:3454:ILE:HG13 | 2.21                     | 0.41              |
| 1:B:3470:ASP:OD1  | 3:F:293:LEU:HG    | 2.20                     | 0.41              |
| 1:B:3729:GLU:O    | 1:B:3730:GLU:C    | 2.64                     | 0.41              |
| 1:B:4723:LEU:HD13 | 1:B:4763:LEU:HB2  | 2.01                     | 0.41              |
| 2:C:79:ASP:OD1    | 2:C:79:ASP:N      | 2.54                     | 0.41              |
| 1:A:73:PHE:CE1    | 1:A:155:MET:SD    | 3.14                     | 0.40              |
| 1:A:484:LEU:HD22  | 1:A:530:LEU:HD11  | 2.03                     | 0.40              |
| 1:A:1118:LEU:HD13 | 1:A:1273:LEU:HG   | 2.03                     | 0.40              |
| 1:A:1499:ILE:HG22 | 1:A:1511:CYS:SG   | 2.60                     | 0.40              |
| 1:A:1819:MET:HA   | 1:A:1822:ILE:HB   | 2.03                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2173:HIS:CD2  | 1:A:2253:LEU:CD1  | 2.87                     | 0.40              |
| 1:A:2410:ASP:HA   | 1:A:2411:PRO:HD3  | 1.94                     | 0.40              |
| 1:A:3044:GLU:O    | 1:A:3049:ASN:ND2  | 2.53                     | 0.40              |
| 1:A:3968:LEU:O    | 1:A:3969:GLN:C    | 2.63                     | 0.40              |
| 1:A:4195:HIS:NE2  | 2:C:35:THR:CG2    | 2.85                     | 0.40              |
| 1:A:4714:LEU:HD11 | 1:A:4754:VAL:CG1  | 2.49                     | 0.40              |
| 1:B:129:LEU:HD23  | 1:B:129:LEU:HA    | 1.88                     | 0.40              |
| 1:B:337:LEU:HD12  | 1:B:337:LEU:HA    | 1.94                     | 0.40              |
| 1:B:484:LEU:HB3   | 1:B:657:PHE:CZ    | 2.56                     | 0.40              |
| 1:B:491:LEU:HD13  | 1:B:521:ILE:HG13  | 2.03                     | 0.40              |
| 1:B:1104:ILE:HG23 | 1:B:1110:LEU:CD1  | 2.51                     | 0.40              |
| 1:B:1236:ILE:CG2  | 1:B:1282:ALA:HB2  | 2.51                     | 0.40              |
| 1:B:1845:LEU:HA   | 1:B:2194:PRO:HA   | 2.02                     | 0.40              |
| 1:B:2316:GLN:HE22 | 3:F:76:GLN:CD     | 2.29                     | 0.40              |
| 1:B:3179:SER:O    | 1:B:3180:ARG:C    | 2.65                     | 0.40              |
| 1:B:3298:ASP:HB3  | 1:B:3398:GLN:CD   | 2.45                     | 0.40              |
| 1:B:4031:SER:HB3  | 3:F:310:GLU:OE2   | 2.21                     | 0.40              |
| 1:B:4059:TRP:CE3  | 3:F:323:LEU:HD21  | 2.56                     | 0.40              |
| 1:B:4307:LYS:HG2  | 1:B:4478:VAL:HG13 | 2.01                     | 0.40              |
| 1:A:112:LEU:HD11  | 1:A:247:LEU:HD12  | 2.04                     | 0.40              |
| 1:A:234:LYS:O     | 1:A:238:VAL:HG23  | 2.21                     | 0.40              |
| 1:A:317:VAL:O     | 1:A:318:LEU:C     | 2.63                     | 0.40              |
| 1:A:671:ARG:HB3   | 1:A:722:LEU:HD11  | 2.03                     | 0.40              |
| 1:A:741:SER:OG    | 1:A:785:ARG:NH1   | 2.54                     | 0.40              |
| 1:A:1025:MET:HE2  | 1:A:1025:MET:HB3  | 1.88                     | 0.40              |
| 1:A:1137:GLU:HG2  | 1:A:1141:LYS:HD2  | 2.04                     | 0.40              |
| 1:A:1204:ILE:HG21 | 1:A:1218:LEU:HD12 | 2.03                     | 0.40              |
| 1:A:1392:GLN:CD   | 1:A:1392:GLN:H    | 2.28                     | 0.40              |
| 1:A:1996:LEU:HB3  | 1:A:2000:ASN:HB3  | 2.03                     | 0.40              |
| 1:A:2060:ILE:HG12 | 1:A:2074:LEU:HD12 | 2.03                     | 0.40              |
| 1:A:2369:GLU:HA   | 1:A:2373:ARG:O    | 2.20                     | 0.40              |
| 1:A:4059:TRP:CE3  | 3:E:323:LEU:HD21  | 2.56                     | 0.40              |
| 1:A:4127:ASN:C    | 1:A:4129:LEU:N    | 2.78                     | 0.40              |
| 1:A:4187:TYR:O    | 1:A:4191:ILE:HG12 | 2.21                     | 0.40              |
| 1:A:4201:ALA:HA   | 1:A:4205:VAL:HG12 | 2.03                     | 0.40              |
| 1:A:4280:ARG:NH1  | 1:A:4285:ASP:OD2  | 2.52                     | 0.40              |
| 1:A:4363:LEU:HD21 | 1:A:4444:MET:HG3  | 2.02                     | 0.40              |
| 1:B:322:ASN:O     | 1:B:323:PRO:C     | 2.63                     | 0.40              |
| 1:B:336:CYS:O     | 1:B:337:LEU:C     | 2.63                     | 0.40              |
| 1:B:684:ALA:HA    | 1:B:734:GLN:HG3   | 2.03                     | 0.40              |
| 1:B:905:THR:HG22  | 1:B:906:PRO:O     | 2.21                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1079:LYS:C    | 1:B:1081:SER:H    | 2.28                     | 0.40              |
| 1:B:2042:PRO:HD3  | 1:B:2088:VAL:O    | 2.21                     | 0.40              |
| 1:B:2220:THR:HG23 | 1:B:2224:GLU:HA   | 2.02                     | 0.40              |
| 1:B:3289:ASN:HA   | 1:B:3292:LYS:NZ   | 2.36                     | 0.40              |
| 1:B:3295:ILE:HD13 | 1:B:3395:LEU:HD23 | 2.03                     | 0.40              |
| 1:B:3742:LEU:HD13 | 1:B:3820:LYS:HG2  | 2.03                     | 0.40              |
| 1:B:4273:LEU:O    | 1:B:4280:ARG:NH2  | 2.53                     | 0.40              |
| 1:B:4716:ARG:HA   | 1:B:4717:PRO:HD3  | 1.92                     | 0.40              |
| 2:D:50:GLN:HA     | 2:D:53:ILE:HG22   | 2.03                     | 0.40              |
| 3:F:65:TYR:HB3    | 3:F:70:PHE:CE2    | 2.56                     | 0.40              |
| 1:A:81:SER:O      | 1:A:85:ILE:HG13   | 2.21                     | 0.40              |
| 1:A:793:ASN:HB3   | 1:A:854:ILE:HG13  | 2.02                     | 0.40              |
| 1:A:864:TYR:C     | 1:A:866:LEU:H     | 2.30                     | 0.40              |
| 1:A:1055:LYS:O    | 1:A:1059:ILE:HG13 | 2.22                     | 0.40              |
| 1:A:1063:MET:SD   | 1:A:1068:ALA:HB2  | 2.62                     | 0.40              |
| 1:A:1806:SER:C    | 1:A:1809:PRO:HD2  | 2.47                     | 0.40              |
| 1:A:3196:GLU:HA   | 1:A:3199:MET:HG2  | 2.02                     | 0.40              |
| 1:A:4325:TYR:CE1  | 1:A:4495:ILE:HA   | 2.56                     | 0.40              |
| 1:B:507:ALA:O     | 1:B:523:ARG:NE    | 2.51                     | 0.40              |
| 1:B:791:LYS:HD3   | 1:B:836:ILE:HG12  | 2.03                     | 0.40              |
| 1:B:833:PHE:HE1   | 1:B:858:LEU:HD22  | 1.87                     | 0.40              |
| 1:B:855:LEU:CD2   | 1:B:1002:TYR:HE2  | 2.34                     | 0.40              |
| 1:B:1110:LEU:H    | 1:B:1175:ALA:HB2  | 1.86                     | 0.40              |
| 1:B:1242:PRO:HB2  | 1:B:1251:PHE:HZ   | 1.87                     | 0.40              |
| 1:B:1528:ASN:HD22 | 1:B:1528:ASN:H    | 1.68                     | 0.40              |
| 1:B:1822:ILE:CG2  | 1:B:1826:PHE:CE2  | 3.04                     | 0.40              |
| 1:B:2702:ILE:HA   | 1:B:3005:MET:HG2  | 2.03                     | 0.40              |
| 1:B:3013:GLU:HG2  | 1:B:3077:SER:HB3  | 2.03                     | 0.40              |
| 1:B:3106:LEU:HG   | 1:B:3110:LYS:HE3  | 2.02                     | 0.40              |
| 1:B:3177:THR:OG1  | 1:B:3178:ASN:N    | 2.55                     | 0.40              |
| 1:B:3304:LEU:HD23 | 1:B:3304:LEU:HA   | 1.93                     | 0.40              |
| 1:B:4132:VAL:HA   | 1:B:4135:THR:HG23 | 2.02                     | 0.40              |
| 1:B:4596:MET:O    | 1:B:4600:GLN:HG2  | 2.21                     | 0.40              |
| 1:A:193:PHE:CZ    | 1:B:816:LEU:HD21  | 2.56                     | 0.40              |
| 1:A:545:ALA:HB1   | 1:A:648:LEU:HG    | 2.04                     | 0.40              |
| 1:A:718:VAL:HG13  | 1:A:760:LEU:HG    | 2.03                     | 0.40              |
| 1:A:918:TRP:HA    | 1:A:918:TRP:CE3   | 2.56                     | 0.40              |
| 1:A:1176:TYR:CD1  | 1:A:1281:ALA:CB   | 3.05                     | 0.40              |
| 1:A:1219:VAL:O    | 1:A:1222:LEU:HB2  | 2.20                     | 0.40              |
| 1:A:1312:ARG:O    | 1:A:1316:PRO:HD3  | 2.21                     | 0.40              |
| 1:A:1447:LEU:HA   | 1:A:1505:GLN:HG3  | 2.04                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2302:GLU:HG3  | 1:A:2343:ASN:HD21 | 1.86                     | 0.40              |
| 1:A:4251:VAL:HB   | 1:A:4254:ILE:HD12 | 2.02                     | 0.40              |
| 1:B:408:LEU:HD13  | 1:B:520:ARG:HB3   | 2.04                     | 0.40              |
| 1:B:952:ALA:O     | 1:B:956:LEU:HG    | 2.21                     | 0.40              |
| 1:B:1109:ILE:HG23 | 1:B:1178:LEU:HD12 | 2.03                     | 0.40              |
| 1:B:1127:ALA:O    | 1:B:1131:VAL:HG22 | 2.21                     | 0.40              |
| 1:B:1314:LEU:HA   | 1:B:1317:LEU:HD12 | 2.02                     | 0.40              |
| 1:B:1474:SER:HA   | 1:B:1485:ILE:CD1  | 2.51                     | 0.40              |
| 1:B:2680:LYS:O    | 1:B:2684:GLN:HG3  | 2.22                     | 0.40              |
| 1:B:2702:ILE:HD11 | 1:B:3001:GLN:CD   | 2.46                     | 0.40              |
| 1:B:3556:TYR:O    | 1:B:3606:LYS:CE   | 2.67                     | 0.40              |
| 1:B:3893:ASN:HB3  | 1:B:3896:LEU:HB2  | 2.03                     | 0.40              |
| 1:B:4274:ARG:HB2  | 1:B:4288:GLN:HE22 | 1.86                     | 0.40              |
| 1:B:4303:GLU:O    | 1:B:4307:LYS:HG3  | 2.21                     | 0.40              |
| 1:B:4325:TYR:O    | 1:B:4329:VAL:HG23 | 2.22                     | 0.40              |
| 1:B:4609:ASN:HB3  | 1:B:4612:VAL:HB   | 2.02                     | 0.40              |
| 2:D:52:MET:O      | 2:D:55:GLU:HB3    | 2.21                     | 0.40              |
| 1:A:268:ARG:O     | 1:A:272:ARG:HG3   | 2.22                     | 0.40              |
| 1:A:659:THR:HA    | 1:A:663:LEU:HB2   | 2.02                     | 0.40              |
| 1:A:1416:ASN:O    | 1:A:1470:ARG:NH1  | 2.52                     | 0.40              |
| 1:A:3034:MET:HG2  | 1:A:3035:ASP:N    | 2.36                     | 0.40              |
| 1:A:3393:THR:HA   | 1:A:3396:VAL:HG12 | 2.04                     | 0.40              |
| 1:A:4601:ILE:HA   | 1:A:4606:VAL:HG11 | 2.02                     | 0.40              |
| 1:B:31:VAL:O      | 1:B:35:PRO:CD     | 2.69                     | 0.40              |
| 1:B:60:GLU:HG3    | 1:B:106:VAL:HG13  | 2.02                     | 0.40              |
| 1:B:747:LEU:HD11  | 1:B:793:ASN:ND2   | 2.37                     | 0.40              |
| 1:B:1424:CYS:O    | 1:B:1428:LEU:HG   | 2.21                     | 0.40              |
| 1:B:1666:PHE:HA   | 1:B:1669:THR:OG1  | 2.21                     | 0.40              |
| 1:B:2311:VAL:HG13 | 3:F:56:LEU:HD11   | 2.02                     | 0.40              |
| 1:B:2686:LEU:CD2  | 1:B:3002:VAL:HG21 | 2.49                     | 0.40              |
| 1:B:3789:SER:O    | 1:B:3797:LEU:HD11 | 2.21                     | 0.40              |
| 1:B:4062:ARG:HB2  | 1:B:4062:ARG:NH1  | 2.37                     | 0.40              |
| 1:B:4316:THR:O    | 1:B:4319:ARG:HB2  | 2.21                     | 0.40              |
| 2:D:67:PRO:HA     | 2:D:70:LEU:HB3    | 2.04                     | 0.40              |
| 2:D:137:VAL:CG1   | 2:D:141:GLU:HB2   | 2.50                     | 0.40              |
| 2:D:143:VAL:O     | 2:D:147:THR:HG23  | 2.22                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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     | 3853/5205 (74%)  | 3738 (97%) | 115 (3%) | 0        | 100         | 100 |
| 1   | B     | 3884/5205 (75%)  | 3762 (97%) | 122 (3%) | 0        | 100         | 100 |
| 2   | C     | 142/149 (95%)    | 136 (96%)  | 6 (4%)   | 0        | 100         | 100 |
| 2   | D     | 139/149 (93%)    | 132 (95%)  | 7 (5%)   | 0        | 100         | 100 |
| 3   | E     | 178/381 (47%)    | 175 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 3   | F     | 178/381 (47%)    | 170 (96%)  | 8 (4%)   | 0        | 100         | 100 |
| All | All   | 8374/11470 (73%) | 8113 (97%) | 261 (3%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 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 PDB entries followed by that with respect to all EM entries.

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     | 3438/4542 (76%) | 3329 (97%) | 109 (3%) | 34          | 58 |
| 1   | B     | 3474/4542 (76%) | 3347 (96%) | 127 (4%) | 30          | 55 |
| 2   | C     | 123/127 (97%)   | 118 (96%)  | 5 (4%)   | 27          | 52 |
| 2   | D     | 122/127 (96%)   | 115 (94%)  | 7 (6%)   | 18          | 45 |
| 3   | E     | 162/330 (49%)   | 161 (99%)  | 1 (1%)   | 78          | 80 |
| 3   | F     | 162/330 (49%)   | 159 (98%)  | 3 (2%)   | 50          | 66 |
| All | All   | 7481/9998 (75%) | 7229 (97%) | 252 (3%) | 33          | 57 |

All (252) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 33   | VAL  |
| 1   | A     | 44   | PHE  |
| 1   | A     | 69   | GLN  |
| 1   | A     | 92   | ILE  |
| 1   | A     | 94   | ARG  |
| 1   | A     | 97   | LEU  |
| 1   | A     | 100  | VAL  |
| 1   | A     | 191  | MET  |
| 1   | A     | 277  | VAL  |
| 1   | A     | 284  | ILE  |
| 1   | A     | 318  | LEU  |
| 1   | A     | 347  | MET  |
| 1   | A     | 401  | GLU  |
| 1   | A     | 444  | VAL  |
| 1   | A     | 530  | LEU  |
| 1   | A     | 686  | LEU  |
| 1   | A     | 722  | LEU  |
| 1   | A     | 771  | GLN  |
| 1   | A     | 799  | VAL  |
| 1   | A     | 807  | ASN  |
| 1   | A     | 813  | MET  |
| 1   | A     | 830  | LEU  |
| 1   | A     | 909  | HIS  |
| 1   | A     | 911  | PHE  |
| 1   | A     | 913  | GLU  |
| 1   | A     | 937  | SER  |
| 1   | A     | 984  | ARG  |
| 1   | A     | 1040 | ARG  |
| 1   | A     | 1045 | LEU  |
| 1   | A     | 1046 | ARG  |
| 1   | A     | 1061 | GLN  |
| 1   | A     | 1063 | MET  |
| 1   | A     | 1072 | LEU  |
| 1   | A     | 1113 | HIS  |
| 1   | A     | 1131 | VAL  |
| 1   | A     | 1154 | ILE  |
| 1   | A     | 1159 | LEU  |
| 1   | A     | 1173 | THR  |
| 1   | A     | 1177 | LEU  |
| 1   | A     | 1214 | LEU  |
| 1   | A     | 1244 | ILE  |
| 1   | A     | 1301 | TRP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1303 | ASP  |
| 1   | A     | 1318 | LEU  |
| 1   | A     | 1384 | LEU  |
| 1   | A     | 1471 | MET  |
| 1   | A     | 1481 | GLN  |
| 1   | A     | 1484 | VAL  |
| 1   | A     | 1485 | ILE  |
| 1   | A     | 1486 | GLN  |
| 1   | A     | 1496 | THR  |
| 1   | A     | 1500 | VAL  |
| 1   | A     | 1528 | ASN  |
| 1   | A     | 1553 | HIS  |
| 1   | A     | 1554 | LEU  |
| 1   | A     | 1556 | LEU  |
| 1   | A     | 1594 | GLU  |
| 1   | A     | 1607 | THR  |
| 1   | A     | 1690 | VAL  |
| 1   | A     | 1714 | PHE  |
| 1   | A     | 1894 | LEU  |
| 1   | A     | 1906 | HIS  |
| 1   | A     | 1950 | VAL  |
| 1   | A     | 1956 | SER  |
| 1   | A     | 2180 | VAL  |
| 1   | A     | 2184 | THR  |
| 1   | A     | 2204 | THR  |
| 1   | A     | 2301 | VAL  |
| 1   | A     | 2475 | LEU  |
| 1   | A     | 2488 | SER  |
| 1   | A     | 2667 | TYR  |
| 1   | A     | 2695 | PHE  |
| 1   | A     | 2698 | LYS  |
| 1   | A     | 2984 | THR  |
| 1   | A     | 2994 | VAL  |
| 1   | A     | 3056 | MET  |
| 1   | A     | 3108 | TYR  |
| 1   | A     | 3141 | LEU  |
| 1   | A     | 3159 | LEU  |
| 1   | A     | 3237 | VAL  |
| 1   | A     | 3286 | ARG  |
| 1   | A     | 3315 | VAL  |
| 1   | A     | 3332 | VAL  |
| 1   | A     | 3458 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 3522 | PHE  |
| 1   | A     | 3536 | ASN  |
| 1   | A     | 3581 | LEU  |
| 1   | A     | 3765 | CYS  |
| 1   | A     | 3793 | ASN  |
| 1   | A     | 3866 | HIS  |
| 1   | A     | 3994 | LEU  |
| 1   | A     | 3999 | MET  |
| 1   | A     | 4007 | VAL  |
| 1   | A     | 4127 | ASN  |
| 1   | A     | 4129 | LEU  |
| 1   | A     | 4135 | THR  |
| 1   | A     | 4230 | THR  |
| 1   | A     | 4277 | VAL  |
| 1   | A     | 4309 | PHE  |
| 1   | A     | 4310 | MET  |
| 1   | A     | 4316 | THR  |
| 1   | A     | 4335 | LEU  |
| 1   | A     | 4400 | LEU  |
| 1   | A     | 4447 | LEU  |
| 1   | A     | 4478 | VAL  |
| 1   | A     | 4505 | LEU  |
| 1   | A     | 4520 | VAL  |
| 1   | A     | 4601 | ILE  |
| 1   | A     | 4616 | LEU  |
| 1   | B     | 33   | VAL  |
| 1   | B     | 37   | LEU  |
| 1   | B     | 70   | TYR  |
| 1   | B     | 86   | THR  |
| 1   | B     | 92   | ILE  |
| 1   | B     | 96   | GLN  |
| 1   | B     | 97   | LEU  |
| 1   | B     | 113  | LEU  |
| 1   | B     | 124  | VAL  |
| 1   | B     | 130  | ILE  |
| 1   | B     | 147  | GLU  |
| 1   | B     | 154  | MET  |
| 1   | B     | 194  | LEU  |
| 1   | B     | 200  | VAL  |
| 1   | B     | 204  | ARG  |
| 1   | B     | 243  | ASN  |
| 1   | B     | 283  | PHE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 312  | THR  |
| 1   | B     | 313  | LEU  |
| 1   | B     | 318  | LEU  |
| 1   | B     | 325  | ARG  |
| 1   | B     | 367  | GLU  |
| 1   | B     | 378  | VAL  |
| 1   | B     | 379  | GLN  |
| 1   | B     | 381  | CYS  |
| 1   | B     | 408  | LEU  |
| 1   | B     | 424  | LEU  |
| 1   | B     | 448  | LEU  |
| 1   | B     | 511  | ILE  |
| 1   | B     | 528  | VAL  |
| 1   | B     | 677  | SER  |
| 1   | B     | 680  | GLU  |
| 1   | B     | 686  | LEU  |
| 1   | B     | 698  | LEU  |
| 1   | B     | 703  | ASP  |
| 1   | B     | 717  | LEU  |
| 1   | B     | 727  | LEU  |
| 1   | B     | 799  | VAL  |
| 1   | B     | 813  | MET  |
| 1   | B     | 830  | LEU  |
| 1   | B     | 844  | MET  |
| 1   | B     | 867  | HIS  |
| 1   | B     | 909  | HIS  |
| 1   | B     | 911  | PHE  |
| 1   | B     | 922  | PHE  |
| 1   | B     | 936  | LEU  |
| 1   | B     | 939  | GLU  |
| 1   | B     | 943  | ASP  |
| 1   | B     | 948  | LEU  |
| 1   | B     | 981  | ASP  |
| 1   | B     | 992  | THR  |
| 1   | B     | 1036 | LEU  |
| 1   | B     | 1040 | ARG  |
| 1   | B     | 1045 | LEU  |
| 1   | B     | 1057 | HIS  |
| 1   | B     | 1112 | LEU  |
| 1   | B     | 1131 | VAL  |
| 1   | B     | 1204 | ILE  |
| 1   | B     | 1212 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 1240 | GLU  |
| 1   | B     | 1299 | ILE  |
| 1   | B     | 1318 | LEU  |
| 1   | B     | 1326 | VAL  |
| 1   | B     | 1334 | LEU  |
| 1   | B     | 1338 | LEU  |
| 1   | B     | 1358 | CYS  |
| 1   | B     | 1387 | GLN  |
| 1   | B     | 1392 | GLN  |
| 1   | B     | 1470 | ARG  |
| 1   | B     | 1474 | SER  |
| 1   | B     | 1486 | GLN  |
| 1   | B     | 1528 | ASN  |
| 1   | B     | 1536 | GLU  |
| 1   | B     | 1549 | GLN  |
| 1   | B     | 1553 | HIS  |
| 1   | B     | 1554 | LEU  |
| 1   | B     | 1557 | HIS  |
| 1   | B     | 1595 | CYS  |
| 1   | B     | 1597 | CYS  |
| 1   | B     | 1664 | CYS  |
| 1   | B     | 1800 | GLN  |
| 1   | B     | 1805 | PHE  |
| 1   | B     | 1817 | PHE  |
| 1   | B     | 1873 | VAL  |
| 1   | B     | 1934 | ASP  |
| 1   | B     | 2300 | ASP  |
| 1   | B     | 2301 | VAL  |
| 1   | B     | 2673 | ASP  |
| 1   | B     | 2676 | ASN  |
| 1   | B     | 2974 | ARG  |
| 1   | B     | 2982 | LEU  |
| 1   | B     | 2985 | LEU  |
| 1   | B     | 2995 | ARG  |
| 1   | B     | 3001 | GLN  |
| 1   | B     | 3002 | VAL  |
| 1   | B     | 3003 | ILE  |
| 1   | B     | 3005 | MET  |
| 1   | B     | 3034 | MET  |
| 1   | B     | 3038 | ASP  |
| 1   | B     | 3045 | ARG  |
| 1   | B     | 3049 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 3050 | GLU  |
| 1   | B     | 3098 | CYS  |
| 1   | B     | 3197 | TYR  |
| 1   | B     | 3285 | GLN  |
| 1   | B     | 3286 | ARG  |
| 1   | B     | 3328 | CYS  |
| 1   | B     | 3458 | LEU  |
| 1   | B     | 3543 | CYS  |
| 1   | B     | 3581 | LEU  |
| 1   | B     | 3968 | LEU  |
| 1   | B     | 4135 | THR  |
| 1   | B     | 4228 | LEU  |
| 1   | B     | 4230 | THR  |
| 1   | B     | 4276 | LEU  |
| 1   | B     | 4277 | VAL  |
| 1   | B     | 4279 | GLN  |
| 1   | B     | 4297 | ASP  |
| 1   | B     | 4329 | VAL  |
| 1   | B     | 4331 | ILE  |
| 1   | B     | 4400 | LEU  |
| 1   | B     | 4447 | LEU  |
| 1   | B     | 4593 | GLN  |
| 1   | B     | 4612 | VAL  |
| 1   | B     | 4634 | LEU  |
| 1   | B     | 4752 | GLU  |
| 1   | B     | 4773 | GLU  |
| 2   | C     | 33   | LEU  |
| 2   | C     | 49   | LEU  |
| 2   | C     | 79   | ASP  |
| 2   | C     | 96   | ASP  |
| 2   | C     | 101  | ILE  |
| 2   | D     | 21   | ASP  |
| 2   | D     | 28   | ILE  |
| 2   | D     | 33   | LEU  |
| 2   | D     | 49   | LEU  |
| 2   | D     | 63   | THR  |
| 2   | D     | 64   | ILE  |
| 2   | D     | 105  | GLU  |
| 3   | E     | 131  | HIS  |
| 3   | F     | 70   | PHE  |
| 3   | F     | 131  | HIS  |
| 3   | F     | 136  | HIS  |

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

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 96   | GLN  |
| 1   | A     | 98   | GLN  |
| 1   | A     | 196  | GLN  |
| 1   | A     | 229  | GLN  |
| 1   | A     | 243  | ASN  |
| 1   | A     | 271  | ASN  |
| 1   | A     | 274  | GLN  |
| 1   | A     | 327  | GLN  |
| 1   | A     | 402  | HIS  |
| 1   | A     | 407  | GLN  |
| 1   | A     | 466  | HIS  |
| 1   | A     | 479  | HIS  |
| 1   | A     | 664  | ASN  |
| 1   | A     | 712  | HIS  |
| 1   | A     | 714  | ASN  |
| 1   | A     | 729  | ASN  |
| 1   | A     | 792  | GLN  |
| 1   | A     | 867  | HIS  |
| 1   | A     | 868  | GLN  |
| 1   | A     | 879  | GLN  |
| 1   | A     | 881  | GLN  |
| 1   | A     | 917  | ASN  |
| 1   | A     | 1067 | HIS  |
| 1   | A     | 1182 | ASN  |
| 1   | A     | 1227 | GLN  |
| 1   | A     | 1253 | ASN  |
| 1   | A     | 1364 | ASN  |
| 1   | A     | 1365 | HIS  |
| 1   | A     | 1418 | ASN  |
| 1   | A     | 1481 | GLN  |
| 1   | A     | 1486 | GLN  |
| 1   | A     | 1493 | GLN  |
| 1   | A     | 1553 | HIS  |
| 1   | A     | 1598 | HIS  |
| 1   | A     | 1682 | HIS  |
| 1   | A     | 1802 | GLN  |
| 1   | A     | 1892 | HIS  |
| 1   | A     | 1916 | HIS  |
| 1   | A     | 2296 | GLN  |
| 1   | A     | 2343 | ASN  |
| 1   | A     | 2990 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 3023 | ASN  |
| 1   | A     | 3148 | HIS  |
| 1   | A     | 3178 | ASN  |
| 1   | A     | 3321 | GLN  |
| 1   | A     | 3397 | ASN  |
| 1   | A     | 3410 | GLN  |
| 1   | A     | 3491 | GLN  |
| 1   | A     | 3536 | ASN  |
| 1   | A     | 3591 | ASN  |
| 1   | A     | 3639 | ASN  |
| 1   | A     | 3683 | GLN  |
| 1   | A     | 3740 | ASN  |
| 1   | A     | 3759 | GLN  |
| 1   | A     | 3835 | GLN  |
| 1   | A     | 4011 | ASN  |
| 1   | A     | 4127 | ASN  |
| 1   | A     | 4161 | GLN  |
| 1   | A     | 4234 | GLN  |
| 1   | A     | 4279 | GLN  |
| 1   | A     | 4490 | ASN  |
| 1   | A     | 4602 | ASN  |
| 1   | B     | 69   | GLN  |
| 1   | B     | 83   | HIS  |
| 1   | B     | 98   | GLN  |
| 1   | B     | 192  | ASN  |
| 1   | B     | 229  | GLN  |
| 1   | B     | 243  | ASN  |
| 1   | B     | 262  | ASN  |
| 1   | B     | 274  | GLN  |
| 1   | B     | 379  | GLN  |
| 1   | B     | 407  | GLN  |
| 1   | B     | 656  | ASN  |
| 1   | B     | 729  | ASN  |
| 1   | B     | 867  | HIS  |
| 1   | B     | 881  | GLN  |
| 1   | B     | 882  | HIS  |
| 1   | B     | 921  | HIS  |
| 1   | B     | 979  | GLN  |
| 1   | B     | 1022 | GLN  |
| 1   | B     | 1097 | GLN  |
| 1   | B     | 1111 | GLN  |
| 1   | B     | 1113 | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 1132 | GLN  |
| 1   | B     | 1227 | GLN  |
| 1   | B     | 1234 | ASN  |
| 1   | B     | 1266 | GLN  |
| 1   | B     | 1306 | ASN  |
| 1   | B     | 1309 | GLN  |
| 1   | B     | 1364 | ASN  |
| 1   | B     | 1387 | GLN  |
| 1   | B     | 1418 | ASN  |
| 1   | B     | 1486 | GLN  |
| 1   | B     | 1493 | GLN  |
| 1   | B     | 1528 | ASN  |
| 1   | B     | 1553 | HIS  |
| 1   | B     | 1558 | ASN  |
| 1   | B     | 1573 | GLN  |
| 1   | B     | 1800 | GLN  |
| 1   | B     | 1925 | GLN  |
| 1   | B     | 2182 | GLN  |
| 1   | B     | 2219 | HIS  |
| 1   | B     | 2258 | GLN  |
| 1   | B     | 2294 | HIS  |
| 1   | B     | 2296 | GLN  |
| 1   | B     | 2316 | GLN  |
| 1   | B     | 2319 | HIS  |
| 1   | B     | 2522 | GLN  |
| 1   | B     | 2524 | GLN  |
| 1   | B     | 2699 | GLN  |
| 1   | B     | 2983 | GLN  |
| 1   | B     | 2990 | ASN  |
| 1   | B     | 3001 | GLN  |
| 1   | B     | 3049 | ASN  |
| 1   | B     | 3209 | GLN  |
| 1   | B     | 3397 | ASN  |
| 1   | B     | 3438 | ASN  |
| 1   | B     | 3491 | GLN  |
| 1   | B     | 3591 | ASN  |
| 1   | B     | 3639 | ASN  |
| 1   | B     | 3683 | GLN  |
| 1   | B     | 3740 | ASN  |
| 1   | B     | 3756 | HIS  |
| 1   | B     | 3835 | GLN  |
| 1   | B     | 3848 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 4002 | ASN  |
| 1   | B     | 4021 | GLN  |
| 1   | B     | 4233 | GLN  |
| 1   | B     | 4490 | ASN  |
| 1   | B     | 4602 | ASN  |
| 1   | B     | 4766 | ASN  |
| 2   | C     | 43   | ASN  |
| 2   | C     | 54   | ASN  |
| 2   | C     | 98   | ASN  |
| 2   | C     | 138  | ASN  |
| 2   | D     | 54   | ASN  |
| 2   | D     | 61   | ASN  |
| 2   | D     | 98   | ASN  |
| 3   | F     | 74   | GLN  |
| 3   | F     | 76   | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 24 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

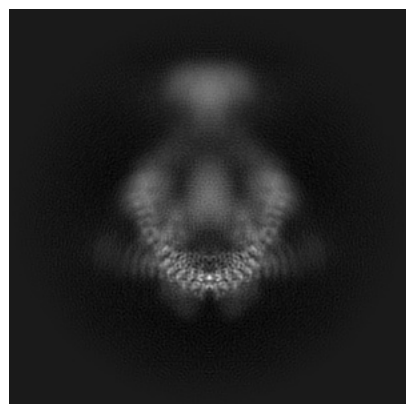
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46686. These allow visual inspection of the internal detail of the map and identification of artifacts.

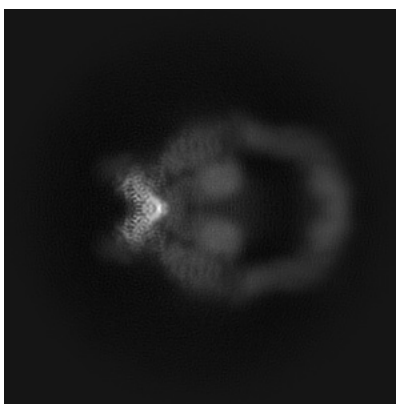
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

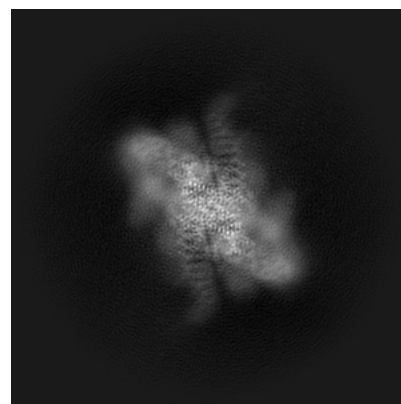
#### 6.1.1 Primary map



X

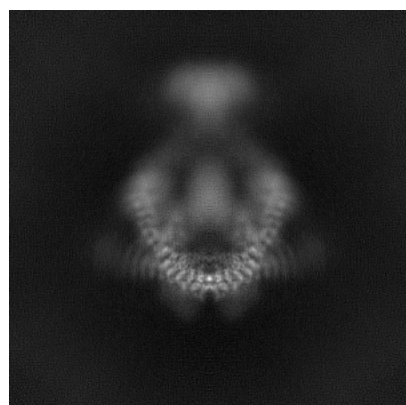


Y

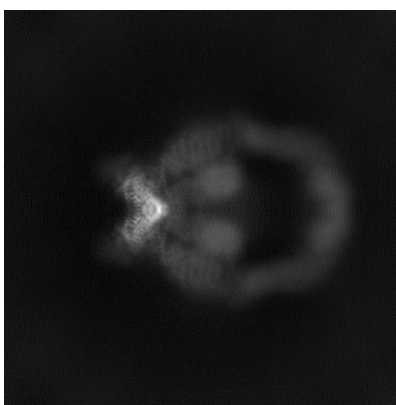


Z

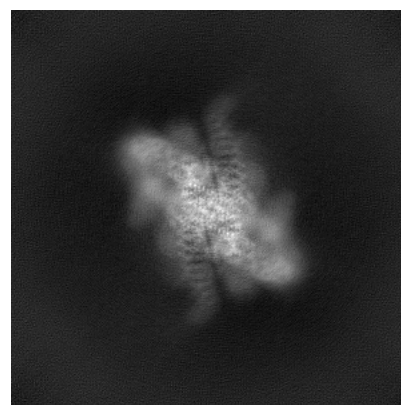
#### 6.1.2 Raw map



X



Y

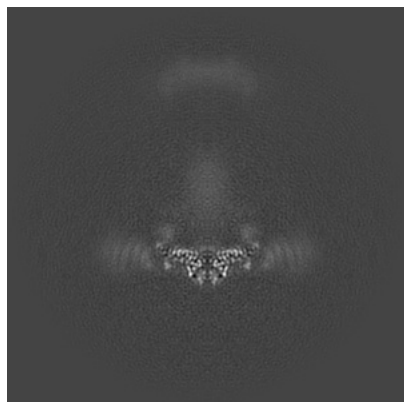


Z

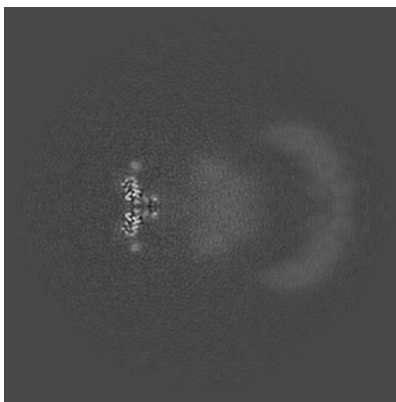
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

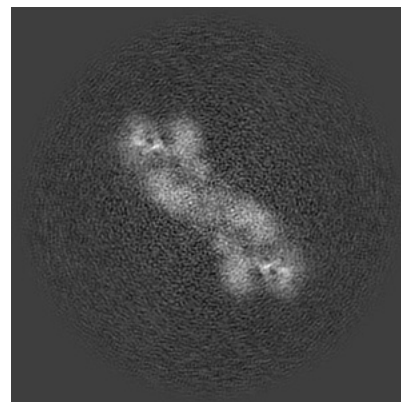
### 6.2.1 Primary map



X Index: 210



Y Index: 210

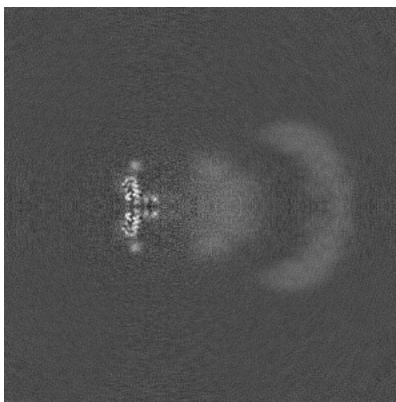


Z Index: 210

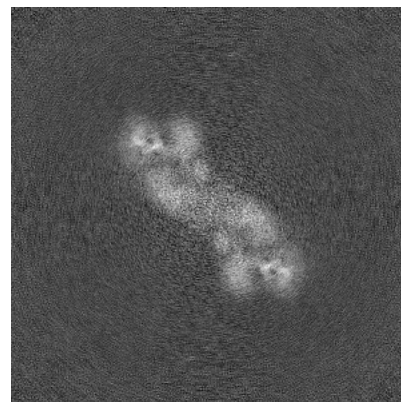
### 6.2.2 Raw map



X Index: 210



Y Index: 210



Z Index: 210

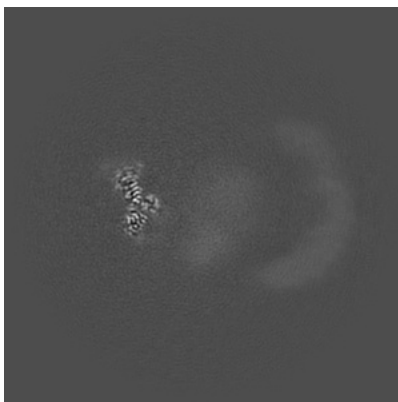
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

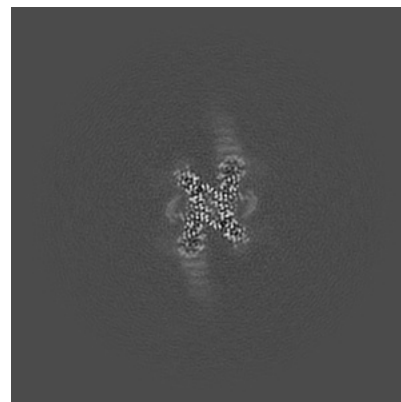
### 6.3.1 Primary map



X Index: 193

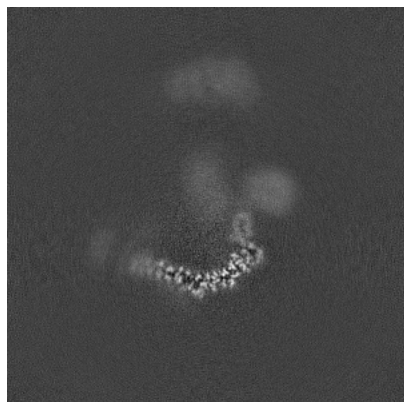


Y Index: 221

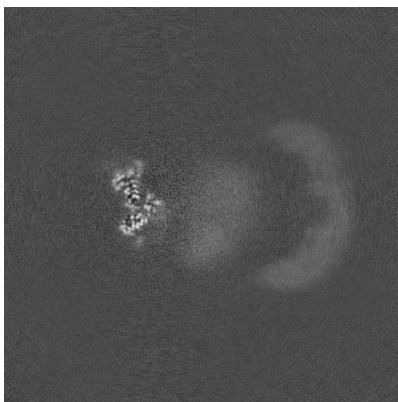


Z Index: 140

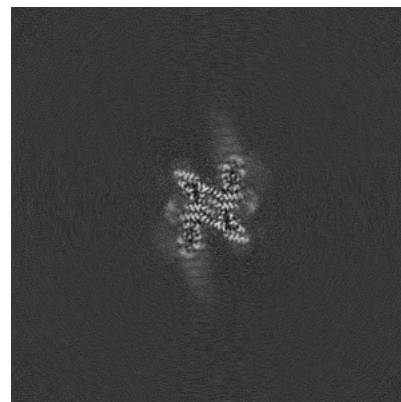
### 6.3.2 Raw map



X Index: 188



Y Index: 218

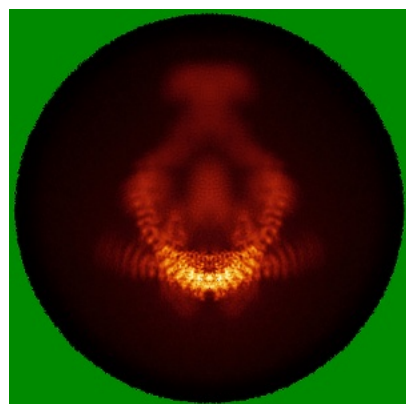


Z Index: 138

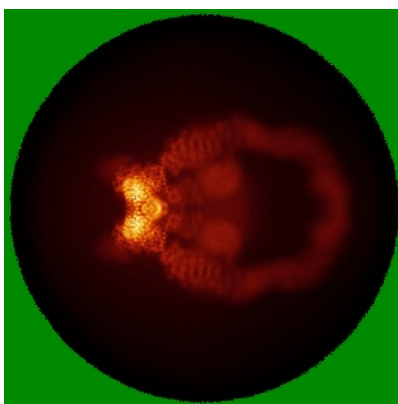
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) ⓘ

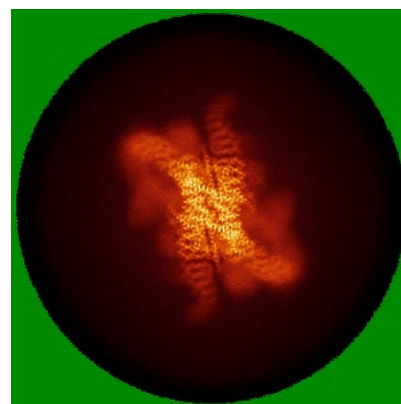
### 6.4.1 Primary map



X

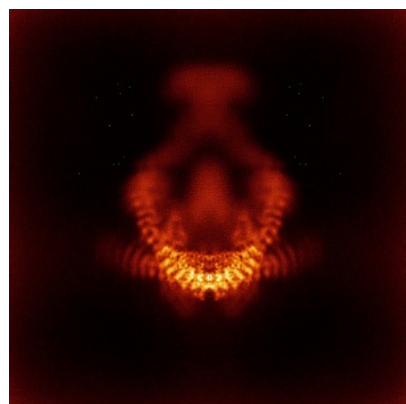


Y

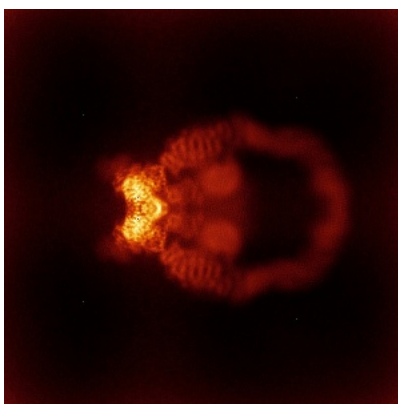


Z

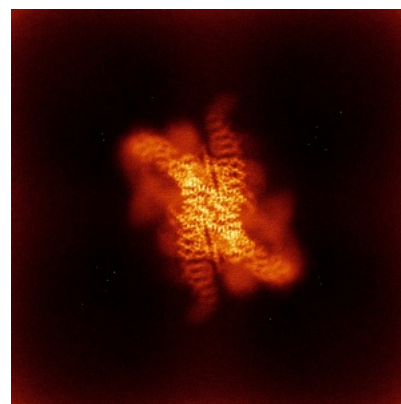
### 6.4.2 Raw map



X



Y

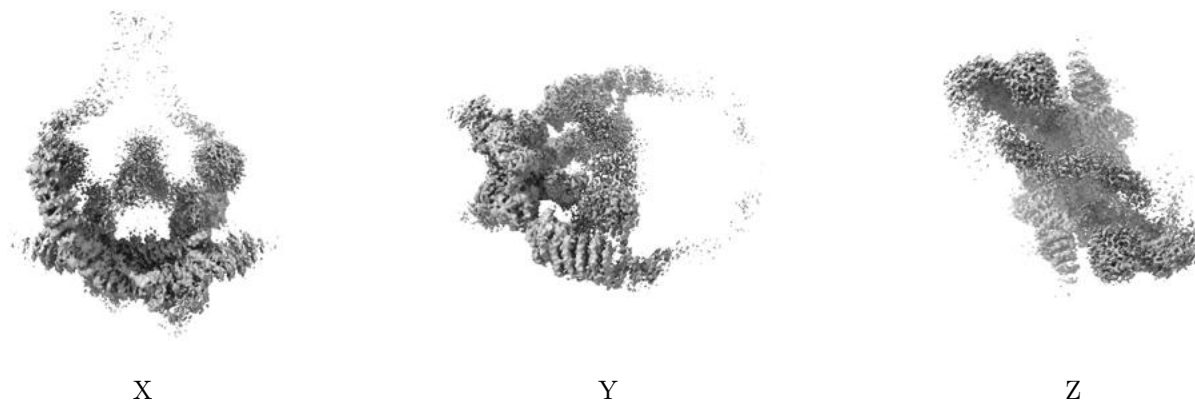


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

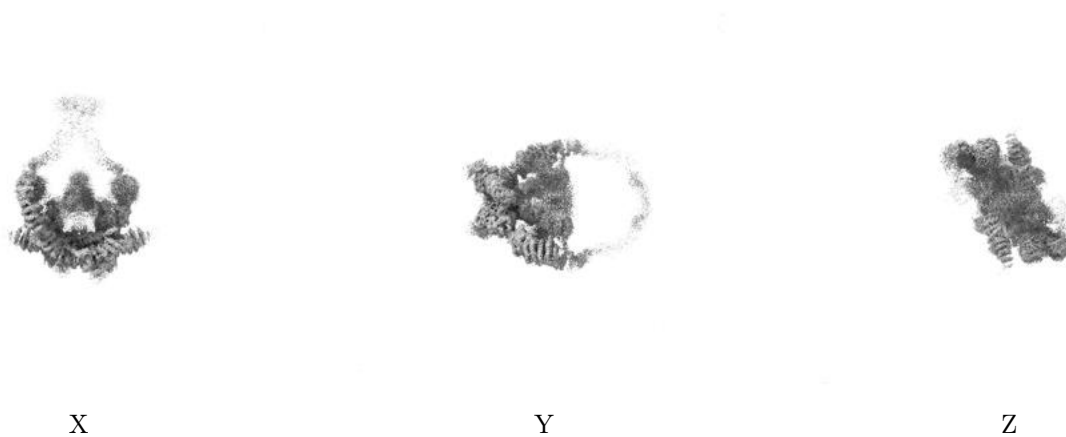
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.13. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

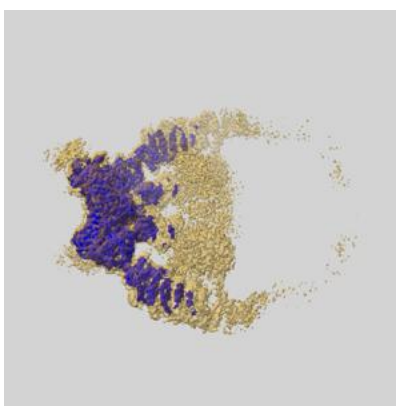
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

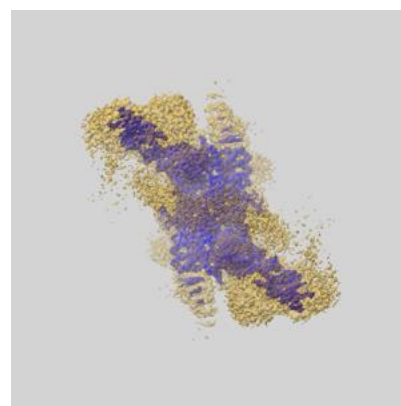
### 6.6.1 emd\_46686\_msk\_1.map [i](#)



X



Y

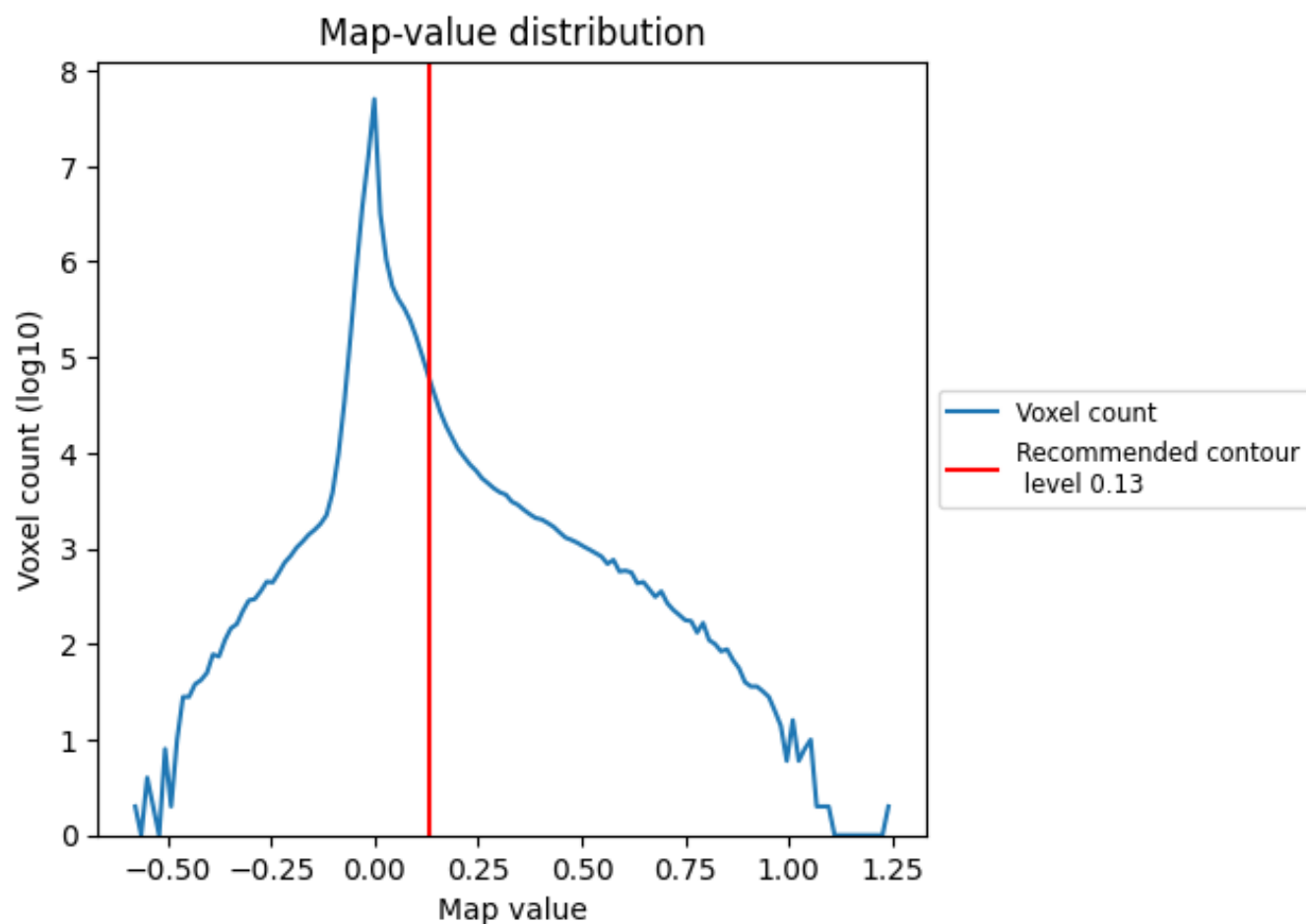


Z

## 7 Map analysis [i](#)

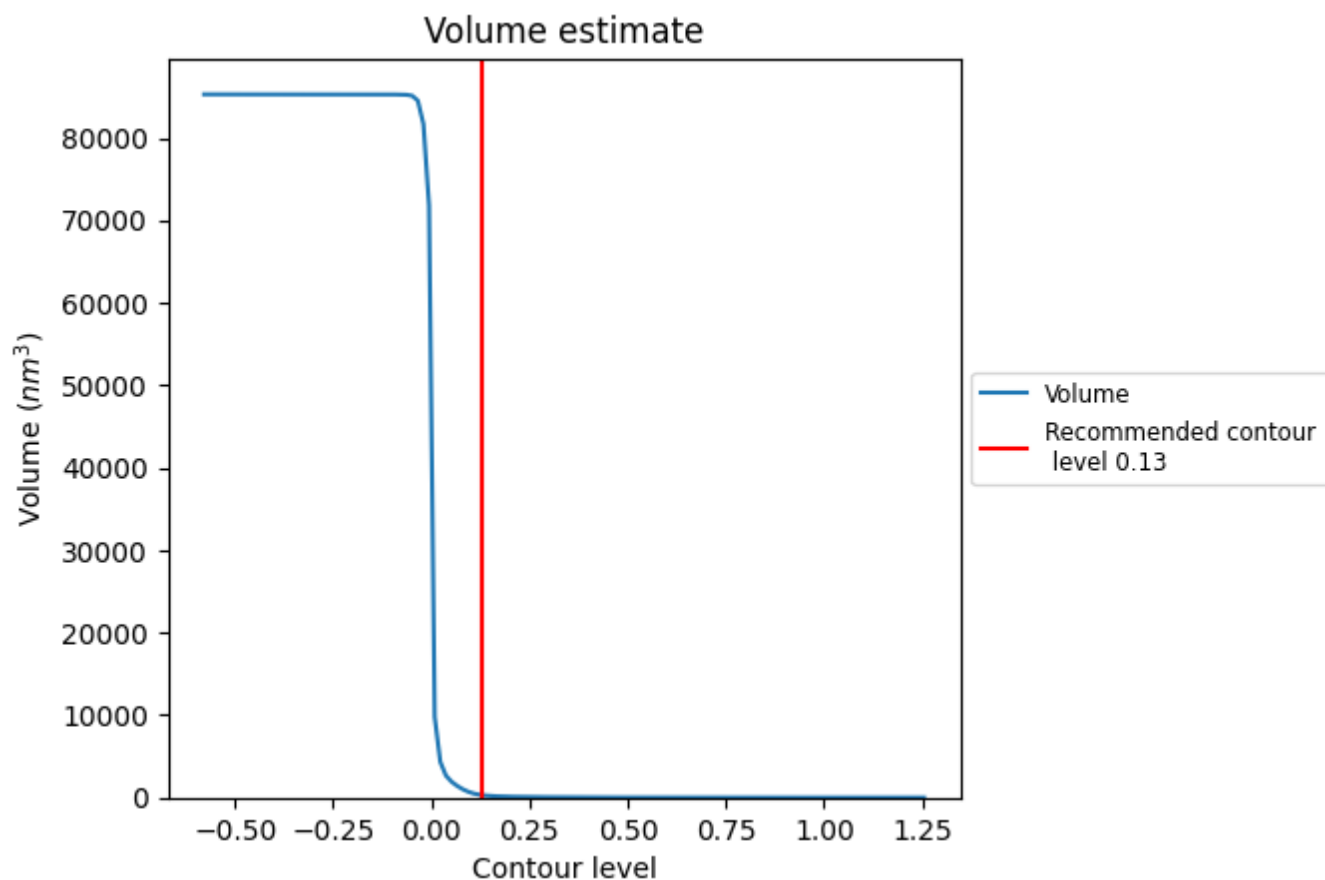
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

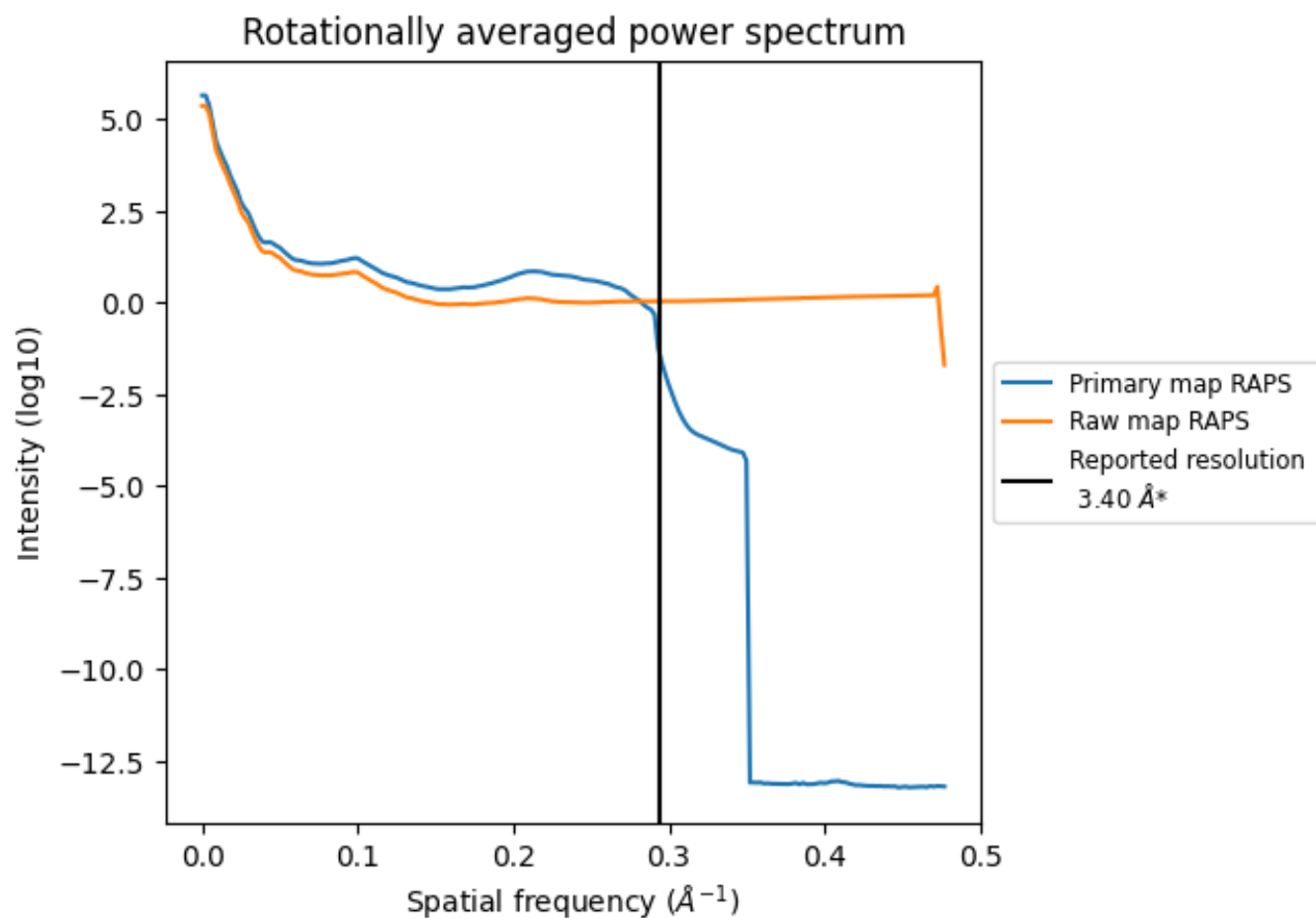
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 296 nm<sup>3</sup>; this corresponds to an approximate mass of 268 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

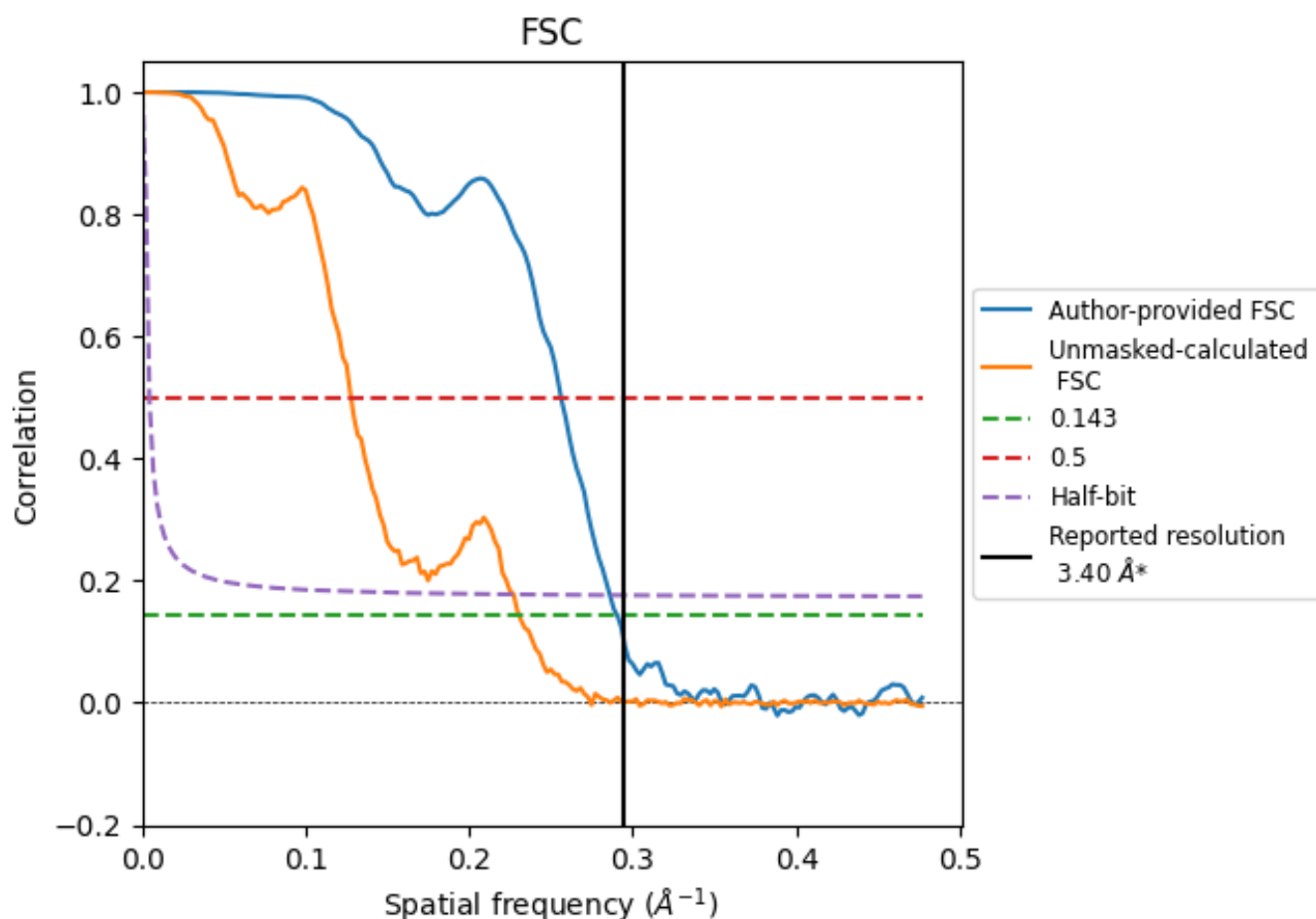


\*Reported resolution corresponds to spatial frequency of 0.294 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.294  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

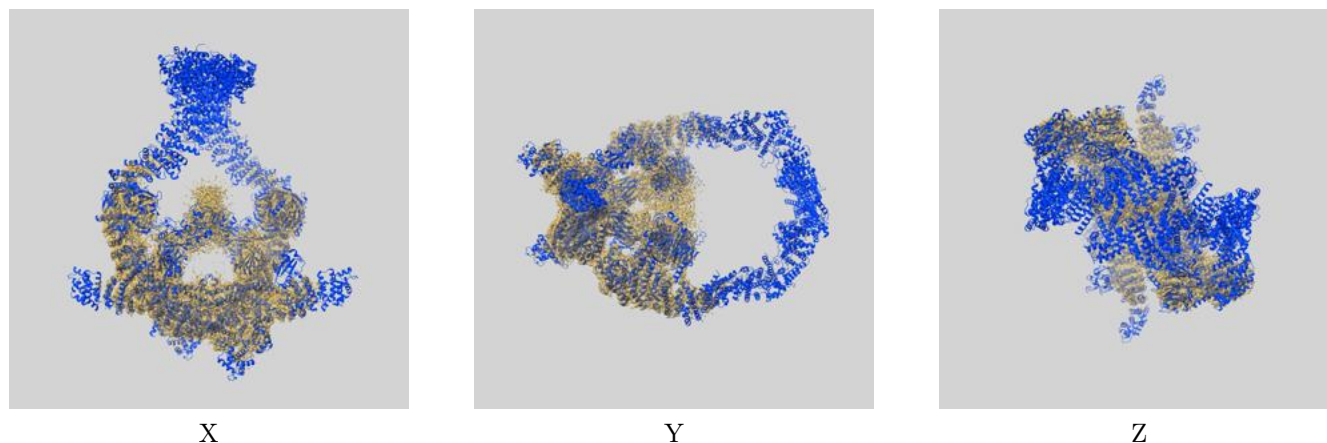
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.40                               | -    | -        |
| Author-provided FSC curve | 3.44                               | 3.90 | 3.50     |
| Unmasked-calculated*      | 4.34                               | 7.83 | 4.40     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.34 differs from the reported value 3.4 by more than 10 %

## 9 Map-model fit [i](#)

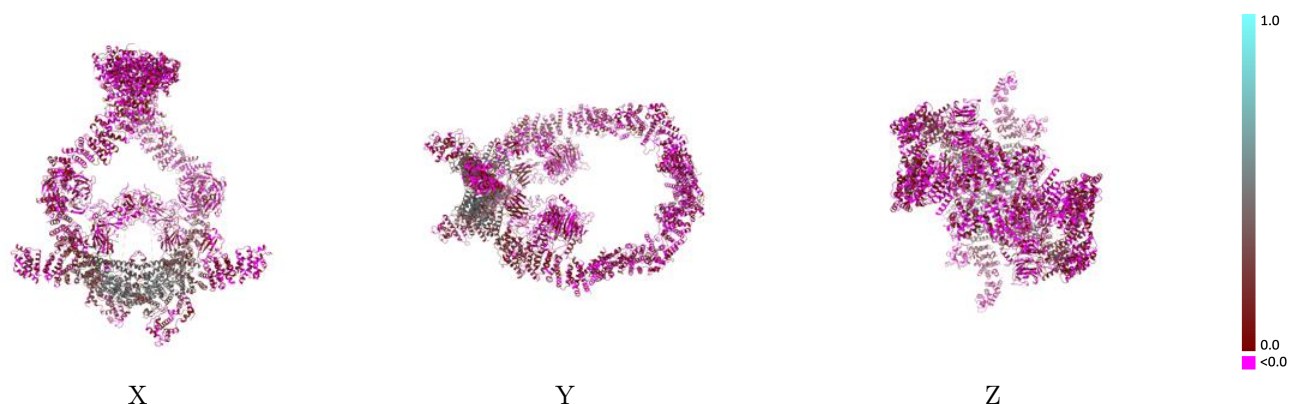
This section contains information regarding the fit between EMDB map EMD-46686 and PDB model 9D9Z. Per-residue inclusion information can be found in section [3](#) on page [6](#).

### 9.1 Map-model overlay [i](#)



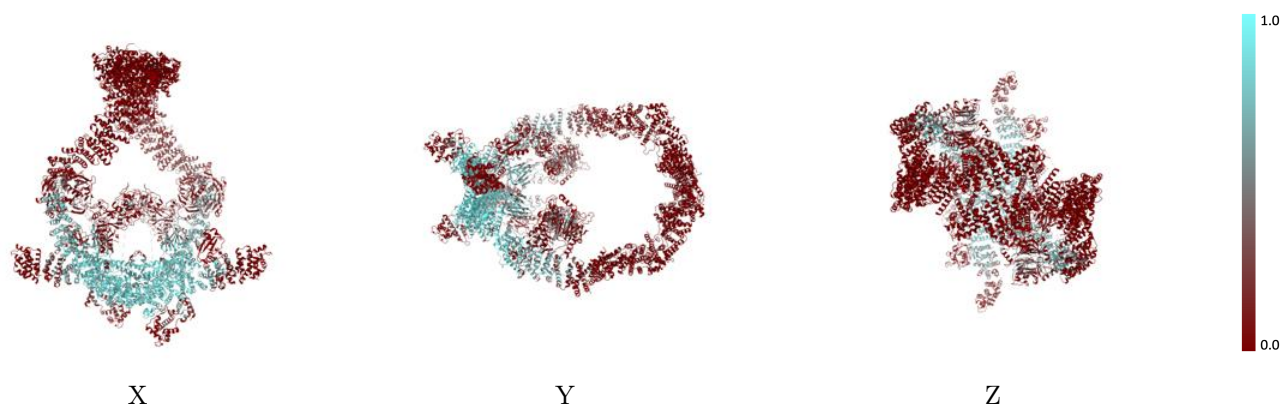
The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



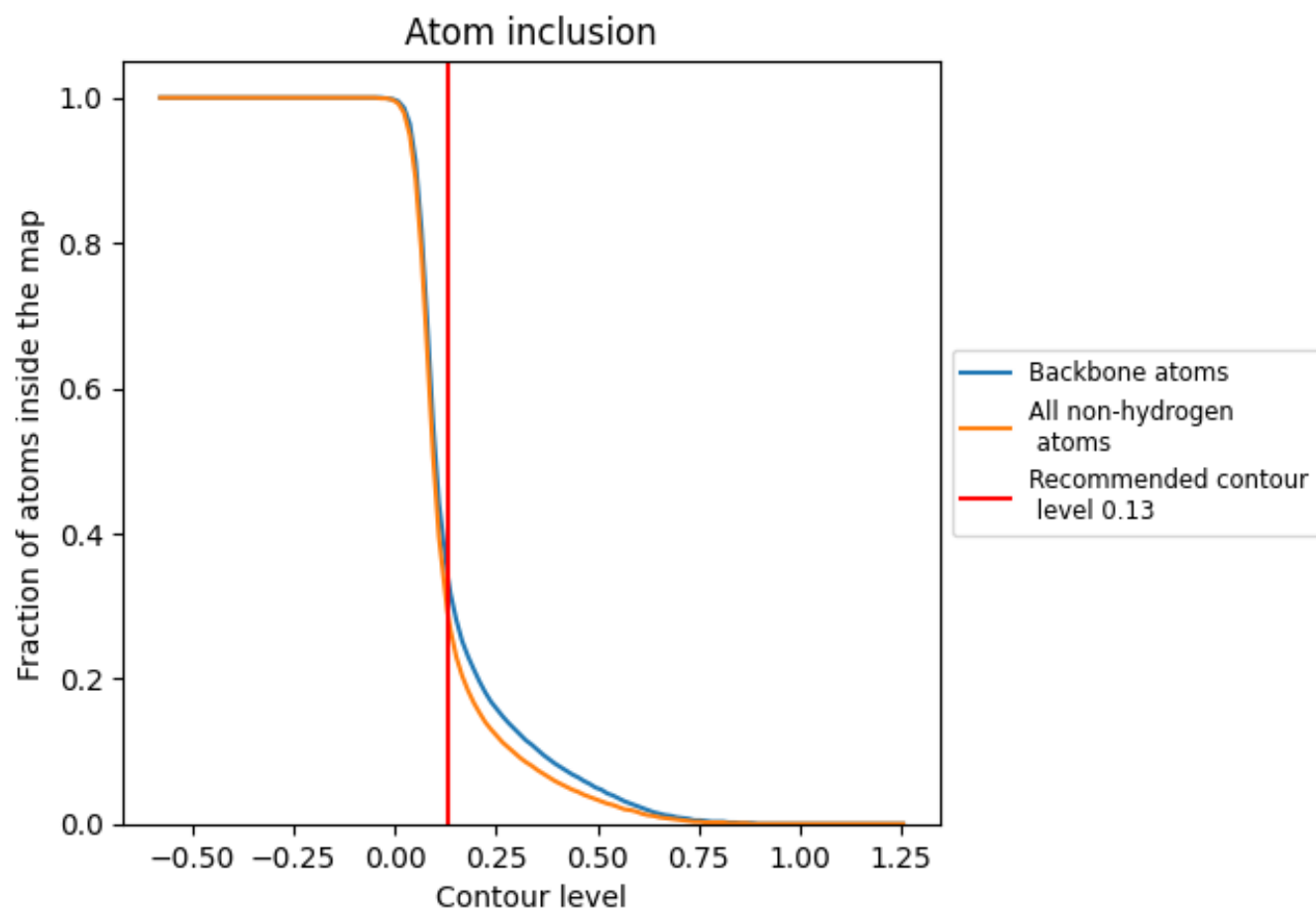
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.13).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 34% of all backbone atoms, 29% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.13) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.2930 | <div></div> 0.1100 |
| A     | <div></div> 0.3000 | <div></div> 0.1120 |
| B     | <div></div> 0.2990 | <div></div> 0.1130 |
| C     | <div></div> 0.1500 | <div></div> 0.0740 |
| D     | <div></div> 0.1350 | <div></div> 0.0820 |
| E     | <div></div> 0.2720 | <div></div> 0.0850 |
| F     | <div></div> 0.2740 | <div></div> 0.0890 |

1.0

0.0

<0.0