



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2023 – 12:52 PM EDT

PDB ID : 3I4M
Title : 8-oxoguanine containing RNA polymerase II elongation complex D
Authors : Damsma, G.E.; Cramer, P.
Deposited on : 2009-07-02
Resolution : 3.70 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

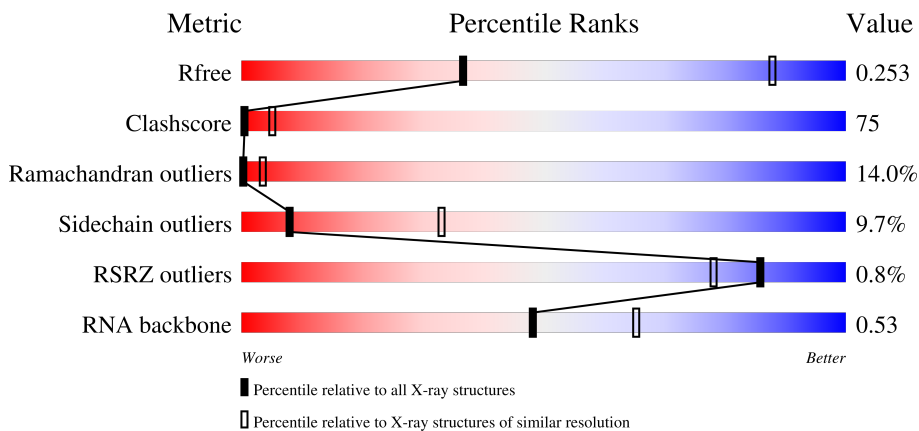
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|--------------------------|--|
| R_{free} | 130704 | 1049 (3.88-3.52) |
| Clashscore | 141614 | 1027 (3.86-3.54) |
| Ramachandran outliers | 138981 | 1069 (3.88-3.52) |
| Sidechain outliers | 138945 | 1065 (3.88-3.52) |
| RSRZ outliers | 127900 | 1578 (3.90-3.50) |
| RNA backbone | 3102 | 1027 (4.40-3.00) |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 1733 | |
| 2 | B | 1224 | |
| 3 | C | 324 | |
| 4 | D | 221 | |

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

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 32355 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 1 | A | 1429 | 11240 | 7079 | 1966 | 2133 | 62 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 2 | B | 1125 | 8942 | 5659 | 1571 | 1657 | 55 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 3 | C | 270 | 2125 | 1336 | 353 | 422 | 14 | 0 | 0 | 0 |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| C | -5 | HIS | - | EXPRESSION TAG | UNP P16370 |
| C | -4 | HIS | - | EXPRESSION TAG | UNP P16370 |
| C | -3 | HIS | - | EXPRESSION TAG | UNP P16370 |
| C | -2 | HIS | - | EXPRESSION TAG | UNP P16370 |
| C | -1 | HIS | - | EXPRESSION TAG | UNP P16370 |
| C | 0 | HIS | - | EXPRESSION TAG | UNP P16370 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 4 | D | 187 | 1504 | 930 | 269 | 301 | 4 | 0 | 0 | 0 |

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 6 | F | 88 | 712 | 455 | 120 | 134 | 3 | 0 | 0 | 0 |

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 8 | H | 137 | 1101 | 693 | 185 | 218 | 5 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 9 | I | 116 | 944 | 581 | 172 | 181 | 10 | 0 | 0 | 0 |

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 11 | K | 116 | 929 | 596 | 158 | 173 | 2 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 12 | L | 47 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 370 | 228 | 73 | 65 | 4 | | | |

- Molecule 13 is a DNA chain called DNA (5'-D(*AP*G*CP*TP*CP*AP*AP*GP*TP*AP*CP*TP*TP*AP*(8OG)P*GP*CP*CP*(BRU)P*GP*GP*TP*CP*AP*TP*T)-3').

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|-----|----|-----|----|---------|---------|-------|
| 13 | T | 21 | Total | Br | C | N | O | P | 0 | 0 | 0 |
| | | | 426 | 1 | 203 | 75 | 127 | 20 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|---------|-------|
| 14 | N | 11 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 224 | 108 | 42 | 64 | 10 | | | |

- Molecule 15 is a RNA chain called RNA (5'-R(*UP*GP*CP*AP*UP*C*UP*UP*CP*CP*AP*GP*GP*CP*CP*U)-3').

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 15 | P | 10 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 205 | 93 | 33 | 70 | 9 | | | |

- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 16 | A | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 17 | A | 2 | Total | Zn | 0 | 0 |
| | | | 2 | 2 | | |
| 17 | B | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 17 | C | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 17 | I | 2 | Total | Zn | 0 | 0 |
| | | | 2 | 2 | | |

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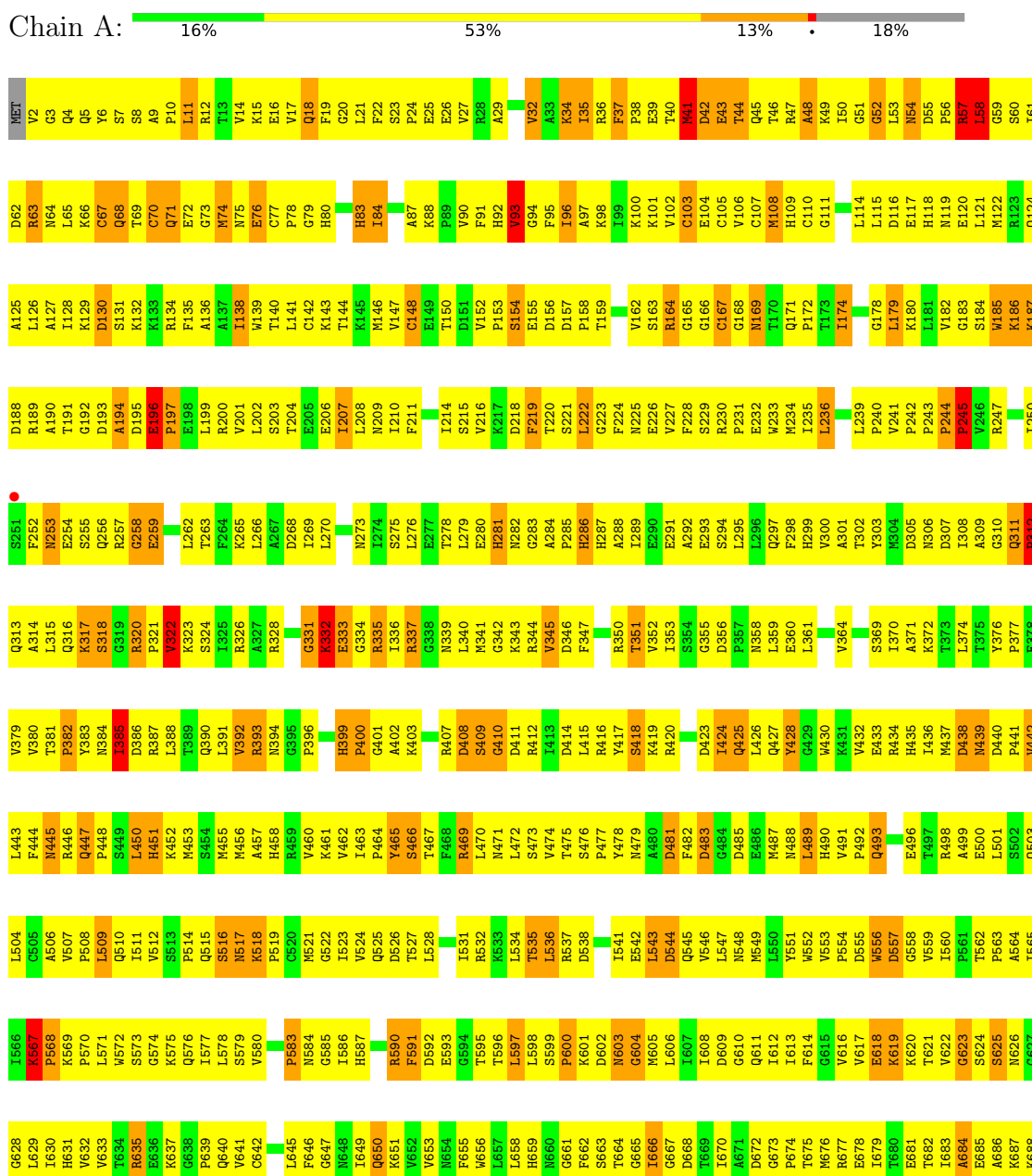
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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|------------|--------------|-----------------|--------------|---------|----------------|----------------|
| 17 | J | 1 | Total 1 | Zn 1 | 0 | 0 |
| 17 | L | 1 | Total 1 | Zn 1 | 0 | 0 |

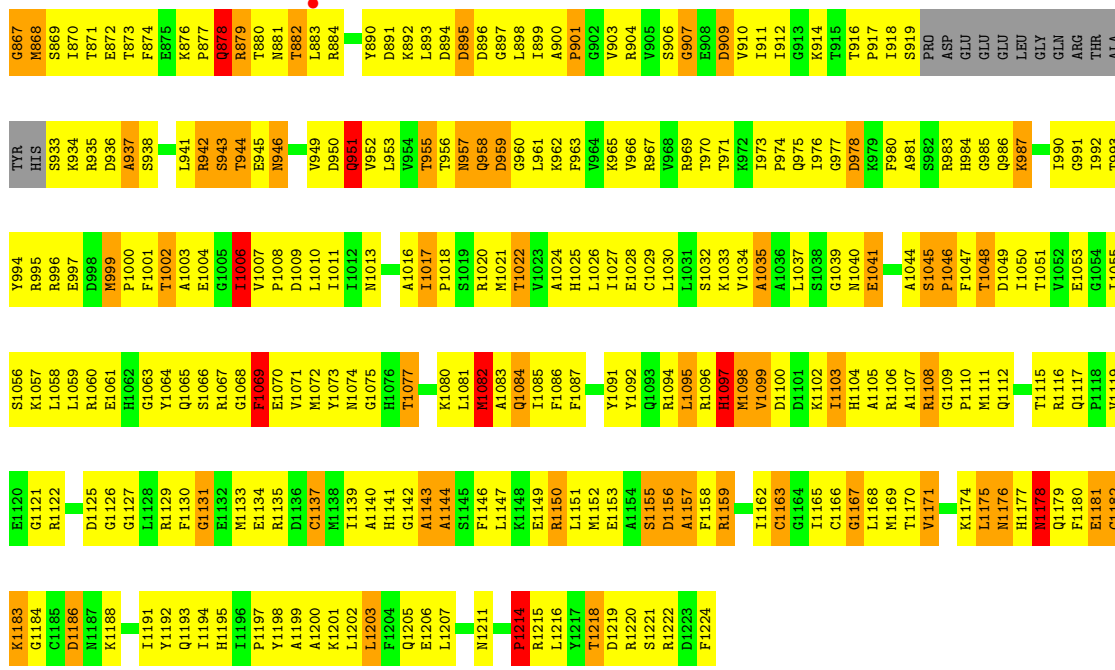
3 Residue-property plots

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

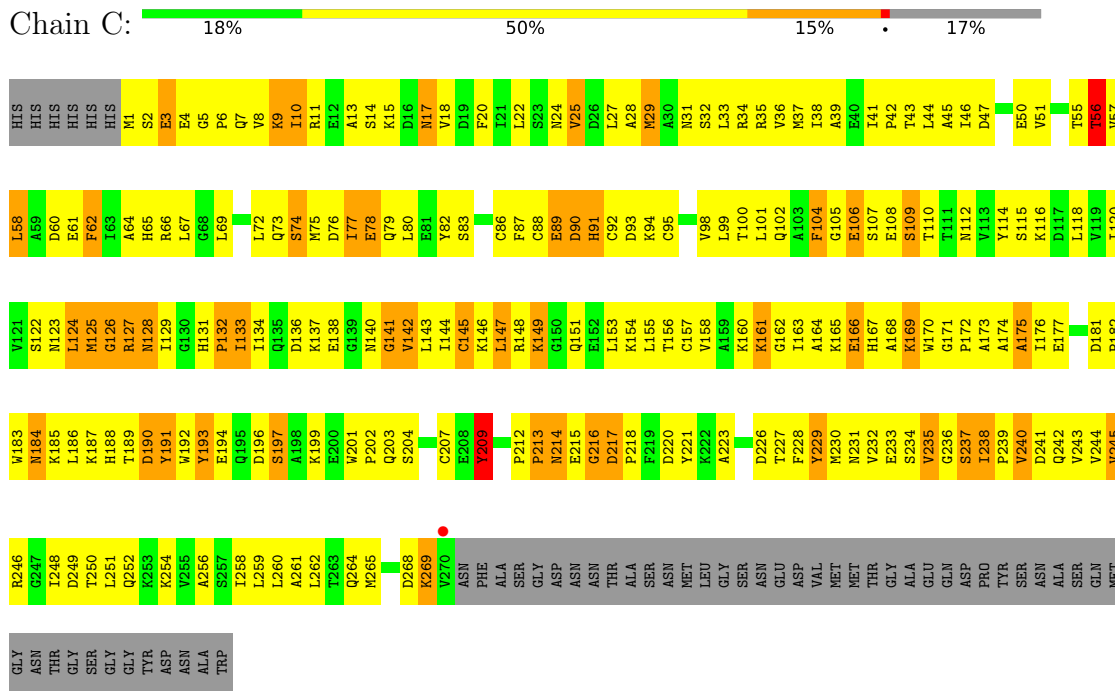
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1



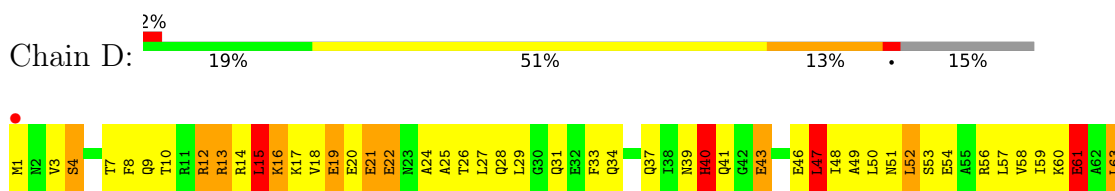
| | | | | | | | | | | | | | | |
|-----|-----|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|------|
| PRO | SER | E1447 | R1386 | V1319 | A1254 | L1192 | E1129 | A1069 | Q1008 | L943 | K880 | A817 | G753 | K689 |
| THR | PRO | E1448 | H1387 | V1320 | E1295 | L1193 | Q1130 | Q1070 | M1009 | R944 | Q881 | M818 | S754 | V690 |
| THR | THR | S1449 | G1388 | I1322 | E1256 | L1194 | Q1131 | A1131 | A1010 | E945 | S882 | G819 | S755 | L691 |
| PRO | TYR | L1450 | F1389 | D1323 | D1257 | R1195 | K1132 | I1072 | Q1011 | E946 | L883 | V946 | I756 | D692 |
| PRO | PRO | L1451 | M1390 | P1324 | E1196 | L1196 | L1133 | G1073 | R1012 | F947 | D884 | R821 | N757 | V693 |
| PRO | PRO | K1452 | R1391 | T1325 | M1259 | L1197 | L1134 | E1074 | D1013 | V948 | T885 | E822 | I758 | T694 |
| TYR | THR | Y1453 | S1392 | G1326 | L1260 | D1198 | I1135 | P1075 | A1014 | D949 | I886 | I825 | A759 | K695 |
| SER | ALA | M1454 | R1393 | I1327 | K1261 | L1199 | I1138 | A1076 | V1015 | G950 | G887 | I826 | G760 | E696 |
| PRO | ASP | T1455 | T1394 | Y1328 | K1262 | A1200 | E1139 | T1077 | T1016 | E951 | G888 | D826 | M761 | A697 |
| THR | TYR | G1395 | G1395 | L1329 | L1263 | A1201 | H1140 | Q1078 | L1017 | A952 | S889 | T827 | S762 | Q698 |
| THR | TYR | L1396 | A1396 | M1330 | E1264 | M1078 | T1141 | M1079 | F1018 | A953 | D890 | A828 | A763 | B699 |
| PRO | GLY | L1397 | L1397 | S1331 | M1265 | T1080 | T1142 | C1019 | C1019 | N954 | A891 | V829 | C764 | N700 |
| PRO | ALA | F1402 | M1398 | F1332 | T1266 | L1081 | L1143 | L1081 | C1020 | P955 | K830 | V829 | V765 | L701 |
| THR | THR | A1403 | A1399 | I1333 | M1267 | ASN | K1144 | THR | L1021 | | T831 | T831 | G766 | L702 |
| SER | SER | C1400 | C1400 | D1334 | S1145 | THR | S1145 | THR | L1022 | Y958 | K895 | A832 | Q767 | T703 |
| PRO | PRO | I1401 | F1402 | I1335 | E1268 | M1209 | V1146 | PHE | | N959 | R896 | A832 | Q768 | A704 |
| THR | THR | F1403 | F1403 | G1336 | E1269 | M1208 | T1147 | THR | R1025 | E960 | R897 | T834 | S769 | K705 |
| PRO | GLY | E1404 | E1404 | L1339 | M1270 | G1210 | HIS | PHE | L1026 | R961 | R898 | G836 | V770 | H706 |
| PRO | ALA | A1405 | A1405 | L1340 | T1272 | V1212 | ALA | ALA | A1027 | R962 | V899 | Y836 | E771 | T709 |
| THR | THR | T1406 | T1406 | G1341 | L1273 | G1213 | GLY | GLY | T1028 | I963 | D900 | I837 | | L710 |
| THR | THR | | | I1341 | E1214 | E1214 | VAL | VAL | R1029 | I964 | L901 | Q838 | R774 | R711 |
| PRO | GLY | I1408 | I1408 | I1342 | I1215 | I1215 | ALA | ALA | R1030 | Q965 | L902 | R839 | I775 | R712 |
| PRO | GLY | L1409 | L1409 | A1343 | I1216 | I1216 | SER | SER | V1031 | N966 | N903 | R840 | A776 | E712 |
| PRO | VAL | F1410 | F1410 | G1344 | E1277 | M1278 | LYS | LYS | L1032 | A967 | T904 | L841 | F777 | S713 |
| THR | THR | E1411 | E1411 | R1345 | Q1218 | Q1218 | K1093 | K1093 | G1033 | Q968 | D905 | V642 | F778 | F714 |
| PRO | SER | A1412 | A1412 | R1345 | T1219 | T1219 | V1094 | V1094 | E1034 | Q969 | H906 | K843 | F779 | E715 |
| PRO | PRO | G1413 | G1413 | L1348 | F1220 | F1220 | T1095 | T1095 | Y1035 | T970 | T907 | A844 | V780 | V718 |
| THR | THR | A1414 | A1414 | Y1349 | K1221 | K1221 | S1096 | S1096 | F971 | L908 | L908 | L845 | D781 | L719 |
| THR | THR | S1415 | S1415 | K1350 | M1222 | M1222 | G1097 | G1097 | L1037 | H972 | D909 | E846 | R782 | R719 |
| PRO | GLY | A1416 | A1416 | E1351 | D1223 | D1223 | S1160 | V1098 | T1038 | R973 | P910 | D847 | T783 | R720 |
| THR | VAL | F1417 | F1417 | Y1352 | L1224 | L1224 | P1099 | P1099 | K1039 | D974 | S911 | I848 | F777 | F721 |
| THR | SER | Y1353 | Y1353 | Y1353 | F1225 | F1225 | V1162 | V1162 | Q1040 | H975 | L912 | M849 | F778 | L722 |
| PRO | SER | M1354 | M1354 | M1354 | I1163 | I1163 | L1101 | L1101 | A1041 | T976 | L913 | H786 | K790 | M723 |
| PRO | VAL | V1355 | V1355 | V1355 | P1164 | P1164 | K1102 | K1102 | F1042 | S979 | E914 | Y852 | F787 | E724 |
| PRO | ASN | I1356 | I1356 | I1356 | E1165 | E1165 | E1103 | E1103 | D1043 | D980 | S915 | D853 | S788 | A725 |
| PRO | ASN | A1357 | A1357 | A1357 | D1166 | D1166 | I1104 | I1104 | V1044 | G916 | G916 | M854 | K797 | R726 |
| PRO | ASP | G1423 | G1423 | G1423 | E1167 | E1167 | L1105 | L1105 | W1045 | L981 | S917 | T855 | D727 | D727 |
| PRO | LEU | V1424 | V1424 | V1424 | E1168 | E1168 | M1106 | M1106 | L1046 | T982 | E918 | T856 | K790 | K728 |
| PRO | ASP | S1425 | S1425 | S1425 | F1169 | F1169 | V1107 | V1107 | S1047 | I983 | I919 | R857 | P794 | A729 |
| PRO | VAL | L1362 | L1362 | L1362 | I1170 | I1170 | A1108 | A1108 | M1048 | K984 | N888 | N858 | E796 | G730 |
| PRO | LYS | Y1363 | Y1363 | Y1363 | H1173 | H1173 | M1109 | M1109 | I1049 | D985 | K924 | S859 | S796 | R731 |
| PRO | ASP | M1364 | M1364 | M1364 | F1174 | F1174 | K1110 | K1110 | E1050 | I986 | G924 | L860 | K797 | L732 |
| PRO | THR | R1365 | R1365 | R1365 | S1175 | S1175 | M1111 | M1111 | A1051 | V987 | L925 | G861 | G798 | A733 |
| PRO | TYR | H1366 | H1366 | H1366 | L1176 | L1176 | K1112 | K1112 | Q1052 | L988 | Q926 | | F799 | E734 |
| PRO | LEU | M1368 | M1368 | M1368 | I1237 | I1237 | T1113 | T1113 | F1053 | | V927 | I864 | V800 | V735 |
| PRO | PRO | A1369 | A1369 | A1369 | L1238 | L1238 | P1114 | P1114 | L1054 | L993 | L928 | Q865 | E801 | M736 |
| PRO | THR | L1370 | L1370 | L1370 | C1240 | C1240 | S1115 | S1115 | R1055 | Q994 | L929 | F866 | N802 | M737 |
| PRO | THR | L1371 | L1371 | L1371 | R1235 | R1235 | L1116 | L1116 | S1056 | E995 | D930 | I867 | S803 | K738 |
| PRO | PRO | L1372 | L1372 | L1372 | K1236 | K1236 | T1117 | T1117 | V1057 | N996 | E931 | Y868 | S803 | K738 |
| PRO | ALA | D1373 | D1373 | D1373 | V1242 | V1242 | V1118 | V1118 | V1058 | L997 | E932 | L740 | Y804 | D739 |
| PRO | VAL | V1374 | V1374 | V1374 | R1244 | R1244 | Y1119 | Y1119 | H1059 | L998 | Y933 | E870 | L805 | L740 |
| PRO | ASP | M1375 | M1375 | M1375 | GLN | GLN | L1120 | L1120 | P1060 | V999 | K934 | E870 | L808 | M741 |
| PRO | PRO | T1376 | T1376 | T1376 | GLU | GLU | L1121 | L1121 | G1061 | Q995 | K934 | D871 | L808 | M742 |
| PRO | THR | L1377 | L1377 | L1377 | SER | SER | E1121 | E1121 | G1062 | L1000 | Q995 | G872 | T809 | M743 |
| PRO | SER | Q1378 | Q1378 | Q1378 | PHE | PHE | P1122 | P1122 | E1062 | R1001 | L936 | M873 | P810 | V743 |
| PRO | PRO | F1441 | F1441 | F1441 | ASP | ASP | H1124 | H1124 | M1063 | G1002 | V937 | D874 | Q811 | K744 |
| PRO | ASP | D1442 | D1442 | D1442 | LEU | LEU | G1124 | G1124 | V1064 | K1003 | K938 | A875 | Q745 | M745 |
| PRO | ALA | V1443 | V1443 | V1443 | ALA | ALA | A1125 | A1125 | G1065 | M1004 | D939 | A876 | F813 | V747 |
| PRO | MET | T1382 | T1382 | T1382 | ALA | ALA | A1126 | A1126 | V1066 | H877 | R940 | A876 | F814 | V747 |
| PRO | PRO | S1383 | S1383 | S1383 | THR | THR | L1127 | L1127 | L1067 | I1006 | K941 | F814 | F814 | S751 |
| PRO | ALA | V1384 | V1384 | V1384 | GLU | GLU | P1190 | P1190 | L1067 | I1006 | K941 | F814 | F814 | S751 |
| PRO | THR | L1385 | L1385 | L1385 | GLU | GLU | M1191 | M1191 | A1068 | I1007 | F942 | E879 | H816 | K752 |

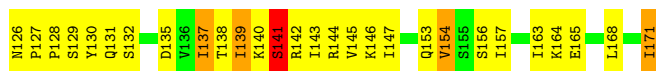


• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

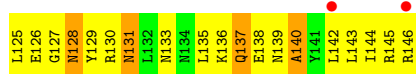
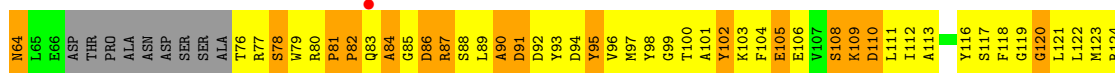
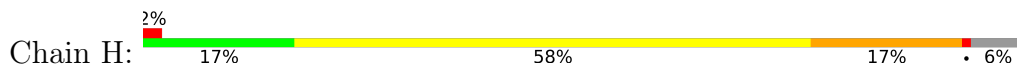


• Molecule 4: DNA-directed RNA polymerase II subunit RPB4

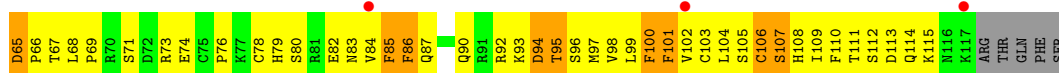




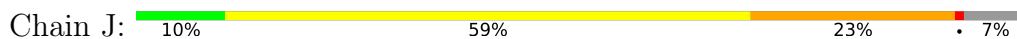
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



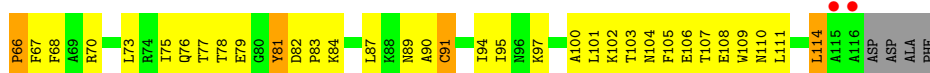
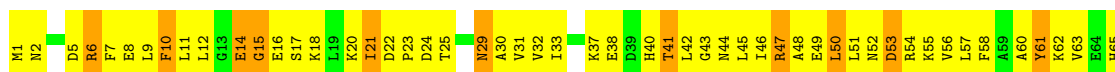
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



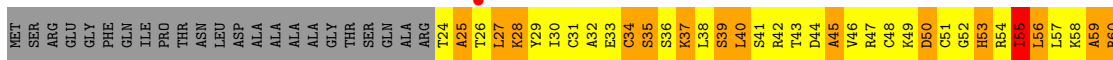
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



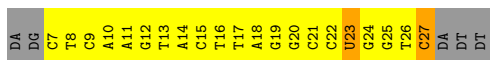
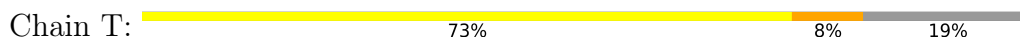
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11



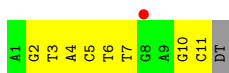
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



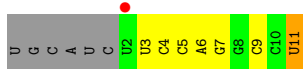
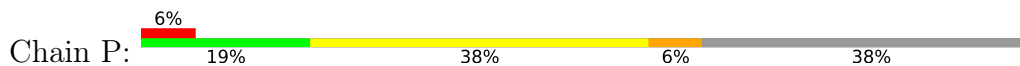
- Molecule 13: DNA (5'-D(*AP*G*CP*TP*CP*AP*AP*GP*TP*AP*CP*TP*TP*AP*(8OG)P*GP*CP*CP*(BRU)P*GP*GP*TP*CP*AP*TP*T)-3')



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



- Molecule 15: RNA (5'-R(*UP*GP*CP*AP*UP*C*UP*UP*CP*CP*AP*GP*GP*CP*CP*U)-3')



4 Data and refinement statistics i

| Property | Value | Source |
|---|---|------------------|
| Space group | C 2 2 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 220.65Å 392.00Å 281.45Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 50.00 – 3.70 49.00 – 3.70 | Depositor EDS |
| % Data completeness (in resolution range) | 99.6 (50.00-3.70) 100.0 (49.00-3.70) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | 0.08 | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.93 (at 3.67Å) | Xtriage |
| Refinement program | CNS 1.2 | Depositor |
| R, R_{free} | 0.225 , 0.258 0.227 , 0.253 | Depositor DCC |
| R_{free} test set | 2439 reflections (1.88%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 114.2 | Xtriage |
| Anisotropy | 0.492 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.30 , 97.9 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$ | Xtriage |
| Estimated twinning fraction | 0.029 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.034 for 1/2*h+1/2*k,3/2*h-1/2*k,-l | Xtriage |
| F_o, F_c correlation | 0.93 | EDS |
| Total number of atoms | 32355 | wwPDB-VP |
| Average B, all atoms (Å ²) | 89.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

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

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 | 0.44 | 0/11441 | 0.74 | 3/15473 (0.0%) |
| 2 | B | 0.41 | 0/9116 | 0.70 | 0/12291 |
| 3 | C | 0.42 | 0/2163 | 0.69 | 0/2930 |
| 4 | D | 0.38 | 0/1516 | 0.63 | 0/2031 |
| 5 | E | 0.39 | 0/1788 | 0.64 | 0/2406 |
| 6 | F | 0.52 | 0/724 | 0.82 | 0/977 |
| 7 | G | 0.44 | 0/1368 | 0.72 | 0/1844 |
| 8 | H | 0.37 | 0/1119 | 0.68 | 0/1514 |
| 9 | I | 0.38 | 0/962 | 0.66 | 0/1295 |
| 10 | J | 0.44 | 0/541 | 0.74 | 0/727 |
| 11 | K | 0.46 | 0/947 | 0.68 | 0/1279 |
| 12 | L | 0.39 | 0/372 | 0.68 | 0/495 |
| 13 | T | 0.56 | 1/426 (0.2%) | 0.87 | 0/650 |
| 14 | N | 0.41 | 0/251 | 0.81 | 0/386 |
| 15 | P | 0.42 | 0/227 | 0.80 | 0/351 |
| All | All | 0.43 | 1/32961 (0.0%) | 0.71 | 3/44649 (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 | 1 |
| 2 | B | 0 | 1 |
| All | All | 0 | 2 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 13 | T | 27 | DC | C1'-N1 | 5.98 | 1.57 | 1.49 |

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1 | A | 567 | LYS | C-N-CD | 5.82 | 140.63 | 128.40 |
| 1 | A | 3 | GLY | N-CA-C | -5.75 | 98.73 | 113.10 |
| 1 | A | 509 | LEU | CA-CB-CG | -5.00 | 103.79 | 115.30 |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|-----------|
| 1 | A | 1035 | TYR | Sidechain |
| 2 | B | 797 | TYR | Sidechain |

5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 11240 | 0 | 11311 | 1819 | 0 |
| 2 | B | 8942 | 0 | 8986 | 1481 | 0 |
| 3 | C | 2125 | 0 | 2090 | 340 | 0 |
| 4 | D | 1504 | 0 | 1518 | 205 | 0 |
| 5 | E | 1752 | 0 | 1776 | 286 | 0 |
| 6 | F | 712 | 0 | 738 | 138 | 0 |
| 7 | G | 1340 | 0 | 1357 | 217 | 0 |
| 8 | H | 1101 | 0 | 1075 | 206 | 0 |
| 9 | I | 944 | 0 | 901 | 162 | 0 |
| 10 | J | 532 | 0 | 542 | 129 | 0 |
| 11 | K | 929 | 0 | 939 | 135 | 0 |
| 12 | L | 370 | 0 | 394 | 90 | 0 |
| 13 | T | 426 | 0 | 236 | 37 | 0 |
| 14 | N | 224 | 0 | 126 | 11 | 0 |
| 15 | P | 205 | 0 | 109 | 8 | 0 |
| 16 | A | 1 | 0 | 0 | 0 | 0 |
| 17 | A | 2 | 0 | 0 | 0 | 0 |
| 17 | B | 1 | 0 | 0 | 0 | 0 |
| 17 | C | 1 | 0 | 0 | 0 | 0 |
| 17 | I | 2 | 0 | 0 | 0 | 0 |
| 17 | J | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 17 | L | 1 | 0 | 0 | 0 | 0 |
| All | All | 32355 | 0 | 32098 | 4821 | 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 75.

All (4821) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:69:LEU:HD13 | 2:B:429:PHE:CD1 | 1.39 | 1.55 |
| 2:B:69:LEU:HD13 | 2:B:429:PHE:CE1 | 1.66 | 1.30 |
| 2:B:577:ALA:HB1 | 2:B:589:VAL:HG11 | 1.24 | 1.17 |
| 2:B:806:THR:HG22 | 2:B:808:ALA:H | 1.08 | 1.16 |
| 2:B:340:ALA:HB3 | 2:B:343:ILE:HG12 | 1.29 | 1.15 |
| 2:B:69:LEU:CD1 | 2:B:429:PHE:CD1 | 2.30 | 1.14 |
| 13:T:16:DT:H2'' | 13:T:17:DT:H5' | 1.29 | 1.13 |
| 2:B:133:LYS:HE3 | 2:B:135:ARG:HH21 | 1.13 | 1.12 |
| 1:A:225:ASN:ND2 | 1:A:228:PHE:H | 1.48 | 1.12 |
| 1:A:41:MET:HB2 | 1:A:49:LYS:HA | 1.32 | 1.12 |
| 1:A:825:ILE:HD11 | 2:B:512:ARG:HB3 | 1.22 | 1.11 |
| 2:B:639:ILE:HD11 | 2:B:691:GLU:HG3 | 1.32 | 1.11 |
| 1:A:567:LYS:HG3 | 8:H:95:TYR:HA | 1.11 | 1.10 |
| 2:B:637:LEU:HD12 | 2:B:693:ILE:HD12 | 1.32 | 1.10 |
| 2:B:622:LYS:HE2 | 9:I:59:VAL:HG22 | 1.28 | 1.10 |
| 3:C:43:THR:HG22 | 3:C:44:LEU:H | 1.02 | 1.09 |
| 1:A:899:VAL:HB | 1:A:929:LEU:HD11 | 1.14 | 1.09 |
| 1:A:768:GLN:HG2 | 1:A:816:HIS:HA | 1.27 | 1.09 |
| 7:G:138:THR:HG22 | 7:G:139:ILE:H | 1.00 | 1.07 |
| 1:A:53:LEU:HD23 | 1:A:54:ASN:N | 1.70 | 1.07 |
| 6:F:109:VAL:HG11 | 6:F:123:LYS:HD2 | 1.30 | 1.06 |
| 3:C:148:ARG:H | 3:C:151:GLN:HG3 | 1.20 | 1.05 |
| 1:A:1244:ARG:HB3 | 1:A:1245:PRO:HA | 1.28 | 1.05 |
| 2:B:244:LEU:HD11 | 2:B:366:GLN:HE22 | 1.20 | 1.05 |
| 2:B:506:GLY:HA2 | 2:B:512:ARG:HH21 | 1.21 | 1.05 |
| 1:A:666:ILE:H | 2:B:1026:LEU:HD13 | 1.21 | 1.05 |
| 12:L:40:LEU:HD13 | 12:L:44:ASP:HB3 | 1.38 | 1.04 |
| 1:A:320:ARG:HB2 | 1:A:320:ARG:HH11 | 1.19 | 1.04 |
| 1:A:12:ARG:HB2 | 2:B:1218:THR:HG22 | 1.39 | 1.04 |
| 2:B:217:ARG:HE | 2:B:405:ARG:HB2 | 1.20 | 1.04 |
| 8:H:12:VAL:HB | 8:H:52:GLN:H | 1.21 | 1.04 |
| 5:E:22:MET:HE3 | 5:E:26:ARG:HH11 | 1.23 | 1.03 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:273:LEU:HB2 | 2:B:276:ILE:HD12 | 1.40 | 1.02 |
| 2:B:1097:HIS:H | 2:B:1098:MET:HE2 | 1.23 | 1.02 |
| 8:H:81:PRO:HB2 | 8:H:82:PRO:CD | 1.89 | 1.02 |
| 8:H:64:ASN:HB2 | 8:H:88:SER:HB2 | 1.41 | 1.02 |
| 1:A:399:HIS:HB3 | 1:A:400:PRO:HD3 | 1.41 | 1.01 |
| 1:A:903:ASN:HD22 | 1:A:904:THR:N | 1.57 | 1.01 |
| 2:B:69:LEU:HB3 | 2:B:429:PHE:HE1 | 1.22 | 1.01 |
| 5:E:78:LEU:HA | 5:E:107:THR:HB | 1.38 | 1.01 |
| 5:E:100:ILE:HG23 | 5:E:105:PHE:HB2 | 1.41 | 1.01 |
| 1:A:1445:ILE:H | 1:A:1445:ILE:HD12 | 1.26 | 1.00 |
| 1:A:590:ARG:HB2 | 1:A:590:ARG:HH11 | 1.24 | 1.00 |
| 3:C:238:ILE:HG23 | 3:C:242:GLN:HB2 | 1.43 | 1.00 |
| 2:B:521:LEU:HD22 | 2:B:633:VAL:HG12 | 1.42 | 1.00 |
| 12:L:32:ALA:HB2 | 12:L:55:ILE:HG13 | 1.44 | 1.00 |
| 1:A:535:THR:HG21 | 1:A:616:VAL:HA | 1.44 | 1.00 |
| 1:A:188:ASP:HB3 | 1:A:191:THR:HB | 1.43 | 0.99 |
| 10:J:5:VAL:HG12 | 10:J:6:ARG:HG3 | 1.43 | 0.99 |
| 3:C:101:LEU:HD13 | 3:C:118:LEU:HD23 | 1.41 | 0.99 |
| 1:A:382:PRO:HD3 | 1:A:428:TYR:HD2 | 1.27 | 0.99 |
| 2:B:1065:GLN:HE21 | 2:B:1067:ARG:N | 1.60 | 0.99 |
| 2:B:503:GLY:HA3 | 2:B:507:LYS:HE2 | 1.45 | 0.98 |
| 9:I:58:VAL:HG13 | 9:I:62:ILE:HD12 | 1.44 | 0.98 |
| 5:E:207:ARG:HB3 | 5:E:207:ARG:HH11 | 1.28 | 0.98 |
| 6:F:76:LYS:HA | 6:F:79:ARG:HD3 | 1.45 | 0.98 |
| 2:B:69:LEU:CD1 | 2:B:429:PHE:CE1 | 2.45 | 0.98 |
| 3:C:148:ARG:N | 3:C:151:GLN:HG3 | 1.78 | 0.98 |
| 1:A:567:LYS:HE2 | 8:H:47:PHE:HB2 | 1.44 | 0.97 |
| 2:B:583:ASN:HD21 | 2:B:628:THR:HG22 | 1.28 | 0.97 |
| 2:B:810:GLU:HA | 2:B:815:ARG:HH22 | 1.29 | 0.97 |
| 6:F:111:LEU:HD12 | 6:F:111:LEU:H | 1.27 | 0.97 |
| 1:A:902:LEU:HG | 1:A:926:GLN:HG3 | 1.45 | 0.97 |
| 8:H:40:LEU:HD22 | 8:H:123:MET:HE3 | 1.46 | 0.97 |
| 1:A:683:ILE:HD13 | 1:A:801:GLU:HG3 | 1.46 | 0.97 |
| 2:B:800:GLN:HB3 | 10:J:52:THR:CG2 | 1.92 | 0.96 |
| 5:E:124:VAL:HG13 | 5:E:132:ILE:HG13 | 1.46 | 0.96 |
| 1:A:1111:MET:HE2 | 1:A:1331:SER:HA | 1.46 | 0.96 |
| 2:B:559:SER:HA | 2:B:563:MET:HB3 | 1.47 | 0.96 |
| 7:G:138:THR:HG22 | 7:G:139:ILE:N | 1.80 | 0.96 |
| 1:A:925:LEU:HD13 | 1:A:983:ILE:HD12 | 1.48 | 0.96 |
| 1:A:666:ILE:HD12 | 1:A:667:GLY:H | 1.31 | 0.95 |
| 1:A:269:ILE:HG12 | 1:A:299:HIS:HB3 | 1.48 | 0.95 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:800:GLN:HB3 | 10:J:52:THR:HG21 | 1.49 | 0.95 |
| 2:B:1099:VAL:HG13 | 2:B:1100:ASP:H | 1.32 | 0.95 |
| 5:E:22:MET:CE | 5:E:26:ARG:HH11 | 1.80 | 0.95 |
| 9:I:85:PHE:H | 9:I:85:PHE:HD2 | 1.08 | 0.95 |
| 2:B:515:HIS:HD2 | 2:B:517:THR:H | 1.01 | 0.95 |
| 6:F:73:ALA:HB1 | 6:F:143:PHE:H | 1.31 | 0.94 |
| 2:B:866:TYR:HB2 | 2:B:870:ILE:HB | 1.49 | 0.94 |
| 8:H:100:THR:HG23 | 8:H:138:GLU:HA | 1.48 | 0.94 |
| 5:E:16:PHE:CZ | 5:E:20:LYS:HE2 | 2.02 | 0.94 |
| 5:E:153:HIS:O | 5:E:154:ILE:HG13 | 1.66 | 0.94 |
| 1:A:308:ILE:HG22 | 1:A:309:ALA:H | 1.33 | 0.94 |
| 10:J:64:ASN:HB3 | 10:J:65:PRO:CD | 1.97 | 0.94 |
| 8:H:128:ASN:H | 8:H:130:ARG:NH1 | 1.65 | 0.94 |
| 1:A:445:ASN:HB2 | 1:A:455:MET:HG2 | 1.49 | 0.94 |
| 1:A:754:SER:H | 1:A:757:ASN:HD22 | 1.13 | 0.94 |
| 8:H:12:VAL:HB | 8:H:52:GLN:N | 1.83 | 0.94 |
| 1:A:320:ARG:HB2 | 1:A:320:ARG:NH1 | 1.83 | 0.94 |
| 8:H:81:PRO:HB2 | 8:H:82:PRO:HD3 | 1.48 | 0.93 |
| 1:A:567:LYS:CG | 8:H:95:TYR:HA | 1.97 | 0.93 |
| 3:C:114:TYR:CD2 | 3:C:140:ASN:HB3 | 2.02 | 0.93 |
| 12:L:27:LEU:HD23 | 12:L:27:LEU:H | 1.34 | 0.93 |
| 2:B:1065:GLN:HE21 | 2:B:1067:ARG:H | 0.96 | 0.93 |
| 1:A:541:ILE:HD13 | 1:A:549:MET:HE1 | 1.51 | 0.93 |
| 1:A:1144:LYS:HB2 | 1:A:1268:LEU:O | 1.68 | 0.93 |
| 4:D:39:ASN:ND2 | 4:D:41:GLN:HB2 | 1.83 | 0.93 |
| 10:J:44:TYR:HA | 10:J:47:ARG:HB2 | 1.51 | 0.93 |
| 11:K:21:ILE:HG23 | 11:K:33:ILE:HG12 | 1.51 | 0.93 |
| 1:A:466:SER:HB3 | 2:B:1103:ILE:HG12 | 1.52 | 0.92 |
| 7:G:127:PRO:HG2 | 7:G:138:THR:HG21 | 1.50 | 0.92 |
| 1:A:720:ARG:O | 1:A:724:GLU:HB2 | 1.70 | 0.92 |
| 1:A:901:LEU:H | 1:A:926:GLN:NE2 | 1.67 | 0.92 |
| 1:A:1424:VAL:HG13 | 1:A:1436:ILE:HD11 | 1.51 | 0.92 |
| 8:H:102:TYR:H | 8:H:102:TYR:HD2 | 1.13 | 0.92 |
| 2:B:115:GLN:HG2 | 2:B:193:LYS:HB2 | 1.48 | 0.92 |
| 1:A:1161:THR:HG22 | 1:A:1163:ILE:H | 1.34 | 0.92 |
| 2:B:520:GLY:H | 2:B:748:ILE:HG22 | 1.34 | 0.92 |
| 3:C:43:THR:HG22 | 3:C:44:LEU:N | 1.85 | 0.92 |
| 8:H:33:GLN:HE21 | 8:H:35:GLN:HB2 | 1.31 | 0.92 |
| 7:G:122:ASN:HB2 | 7:G:131:GLN:HE21 | 1.34 | 0.91 |
| 2:B:911:ILE:HD11 | 2:B:941:LEU:HD13 | 1.52 | 0.91 |
| 1:A:897:TYR:HD2 | 1:A:936:LEU:HD13 | 1.34 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:69:LEU:HB3 | 2:B:429:PHE:CE1 | 2.05 | 0.91 |
| 1:A:1208:THR:HB | 1:A:1211:GLN:HG3 | 1.52 | 0.91 |
| 1:A:1004:ASN:ND2 | 5:E:167:ARG:HD2 | 1.86 | 0.91 |
| 7:G:7:LEU:HB2 | 7:G:74:TYR:CE2 | 2.04 | 0.91 |
| 1:A:49:LYS:HZ1 | 1:A:61:ILE:HG13 | 1.34 | 0.91 |
| 1:A:441:PRO:HG3 | 1:A:498:ARG:HB2 | 1.51 | 0.91 |
| 3:C:203:GLN:HG2 | 3:C:207:CYS:SG | 2.10 | 0.91 |
| 1:A:225:ASN:HD22 | 1:A:228:PHE:N | 1.68 | 0.91 |
| 11:K:12:LEU:H | 11:K:12:LEU:HD12 | 1.33 | 0.91 |
| 1:A:470:LEU:HD13 | 1:A:487:MET:HE1 | 1.52 | 0.90 |
| 3:C:258:ILE:HD11 | 11:K:42:LEU:HD11 | 1.52 | 0.90 |
| 1:A:335:ARG:HD3 | 2:B:1202:LEU:HD23 | 1.54 | 0.90 |
| 2:B:69:LEU:HD22 | 2:B:429:PHE:CE1 | 2.07 | 0.90 |
| 1:A:442:VAL:HG12 | 1:A:490:HIS:O | 1.71 | 0.90 |
| 2:B:410:GLY:HA2 | 2:B:413:LEU:HD12 | 1.52 | 0.89 |
| 2:B:642:ASP:HA | 2:B:649:LYS:HA | 1.52 | 0.89 |
| 3:C:39:ALA:HA | 3:C:164:ALA:HB3 | 1.54 | 0.89 |
| 1:A:1409:LEU:HD13 | 2:B:1207:LEU:HD11 | 1.54 | 0.89 |
| 11:K:47:ARG:HB3 | 11:K:47:ARG:HH11 | 1.34 | 0.89 |
| 2:B:515:HIS:CD2 | 2:B:517:THR:H | 1.90 | 0.89 |
| 4:D:3:VAL:HG21 | 7:G:10:ASN:HB2 | 1.52 | 0.89 |
| 1:A:14:VAL:H | 1:A:1432:GLN:HE22 | 1.14 | 0.89 |
| 1:A:1369:ALA:O | 1:A:1372:VAL:HG12 | 1.72 | 0.89 |
| 2:B:384:ARG:HA | 2:B:387:LEU:HD22 | 1.52 | 0.89 |
| 2:B:999:MET:HG3 | 2:B:1000:PRO:HD2 | 1.55 | 0.89 |
| 5:E:117:THR:HG22 | 5:E:119:SER:H | 1.37 | 0.89 |
| 3:C:57:VAL:HG11 | 10:J:60:PHE:HB3 | 1.53 | 0.89 |
| 3:C:77:ILE:H | 3:C:129:ILE:HD11 | 1.36 | 0.89 |
| 1:A:1308:THR:HG23 | 1:A:1309:ASP:N | 1.84 | 0.89 |
| 3:C:43:THR:CG2 | 3:C:44:LEU:H | 1.85 | 0.88 |
| 7:G:138:THR:CG2 | 7:G:139:ILE:H | 1.82 | 0.88 |
| 1:A:18:GLN:HG2 | 1:A:1418:LEU:HD13 | 1.55 | 0.88 |
| 1:A:537:ARG:HD2 | 8:H:20:TYR:HE1 | 1.37 | 0.88 |
| 1:A:1153:TYR:HB2 | 1:A:1192:LEU:HD23 | 1.55 | 0.88 |
| 2:B:193:LYS:NZ | 12:L:32:ALA:HB1 | 1.88 | 0.88 |
| 1:A:335:ARG:HD2 | 2:B:1206:GLU:OE1 | 1.73 | 0.88 |
| 1:A:1227:ILE:HG22 | 1:A:1228:TRP:H | 1.37 | 0.88 |
| 1:A:568:PRO:HG2 | 8:H:46:LEU:HD22 | 1.55 | 0.88 |
| 1:A:946:VAL:HG13 | 5:E:201:LYS:HB3 | 1.55 | 0.88 |
| 5:E:17:ARG:NH1 | 5:E:17:ARG:HB2 | 1.88 | 0.88 |
| 2:B:880:THR:HB | 2:B:934:LYS:CE | 2.04 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1420:ASP:CB | 1:A:1422:ARG:HG3 | 2.02 | 0.88 |
| 5:E:171:LYS:HG2 | 5:E:174:GLN:OE1 | 1.74 | 0.88 |
| 1:A:71:GLN:HG3 | 1:A:72:GLU:HG2 | 1.56 | 0.88 |
| 4:D:164:ILE:HG23 | 4:D:168:LYS:HD2 | 1.56 | 0.88 |
| 1:A:1030:ARG:HG3 | 1:A:1034:GLU:OE2 | 1.75 | 0.88 |
| 2:B:539:LEU:H | 2:B:539:LEU:HD12 | 1.38 | 0.88 |
| 2:B:69:LEU:O | 2:B:70:ILE:HG13 | 1.74 | 0.87 |
| 1:A:630:ILE:HD11 | 1:A:646:PHE:CZ | 2.09 | 0.87 |
| 1:A:665:GLY:O | 1:A:667:GLY:N | 2.06 | 0.87 |
| 2:B:299:GLU:HB3 | 2:B:571:PRO:HG3 | 1.57 | 0.87 |
| 5:E:17:ARG:HB2 | 5:E:17:ARG:HH11 | 1.37 | 0.87 |
| 1:A:899:VAL:HB | 1:A:929:LEU:CD1 | 2.04 | 0.87 |
| 1:A:1101:LEU:HB2 | 1:A:1355:VAL:HG11 | 1.55 | 0.87 |
| 2:B:1065:GLN:NE2 | 2:B:1067:ARG:H | 1.73 | 0.87 |
| 1:A:901:LEU:H | 1:A:926:GLN:HE21 | 1.19 | 0.87 |
| 12:L:61:THR:HG21 | 12:L:63:ARG:HE | 1.38 | 0.87 |
| 3:C:175:ALA:HB2 | 10:J:10:CYS:HB2 | 1.57 | 0.87 |
| 1:A:899:VAL:HG13 | 1:A:908:LEU:HD21 | 1.55 | 0.87 |
| 1:A:182:VAL:HG22 | 1:A:201:VAL:HA | 1.55 | 0.86 |
| 12:L:55:ILE:HD13 | 12:L:55:ILE:H | 1.40 | 0.86 |
| 2:B:810:GLU:CA | 2:B:815:ARG:HH22 | 1.88 | 0.86 |
| 1:A:1323:ASP:OD1 | 1:A:1325:THR:HG22 | 1.74 | 0.86 |
| 13:T:15:DC:H2'' | 13:T:16:DT:H72 | 1.55 | 0.86 |
| 1:A:40:THR:HG22 | 1:A:41:MET:HG3 | 1.54 | 0.86 |
| 1:A:1242:VAL:HG12 | 1:A:1243:VAL:H | 1.39 | 0.86 |
| 2:B:278:GLN:HG2 | 2:B:279:ASP:H | 1.38 | 0.86 |
| 9:I:82:GLU:HB3 | 9:I:104:LEU:HD12 | 1.58 | 0.86 |
| 1:A:567:LYS:HG3 | 8:H:95:TYR:CA | 2.03 | 0.86 |
| 2:B:801:LYS:O | 10:J:52:THR:HG23 | 1.75 | 0.86 |
| 12:L:34:CYS:HB3 | 12:L:51:CYS:SG | 2.15 | 0.86 |
| 5:E:3:GLN:HG3 | 5:E:5:ASN:H | 1.40 | 0.86 |
| 4:D:70:PHE:O | 4:D:74:GLN:HG3 | 1.75 | 0.85 |
| 1:A:616:VAL:HG12 | 1:A:617:VAL:H | 1.42 | 0.85 |
| 5:E:85:GLU:HB2 | 5:E:88:VAL:HG22 | 1.56 | 0.85 |
| 6:F:103:MET:CE | 7:G:66:GLY:H | 1.89 | 0.85 |
| 1:A:34:LYS:HZ1 | 1:A:57:ARG:NH2 | 1.74 | 0.85 |
| 2:B:287:ARG:HG2 | 2:B:292:ILE:HA | 1.56 | 0.85 |
| 9:I:65:ASP:HB3 | 9:I:68:LEU:HD12 | 1.56 | 0.85 |
| 13:T:15:DC:C2' | 13:T:16:DT:H72 | 2.05 | 0.85 |
| 1:A:298:PHE:HZ | 1:A:314:ALA:HB2 | 1.39 | 0.85 |
| 1:A:390:GLN:O | 1:A:394:ASN:HB2 | 1.75 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:738:LYS:HB2 | 1:A:740:LEU:HG | 1.58 | 0.85 |
| 6:F:72:LYS:HA | 6:F:72:LYS:HE3 | 1.59 | 0.85 |
| 8:H:100:THR:OG1 | 8:H:138:GLU:HG3 | 1.76 | 0.85 |
| 1:A:1261:LYS:O | 1:A:1264:GLU:HB3 | 1.76 | 0.85 |
| 3:C:244:VAL:O | 3:C:248:ILE:HG13 | 1.75 | 0.85 |
| 1:A:875:ALA:HB2 | 1:A:1366:ARG:HD2 | 1.58 | 0.85 |
| 1:A:134:ARG:HG2 | 1:A:138:ILE:HD11 | 1.56 | 0.85 |
| 7:G:45:ILE:HA | 7:G:78:VAL:HG12 | 1.58 | 0.85 |
| 2:B:882:THR:HG22 | 2:B:884:ARG:HB2 | 1.56 | 0.85 |
| 11:K:49:GLU:OE2 | 11:K:97:LYS:HE3 | 1.76 | 0.85 |
| 5:E:156:LEU:HD12 | 5:E:195:VAL:HB | 1.57 | 0.84 |
| 1:A:913:LEU:HD12 | 1:A:914:GLU:H | 1.40 | 0.84 |
| 2:B:640:VAL:HG22 | 2:B:651:LEU:HD23 | 1.57 | 0.84 |
| 1:A:42:ASP:O | 1:A:44:THR:N | 2.11 | 0.84 |
| 2:B:289:LEU:HD13 | 2:B:375:ALA:HB2 | 1.58 | 0.84 |
| 2:B:880:THR:HB | 2:B:934:LYS:HD3 | 1.58 | 0.84 |
| 2:B:1119:VAL:O | 2:B:1126:GLY:HA3 | 1.78 | 0.84 |
| 2:B:69:LEU:HD13 | 2:B:429:PHE:HD1 | 1.11 | 0.84 |
| 11:K:65:HIS:CD2 | 11:K:67:PHE:H | 1.96 | 0.84 |
| 2:B:604:ARG:HG3 | 2:B:611:PRO:HA | 1.58 | 0.84 |
| 3:C:147:LEU:HB2 | 3:C:151:GLN:HB2 | 1.59 | 0.84 |
| 1:A:49:LYS:HZ1 | 1:A:61:ILE:N | 1.75 | 0.84 |
| 3:C:32:SER:O | 3:C:36:VAL:HG23 | 1.78 | 0.84 |
| 1:A:53:LEU:HD23 | 1:A:54:ASN:H | 1.40 | 0.84 |
| 6:F:73:ALA:CB | 6:F:143:PHE:H | 1.90 | 0.84 |
| 1:A:414:ASP:OD1 | 1:A:416:ARG:HG2 | 1.78 | 0.84 |
| 1:A:1404:GLU:HB2 | 1:A:1408:ILE:HD12 | 1.58 | 0.83 |
| 12:L:55:ILE:O | 12:L:56:LEU:HB2 | 1.77 | 0.83 |
| 5:E:19:VAL:O | 5:E:23:VAL:HG23 | 1.77 | 0.83 |
| 1:A:563:PRO:HG3 | 1:A:572:TRP:CZ2 | 2.13 | 0.83 |
| 1:A:981:LEU:HD21 | 1:A:1039:LYS:HA | 1.59 | 0.83 |
| 1:A:1420:ASP:HB2 | 1:A:1422:ARG:HG3 | 1.59 | 0.83 |
| 2:B:882:THR:CG2 | 2:B:884:ARG:HB2 | 2.08 | 0.83 |
| 2:B:1180:PHE:HB3 | 2:B:1191:ILE:HD12 | 1.59 | 0.83 |
| 3:C:47:ASP:HA | 12:L:69:ALA:HB3 | 1.60 | 0.83 |
| 8:H:64:ASN:HD22 | 8:H:88:SER:CB | 1.90 | 0.83 |
| 1:A:738:LYS:H | 1:A:738:LYS:HD2 | 1.42 | 0.83 |
| 2:B:526:GLU:HG2 | 2:B:538:ASN:HD22 | 1.43 | 0.83 |
| 2:B:652:LYS:O | 2:B:689:LEU:HD22 | 1.78 | 0.83 |
| 2:B:1084:GLN:N | 2:B:1084:GLN:NE2 | 2.26 | 0.83 |
| 8:H:129:TYR:H | 8:H:130:ARG:HH11 | 1.27 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:32:VAL:O | 1:A:57:ARG:HD3 | 1.78 | 0.83 |
| 1:A:332:LYS:HG3 | 1:A:333:GLU:OE2 | 1.77 | 0.83 |
| 2:B:593:PRO:HG2 | 2:B:617:ARG:CZ | 2.09 | 0.83 |
| 2:B:121:ASN:HA | 2:B:207:GLY:HA2 | 1.58 | 0.83 |
| 1:A:1189:SER:O | 1:A:1241:ARG:HD3 | 1.79 | 0.82 |
| 2:B:101:MET:HB2 | 2:B:169:ARG:HH22 | 1.44 | 0.82 |
| 7:G:1:MET:SD | 7:G:2:PHE:N | 2.52 | 0.82 |
| 12:L:32:ALA:CB | 12:L:55:ILE:HG13 | 2.09 | 0.82 |
| 5:E:114:ASN:O | 5:E:115:ASN:HB3 | 1.76 | 0.82 |
| 1:A:1095:THR:HG22 | 1:A:1100:ARG:HB2 | 1.61 | 0.82 |
| 2:B:309:GLN:OE1 | 9:I:52:ILE:HD11 | 1.79 | 0.82 |
| 2:B:770:GLN:CD | 2:B:983:ARG:HA | 1.98 | 0.82 |
| 1:A:196:GLU:HB2 | 1:A:197:PRO:HD2 | 1.61 | 0.82 |
| 1:A:351:THR:HB | 2:B:1103:ILE:CD1 | 2.09 | 0.82 |
| 1:A:590:ARG:HH11 | 1:A:590:ARG:CB | 1.91 | 0.82 |
| 1:A:709:THR:HG22 | 1:A:711:ARG:H | 1.45 | 0.82 |
| 2:B:277:LYS:HG3 | 2:B:338:GLY:HA2 | 1.60 | 0.82 |
| 2:B:1084:GLN:HE21 | 2:B:1084:GLN:H | 1.24 | 0.82 |
| 7:G:62:LEU:HB3 | 7:G:63:PRO:HD2 | 1.61 | 0.82 |
| 1:A:69:THR:O | 1:A:71:GLN:N | 2.13 | 0.82 |
| 1:A:770:VAL:HA | 1:A:822:GLU:OE1 | 1.79 | 0.82 |
| 2:B:815:ARG:HD3 | 2:B:1041:GLU:OE2 | 1.79 | 0.82 |
| 2:B:1095:LEU:H | 2:B:1095:LEU:HD12 | 1.45 | 0.82 |
| 2:B:850:LEU:HD12 | 2:B:851:PHE:N | 1.94 | 0.82 |
| 2:B:1099:VAL:HG13 | 2:B:1100:ASP:N | 1.95 | 0.82 |
| 7:G:49:LEU:HD21 | 7:G:77:VAL:HG23 | 1.61 | 0.82 |
| 1:A:1244:ARG:HB3 | 1:A:1245:PRO:CA | 2.08 | 0.82 |
| 2:B:65:GLU:HG3 | 2:B:66:ASP:H | 1.45 | 0.82 |
| 2:B:515:HIS:HD2 | 2:B:517:THR:N | 1.77 | 0.82 |
| 2:B:830:TYR:CE2 | 2:B:1000:PRO:HD3 | 2.15 | 0.82 |
| 2:B:1084:GLN:N | 2:B:1084:GLN:HE21 | 1.77 | 0.82 |
| 9:I:26:LEU:HD23 | 9:I:37:GLU:HA | 1.59 | 0.82 |
| 3:C:142:VAL:H | 10:J:16:ASP:HB3 | 1.45 | 0.82 |
| 1:A:855:THR:HG21 | 1:A:857:ARG:HE | 1.44 | 0.81 |
| 1:A:1116:LEU:HB3 | 1:A:1308:THR:CG2 | 2.10 | 0.81 |
| 1:A:225:ASN:HD22 | 1:A:228:PHE:H | 0.83 | 0.81 |
| 3:C:133:ILE:HG21 | 3:C:236:GLY:HA3 | 1.62 | 0.81 |
| 7:G:87:VAL:HB | 7:G:103:VAL:HG11 | 1.61 | 0.81 |
| 1:A:49:LYS:NZ | 1:A:61:ILE:HG13 | 1.94 | 0.81 |
| 1:A:1260:LEU:HD12 | 1:A:1260:LEU:O | 1.81 | 0.81 |
| 2:B:69:LEU:CB | 2:B:429:PHE:HE1 | 1.93 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:567:LYS:CE | 8:H:47:PHE:HB2 | 2.11 | 0.81 |
| 1:A:590:ARG:HB3 | 1:A:605:MET:H | 1.46 | 0.81 |
| 2:B:69:LEU:HD22 | 2:B:429:PHE:CZ | 2.16 | 0.81 |
| 2:B:622:LYS:CE | 9:I:59:VAL:HG22 | 2.11 | 0.81 |
| 5:E:128:PRO:HA | 5:E:129:PRO:O | 1.79 | 0.81 |
| 10:J:64:ASN:HB3 | 10:J:65:PRO:HD2 | 1.61 | 0.81 |
| 1:A:107:CYS:HA | 1:A:171:GLN:OE1 | 1.79 | 0.81 |
| 1:A:1438:THR:HB | 2:B:1144:ALA:HB3 | 1.63 | 0.81 |
| 2:B:289:LEU:HD13 | 2:B:375:ALA:CB | 2.09 | 0.81 |
| 2:B:579:ARG:HB2 | 2:B:586:TRP:NE1 | 1.95 | 0.81 |
| 7:G:125:SER:OG | 7:G:128:PRO:HA | 1.80 | 0.81 |
| 1:A:1002:GLY:HA3 | 1:A:1007:ILE:HG21 | 1.60 | 0.81 |
| 2:B:1017:ILE:HB | 2:B:1018:PRO:HD3 | 1.61 | 0.81 |
| 8:H:93:TYR:HB3 | 8:H:144:ILE:O | 1.80 | 0.81 |
| 2:B:637:LEU:O | 2:B:690:VAL:HG13 | 1.81 | 0.80 |
| 9:I:35:VAL:HG12 | 9:I:36:GLU:N | 1.96 | 0.80 |
| 1:A:180:LYS:HZ2 | 1:A:294:SER:HB3 | 1.46 | 0.80 |
| 2:B:1182:CYS:O | 2:B:1182:CYS:SG | 2.38 | 0.80 |
| 2:B:882:THR:HG21 | 2:B:935:ARG:HA | 1.63 | 0.80 |
| 1:A:321:PRO:O | 1:A:322:VAL:HG12 | 1.81 | 0.80 |
| 2:B:365:THR:OG1 | 2:B:367:LEU:HG | 1.81 | 0.80 |
| 2:B:1002:THR:HG23 | 2:B:1006:ILE:HG13 | 1.62 | 0.80 |
| 2:B:1150:ARG:HG3 | 2:B:1150:ARG:HH11 | 1.45 | 0.80 |
| 1:A:779:PHE:HE1 | 1:A:785:PRO:HD3 | 1.45 | 0.80 |
| 2:B:217:ARG:NE | 2:B:405:ARG:HB2 | 1.97 | 0.80 |
| 6:F:77:ASP:O | 6:F:78:GLN:HB2 | 1.79 | 0.80 |
| 8:H:101:ALA:HB2 | 8:H:116:TYR:CZ | 2.15 | 0.80 |
| 1:A:600:PRO:HG2 | 1:A:601:LYS:H | 1.44 | 0.80 |
| 2:B:336:ARG:HE | 2:B:348:ARG:HH12 | 1.25 | 0.80 |
| 3:C:8:VAL:HG12 | 3:C:9:LYS:H | 1.46 | 0.80 |
| 1:A:93:VAL:HG22 | 1:A:301:ALA:HA | 1.62 | 0.80 |
| 2:B:957:ASN:HD22 | 2:B:961:LEU:HB2 | 1.47 | 0.80 |
| 2:B:1084:GLN:HG2 | 3:C:201:TRP:CZ2 | 2.17 | 0.80 |
| 2:B:1159:ARG:HB3 | 2:B:1159:ARG:HH11 | 1.46 | 0.80 |
| 7:G:15:PRO:HA | 7:G:18:PHE:CD1 | 2.17 | 0.80 |
| 1:A:23:SER:HA | 1:A:233:TRP:NE1 | 1.96 | 0.80 |
| 1:A:1130:GLN:HE21 | 1:A:1134:ILE:HD11 | 1.47 | 0.80 |
| 1:A:1444:MET:HE1 | 6:F:135:ARG:HB2 | 1.64 | 0.80 |
| 3:C:98:VAL:C | 3:C:99:LEU:HD23 | 2.02 | 0.80 |
| 5:E:52:ARG:HB3 | 5:E:53:PRO:HD2 | 1.64 | 0.80 |
| 2:B:422:LYS:O | 2:B:426:LYS:HG2 | 1.80 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:47:LEU:HD13 | 4:D:48:ILE:H | 1.46 | 0.79 |
| 13:T:15:DC:H2" | 13:T:16:DT:C7 | 2.12 | 0.79 |
| 1:A:115:LEU:O | 1:A:122:MET:HG2 | 1.83 | 0.79 |
| 3:C:45:ALA:HA | 3:C:72:LEU:HD12 | 1.64 | 0.79 |
| 12:L:61:THR:HG22 | 12:L:63:ARG:H | 1.47 | 0.79 |
| 2:B:343:ILE:HG23 | 2:B:347:LYS:HE2 | 1.62 | 0.79 |
| 2:B:824:ILE:HG22 | 2:B:1087:PHE:CE2 | 2.18 | 0.79 |
| 6:F:103:MET:HE2 | 7:G:66:GLY:H | 1.47 | 0.79 |
| 10:J:9:SER:HB2 | 10:J:45:CYS:HB2 | 1.64 | 0.79 |
| 1:A:1206:ASP:HB3 | 1:A:1274:ARG:HH12 | 1.45 | 0.79 |
| 1:A:1254:ALA:O | 1:A:1255:GLU:HB2 | 1.81 | 0.79 |
| 11:K:53:ASP:HB3 | 11:K:56:VAL:HG23 | 1.64 | 0.79 |
| 2:B:133:LYS:HE3 | 2:B:135:ARG:NH2 | 1.95 | 0.79 |
| 2:B:46:GLN:HB2 | 2:B:408:LEU:HD21 | 1.65 | 0.79 |
| 1:A:21:LEU:HD11 | 1:A:1414:ALA:HA | 1.65 | 0.79 |
| 2:B:995:ARG:HH12 | 3:C:165:LYS:HG2 | 1.47 | 0.79 |
| 4:D:8:PHE:CD2 | 7:G:6:ASP:HB2 | 2.18 | 0.79 |
| 11:K:6:ARG:O | 11:K:9:LEU:HG | 1.81 | 0.79 |
| 7:G:7:LEU:HB2 | 7:G:74:TYR:HE2 | 1.43 | 0.79 |
| 11:K:12:LEU:HD12 | 11:K:12:LEU:N | 1.97 | 0.79 |
| 1:A:148:CYS:O | 1:A:168:GLY:HA2 | 1.82 | 0.78 |
| 2:B:35:SER:HA | 2:B:811:TYR:HE2 | 1.48 | 0.78 |
| 3:C:39:ALA:CA | 3:C:164:ALA:HB3 | 2.12 | 0.78 |
| 3:C:238:ILE:HD11 | 3:C:246:ARG:HH11 | 1.47 | 0.78 |
| 8:H:44:VAL:HG13 | 8:H:48:PRO:HA | 1.63 | 0.78 |
| 12:L:30:ILE:O | 12:L:56:LEU:HA | 1.82 | 0.78 |
| 1:A:92:HIS:HB2 | 1:A:236:LEU:HD21 | 1.63 | 0.78 |
| 1:A:982:THR:H | 1:A:985:ASP:HB2 | 1.47 | 0.78 |
| 3:C:73:GLN:HE21 | 3:C:74:SER:H | 1.29 | 0.78 |
| 7:G:88:ASP:HB3 | 7:G:144:ARG:HA | 1.66 | 0.78 |
| 1:A:372:LYS:HA | 1:A:435:HIS:ND1 | 1.98 | 0.78 |
| 2:B:880:THR:CB | 2:B:934:LYS:HD3 | 2.12 | 0.78 |
| 3:C:235:VAL:HG12 | 10:J:13:VAL:HG23 | 1.64 | 0.78 |
| 7:G:128:PRO:O | 7:G:138:THR:HG23 | 1.83 | 0.78 |
| 2:B:1162:ILE:HD11 | 2:B:1194:ILE:HD13 | 1.64 | 0.78 |
| 5:E:207:ARG:HB3 | 5:E:207:ARG:NH1 | 1.98 | 0.78 |
| 8:H:27:GLU:HG2 | 8:H:39:THR:HA | 1.66 | 0.78 |
| 12:L:28:LYS:HB2 | 12:L:39:SER:HB2 | 1.65 | 0.78 |
| 5:E:109:ILE:HG22 | 5:E:110:PHE:H | 1.47 | 0.78 |
| 13:T:13:DT:H2" | 13:T:14:DA:OP2 | 1.83 | 0.78 |
| 1:A:84:ILE:HD11 | 1:A:270:LEU:HD13 | 1.65 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:412:LEU:HB3 | 2:B:466:TRP:HE1 | 1.48 | 0.78 |
| 2:B:579:ARG:HB2 | 2:B:586:TRP:HE1 | 1.46 | 0.78 |
| 4:D:18:VAL:O | 4:D:19:GLU:HB2 | 1.82 | 0.78 |
| 10:J:1:MET:N | 10:J:57:ILE:H | 1.82 | 0.78 |
| 1:A:567:LYS:HB3 | 1:A:568:PRO:HD3 | 1.65 | 0.78 |
| 2:B:549:THR:HB | 2:B:628:THR:OG1 | 1.84 | 0.78 |
| 2:B:613:VAL:HG13 | 2:B:627:PHE:O | 1.84 | 0.78 |
| 8:H:41:ASP:O | 8:H:42:ILE:HG13 | 1.84 | 0.78 |
| 1:A:1004:ASN:HD21 | 5:E:167:ARG:HD2 | 1.46 | 0.78 |
| 2:B:294:ASP:O | 2:B:296:GLU:N | 2.17 | 0.78 |
| 11:K:30:ALA:HB2 | 11:K:76:GLN:HG3 | 1.64 | 0.78 |
| 1:A:320:ARG:HH11 | 1:A:320:ARG:CB | 1.97 | 0.78 |
| 1:A:1100:ARG:NH2 | 1:A:1351:GLU:HG2 | 1.99 | 0.78 |
| 2:B:70:ILE:O | 2:B:137:TYR:HB2 | 1.84 | 0.78 |
| 2:B:244:LEU:HD11 | 2:B:366:GLN:NE2 | 1.97 | 0.78 |
| 2:B:880:THR:HB | 2:B:934:LYS:CD | 2.12 | 0.78 |
| 2:B:882:THR:HG22 | 2:B:884:ARG:H | 1.49 | 0.78 |
| 1:A:696:GLU:OE2 | 1:A:702:LEU:HD21 | 1.83 | 0.77 |
| 8:H:25:ARG:HA | 8:H:41:ASP:HA | 1.65 | 0.77 |
| 8:H:80:ARG:HH11 | 11:K:57:LEU:HD21 | 1.49 | 0.77 |
| 2:B:1095:LEU:HD12 | 2:B:1095:LEU:N | 1.99 | 0.77 |
| 4:D:40:HIS:CB | 7:G:73:LYS:HZ2 | 1.97 | 0.77 |
| 5:E:109:ILE:HG22 | 5:E:110:PHE:N | 1.99 | 0.77 |
| 8:H:128:ASN:H | 8:H:130:ARG:HH11 | 1.30 | 0.77 |
| 1:A:56:PRO:O | 1:A:57:ARG:HG3 | 1.84 | 0.77 |
| 1:A:541:ILE:HD13 | 1:A:549:MET:CE | 2.14 | 0.77 |
| 1:A:567:LYS:HD3 | 1:A:568:PRO:HD3 | 1.65 | 0.77 |
| 1:A:629:LEU:O | 1:A:633:VAL:HG23 | 1.83 | 0.77 |
| 1:A:635:ARG:HH11 | 1:A:635:ARG:HA | 1.50 | 0.77 |
| 2:B:611:PRO:HG2 | 2:B:685:LEU:HD21 | 1.67 | 0.77 |
| 4:D:139:LYS:HE2 | 4:D:143:ASN:HD21 | 1.47 | 0.77 |
| 11:K:55:LYS:HB3 | 11:K:81:TYR:CD1 | 2.20 | 0.77 |
| 2:B:277:LYS:O | 2:B:278:GLN:HB2 | 1.83 | 0.77 |
| 3:C:38:ILE:HA | 3:C:173:ALA:HB2 | 1.66 | 0.77 |
| 3:C:46:ILE:HG13 | 3:C:72:LEU:HD11 | 1.66 | 0.77 |
| 1:A:1175:SER:O | 1:A:1176:LEU:HB2 | 1.84 | 0.77 |
| 2:B:723:VAL:HG12 | 2:B:724:ASP:H | 1.49 | 0.77 |
| 8:H:130:ARG:N | 8:H:130:ARG:HD2 | 1.98 | 0.77 |
| 9:I:7:CYS:HB3 | 9:I:14:LEU:HD21 | 1.66 | 0.77 |
| 1:A:284:ALA:C | 1:A:286:HIS:H | 1.88 | 0.77 |
| 1:A:1325:THR:O | 5:E:148:GLU:HB2 | 1.84 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1444:MET:HG3 | 7:G:60:ARG:HA | 1.66 | 0.77 |
| 1:A:189:ARG:HA | 1:A:195:ASP:HA | 1.65 | 0.77 |
| 1:A:477:PRO:HG2 | 1:A:521:MET:HG2 | 1.67 | 0.77 |
| 1:A:1343:ALA:HB2 | 5:E:150:VAL:HG22 | 1.64 | 0.77 |
| 1:A:49:LYS:NZ | 1:A:61:ILE:H | 1.82 | 0.77 |
| 11:K:31:VAL:HG12 | 11:K:32:VAL:H | 1.50 | 0.77 |
| 11:K:55:LYS:HB3 | 11:K:81:TYR:HD1 | 1.49 | 0.77 |
| 11:K:107:THR:O | 11:K:111:LEU:HG | 1.85 | 0.77 |
| 1:A:11:LEU:C | 1:A:11:LEU:HD12 | 2.05 | 0.77 |
| 1:A:590:ARG:HH21 | 1:A:620:LYS:HB3 | 1.48 | 0.77 |
| 1:A:899:VAL:HG22 | 1:A:1029:ARG:HG2 | 1.65 | 0.77 |
| 1:A:1115:SER:C | 1:A:1308:THR:HG22 | 2.04 | 0.77 |
| 2:B:464:GLY:O | 2:B:477:ALA:HA | 1.85 | 0.77 |
| 15:P:3:U:H2' | 15:P:4:C:C6 | 2.20 | 0.77 |
| 1:A:1160:SER:HA | 1:A:1170:ILE:HD13 | 1.65 | 0.76 |
| 1:A:1308:THR:HG23 | 1:A:1310:GLY:H | 1.50 | 0.76 |
| 2:B:506:GLY:HA2 | 2:B:512:ARG:NH2 | 1.99 | 0.76 |
| 2:B:906:SER:O | 2:B:941:LEU:HD23 | 1.83 | 0.76 |
| 7:G:119:LEU:HD12 | 7:G:131:GLN:O | 1.85 | 0.76 |
| 11:K:31:VAL:HG12 | 11:K:32:VAL:N | 2.00 | 0.76 |
| 1:A:343:LYS:NZ | 2:B:1151:LEU:HD12 | 2.00 | 0.76 |
| 2:B:800:GLN:HB3 | 10:J:52:THR:HG22 | 1.67 | 0.76 |
| 2:B:1069:PHE:H | 2:B:1069:PHE:HD1 | 1.31 | 0.76 |
| 3:C:235:VAL:HG11 | 10:J:6:ARG:HH21 | 1.49 | 0.76 |
| 11:K:46:ILE:O | 11:K:50:LEU:HB2 | 1.85 | 0.76 |
| 1:A:12:ARG:HD2 | 2:B:1218:THR:HB | 1.67 | 0.76 |
| 1:A:837:ILE:HA | 1:A:840:ARG:HD3 | 1.67 | 0.76 |
| 2:B:745:PRO:O | 2:B:748:ILE:HG12 | 1.84 | 0.76 |
| 4:D:8:PHE:HD2 | 7:G:6:ASP:HB2 | 1.50 | 0.76 |
| 13:T:16:DT:C2' | 13:T:17:DT:H5' | 2.14 | 0.76 |
| 1:A:577:ILE:O | 1:A:580:VAL:HG23 | 1.85 | 0.76 |
| 1:A:869:GLY:O | 5:E:204:THR:HG21 | 1.86 | 0.76 |
| 2:B:326:ASP:OD2 | 2:B:328:GLU:HB3 | 1.85 | 0.76 |
| 2:B:803:LEU:HD12 | 2:B:1032:SER:HB3 | 1.67 | 0.76 |
| 1:A:115:LEU:HG | 1:A:142:CYS:HB3 | 1.68 | 0.76 |
| 1:A:381:THR:C | 1:A:383:TYR:H | 1.88 | 0.76 |
| 1:A:754:SER:N | 1:A:757:ASN:HD22 | 1.83 | 0.76 |
| 2:B:314:LEU:O | 2:B:318:VAL:HG23 | 1.84 | 0.76 |
| 2:B:755:ILE:HG23 | 2:B:809:MET:HE3 | 1.65 | 0.76 |
| 1:A:852:TYR:CD2 | 1:A:1060:PRO:HB2 | 2.21 | 0.76 |
| 1:A:392:VAL:HG13 | 1:A:415:LEU:HD11 | 1.68 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:670:ILE:HG23 | 1:A:805:LEU:HD21 | 1.67 | 0.76 |
| 1:A:866:PHE:C | 1:A:867:ILE:HD12 | 2.06 | 0.76 |
| 2:B:821:GLN:HE22 | 2:B:851:PHE:H | 1.33 | 0.76 |
| 2:B:1224:PHE:CE1 | 5:E:171:LYS:HG3 | 2.21 | 0.76 |
| 3:C:92:CYS:SG | 3:C:94:LYS:HB2 | 2.26 | 0.76 |
| 8:H:42:ILE:HG23 | 8:H:95:TYR:HE1 | 1.50 | 0.76 |
| 1:A:1101:LEU:O | 1:A:1101:LEU:HD12 | 1.85 | 0.76 |
| 1:A:1315:GLU:C | 1:A:1317:MET:H | 1.88 | 0.75 |
| 2:B:758:PHE:CE1 | 2:B:1027:ILE:HG22 | 2.21 | 0.75 |
| 10:J:57:ILE:HA | 10:J:60:PHE:HD2 | 1.51 | 0.75 |
| 1:A:34:LYS:NZ | 1:A:57:ARG:HH21 | 1.84 | 0.75 |
| 1:A:504:LEU:HD11 | 6:F:91:ALA:CB | 2.15 | 0.75 |
| 1:A:836:TYR:CE2 | 1:A:840:ARG:HD2 | 2.22 | 0.75 |
| 2:B:757:PRO:HG3 | 2:B:1028:GLU:OE2 | 1.87 | 0.75 |
| 2:B:834:ASN:HA | 2:B:838:SER:O | 1.86 | 0.75 |
| 5:E:113:GLN:HA | 5:E:137:GLU:HG3 | 1.68 | 0.75 |
| 1:A:35:ILE:HG22 | 1:A:84:ILE:HD12 | 1.68 | 0.75 |
| 1:A:857:ARG:NH1 | 6:F:139:PRO:HB2 | 2.00 | 0.75 |
| 2:B:654:ARG:H | 2:B:657:HIS:HD2 | 1.32 | 0.75 |
| 7:G:1:MET:SD | 7:G:79:PHE:HD1 | 2.09 | 0.75 |
| 2:B:359:GLU:O | 2:B:362:PRO:HD3 | 1.86 | 0.75 |
| 2:B:516:ASN:HD22 | 2:B:516:ASN:N | 1.83 | 0.75 |
| 2:B:777:ALA:HA | 2:B:1095:LEU:HA | 1.66 | 0.75 |
| 5:E:212:ARG:HH11 | 5:E:212:ARG:HG3 | 1.50 | 0.75 |
| 1:A:34:LYS:NZ | 1:A:57:ARG:NH2 | 2.35 | 0.75 |
| 2:B:806:THR:HG22 | 2:B:808:ALA:N | 1.94 | 0.75 |
| 4:D:47:LEU:O | 4:D:48:ILE:HD13 | 1.87 | 0.75 |
| 7:G:97:HIS:HA | 7:G:112:LYS:HE2 | 1.68 | 0.75 |
| 1:A:43:GLU:HB2 | 1:A:46:THR:HB | 1.67 | 0.75 |
| 1:A:583:PRO:HG2 | 1:A:586:ILE:HG13 | 1.69 | 0.75 |
| 4:D:40:HIS:HB3 | 7:G:73:LYS:HZ2 | 1.52 | 0.75 |
| 2:B:97:VAL:HG22 | 2:B:128:LEU:HG | 1.68 | 0.75 |
| 2:B:336:ARG:HE | 2:B:348:ARG:NH1 | 1.84 | 0.75 |
| 2:B:855:PHE:HD1 | 2:B:856:PHE:N | 1.84 | 0.75 |
| 4:D:144:THR:HG21 | 7:G:46:LEU:HD13 | 1.69 | 0.75 |
| 3:C:89:GLU:O | 3:C:90:ASP:HB3 | 1.86 | 0.75 |
| 8:H:99:GLY:HA3 | 8:H:118:PHE:HA | 1.69 | 0.75 |
| 10:J:23:ASN:C | 10:J:25:LEU:H | 1.90 | 0.75 |
| 13:T:26:DT:H2" | 13:T:27:DC:OP2 | 1.87 | 0.75 |
| 1:A:335:ARG:CD | 2:B:1202:LEU:HD23 | 2.16 | 0.74 |
| 1:A:809:THR:H | 1:A:812:GLU:HB2 | 1.52 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:G:28:THR:O | 7:G:32:GLU:HG3 | 1.88 | 0.74 |
| 1:A:463:ILE:HB | 1:A:464:PRO:HD2 | 1.70 | 0.74 |
| 1:A:1394:THR:HG21 | 1:A:1398:MET:SD | 2.26 | 0.74 |
| 5:E:92:THR:O | 5:E:95:THR:HB | 1.87 | 0.74 |
| 1:A:1255:GLU:OE1 | 1:A:1258:HIS:HB2 | 1.88 | 0.74 |
| 2:B:69:LEU:CG | 2:B:429:PHE:CE1 | 2.69 | 0.74 |
| 3:C:36:VAL:HG21 | 3:C:251:LEU:HB2 | 1.68 | 0.74 |
| 3:C:242:GLN:HA | 3:C:245:VAL:HG23 | 1.68 | 0.74 |
| 5:E:23:VAL:HG13 | 5:E:78:LEU:HD13 | 1.70 | 0.74 |
| 10:J:44:TYR:H | 10:J:44:TYR:HD2 | 1.31 | 0.74 |
| 1:A:298:PHE:CZ | 1:A:314:ALA:HB2 | 2.22 | 0.74 |
| 1:A:940:ARG:HG2 | 1:A:940:ARG:HH11 | 1.51 | 0.74 |
| 2:B:850:LEU:HD12 | 2:B:851:PHE:H | 1.52 | 0.74 |
| 2:B:957:ASN:O | 2:B:959:ASP:N | 2.20 | 0.74 |
| 3:C:93:ASP:OD1 | 3:C:122:SER:HB2 | 1.88 | 0.74 |
| 11:K:7:PHE:HB2 | 11:K:11:LEU:HD23 | 1.69 | 0.74 |
| 1:A:22:PHE:HB2 | 2:B:1211:ASN:OD1 | 1.88 | 0.74 |
| 1:A:1280:GLU:O | 1:A:1309:ASP:HB3 | 1.88 | 0.74 |
| 1:A:132:LYS:HE2 | 1:A:1411:GLU:OE1 | 1.87 | 0.74 |
| 2:B:378:LEU:O | 2:B:382:ILE:HG13 | 1.87 | 0.74 |
| 2:B:1180:PHE:HB3 | 2:B:1191:ILE:CD1 | 2.17 | 0.74 |
| 12:L:28:LYS:HD2 | 12:L:39:SER:OG | 1.87 | 0.74 |
| 15:P:3:U:H2' | 15:P:4:C:H6 | 1.53 | 0.74 |
| 1:A:868:TYR:CE1 | 1:A:1064:VAL:HG11 | 2.23 | 0.74 |
| 1:A:1006:ILE:HD11 | 5:E:163:GLU:HG3 | 1.70 | 0.73 |
| 1:A:464:PRO:HG2 | 1:A:465:TYR:HD1 | 1.52 | 0.73 |
| 1:A:483:ASP:OD2 | 15:P:11:U:H5'' | 1.88 | 0.73 |
| 2:B:526:GLU:HG2 | 2:B:538:ASN:ND2 | 2.03 | 0.73 |
| 1:A:7:SER:CB | 2:B:1175:LEU:HD22 | 2.17 | 0.73 |
| 1:A:105:CYS:O | 1:A:114:LEU:HG | 1.88 | 0.73 |
| 1:A:889:SER:HB3 | 1:A:1297:GLU:HG3 | 1.70 | 0.73 |
| 5:E:180:ARG:HH21 | 5:E:192:ARG:HB2 | 1.52 | 0.73 |
| 1:A:239:LEU:HD12 | 1:A:240:PRO:HD2 | 1.70 | 0.73 |
| 1:A:825:ILE:HD11 | 2:B:512:ARG:CB | 2.13 | 0.73 |
| 1:A:1391:ARG:HD2 | 1:A:1391:ARG:C | 2.08 | 0.73 |
| 2:B:1006:ILE:HG22 | 10:J:45:CYS:HB3 | 1.69 | 0.73 |
| 3:C:50:GLU:HG2 | 12:L:64:LEU:HD22 | 1.71 | 0.73 |
| 11:K:61:TYR:C | 11:K:61:TYR:CD2 | 2.61 | 0.73 |
| 1:A:450:LEU:HD13 | 1:A:1074:GLU:HG2 | 1.69 | 0.73 |
| 2:B:23:ALA:HB1 | 2:B:24:PRO:HD2 | 1.69 | 0.73 |
| 3:C:128:ASN:O | 3:C:129:ILE:HG13 | 1.88 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:H:109:LYS:HD2 | 8:H:111:LEU:HD11 | 1.71 | 0.73 |
| 12:L:60:ARG:HH21 | 12:L:65:VAL:HG21 | 1.52 | 0.73 |
| 1:A:288:ALA:HA | 1:A:291:GLU:OE2 | 1.87 | 0.73 |
| 1:A:14:VAL:N | 1:A:1432:GLN:HE22 | 1.85 | 0.73 |
| 1:A:351:THR:HB | 2:B:1103:ILE:HD12 | 1.69 | 0.73 |
| 1:A:591:PHE:HA | 1:A:595:THR:HG21 | 1.70 | 0.73 |
| 1:A:1219:THR:HG21 | 1:A:1271:ILE:HD11 | 1.71 | 0.73 |
| 3:C:112:ASN:HB3 | 3:C:114:TYR:CE1 | 2.24 | 0.73 |
| 9:I:111:THR:HG22 | 9:I:112:SER:H | 1.54 | 0.73 |
| 1:A:10:PRO:HB3 | 4:D:3:VAL:HA | 1.71 | 0.73 |
| 1:A:49:LYS:HZ1 | 1:A:61:ILE:H | 1.32 | 0.73 |
| 3:C:22:LEU:HD13 | 3:C:230:MET:CE | 2.19 | 0.73 |
| 6:F:79:ARG:NH2 | 6:F:150:GLU:OE1 | 2.22 | 0.73 |
| 1:A:438:ASP:OD2 | 1:A:461:LYS:HD2 | 1.89 | 0.72 |
| 1:A:464:PRO:HG2 | 1:A:465:TYR:CD1 | 2.23 | 0.72 |
| 1:A:506:ALA:HB1 | 1:A:508:PRO:HD2 | 1.71 | 0.72 |
| 1:A:682:THR:CG2 | 1:A:728:LYS:HE3 | 2.19 | 0.72 |
| 8:H:100:THR:HG22 | 8:H:101:ALA:N | 2.03 | 0.72 |
| 1:A:34:LYS:HB3 | 1:A:36:ARG:HH21 | 1.52 | 0.72 |
| 1:A:896:ARG:NH2 | 1:A:1030:ARG:HE | 1.86 | 0.72 |
| 1:A:1116:LEU:N | 1:A:1308:THR:HG22 | 2.03 | 0.72 |
| 2:B:708:GLU:HG3 | 2:B:709:ASP:H | 1.53 | 0.72 |
| 2:B:1097:HIS:N | 2:B:1098:MET:HE2 | 2.02 | 0.72 |
| 11:K:65:HIS:HD2 | 11:K:67:PHE:H | 1.36 | 0.72 |
| 1:A:335:ARG:HA | 1:A:335:ARG:HE | 1.54 | 0.72 |
| 1:A:511:ILE:HA | 1:A:521:MET:HE3 | 1.69 | 0.72 |
| 1:A:535:THR:HG23 | 1:A:575:LYS:HG2 | 1.71 | 0.72 |
| 1:A:1015:VAL:HG12 | 1:A:1019:CYS:SG | 2.29 | 0.72 |
| 2:B:193:LYS:HZ1 | 12:L:32:ALA:HB1 | 1.54 | 0.72 |
| 2:B:364:ILE:O | 2:B:365:THR:HB | 1.89 | 0.72 |
| 10:J:1:MET:N | 10:J:56:LEU:N | 2.36 | 0.72 |
| 1:A:534:LEU:O | 1:A:574:GLY:HA3 | 1.90 | 0.72 |
| 1:A:802:ASN:ND2 | 2:B:728:ARG:HB2 | 2.04 | 0.72 |
| 1:A:1420:ASP:O | 1:A:1421:CYS:HB2 | 1.88 | 0.72 |
| 5:E:190:LEU:HD12 | 5:E:214:CYS:HB2 | 1.72 | 0.72 |
| 1:A:50:ILE:O | 1:A:52:GLY:N | 2.23 | 0.72 |
| 1:A:967:ALA:HA | 1:A:1044:TRP:CZ3 | 2.24 | 0.72 |
| 1:A:1101:LEU:HD11 | 1:A:1105:LEU:HD11 | 1.72 | 0.72 |
| 4:D:119:ARG:HD3 | 4:D:221:TYR:CD2 | 2.25 | 0.72 |
| 5:E:61:GLN:HG3 | 5:E:78:LEU:O | 1.89 | 0.72 |
| 8:H:129:TYR:H | 8:H:130:ARG:NH1 | 1.87 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:399:HIS:CB | 1:A:400:PRO:HD3 | 2.20 | 0.72 |
| 1:A:1193:LEU:HB2 | 1:A:1260:LEU:HD11 | 1.71 | 0.72 |
| 2:B:1150:ARG:HH11 | 2:B:1150:ARG:CG | 2.03 | 0.72 |
| 5:E:23:VAL:O | 5:E:28:TYR:HB2 | 1.89 | 0.72 |
| 1:A:382:PRO:HB3 | 1:A:428:TYR:HE2 | 1.53 | 0.72 |
| 1:A:557:ASP:OD2 | 1:A:559:VAL:HB | 1.88 | 0.72 |
| 1:A:890:ASP:H | 1:A:1296:GLY:HA3 | 1.54 | 0.72 |
| 4:D:24:ALA:C | 4:D:26:THR:H | 1.92 | 0.72 |
| 6:F:79:ARG:HG3 | 6:F:144:GLU:HG2 | 1.72 | 0.72 |
| 1:A:470:LEU:HD23 | 1:A:470:LEU:H | 1.51 | 0.72 |
| 1:A:1152:ILE:HD11 | 9:I:44:TYR:CD2 | 2.25 | 0.72 |
| 3:C:44:LEU:HB2 | 3:C:77:ILE:HD11 | 1.71 | 0.72 |
| 2:B:269:ILE:HD11 | 2:B:386:LEU:HD21 | 1.72 | 0.72 |
| 2:B:810:GLU:HA | 2:B:815:ARG:NH2 | 2.02 | 0.72 |
| 2:B:906:SER:HA | 2:B:946:ASN:HB2 | 1.70 | 0.72 |
| 12:L:30:ILE:O | 12:L:56:LEU:HD23 | 1.90 | 0.72 |
| 1:A:763:ALA:O | 1:A:803:SER:HB3 | 1.90 | 0.71 |
| 2:B:547:VAL:HG12 | 2:B:612:GLU:OE2 | 1.89 | 0.71 |
| 4:D:119:ARG:HG2 | 4:D:120:GLU:N | 2.04 | 0.71 |
| 3:C:236:GLY:O | 3:C:238:ILE:N | 2.23 | 0.71 |
| 6:F:99:LEU:O | 6:F:103:MET:HG2 | 1.90 | 0.71 |
| 9:I:105:SER:O | 9:I:106:CYS:HB3 | 1.89 | 0.71 |
| 1:A:722:LEU:H | 1:A:722:LEU:HD12 | 1.53 | 0.71 |
| 2:B:1106:ARG:NH1 | 2:B:1110:PRO:HG2 | 2.05 | 0.71 |
| 3:C:22:LEU:HD13 | 3:C:230:MET:HE3 | 1.73 | 0.71 |
| 5:E:195:VAL:HG12 | 5:E:196:VAL:H | 1.54 | 0.71 |
| 1:A:356:ASP:HB2 | 1:A:469:ARG:NH1 | 2.05 | 0.71 |
| 1:A:903:ASN:HD22 | 1:A:904:THR:H | 1.39 | 0.71 |
| 2:B:862:GLN:HG2 | 2:B:963:PHE:HD1 | 1.56 | 0.71 |
| 3:C:75:MET:HB3 | 3:C:128:ASN:HB3 | 1.72 | 0.71 |
| 9:I:74:GLU:HA | 9:I:80:SER:O | 1.90 | 0.71 |
| 13:T:9:DC:H2" | 13:T:10:DA:C8 | 2.25 | 0.71 |
| 1:A:1116:LEU:HD13 | 1:A:1329:THR:HB | 1.73 | 0.71 |
| 1:A:1436:ILE:HD13 | 2:B:1139:ILE:HG23 | 1.73 | 0.71 |
| 2:B:582:VAL:HB | 2:B:587:HIS:HD2 | 1.54 | 0.71 |
| 8:H:64:ASN:OD1 | 8:H:90:ALA:N | 2.20 | 0.71 |
| 12:L:61:THR:HG21 | 12:L:63:ARG:NE | 2.05 | 0.71 |
| 1:A:32:VAL:HG23 | 1:A:57:ARG:HB2 | 1.71 | 0.71 |
| 1:A:567:LYS:HD2 | 8:H:95:TYR:CD2 | 2.26 | 0.71 |
| 2:B:60:GLN:O | 2:B:63:ILE:HG22 | 1.90 | 0.71 |
| 2:B:412:LEU:HB3 | 2:B:466:TRP:NE1 | 2.06 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:C:147:LEU:HB2 | 3:C:151:GLN:CB | 2.21 | 0.71 |
| 5:E:44:ALA:O | 5:E:45:LYS:HB2 | 1.90 | 0.71 |
| 8:H:89:LEU:HB3 | 8:H:91:ASP:OD1 | 1.90 | 0.71 |
| 8:H:101:ALA:HB2 | 8:H:116:TYR:CE2 | 2.24 | 0.71 |
| 9:I:76:PRO:HD2 | 9:I:108:HIS:HD2 | 1.54 | 0.71 |
| 1:A:853:ASP:O | 1:A:854:ASN:HB2 | 1.89 | 0.71 |
| 1:A:868:TYR:OH | 1:A:1366:ARG:HD3 | 1.89 | 0.71 |
| 2:B:126:SER:OG | 2:B:172:ILE:HD11 | 1.91 | 0.71 |
| 6:F:79:ARG:HB2 | 6:F:79:ARG:HH11 | 1.55 | 0.71 |
| 9:I:71:SER:OG | 9:I:83:ASN:HB2 | 1.90 | 0.71 |
| 1:A:96:ILE:CG2 | 1:A:97:ALA:N | 2.53 | 0.71 |
| 1:A:184:SER:HB3 | 1:A:199:LEU:HD23 | 1.73 | 0.71 |
| 1:A:524:VAL:HG12 | 1:A:525:GLN:N | 2.04 | 0.71 |
| 1:A:816:HIS:CD2 | 2:B:764:SER:HB2 | 2.26 | 0.71 |
| 1:A:1032:LEU:O | 1:A:1036:ARG:HD3 | 1.91 | 0.71 |
| 5:E:63:ASN:HB3 | 5:E:64:PRO:HD2 | 1.73 | 0.71 |
| 9:I:58:VAL:HG13 | 9:I:62:ILE:CD1 | 2.20 | 0.71 |
| 1:A:225:ASN:ND2 | 1:A:228:PHE:N | 2.31 | 0.71 |
| 1:A:356:ASP:HB2 | 1:A:469:ARG:HH12 | 1.56 | 0.71 |
| 1:A:438:ASP:O | 1:A:439:ASN:HB2 | 1.90 | 0.71 |
| 1:A:963:ILE:HD11 | 1:A:1048:ASN:CB | 2.21 | 0.71 |
| 6:F:109:VAL:HG12 | 6:F:110:ASP:N | 2.06 | 0.71 |
| 8:H:95:TYR:CE2 | 8:H:97:MET:HG3 | 2.26 | 0.71 |
| 12:L:61:THR:CG2 | 12:L:63:ARG:HE | 2.03 | 0.71 |
| 14:N:3:DT:H1' | 14:N:4:DA:C8 | 2.25 | 0.71 |
| 1:A:34:LYS:HZ1 | 1:A:57:ARG:HH21 | 1.34 | 0.71 |
| 2:B:701:ILE:HD11 | 2:B:703:ILE:HD11 | 1.71 | 0.71 |
| 2:B:713:ALA:HB1 | 2:B:714:GLU:OE1 | 1.91 | 0.71 |
| 3:C:73:GLN:NE2 | 3:C:74:SER:H | 1.87 | 0.71 |
| 1:A:117:GLU:H | 1:A:117:GLU:CD | 1.93 | 0.70 |
| 1:A:722:LEU:HD23 | 1:A:799:PHE:CD1 | 2.26 | 0.70 |
| 1:A:960:ILE:O | 1:A:963:ILE:HG22 | 1.91 | 0.70 |
| 1:A:1006:ILE:CD1 | 5:E:163:GLU:HG3 | 2.21 | 0.70 |
| 1:A:1107:VAL:HG12 | 1:A:1107:VAL:O | 1.91 | 0.70 |
| 2:B:291:ILE:HD13 | 2:B:300:HIS:NE2 | 2.05 | 0.70 |
| 2:B:583:ASN:ND2 | 2:B:628:THR:HG22 | 2.05 | 0.70 |
| 7:G:23:LYS:HG3 | 7:G:56:ILE:HD11 | 1.73 | 0.70 |
| 1:A:41:MET:HB2 | 1:A:49:LYS:CA | 2.17 | 0.70 |
| 1:A:381:THR:O | 1:A:383:TYR:N | 2.24 | 0.70 |
| 1:A:515:GLN:HA | 1:A:1367:HIS:HE2 | 1.57 | 0.70 |
| 1:A:616:VAL:HG12 | 1:A:617:VAL:N | 2.05 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:903:ASN:ND2 | 1:A:904:THR:N | 2.37 | 0.70 |
| 2:B:294:ASP:C | 2:B:296:GLU:H | 1.95 | 0.70 |
| 2:B:977:GLY:HA3 | 2:B:1099:VAL:HB | 1.73 | 0.70 |
| 4:D:9:GLN:NE2 | 4:D:31:GLN:HE21 | 1.89 | 0.70 |
| 8:H:64:ASN:HD22 | 8:H:88:SER:HB2 | 1.55 | 0.70 |
| 9:I:13:MET:CE | 9:I:14:LEU:H | 2.04 | 0.70 |
| 1:A:49:LYS:HZ1 | 1:A:61:ILE:CG1 | 2.04 | 0.70 |
| 1:A:144:THR:O | 1:A:146:MET:HG3 | 1.90 | 0.70 |
| 1:A:535:THR:CG2 | 1:A:616:VAL:HA | 2.20 | 0.70 |
| 1:A:567:LYS:CB | 1:A:568:PRO:HD3 | 2.21 | 0.70 |
| 1:A:1027:ALA:O | 1:A:1031:VAL:HG23 | 1.91 | 0.70 |
| 11:K:63:VAL:HG23 | 11:K:63:VAL:O | 1.92 | 0.70 |
| 1:A:466:SER:HB2 | 2:B:1099:VAL:CG2 | 2.21 | 0.70 |
| 1:A:834:THR:HG21 | 1:A:1077:THR:HG23 | 1.72 | 0.70 |
| 4:D:119:ARG:HD3 | 4:D:221:TYR:CE2 | 2.26 | 0.70 |
| 1:A:896:ARG:NH2 | 1:A:1030:ARG:HH21 | 1.89 | 0.70 |
| 2:B:112:LEU:HD12 | 2:B:113:TYR:H | 1.57 | 0.70 |
| 2:B:613:VAL:HG22 | 2:B:628:THR:HA | 1.73 | 0.70 |
| 5:E:22:MET:HE3 | 5:E:26:ARG:NH1 | 2.04 | 0.70 |
| 6:F:132:LEU:HD21 | 7:G:61:ILE:HD11 | 1.72 | 0.70 |
| 8:H:129:TYR:N | 8:H:130:ARG:HH11 | 1.89 | 0.70 |
| 1:A:37:PHE:N | 1:A:37:PHE:HD1 | 1.89 | 0.70 |
| 1:A:382:PRO:HD3 | 1:A:428:TYR:CD2 | 2.19 | 0.70 |
| 1:A:885:THR:HG22 | 1:A:885:THR:O | 1.91 | 0.70 |
| 2:B:229:ALA:HB1 | 2:B:231:PRO:HD2 | 1.72 | 0.70 |
| 2:B:603:LEU:HD13 | 2:B:608:ASP:HB3 | 1.74 | 0.70 |
| 9:I:35:VAL:HG12 | 9:I:36:GLU:H | 1.56 | 0.70 |
| 9:I:85:PHE:HD2 | 9:I:85:PHE:N | 1.87 | 0.70 |
| 10:J:24:LEU:HD12 | 10:J:39:LEU:HD11 | 1.73 | 0.70 |
| 12:L:38:LEU:O | 12:L:39:SER:HB3 | 1.92 | 0.70 |
| 1:A:332:LYS:H | 1:A:337:ARG:CB | 2.05 | 0.70 |
| 1:A:1057:VAL:HG12 | 1:A:1058:VAL:N | 2.06 | 0.70 |
| 1:A:1066:VAL:O | 1:A:1070:GLN:HG3 | 1.91 | 0.70 |
| 2:B:69:LEU:CD2 | 2:B:429:PHE:CE1 | 2.74 | 0.70 |
| 2:B:244:LEU:HD21 | 2:B:366:GLN:HE21 | 1.56 | 0.70 |
| 3:C:5:GLY:O | 3:C:7:GLN:HG3 | 1.92 | 0.70 |
| 3:C:107:SER:O | 3:C:109:SER:N | 2.23 | 0.70 |
| 9:I:111:THR:HG22 | 9:I:112:SER:N | 2.06 | 0.70 |
| 2:B:918:ILE:HD12 | 2:B:935:ARG:CZ | 2.22 | 0.70 |
| 1:A:230:ARG:H | 1:A:233:TRP:HE3 | 1.38 | 0.70 |
| 1:A:252:PHE:O | 1:A:256:GLN:HB2 | 1.92 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:340:LEU:HD13 | 1:A:1429:ILE:HG23 | 1.74 | 0.70 |
| 1:A:774:ARG:NH1 | 1:A:797:LYS:HG3 | 2.07 | 0.70 |
| 1:A:1036:ARG:HG2 | 1:A:1036:ARG:HH11 | 1.56 | 0.70 |
| 1:A:1149:ALA:HB2 | 9:I:47:GLU:HA | 1.74 | 0.70 |
| 1:A:1420:ASP:HB3 | 1:A:1422:ARG:HG3 | 1.72 | 0.70 |
| 3:C:73:GLN:HE21 | 3:C:75:MET:N | 1.89 | 0.70 |
| 3:C:259:LEU:HD21 | 11:K:91:CYS:HB3 | 1.73 | 0.70 |
| 7:G:122:ASN:ND2 | 7:G:125:SER:HB3 | 2.07 | 0.70 |
| 8:H:118:PHE:O | 8:H:120:GLY:N | 2.25 | 0.70 |
| 8:H:125:LEU:HG | 8:H:126:GLU:H | 1.55 | 0.70 |
| 1:A:317:LYS:O | 1:A:318:SER:HB3 | 1.92 | 0.69 |
| 1:A:596:THR:C | 1:A:598:LEU:H | 1.95 | 0.69 |
| 2:B:172:ILE:HD13 | 2:B:178:ASN:HD22 | 1.56 | 0.69 |
| 1:A:35:ILE:HG22 | 1:A:35:ILE:O | 1.92 | 0.69 |
| 1:A:96:ILE:HG22 | 1:A:97:ALA:H | 1.57 | 0.69 |
| 1:A:332:LYS:H | 1:A:337:ARG:HB2 | 1.57 | 0.69 |
| 1:A:567:LYS:HB2 | 8:H:96:VAL:H | 1.56 | 0.69 |
| 1:A:885:THR:O | 1:A:940:ARG:HD2 | 1.91 | 0.69 |
| 1:A:1116:LEU:HB3 | 1:A:1308:THR:HG21 | 1.73 | 0.69 |
| 2:B:1095:LEU:H | 2:B:1095:LEU:CD1 | 2.03 | 0.69 |
| 5:E:153:HIS:HB3 | 5:E:196:VAL:CG1 | 2.22 | 0.69 |
| 6:F:147:SER:OG | 6:F:150:GLU:HG3 | 1.91 | 0.69 |
| 12:L:53:HIS:HB3 | 12:L:55:ILE:CD1 | 2.22 | 0.69 |
| 1:A:12:ARG:HB2 | 2:B:1218:THR:CG2 | 2.20 | 0.69 |
| 1:A:202:LEU:HA | 1:A:206:GLU:OE1 | 1.92 | 0.69 |
| 1:A:883:LEU:HD11 | 1:A:1017:LEU:HD11 | 1.75 | 0.69 |
| 2:B:405:ARG:NE | 2:B:632:ARG:HG2 | 2.07 | 0.69 |
| 2:B:637:LEU:HD21 | 2:B:742:GLU:OE2 | 1.92 | 0.69 |
| 2:B:1007:VAL:CG2 | 2:B:1008:PRO:HD2 | 2.22 | 0.69 |
| 5:E:117:THR:HG22 | 5:E:119:SER:N | 2.07 | 0.69 |
| 8:H:15:VAL:HG13 | 8:H:26:ILE:HG12 | 1.72 | 0.69 |
| 8:H:38:LEU:HD12 | 8:H:124:ARG:O | 1.92 | 0.69 |
| 8:H:104:PHE:CZ | 8:H:136:LYS:HA | 2.27 | 0.69 |
| 2:B:189:LEU:HD13 | 2:B:196:PRO:HA | 1.74 | 0.69 |
| 2:B:1215:ARG:O | 2:B:1216:LEU:HD23 | 1.91 | 0.69 |
| 8:H:106:GLU:HG2 | 8:H:112:ILE:HG12 | 1.71 | 0.69 |
| 1:A:829:VAL:C | 1:A:831:THR:H | 1.93 | 0.69 |
| 1:A:1081:LEU:HD11 | 1:A:1097:GLY:HA3 | 1.73 | 0.69 |
| 2:B:175:ARG:HG2 | 2:B:175:ARG:HH11 | 1.56 | 0.69 |
| 2:B:654:ARG:H | 2:B:657:HIS:CD2 | 2.10 | 0.69 |
| 2:B:746:SER:HB2 | 2:B:1046:PRO:HG2 | 1.74 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1164:PRO:HG2 | 1:A:1165:GLU:H | 1.55 | 0.69 |
| 2:B:911:ILE:HD11 | 2:B:941:LEU:CD1 | 2.23 | 0.69 |
| 2:B:999:MET:HB3 | 2:B:1007:VAL:HG21 | 1.73 | 0.69 |
| 4:D:155:ARG:HD3 | 4:D:221:TYR:CZ | 2.27 | 0.69 |
| 5:E:173:SER:O | 5:E:175:LEU:N | 2.24 | 0.69 |
| 1:A:913:LEU:CD1 | 1:A:914:GLU:H | 2.06 | 0.69 |
| 12:L:53:HIS:O | 12:L:55:ILE:HD13 | 1.91 | 0.69 |
| 1:A:49:LYS:NZ | 1:A:61:ILE:N | 2.41 | 0.69 |
| 1:A:608:ILE:HB | 1:A:613:ILE:HD11 | 1.73 | 0.69 |
| 2:B:497:ARG:HH22 | 2:B:775:LYS:CE | 2.04 | 0.69 |
| 3:C:212:PRO:HB3 | 3:C:213:PRO:HD2 | 1.74 | 0.69 |
| 7:G:30:LEU:HD13 | 7:G:72:VAL:HG11 | 1.73 | 0.69 |
| 12:L:26:THR:HG23 | 12:L:62:LYS:NZ | 2.07 | 0.69 |
| 2:B:430:ARG:O | 2:B:434:ARG:HD2 | 1.93 | 0.69 |
| 10:J:48:ARG:HE | 10:J:49:MET:HE2 | 1.57 | 0.69 |
| 1:A:552:TRP:HE3 | 1:A:651:LYS:HB3 | 1.57 | 0.69 |
| 1:A:567:LYS:CG | 1:A:568:PRO:HD3 | 2.22 | 0.69 |
| 1:A:852:TYR:CD1 | 6:F:136:ARG:HB3 | 2.28 | 0.69 |
| 2:B:213:ILE:HD11 | 2:B:497:ARG:HB3 | 1.74 | 0.69 |
| 2:B:1000:PRO:O | 2:B:1007:VAL:HG23 | 1.92 | 0.69 |
| 2:B:1142:GLY:HA3 | 6:F:88:TYR:HE2 | 1.58 | 0.69 |
| 3:C:137:LYS:HB2 | 3:C:138:GLU:OE1 | 1.92 | 0.69 |
| 7:G:127:PRO:HG3 | 7:G:139:ILE:CD1 | 2.23 | 0.69 |
| 7:G:139:ILE:HG22 | 7:G:140:LYS:HD3 | 1.75 | 0.69 |
| 1:A:709:THR:HB | 1:A:712:GLU:H | 1.58 | 0.68 |
| 1:A:870:GLU:O | 5:E:205:SER:HB3 | 1.93 | 0.68 |
| 6:F:75:PRO:HG2 | 6:F:77:ASP:O | 1.93 | 0.68 |
| 6:F:106:PRO:HG2 | 7:G:18:PHE:O | 1.93 | 0.68 |
| 1:A:90:VAL:HG13 | 1:A:297:GLN:CD | 2.13 | 0.68 |
| 1:A:630:ILE:HD11 | 1:A:646:PHE:HZ | 1.55 | 0.68 |
| 2:B:483:LEU:HD11 | 2:B:491:THR:HG23 | 1.75 | 0.68 |
| 2:B:1159:ARG:HB3 | 2:B:1159:ARG:NH1 | 2.08 | 0.68 |
| 3:C:235:VAL:HG11 | 10:J:6:ARG:NH2 | 2.07 | 0.68 |
| 4:D:134:THR:HG22 | 4:D:136:GLY:H | 1.58 | 0.68 |
| 1:A:504:LEU:HD11 | 6:F:91:ALA:HB1 | 1.75 | 0.68 |
| 2:B:100:PRO:HA | 2:B:125:SER:O | 1.93 | 0.68 |
| 2:B:273:LEU:HD12 | 2:B:276:ILE:HD12 | 1.75 | 0.68 |
| 2:B:751:VAL:HG13 | 2:B:812:LEU:HD22 | 1.75 | 0.68 |
| 3:C:100:THR:HG22 | 3:C:101:LEU:H | 1.57 | 0.68 |
| 1:A:475:THR:HG23 | 1:A:476:SER:N | 2.08 | 0.68 |
| 1:A:866:PHE:HE1 | 5:E:211:TYR:H | 1.41 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:273:LEU:CB | 2:B:276:ILE:HD12 | 2.21 | 0.68 |
| 2:B:364:ILE:HG12 | 2:B:585:VAL:HG13 | 1.76 | 0.68 |
| 2:B:879:ARG:NH1 | 2:B:883:LEU:HD22 | 2.07 | 0.68 |
| 2:B:955:THR:CG2 | 2:B:956:THR:N | 2.56 | 0.68 |
| 3:C:184:ASN:ND2 | 3:C:187:LYS:HA | 2.08 | 0.68 |
| 1:A:382:PRO:HB3 | 1:A:428:TYR:CE2 | 2.27 | 0.68 |
| 1:A:1100:ARG:HH21 | 1:A:1351:GLU:HG2 | 1.58 | 0.68 |
| 2:B:852:ARG:HH22 | 12:L:70:ARG:C | 1.97 | 0.68 |
| 4:D:170:THR:C | 4:D:172:LEU:H | 1.97 | 0.68 |
| 14:N:2:DG:H4' | 14:N:3:DT:OP1 | 1.94 | 0.68 |
| 1:A:2:VAL:HG11 | 2:B:1157:ALA:HB1 | 1.74 | 0.68 |
| 1:A:883:LEU:HD23 | 1:A:1021:LEU:HD13 | 1.76 | 0.68 |
| 2:B:497:ARG:HH22 | 2:B:775:LYS:HE2 | 1.58 | 0.68 |
| 2:B:863:GLU:OE2 | 2:B:873:THR:HA | 1.94 | 0.68 |
| 8:H:84:ALA:HB2 | 8:H:87:ARG:HD2 | 1.75 | 0.68 |
| 1:A:857:ARG:HD3 | 1:A:861:GLY:O | 1.94 | 0.68 |
| 2:B:638:PHE:HA | 2:B:690:VAL:HG22 | 1.74 | 0.68 |
| 5:E:111:VAL:HG12 | 5:E:137:GLU:HG2 | 1.76 | 0.68 |
| 1:A:285:PRO:HG2 | 1:A:288:ALA:HB3 | 1.75 | 0.68 |
| 1:A:427:GLN:HB2 | 1:A:430:TRP:CD1 | 2.28 | 0.68 |
| 1:A:658:LEU:HD23 | 1:A:659:HIS:CE1 | 2.29 | 0.68 |
| 1:A:852:TYR:CE2 | 1:A:1060:PRO:HB2 | 2.27 | 0.68 |
| 1:A:1339:LEU:HD13 | 5:E:147:HIS:CD2 | 2.29 | 0.68 |
| 2:B:423:LYS:HA | 2:B:426:LYS:HE2 | 1.76 | 0.68 |
| 2:B:1007:VAL:HG22 | 2:B:1008:PRO:HD2 | 1.76 | 0.68 |
| 3:C:66:ARG:NH2 | 10:J:3:VAL:O | 2.25 | 0.68 |
| 6:F:109:VAL:HG11 | 6:F:123:LYS:CD | 2.15 | 0.68 |
| 11:K:87:LEU:O | 11:K:91:CYS:HB2 | 1.94 | 0.68 |
| 1:A:528:LEU:O | 1:A:531:ILE:HG22 | 1.93 | 0.68 |
| 2:B:60:GLN:NE2 | 2:B:95:ILE:HG22 | 2.08 | 0.68 |
| 2:B:167:ILE:HD12 | 2:B:167:ILE:N | 2.09 | 0.68 |
| 2:B:520:GLY:N | 2:B:748:ILE:HG22 | 2.09 | 0.68 |
| 8:H:111:LEU:HA | 8:H:127:GLY:O | 1.93 | 0.68 |
| 1:A:11:LEU:HD12 | 1:A:11:LEU:O | 1.94 | 0.68 |
| 2:B:114:PRO:HG3 | 2:B:181:LEU:HD11 | 1.76 | 0.68 |
| 2:B:582:VAL:HA | 2:B:626:ILE:HB | 1.74 | 0.68 |
| 7:G:102:GLN:HG3 | 7:G:106:MET:O | 1.94 | 0.68 |
| 1:A:910:PRO:HB3 | 1:A:916:GLY:HA3 | 1.75 | 0.67 |
| 1:A:1308:THR:HG21 | 1:A:1310:GLY:O | 1.94 | 0.67 |
| 3:C:80:LEU:HD11 | 3:C:95:CYS:C | 2.14 | 0.67 |
| 1:A:84:ILE:O | 1:A:84:ILE:HG23 | 1.93 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:402:ALA:CB | 1:A:434:ARG:HA | 2.25 | 0.67 |
| 1:A:447:GLN:NE2 | 13:T:20:DG:H4' | 2.09 | 0.67 |
| 1:A:825:ILE:CG2 | 1:A:826:ASP:N | 2.58 | 0.67 |
| 1:A:903:ASN:HD22 | 1:A:903:ASN:C | 1.97 | 0.67 |
| 1:A:981:LEU:CD2 | 1:A:1039:LYS:HA | 2.23 | 0.67 |
| 1:A:1127:ASP:CG | 1:A:1130:GLN:HB2 | 2.15 | 0.67 |
| 1:A:1262:LYS:C | 1:A:1264:GLU:H | 1.97 | 0.67 |
| 2:B:519:TRP:HE1 | 2:B:635:ARG:NH2 | 1.92 | 0.67 |
| 2:B:855:PHE:HD1 | 2:B:855:PHE:C | 1.97 | 0.67 |
| 3:C:146:LYS:HB2 | 10:J:61:LEU:HD11 | 1.77 | 0.67 |
| 3:C:193:TYR:HD2 | 3:C:197:SER:HB3 | 1.60 | 0.67 |
| 12:L:40:LEU:HD22 | 12:L:44:ASP:CG | 2.15 | 0.67 |
| 1:A:216:VAL:O | 1:A:219:PHE:HB2 | 1.94 | 0.67 |
| 1:A:353:ILE:HD13 | 1:A:487:MET:HE2 | 1.75 | 0.67 |
| 2:B:408:LEU:HD22 | 2:B:545:ILE:HD12 | 1.77 | 0.67 |
| 3:C:123:ASN:HD21 | 3:C:125:MET:HA | 1.60 | 0.67 |
| 8:H:4:THR:HG22 | 8:H:5:LEU:H | 1.59 | 0.67 |
| 8:H:89:LEU:C | 8:H:91:ASP:H | 1.98 | 0.67 |
| 1:A:1224:LEU:HD11 | 1:A:1240:CYS:HB2 | 1.75 | 0.67 |
| 2:B:1181:GLU:O | 2:B:1182:CYS:HB3 | 1.93 | 0.67 |
| 3:C:77:ILE:N | 3:C:129:ILE:HD11 | 2.08 | 0.67 |
| 3:C:99:LEU:HD22 | 3:C:120:ILE:HG12 | 1.75 | 0.67 |
| 5:E:195:VAL:HG12 | 5:E:196:VAL:N | 2.09 | 0.67 |
| 2:B:98:THR:O | 2:B:126:SER:HB2 | 1.95 | 0.67 |
| 2:B:168:GLY:HA2 | 2:B:454:THR:OG1 | 1.94 | 0.67 |
| 3:C:77:ILE:HG22 | 3:C:78:GLU:N | 2.09 | 0.67 |
| 4:D:69:ALA:HA | 4:D:72:ARG:HD2 | 1.77 | 0.67 |
| 5:E:15:ALA:O | 5:E:19:VAL:HG23 | 1.94 | 0.67 |
| 7:G:96:GLN:O | 7:G:112:LYS:HD3 | 1.94 | 0.67 |
| 1:A:446:ARG:HB2 | 1:A:487:MET:SD | 2.33 | 0.67 |
| 2:B:193:LYS:HZ2 | 12:L:32:ALA:HB1 | 1.57 | 0.67 |
| 2:B:288:ALA:HA | 2:B:331:LEU:HD12 | 1.74 | 0.67 |
| 2:B:810:GLU:CB | 2:B:815:ARG:HH22 | 2.06 | 0.67 |
| 2:B:999:MET:HE2 | 2:B:999:MET:HA | 1.77 | 0.67 |
| 3:C:238:ILE:CG2 | 3:C:242:GLN:HB2 | 2.20 | 0.67 |
| 4:D:39:ASN:HD22 | 4:D:41:GLN:HB2 | 1.60 | 0.67 |
| 5:E:154:ILE:H | 5:E:196:VAL:HG13 | 1.58 | 0.67 |
| 9:I:17:ARG:HG3 | 9:I:28:GLU:OE1 | 1.95 | 0.67 |
| 1:A:416:ARG:NH1 | 1:A:417:TYR:HE2 | 1.93 | 0.67 |
| 2:B:25:ILE:HG23 | 2:B:658:ILE:HD11 | 1.76 | 0.67 |
| 2:B:515:HIS:H | 2:B:518:HIS:CD2 | 2.12 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:596:LEU:O | 2:B:600:LEU:HG | 1.94 | 0.67 |
| 2:B:999:MET:HA | 2:B:999:MET:CE | 2.25 | 0.67 |
| 8:H:55:LEU:HB3 | 8:H:144:ILE:HG23 | 1.76 | 0.67 |
| 10:J:36:LEU:HB2 | 10:J:47:ARG:HH12 | 1.60 | 0.67 |
| 1:A:37:PHE:N | 1:A:37:PHE:CD1 | 2.60 | 0.67 |
| 1:A:606:LEU:HG | 1:A:613:ILE:HB | 1.76 | 0.67 |
| 2:B:133:LYS:CE | 2:B:135:ARG:HH21 | 2.01 | 0.67 |
| 3:C:56:THR:HG21 | 3:C:145:CYS:SG | 2.34 | 0.67 |
| 1:A:552:TRP:CE3 | 1:A:651:LYS:HB3 | 2.29 | 0.67 |
| 1:A:855:THR:HG21 | 1:A:857:ARG:NE | 2.08 | 0.67 |
| 1:A:1264:GLU:HG3 | 1:A:1265:ASN:N | 2.10 | 0.67 |
| 2:B:383:ASN:C | 2:B:387:LEU:HD13 | 2.15 | 0.67 |
| 2:B:546:SER:OG | 2:B:631:GLY:N | 2.27 | 0.67 |
| 2:B:616:ILE:HD12 | 2:B:616:ILE:N | 2.10 | 0.67 |
| 2:B:744:HIS:HD2 | 2:B:746:SER:OG | 1.78 | 0.67 |
| 2:B:1084:GLN:HG2 | 3:C:201:TRP:HZ2 | 1.59 | 0.67 |
| 7:G:48:VAL:HA | 7:G:76:ALA:HB2 | 1.75 | 0.67 |
| 1:A:802:ASN:HD21 | 2:B:729:ILE:H | 1.41 | 0.67 |
| 1:A:1148:ILE:HD11 | 1:A:1198:ASP:HA | 1.76 | 0.67 |
| 1:A:1227:ILE:HG22 | 1:A:1228:TRP:N | 2.07 | 0.67 |
| 2:B:29:ASP:CG | 2:B:658:ILE:HD13 | 2.14 | 0.67 |
| 2:B:1201:LYS:HE2 | 2:B:1205:GLN:OE1 | 1.94 | 0.67 |
| 3:C:35:ARG:NH1 | 11:K:41:THR:OG1 | 2.27 | 0.67 |
| 5:E:157:SER:OG | 5:E:160:GLU:HG3 | 1.95 | 0.67 |
| 1:A:451:HIS:O | 2:B:1137:CYS:SG | 2.52 | 0.66 |
| 1:A:1151:GLU:OE2 | 9:I:45:ARG:HD2 | 1.96 | 0.66 |
| 1:A:1313:LEU:HD23 | 1:A:1338:VAL:HG21 | 1.75 | 0.66 |
| 2:B:822:ASN:HD21 | 10:J:52:THR:HG21 | 1.60 | 0.66 |
| 3:C:3:GLU:HG3 | 11:K:104:ASN:OD1 | 1.95 | 0.66 |
| 4:D:8:PHE:CZ | 4:D:37:GLN:HB2 | 2.30 | 0.66 |
| 8:H:15:VAL:HA | 8:H:26:ILE:HG23 | 1.76 | 0.66 |
| 9:I:73:ARG:HH12 | 9:I:112:SER:HB3 | 1.60 | 0.66 |
| 11:K:45:LEU:HG | 11:K:94:ILE:HD13 | 1.77 | 0.66 |
| 11:K:67:PHE:C | 11:K:68:PHE:HD2 | 1.98 | 0.66 |
| 2:B:593:PRO:HA | 2:B:596:LEU:HB3 | 1.76 | 0.66 |
| 2:B:1080:LYS:HD2 | 3:C:188:HIS:HB2 | 1.77 | 0.66 |
| 3:C:238:ILE:CD1 | 3:C:246:ARG:HH11 | 2.08 | 0.66 |
| 4:D:208:GLU:HG3 | 4:D:212:LYS:HE3 | 1.77 | 0.66 |
| 5:E:124:VAL:CG1 | 5:E:132:ILE:HG13 | 2.23 | 0.66 |
| 1:A:868:TYR:HD2 | 1:A:1058:VAL:HG21 | 1.60 | 0.66 |
| 1:A:929:LEU:HD23 | 1:A:983:ILE:CG2 | 2.26 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:F:136:ARG:O | 6:F:143:PHE:HB2 | 1.95 | 0.66 |
| 1:A:345:VAL:HG21 | 2:B:1150:ARG:HH22 | 1.61 | 0.66 |
| 1:A:524:VAL:HG12 | 1:A:525:GLN:H | 1.59 | 0.66 |
| 1:A:698:GLN:HA | 9:I:97:MET:O | 1.96 | 0.66 |
| 1:A:833:GLU:HG2 | 1:A:1102:LYS:HD2 | 1.76 | 0.66 |
| 1:A:1191:TRP:HB3 | 1:A:1260:LEU:HD23 | 1.77 | 0.66 |
| 1:A:1291:VAL:HG13 | 1:A:1292:PRO:HD2 | 1.77 | 0.66 |
| 2:B:273:LEU:O | 2:B:276:ILE:HB | 1.95 | 0.66 |
| 2:B:527:THR:OG1 | 2:B:528:PRO:HD2 | 1.95 | 0.66 |
| 2:B:755:ILE:HG23 | 2:B:809:MET:CE | 2.26 | 0.66 |
| 3:C:36:VAL:HG21 | 3:C:251:LEU:HD13 | 1.77 | 0.66 |
| 3:C:73:GLN:HE21 | 3:C:75:MET:H | 1.43 | 0.66 |
| 4:D:40:HIS:HB2 | 7:G:73:LYS:CE | 2.26 | 0.66 |
| 4:D:53:SER:HB3 | 4:D:152:SER:HB2 | 1.78 | 0.66 |
| 8:H:102:TYR:HD2 | 8:H:102:TYR:N | 1.91 | 0.66 |
| 1:A:1057:VAL:HG12 | 1:A:1058:VAL:H | 1.61 | 0.66 |
| 2:B:230:ALA:N | 2:B:231:PRO:HD2 | 2.11 | 0.66 |
| 2:B:511:PRO:O | 2:B:513:GLN:N | 2.28 | 0.66 |
| 1:A:116:ASP:OD2 | 1:A:164:ARG:HD2 | 1.95 | 0.66 |
| 1:A:1124:HIS:HB2 | 1:A:1130:GLN:HG2 | 1.78 | 0.66 |
| 2:B:487:THR:HG22 | 2:B:488:TYR:N | 2.10 | 0.66 |
| 2:B:859:TYR:CZ | 2:B:941:LEU:HD12 | 2.29 | 0.66 |
| 3:C:115:SER:O | 3:C:118:LEU:HG | 1.96 | 0.66 |
| 8:H:100:THR:HG23 | 8:H:138:GLU:CA | 2.22 | 0.66 |
| 10:J:24:LEU:HA | 10:J:28:ASP:HB2 | 1.77 | 0.66 |
| 1:A:106:VAL:HG12 | 1:A:107:CYS:H | 1.58 | 0.66 |
| 1:A:456:MET:HE2 | 1:A:507:VAL:HA | 1.76 | 0.66 |
| 1:A:903:ASN:ND2 | 1:A:905:ASP:H | 1.93 | 0.66 |
| 2:B:102:VAL:HB | 2:B:110:HIS:HB3 | 1.76 | 0.66 |
| 5:E:23:VAL:HG13 | 5:E:78:LEU:CD1 | 2.25 | 0.66 |
| 6:F:76:LYS:HA | 6:F:79:ARG:CD | 2.25 | 0.66 |
| 9:I:13:MET:HE2 | 9:I:14:LEU:H | 1.59 | 0.66 |
| 10:J:1:MET:H1 | 10:J:57:ILE:H | 1.40 | 0.66 |
| 1:A:14:VAL:H | 1:A:1432:GLN:NE2 | 1.92 | 0.66 |
| 2:B:276:ILE:HA | 2:B:337:ARG:O | 1.95 | 0.66 |
| 2:B:583:ASN:HD21 | 2:B:628:THR:CG2 | 2.08 | 0.66 |
| 2:B:1072:MET:CE | 2:B:1085:ILE:HB | 2.25 | 0.66 |
| 1:A:79:GLY:HA3 | 1:A:243:PRO:CG | 2.26 | 0.66 |
| 1:A:265:LYS:HD3 | 1:A:302:THR:HG23 | 1.76 | 0.66 |
| 1:A:372:LYS:HA | 1:A:435:HIS:HD1 | 1.57 | 0.66 |
| 1:A:567:LYS:CD | 1:A:568:PRO:HD3 | 2.25 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:596:THR:O | 1:A:598:LEU:N | 2.28 | 0.66 |
| 1:A:899:VAL:CG1 | 1:A:908:LEU:HD21 | 2.25 | 0.66 |
| 1:A:979:SER:OG | 1:A:980:ASP:N | 2.28 | 0.66 |
| 1:A:1312:ASN:O | 1:A:1316:VAL:HG23 | 1.95 | 0.66 |
| 2:B:648:HIS:CG | 2:B:649:LYS:H | 2.13 | 0.66 |
| 2:B:827:ILE:O | 2:B:828:ALA:HB2 | 1.95 | 0.66 |
| 2:B:853:SER:O | 2:B:854:LEU:HD23 | 1.96 | 0.66 |
| 2:B:860:MET:HG3 | 2:B:965:LYS:HG2 | 1.78 | 0.66 |
| 2:B:996:ARG:NH1 | 3:C:38:ILE:HG23 | 2.11 | 0.66 |
| 3:C:166:GLU:HG3 | 11:K:10:PHE:HZ | 1.60 | 0.66 |
| 3:C:181:ASP:CG | 3:C:186:LEU:HD13 | 2.15 | 0.66 |
| 5:E:144:ILE:HG13 | 5:E:145:THR:N | 2.10 | 0.66 |
| 7:G:27:LYS:HE2 | 7:G:54:ILE:HB | 1.78 | 0.66 |
| 7:G:49:LEU:HG | 7:G:76:ALA:HA | 1.78 | 0.66 |
| 13:T:21:DC:H2'' | 13:T:22:DC:H5' | 1.76 | 0.66 |
| 1:A:41:MET:CB | 1:A:49:LYS:HA | 2.18 | 0.66 |
| 1:A:129:LYS:O | 1:A:130:ASP:HB2 | 1.95 | 0.66 |
| 1:A:442:VAL:O | 1:A:457:ALA:HA | 1.96 | 0.66 |
| 2:B:220:GLY:O | 2:B:222:ILE:HG13 | 1.96 | 0.66 |
| 2:B:613:VAL:HG13 | 2:B:628:THR:HA | 1.78 | 0.66 |
| 2:B:975:GLN:O | 2:B:990:ILE:HD12 | 1.95 | 0.66 |
| 2:B:1108:ARG:HG2 | 2:B:1109:GLY:N | 2.11 | 0.66 |
| 2:B:1202:LEU:O | 2:B:1206:GLU:HG3 | 1.96 | 0.66 |
| 3:C:238:ILE:HG22 | 3:C:243:VAL:HG23 | 1.77 | 0.66 |
| 4:D:148:LEU:O | 4:D:152:SER:HB3 | 1.95 | 0.66 |
| 6:F:111:LEU:H | 6:F:111:LEU:CD1 | 2.07 | 0.66 |
| 8:H:135:LEU:HD22 | 8:H:137:GLN:HE21 | 1.61 | 0.66 |
| 10:J:48:ARG:HD2 | 10:J:49:MET:N | 2.10 | 0.66 |
| 1:A:96:ILE:HG22 | 1:A:97:ALA:N | 2.11 | 0.65 |
| 3:C:239:PRO:HB2 | 3:C:241:ASP:OD1 | 1.96 | 0.65 |
| 9:I:31:THR:O | 9:I:32:CYS:HB3 | 1.96 | 0.65 |
| 10:J:9:SER:CB | 10:J:45:CYS:HB2 | 2.25 | 0.65 |
| 1:A:38:PRO:HA | 1:A:270:LEU:HD23 | 1.76 | 0.65 |
| 1:A:57:ARG:HG2 | 1:A:57:ARG:HH11 | 1.60 | 0.65 |
| 1:A:310:GLY:O | 1:A:312:PRO:HD2 | 1.95 | 0.65 |
| 1:A:547:LEU:HD22 | 11:K:58:PHE:CE1 | 2.32 | 0.65 |
| 1:A:1198:ASP:HB3 | 1:A:1201:ALA:HB3 | 1.77 | 0.65 |
| 1:A:1438:THR:HB | 2:B:1144:ALA:CB | 2.25 | 0.65 |
| 2:B:345:LYS:O | 2:B:348:ARG:HG2 | 1.96 | 0.65 |
| 2:B:515:HIS:CD2 | 2:B:516:ASN:N | 2.64 | 0.65 |
| 3:C:83:SER:HA | 3:C:95:CYS:HB2 | 1.78 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:130:LEU:O | 4:D:132:GLN:N | 2.28 | 0.65 |
| 11:K:7:PHE:C | 11:K:9:LEU:H | 2.00 | 0.65 |
| 1:A:7:SER:HB3 | 2:B:1175:LEU:HD22 | 1.78 | 0.65 |
| 1:A:253:ASN:HD22 | 1:A:256:GLN:NE2 | 1.94 | 0.65 |
| 1:A:1028:THR:O | 1:A:1032:LEU:HD12 | 1.96 | 0.65 |
| 1:A:1237:ILE:HG22 | 1:A:1238:ILE:N | 2.11 | 0.65 |
| 2:B:314:LEU:O | 2:B:317:CYS:HB3 | 1.97 | 0.65 |
| 2:B:464:GLY:C | 2:B:465:ASN:HD22 | 1.99 | 0.65 |
| 3:C:18:VAL:HG23 | 3:C:240:VAL:CG1 | 2.26 | 0.65 |
| 3:C:161:LYS:HG3 | 3:C:162:GLY:N | 2.12 | 0.65 |
| 5:E:96:PHE:O | 5:E:99:HIS:HB3 | 1.96 | 0.65 |
| 11:K:50:LEU:HD11 | 11:K:75:ILE:HD13 | 1.77 | 0.65 |
| 1:A:836:TYR:CD2 | 1:A:840:ARG:HD2 | 2.31 | 0.65 |
| 1:A:1225:PHE:CZ | 1:A:1227:ILE:HD11 | 2.32 | 0.65 |
| 2:B:102:VAL:O | 2:B:102:VAL:HG12 | 1.96 | 0.65 |
| 2:B:282:ILE:HD11 | 2:B:317:CYS:SG | 2.36 | 0.65 |
| 2:B:605:ARG:NH1 | 2:B:639:ILE:HG21 | 2.10 | 0.65 |
| 1:A:55:ASP:C | 1:A:57:ARG:H | 2.00 | 0.65 |
| 1:A:1392:SER:O | 1:A:1394:THR:N | 2.29 | 0.65 |
| 1:A:1447:GLU:OE2 | 7:G:23:LYS:HB2 | 1.97 | 0.65 |
| 2:B:773:MET:SD | 2:B:987:LYS:HG2 | 2.37 | 0.65 |
| 2:B:978:ASP:OD2 | 2:B:1098:MET:HG2 | 1.96 | 0.65 |
| 5:E:28:TYR:C | 5:E:65:THR:HG22 | 2.17 | 0.65 |
| 7:G:1:MET:HG2 | 7:G:85:GLU:OE2 | 1.96 | 0.65 |
| 11:K:53:ASP:HB3 | 11:K:56:VAL:CG2 | 2.27 | 0.65 |
| 12:L:55:ILE:HG12 | 12:L:56:LEU:N | 2.11 | 0.65 |
| 1:A:7:SER:HB2 | 2:B:1175:LEU:HD22 | 1.77 | 0.65 |
| 1:A:276:LEU:HD13 | 1:A:293:GLU:HA | 1.79 | 0.65 |
| 1:A:858:ASN:C | 1:A:858:ASN:HD22 | 1.98 | 0.65 |
| 2:B:806:THR:HG23 | 2:B:1046:PRO:HD3 | 1.78 | 0.65 |
| 2:B:955:THR:HG22 | 2:B:956:THR:O | 1.96 | 0.65 |
| 5:E:198:ILE:H | 5:E:198:ILE:HD12 | 1.60 | 0.65 |
| 8:H:64:ASN:CB | 8:H:88:SER:HB2 | 2.21 | 0.65 |
| 1:A:466:SER:HB2 | 2:B:1099:VAL:HG21 | 1.79 | 0.65 |
| 1:A:565:ILE:HG22 | 1:A:565:ILE:O | 1.97 | 0.65 |
| 1:A:630:ILE:HG23 | 1:A:631:HIS:N | 2.11 | 0.65 |
| 1:A:848:ILE:HA | 1:A:857:ARG:O | 1.95 | 0.65 |
| 2:B:508:LEU:O | 2:B:509:ALA:HB2 | 1.97 | 0.65 |
| 5:E:7:ARG:HD2 | 5:E:7:ARG:C | 2.17 | 0.65 |
| 5:E:124:VAL:N | 5:E:125:PRO:HD2 | 2.12 | 0.65 |
| 8:H:40:LEU:HD13 | 8:H:123:MET:HB2 | 1.77 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:I:8:ARG:HG3 | 9:I:34:TYR:CE1 | 2.32 | 0.65 |
| 11:K:18:LYS:NZ | 11:K:38:GLU:HG2 | 2.11 | 0.65 |
| 1:A:91:PHE:HB3 | 1:A:96:ILE:HD12 | 1.79 | 0.65 |
| 1:A:739:ASP:OD2 | 8:H:19:ARG:HD2 | 1.97 | 0.65 |
| 1:A:855:THR:CG2 | 1:A:857:ARG:HE | 2.10 | 0.65 |
| 2:B:589:VAL:HG12 | 2:B:590:HIS:N | 2.12 | 0.65 |
| 2:B:843:GLN:N | 2:B:994:TYR:O | 2.19 | 0.65 |
| 2:B:1162:ILE:HD11 | 2:B:1194:ILE:CD1 | 2.26 | 0.65 |
| 5:E:197:LYS:HG2 | 5:E:199:ILE:HG13 | 1.78 | 0.65 |
| 8:H:135:LEU:HD22 | 8:H:137:GLN:NE2 | 2.12 | 0.65 |
| 9:I:7:CYS:N | 9:I:14:LEU:HD21 | 2.12 | 0.65 |
| 11:K:12:LEU:HD23 | 11:K:16:GLU:O | 1.96 | 0.65 |
| 13:T:7:DC:H2'' | 13:T:8:DT:C5 | 2.32 | 0.65 |
| 1:A:35:ILE:HB | 1:A:83:HIS:O | 1.97 | 0.65 |
| 1:A:767:GLN:HB2 | 1:A:799:PHE:HD1 | 1.60 | 0.65 |
| 1:A:785:PRO:HG2 | 1:A:786:HIS:CD2 | 2.32 | 0.65 |
| 1:A:898:ARG:HD2 | 1:A:899:VAL:N | 2.12 | 0.65 |
| 2:B:165:VAL:HG11 | 2:B:448:ILE:CD1 | 2.27 | 0.65 |
| 2:B:449:ASN:O | 2:B:451:LYS:N | 2.30 | 0.65 |
| 4:D:123:LEU:O | 4:D:127:ASP:HB2 | 1.97 | 0.65 |
| 7:G:13:LEU:HD23 | 7:G:14:HIS:H | 1.60 | 0.65 |
| 1:A:567:LYS:HZ3 | 8:H:95:TYR:CB | 2.09 | 0.65 |
| 1:A:954:TRP:HB3 | 1:A:955:PRO:HD2 | 1.78 | 0.65 |
| 1:A:1208:THR:HB | 1:A:1211:GLN:CG | 2.26 | 0.65 |
| 2:B:38:PHE:HD1 | 2:B:811:TYR:CD2 | 2.15 | 0.65 |
| 2:B:867:GLY:C | 2:B:869:SER:H | 1.99 | 0.65 |
| 3:C:167:HIS:ND1 | 3:C:169:LYS:HG2 | 2.11 | 0.65 |
| 5:E:198:ILE:HD12 | 5:E:198:ILE:N | 2.12 | 0.65 |
| 6:F:70:LYS:O | 6:F:72:LYS:HD2 | 1.96 | 0.65 |
| 1:A:35:ILE:CG2 | 1:A:84:ILE:HD12 | 2.27 | 0.64 |
| 1:A:565:ILE:O | 1:A:570:PRO:HA | 1.97 | 0.64 |
| 1:A:962:ARG:HA | 1:A:965:GLN:HB2 | 1.77 | 0.64 |
| 2:B:26:THR:HA | 2:B:708:GLU:OE1 | 1.96 | 0.64 |
| 2:B:100:PRO:HD2 | 2:B:180:TYR:CE1 | 2.32 | 0.64 |
| 2:B:766:ARG:HG3 | 2:B:1022:THR:HG23 | 1.78 | 0.64 |
| 3:C:261:ALA:O | 3:C:265:MET:HB2 | 1.97 | 0.64 |
| 5:E:111:VAL:CG1 | 5:E:137:GLU:HG2 | 2.27 | 0.64 |
| 5:E:202:SER:OG | 5:E:204:THR:HG22 | 1.97 | 0.64 |
| 7:G:59:GLY:HA3 | 7:G:70:PHE:CD2 | 2.31 | 0.64 |
| 8:H:100:THR:HG22 | 8:H:101:ALA:H | 1.60 | 0.64 |
| 11:K:21:ILE:CG2 | 11:K:33:ILE:HG12 | 2.26 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:34:LYS:CB | 1:A:36:ARG:HH21 | 2.10 | 0.64 |
| 1:A:172:PRO:HD3 | 1:A:185:TRP:NE1 | 2.12 | 0.64 |
| 1:A:381:THR:HG23 | 1:A:382:PRO:HD2 | 1.78 | 0.64 |
| 1:A:469:ARG:HB3 | 1:A:469:ARG:HH11 | 1.60 | 0.64 |
| 1:A:967:ALA:HA | 1:A:1044:TRP:HZ3 | 1.62 | 0.64 |
| 11:K:102:LYS:O | 11:K:106:GLU:HG3 | 1.97 | 0.64 |
| 1:A:474:VAL:HG22 | 1:A:474:VAL:O | 1.96 | 0.64 |
| 1:A:828:ALA:HB2 | 2:B:530:GLY:HA2 | 1.79 | 0.64 |
| 1:A:1341:ILE:HG23 | 1:A:1342:GLU:N | 2.11 | 0.64 |
| 2:B:1099:VAL:CG1 | 2:B:1100:ASP:H | 2.08 | 0.64 |
| 6:F:79:ARG:HG3 | 6:F:144:GLU:CG | 2.27 | 0.64 |
| 2:B:597:MET:HA | 2:B:597:MET:CE | 2.27 | 0.64 |
| 2:B:870:ILE:HG22 | 2:B:917:PRO:HG2 | 1.78 | 0.64 |
| 3:C:56:THR:HG22 | 3:C:57:VAL:H | 1.61 | 0.64 |
| 4:D:22:GLU:H | 4:D:22:GLU:CD | 2.01 | 0.64 |
| 8:H:44:VAL:O | 8:H:44:VAL:HG12 | 1.96 | 0.64 |
| 11:K:68:PHE:HB3 | 11:K:70:ARG:NH1 | 2.12 | 0.64 |
| 12:L:28:LYS:CB | 12:L:39:SER:HB2 | 2.27 | 0.64 |
| 1:A:106:VAL:HG12 | 1:A:107:CYS:N | 2.13 | 0.64 |
| 1:A:172:PRO:HB3 | 1:A:185:TRP:CD2 | 2.33 | 0.64 |
| 1:A:315:LEU:HD13 | 2:B:471:LYS:HB3 | 1.78 | 0.64 |
| 1:A:370:ILE:HG12 | 2:B:1105:ALA:HB2 | 1.79 | 0.64 |
| 1:A:590:ARG:HB3 | 1:A:605:MET:N | 2.12 | 0.64 |
| 1:A:809:THR:HG23 | 1:A:812:GLU:OE1 | 1.97 | 0.64 |
| 1:A:1242:VAL:HG12 | 1:A:1243:VAL:N | 2.12 | 0.64 |
| 1:A:1438:THR:HG23 | 6:F:92:ARG:HB2 | 1.79 | 0.64 |
| 2:B:90:ILE:HD12 | 2:B:432:MET:SD | 2.38 | 0.64 |
| 11:K:50:LEU:HD11 | 11:K:75:ILE:CD1 | 2.28 | 0.64 |
| 1:A:506:ALA:HB3 | 1:A:509:LEU:HD12 | 1.79 | 0.64 |
| 2:B:51:PHE:O | 2:B:54:PHE:HB3 | 1.97 | 0.64 |
| 2:B:243:ALA:CB | 2:B:251:ILE:HG12 | 2.28 | 0.64 |
| 2:B:865:LYS:HG3 | 2:B:961:LEU:HD21 | 1.77 | 0.64 |
| 2:B:1002:THR:HG21 | 2:B:1006:ILE:HD12 | 1.80 | 0.64 |
| 2:B:1186:ASP:O | 4:D:17:LYS:HE2 | 1.97 | 0.64 |
| 1:A:675:THR:OG1 | 1:A:736:ASN:ND2 | 2.29 | 0.64 |
| 2:B:288:ALA:HA | 2:B:331:LEU:CD1 | 2.27 | 0.64 |
| 2:B:604:ARG:C | 2:B:606:LYS:H | 1.98 | 0.64 |
| 2:B:642:ASP:CA | 2:B:649:LYS:HG3 | 2.28 | 0.64 |
| 2:B:918:ILE:CG2 | 2:B:919:SER:N | 2.61 | 0.64 |
| 7:G:13:LEU:HD21 | 7:G:17:PHE:CD1 | 2.33 | 0.64 |
| 1:A:135:PHE:CD1 | 1:A:222:LEU:HD22 | 2.33 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:185:TRP:HE3 | 1:A:185:TRP:H | 1.46 | 0.64 |
| 1:A:637:LYS:HB3 | 1:A:641:VAL:HG21 | 1.79 | 0.64 |
| 2:B:123:THR:OG1 | 2:B:458:LYS:HE2 | 1.98 | 0.64 |
| 2:B:502:ILE:H | 2:B:502:ILE:HD12 | 1.62 | 0.64 |
| 2:B:863:GLU:O | 2:B:961:LEU:HD22 | 1.98 | 0.64 |
| 2:B:891:ASP:C | 2:B:893:LEU:H | 2.00 | 0.64 |
| 2:B:1174:LYS:O | 2:B:1176:ASN:N | 2.31 | 0.64 |
| 5:E:54:GLN:O | 5:E:57:MET:HB3 | 1.97 | 0.64 |
| 8:H:91:ASP:O | 8:H:93:TYR:N | 2.25 | 0.64 |
| 9:I:2:THR:HG22 | 9:I:3:THR:N | 2.13 | 0.64 |
| 1:A:39:GLU:OE1 | 1:A:50:ILE:HD12 | 1.98 | 0.64 |
| 1:A:90:VAL:HG13 | 1:A:297:GLN:OE1 | 1.97 | 0.64 |
| 1:A:666:ILE:HD12 | 1:A:667:GLY:N | 2.08 | 0.64 |
| 1:A:666:ILE:N | 2:B:1026:LEU:HD13 | 2.03 | 0.64 |
| 1:A:868:TYR:CD2 | 1:A:1058:VAL:HG21 | 2.33 | 0.64 |
| 1:A:900:ASP:HA | 1:A:926:GLN:NE2 | 2.12 | 0.64 |
| 2:B:25:ILE:HD11 | 2:B:653:VAL:C | 2.18 | 0.64 |
| 2:B:515:HIS:CD2 | 2:B:516:ASN:H | 2.16 | 0.64 |
| 2:B:822:ASN:ND2 | 10:J:52:THR:HG21 | 2.13 | 0.64 |
| 2:B:855:PHE:C | 2:B:855:PHE:CD1 | 2.69 | 0.64 |
| 2:B:899:ILE:HD11 | 2:B:911:ILE:HA | 1.78 | 0.64 |
| 2:B:1110:PRO:HG3 | 2:B:1125:ASP:HB3 | 1.78 | 0.64 |
| 2:B:1159:ARG:HE | 2:B:1193:GLN:HE21 | 1.44 | 0.64 |
| 11:K:82:ASP:OD1 | 11:K:84:LYS:HG3 | 1.98 | 0.64 |
| 1:A:547:LEU:HD22 | 11:K:58:PHE:CD1 | 2.32 | 0.64 |
| 1:A:1130:GLN:O | 1:A:1134:ILE:HG13 | 1.97 | 0.64 |
| 2:B:135:ARG:HB2 | 2:B:137:TYR:CE1 | 2.33 | 0.64 |
| 2:B:387:LEU:O | 2:B:392:ARG:HB2 | 1.98 | 0.64 |
| 2:B:791:THR:HA | 2:B:858:SER:HB2 | 1.79 | 0.64 |
| 2:B:953:LEU:HD23 | 2:B:965:LYS:O | 1.98 | 0.64 |
| 3:C:8:VAL:O | 3:C:9:LYS:HD2 | 1.98 | 0.64 |
| 4:D:60:LYS:CE | 4:D:126:ILE:HD11 | 2.28 | 0.64 |
| 1:A:963:ILE:HD11 | 1:A:1048:ASN:HB2 | 1.78 | 0.63 |
| 1:A:1191:TRP:CE3 | 1:A:1191:TRP:HA | 2.32 | 0.63 |
| 2:B:758:PHE:CZ | 2:B:1044:ALA:HA | 2.33 | 0.63 |
| 2:B:847:ASP:C | 2:B:849:GLY:H | 2.00 | 0.63 |
| 2:B:899:ILE:CD1 | 2:B:911:ILE:HA | 2.28 | 0.63 |
| 2:B:1034:VAL:HG12 | 2:B:1035:ALA:N | 2.14 | 0.63 |
| 4:D:9:GLN:HE21 | 4:D:31:GLN:NE2 | 1.95 | 0.63 |
| 11:K:47:ARG:HH11 | 11:K:47:ARG:CB | 2.09 | 0.63 |
| 1:A:515:GLN:HA | 1:A:1367:HIS:NE2 | 2.13 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1308:THR:HG23 | 1:A:1309:ASP:H | 1.62 | 0.63 |
| 1:A:1364:ASN:HD22 | 1:A:1365:TYR:N | 1.97 | 0.63 |
| 2:B:1002:THR:CG2 | 2:B:1006:ILE:HG13 | 2.27 | 0.63 |
| 3:C:242:GLN:HA | 3:C:245:VAL:CG2 | 2.28 | 0.63 |
| 4:D:9:GLN:HE21 | 4:D:31:GLN:HE21 | 1.43 | 0.63 |
| 4:D:56:ARG:NH2 | 4:D:155:ARG:HA | 2.12 | 0.63 |
| 8:H:139:ASN:O | 8:H:140:ALA:HB2 | 1.97 | 0.63 |
| 12:L:32:ALA:HB3 | 12:L:33:GLU:OE2 | 1.99 | 0.63 |
| 1:A:1142:THR:HA | 1:A:1273:LEU:HD13 | 1.78 | 0.63 |
| 1:A:1187:GLN:HG3 | 1:A:1188:GLN:HG3 | 1.79 | 0.63 |
| 3:C:148:ARG:H | 3:C:151:GLN:CG | 2.06 | 0.63 |
| 8:H:142:LEU:C | 8:H:143:LEU:HD12 | 2.18 | 0.63 |
| 10:J:14:VAL:O | 10:J:14:VAL:HG12 | 1.96 | 0.63 |
| 2:B:653:VAL:HG22 | 2:B:689:LEU:HB3 | 1.80 | 0.63 |
| 2:B:1096:ARG:O | 2:B:1097:HIS:HB2 | 1.98 | 0.63 |
| 4:D:139:LYS:HE2 | 4:D:143:ASN:ND2 | 2.13 | 0.63 |
| 5:E:165:LEU:N | 5:E:165:LEU:HD23 | 2.13 | 0.63 |
| 5:E:204:THR:HG23 | 5:E:205:SER:N | 2.13 | 0.63 |
| 1:A:93:VAL:HG21 | 1:A:301:ALA:O | 1.99 | 0.63 |
| 1:A:1100:ARG:HH22 | 1:A:1111:MET:CE | 2.11 | 0.63 |
| 2:B:99:LYS:HA | 2:B:178:ASN:HD21 | 1.63 | 0.63 |
| 2:B:114:PRO:HG2 | 2:B:115:GLN:H | 1.63 | 0.63 |
| 2:B:217:ARG:HD2 | 2:B:217:ARG:C | 2.19 | 0.63 |
| 2:B:343:ILE:HG23 | 2:B:347:LYS:CE | 2.28 | 0.63 |
| 2:B:637:LEU:C | 2:B:690:VAL:HG13 | 2.19 | 0.63 |
| 2:B:1096:ARG:O | 2:B:1097:HIS:CB | 2.47 | 0.63 |
| 4:D:60:LYS:HE3 | 4:D:126:ILE:HD11 | 1.79 | 0.63 |
| 12:L:26:THR:HG23 | 12:L:62:LYS:HZ3 | 1.64 | 0.63 |
| 1:A:55:ASP:CG | 1:A:55:ASP:O | 2.36 | 0.63 |
| 1:A:901:LEU:N | 1:A:926:GLN:HE21 | 1.95 | 0.63 |
| 1:A:1364:ASN:HD22 | 1:A:1364:ASN:C | 1.98 | 0.63 |
| 5:E:117:THR:HB | 5:E:120:ALA:CB | 2.29 | 0.63 |
| 5:E:180:ARG:NH2 | 5:E:192:ARG:HD2 | 2.14 | 0.63 |
| 5:E:116:ILE:HG22 | 5:E:117:THR:N | 2.12 | 0.63 |
| 7:G:34:VAL:CG1 | 7:G:45:ILE:HG21 | 2.28 | 0.63 |
| 1:A:535:THR:HG22 | 1:A:575:LYS:HE2 | 1.81 | 0.63 |
| 1:A:877:HIS:ND1 | 1:A:1056:SER:HA | 2.14 | 0.63 |
| 2:B:244:LEU:HD21 | 2:B:366:GLN:NE2 | 2.14 | 0.63 |
| 2:B:363:HIS:O | 2:B:364:ILE:HB | 1.98 | 0.63 |
| 5:E:204:THR:HG23 | 5:E:205:SER:H | 1.64 | 0.63 |
| 1:A:87:ALA:HB3 | 1:A:276:LEU:HD23 | 1.79 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:332:LYS:C | 1:A:334:GLY:H | 2.02 | 0.63 |
| 2:B:276:ILE:HD13 | 2:B:280:ILE:HD11 | 1.80 | 0.63 |
| 2:B:383:ASN:O | 2:B:387:LEU:HD13 | 1.98 | 0.63 |
| 2:B:686:ASN:C | 2:B:688:GLY:H | 2.02 | 0.63 |
| 2:B:857:ARG:HD2 | 2:B:945:GLU:OE1 | 1.97 | 0.63 |
| 3:C:13:ALA:O | 11:K:114:LEU:HD13 | 1.99 | 0.63 |
| 5:E:159:ASP:HA | 5:E:162:ARG:NH2 | 2.13 | 0.63 |
| 5:E:167:ARG:O | 5:E:168:TYR:HD2 | 1.82 | 0.63 |
| 5:E:198:ILE:HD11 | 5:E:212:ARG:HB2 | 1.81 | 0.63 |
| 7:G:27:LYS:O | 7:G:31:LEU:HG | 1.98 | 0.63 |
| 1:A:41:MET:SD | 1:A:42:ASP:N | 2.71 | 0.62 |
| 1:A:278:THR:HG23 | 1:A:282:ASN:HD22 | 1.63 | 0.62 |
| 1:A:343:LYS:HE2 | 2:B:1156:ASP:HB2 | 1.81 | 0.62 |
| 1:A:451:HIS:CD2 | 1:A:1074:GLU:HG3 | 2.33 | 0.62 |
| 1:A:1094:VAL:HG12 | 1:A:1113:THR:HG21 | 1.80 | 0.62 |
| 2:B:90:ILE:HG23 | 2:B:133:LYS:O | 1.99 | 0.62 |
| 2:B:357:GLN:O | 2:B:366:GLN:HA | 1.98 | 0.62 |
| 3:C:209:TYR:HD1 | 3:C:209:TYR:H | 1.47 | 0.62 |
| 6:F:118:LEU:O | 6:F:122:MET:HG3 | 1.99 | 0.62 |
| 8:H:36:CYS:HA | 8:H:126:GLU:O | 1.98 | 0.62 |
| 8:H:144:ILE:HG22 | 8:H:145:ARG:N | 2.14 | 0.62 |
| 2:B:578:THR:H | 2:B:589:VAL:CG1 | 2.12 | 0.62 |
| 2:B:596:LEU:HD11 | 2:B:600:LEU:HD11 | 1.81 | 0.62 |
| 3:C:238:ILE:HD13 | 3:C:246:ARG:HD2 | 1.80 | 0.62 |
| 7:G:142:ARG:HB3 | 7:G:171:ILE:HD11 | 1.80 | 0.62 |
| 1:A:266:LEU:HD21 | 1:A:303:TYR:CE1 | 2.35 | 0.62 |
| 1:A:645:LEU:O | 1:A:649:ILE:HG13 | 2.00 | 0.62 |
| 1:A:847:ASP:O | 1:A:858:ASN:HA | 2.00 | 0.62 |
| 1:A:1436:ILE:O | 1:A:1437:GLY:C | 2.37 | 0.62 |
| 2:B:351:TYR:O | 2:B:355:ILE:HG13 | 2.00 | 0.62 |
| 5:E:93:MET:HE1 | 5:E:123:LEU:HB2 | 1.81 | 0.62 |
| 5:E:168:TYR:HB3 | 5:E:170:LEU:HG | 1.81 | 0.62 |
| 8:H:105:GLU:O | 8:H:112:ILE:HG23 | 1.99 | 0.62 |
| 1:A:79:GLY:HA3 | 1:A:243:PRO:HG3 | 1.80 | 0.62 |
| 1:A:335:ARG:O | 1:A:339:ASN:HB2 | 1.97 | 0.62 |
| 2:B:614:SER:HB3 | 2:B:694:ASP:HB2 | 1.81 | 0.62 |
| 2:B:797:TYR:HE1 | 2:B:971:THR:HG23 | 1.64 | 0.62 |
| 2:B:862:GLN:HG2 | 2:B:963:PHE:CD1 | 2.34 | 0.62 |
| 2:B:1072:MET:HE3 | 2:B:1085:ILE:HB | 1.81 | 0.62 |
| 3:C:31:ASN:O | 3:C:35:ARG:HG3 | 2.00 | 0.62 |
| 9:I:86:PHE:CE1 | 9:I:100:PHE:HB2 | 2.34 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:427:GLN:HG3 | 1:A:430:TRP:CZ2 | 2.33 | 0.62 |
| 2:B:69:LEU:CB | 2:B:429:PHE:CE1 | 2.74 | 0.62 |
| 2:B:449:ASN:O | 2:B:450:ALA:C | 2.38 | 0.62 |
| 3:C:65:HIS:CE1 | 3:C:69:LEU:HD11 | 2.35 | 0.62 |
| 5:E:145:THR:HG21 | 5:E:187:TYR:CE2 | 2.34 | 0.62 |
| 8:H:4:THR:HG22 | 8:H:5:LEU:N | 2.15 | 0.62 |
| 8:H:32:THR:HG22 | 8:H:33:GLN:H | 1.65 | 0.62 |
| 12:L:55:ILE:O | 12:L:56:LEU:CB | 2.48 | 0.62 |
| 1:A:466:SER:O | 2:B:1103:ILE:HD11 | 1.98 | 0.62 |
| 1:A:472:LEU:O | 1:A:475:THR:HB | 1.99 | 0.62 |
| 1:A:475:THR:CG2 | 1:A:476:SER:N | 2.62 | 0.62 |
| 1:A:646:PHE:O | 1:A:650:GLN:HB2 | 1.99 | 0.62 |
| 2:B:232:SER:O | 2:B:261:ARG:HD3 | 1.99 | 0.62 |
| 8:H:30:SER:HB2 | 8:H:36:CYS:HB3 | 1.81 | 0.62 |
| 1:A:1152:ILE:HD11 | 9:I:44:TYR:HD2 | 1.64 | 0.62 |
| 1:A:1424:VAL:HG11 | 2:B:1139:ILE:HD13 | 1.79 | 0.62 |
| 2:B:105:SER:O | 2:B:106:ASP:HB2 | 1.99 | 0.62 |
| 2:B:221:ASN:N | 2:B:241:ARG:O | 2.31 | 0.62 |
| 2:B:284:ILE:HD13 | 2:B:333:PHE:CD2 | 2.35 | 0.62 |
| 2:B:510:LYS:CB | 2:B:511:PRO:HD3 | 2.30 | 0.62 |
| 2:B:768:THR:O | 2:B:771:SER:HB2 | 1.99 | 0.62 |
| 2:B:871:THR:O | 2:B:917:PRO:HG3 | 1.98 | 0.62 |
| 2:B:898:LEU:HD13 | 2:B:952:VAL:HG11 | 1.80 | 0.62 |
| 7:G:23:LYS:HG3 | 7:G:56:ILE:CD1 | 2.30 | 0.62 |
| 9:I:80:SER:OG | 9:I:105:SER:HB2 | 2.00 | 0.62 |
| 1:A:247:ARG:NH1 | 1:A:263:THR:HG23 | 2.15 | 0.62 |
| 1:A:399:HIS:HB3 | 1:A:400:PRO:CD | 2.25 | 0.62 |
| 1:A:1109:LYS:O | 1:A:1110:ASN:HB3 | 2.00 | 0.62 |
| 1:A:1161:THR:HG22 | 1:A:1163:ILE:N | 2.11 | 0.62 |
| 2:B:1177:HIS:C | 2:B:1178:ASN:HD22 | 2.03 | 0.62 |
| 7:G:145:VAL:HG12 | 7:G:146:LYS:N | 2.15 | 0.62 |
| 1:A:110:CYS:HB3 | 1:A:167:CYS:SG | 2.40 | 0.62 |
| 1:A:268:ASP:HB3 | 1:A:299:HIS:CE1 | 2.35 | 0.62 |
| 1:A:899:VAL:CG2 | 1:A:1029:ARG:HG2 | 2.29 | 0.62 |
| 1:A:1118:VAL:HG12 | 1:A:1327:ILE:HG13 | 1.81 | 0.62 |
| 2:B:99:LYS:HB3 | 2:B:100:PRO:HD2 | 1.81 | 0.62 |
| 2:B:196:PRO:HG2 | 2:B:197:PHE:H | 1.65 | 0.62 |
| 2:B:258:LEU:HG | 2:B:258:LEU:O | 2.00 | 0.62 |
| 2:B:282:ILE:HD12 | 2:B:382:ILE:HD13 | 1.82 | 0.62 |
| 2:B:916:THR:HB | 2:B:935:ARG:CG | 2.30 | 0.62 |
| 6:F:72:LYS:HE3 | 6:F:72:LYS:CA | 2.30 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:K:21:ILE:HG22 | 11:K:31:VAL:CG1 | 2.29 | 0.62 |
| 1:A:188:ASP:CB | 1:A:191:THR:HB | 2.25 | 0.62 |
| 1:A:1329:THR:CG2 | 1:A:1335:ILE:HG13 | 2.30 | 0.62 |
| 1:A:1345:ARG:NH1 | 5:E:200:ARG:HH22 | 1.98 | 0.62 |
| 1:A:1371:LEU:O | 1:A:1375:MET:HG3 | 2.00 | 0.62 |
| 2:B:128:LEU:HB2 | 2:B:167:ILE:O | 2.00 | 0.62 |
| 2:B:549:THR:HG22 | 2:B:550:ASP:H | 1.64 | 0.62 |
| 2:B:801:LYS:O | 10:J:52:THR:CG2 | 2.47 | 0.62 |
| 7:G:18:PHE:HA | 7:G:22:MET:CE | 2.30 | 0.62 |
| 8:H:40:LEU:HG | 8:H:41:ASP:O | 1.98 | 0.62 |
| 8:H:82:PRO:HG3 | 11:K:54:ARG:HH11 | 1.65 | 0.62 |
| 9:I:78:CYS:O | 9:I:80:SER:N | 2.32 | 0.62 |
| 1:A:847:ASP:HB3 | 1:A:1424:VAL:HG23 | 1.81 | 0.61 |
| 2:B:351:TYR:CZ | 2:B:355:ILE:HD11 | 2.35 | 0.61 |
| 2:B:593:PRO:HG2 | 2:B:617:ARG:NH1 | 2.15 | 0.61 |
| 2:B:903:VAL:HG12 | 2:B:904:ARG:N | 2.15 | 0.61 |
| 5:E:83:CYS:C | 5:E:85:GLU:H | 2.04 | 0.61 |
| 5:E:89:GLY:HA2 | 5:E:117:THR:OG1 | 1.99 | 0.61 |
| 8:H:4:THR:HA | 8:H:60:ALA:HB2 | 1.80 | 0.61 |
| 11:K:41:THR:HG22 | 11:K:42:LEU:N | 2.14 | 0.61 |
| 11:K:60:ALA:O | 11:K:73:LEU:HD12 | 1.99 | 0.61 |
| 11:K:61:TYR:C | 11:K:61:TYR:HD2 | 2.02 | 0.61 |
| 12:L:55:ILE:HG12 | 12:L:56:LEU:H | 1.65 | 0.61 |
| 1:A:523:ILE:HG23 | 1:A:527:THR:HB | 1.82 | 0.61 |
| 1:A:929:LEU:HD23 | 1:A:983:ILE:HG23 | 1.82 | 0.61 |
| 1:A:1100:ARG:HH21 | 1:A:1351:GLU:CG | 2.12 | 0.61 |
| 2:B:243:ALA:HA | 2:B:250:PHE:O | 2.00 | 0.61 |
| 2:B:807:ARG:HG2 | 2:B:1045:SER:OG | 1.99 | 0.61 |
| 5:E:100:ILE:CG2 | 5:E:105:PHE:HB2 | 2.25 | 0.61 |
| 6:F:86:THR:OG1 | 6:F:89:GLU:HG3 | 2.00 | 0.61 |
| 9:I:6:PHE:HB3 | 9:I:12:ASN:O | 2.00 | 0.61 |
| 11:K:7:PHE:O | 11:K:9:LEU:N | 2.33 | 0.61 |
| 1:A:541:ILE:HG22 | 1:A:546:VAL:HG23 | 1.83 | 0.61 |
| 1:A:986:ILE:HD12 | 1:A:1032:LEU:HD11 | 1.83 | 0.61 |
| 1:A:1018:PHE:O | 1:A:1021:LEU:HB3 | 2.01 | 0.61 |
| 1:A:1276:VAL:HG12 | 1:A:1277:GLU:H | 1.65 | 0.61 |
| 1:A:1315:GLU:O | 1:A:1317:MET:N | 2.33 | 0.61 |
| 2:B:286:PHE:HA | 2:B:289:LEU:HD12 | 1.83 | 0.61 |
| 2:B:378:LEU:O | 2:B:378:LEU:HD12 | 2.00 | 0.61 |
| 2:B:393:LYS:HA | 2:B:393:LYS:HE3 | 1.81 | 0.61 |
| 2:B:510:LYS:HG3 | 2:B:511:PRO:HD3 | 1.81 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:D:40:HIS:CB | 7:G:73:LYS:NZ | 2.63 | 0.61 |
| 8:H:14:GLU:HG2 | 8:H:15:VAL:N | 2.13 | 0.61 |
| 9:I:53:GLY:HA2 | 9:I:56:ALA:HB2 | 1.82 | 0.61 |
| 11:K:12:LEU:H | 11:K:12:LEU:CD1 | 2.10 | 0.61 |
| 1:A:233:TRP:C | 1:A:235:ILE:H | 2.03 | 0.61 |
| 1:A:1155:ASP:OD2 | 1:A:1161:THR:HA | 2.01 | 0.61 |
| 2:B:56:ASP:HB2 | 2:B:57:TYR:HD1 | 1.65 | 0.61 |
| 2:B:273:LEU:HB2 | 2:B:276:ILE:CD1 | 2.24 | 0.61 |
| 4:D:63:LEU:HD13 | 4:D:133:THR:OG1 | 2.00 | 0.61 |
| 4:D:144:THR:O | 4:D:148:LEU:HB2 | 2.00 | 0.61 |
| 5:E:103:LYS:HB3 | 5:E:105:PHE:CE2 | 2.35 | 0.61 |
| 11:K:1:MET:HG3 | 11:K:2:ASN:N | 2.15 | 0.61 |
| 13:T:15:DC:H2'' | 13:T:16:DT:OP2 | 2.01 | 0.61 |
| 1:A:115:LEU:O | 1:A:122:MET:HE2 | 2.00 | 0.61 |
| 1:A:830:LYS:HE2 | 1:A:1081:LEU:HB2 | 1.82 | 0.61 |
| 1:A:849:MET:HE1 | 1:A:1061:GLY:HA2 | 1.82 | 0.61 |
| 1:A:1199:ARG:NH2 | 1:A:1234:GLU:HA | 2.16 | 0.61 |
| 2:B:190:TYR:CE2 | 10:J:62:ARG:HB3 | 2.34 | 0.61 |
| 2:B:497:ARG:NH2 | 2:B:775:LYS:HE2 | 2.14 | 0.61 |
| 2:B:737:THR:CG2 | 9:I:66:PRO:HA | 2.31 | 0.61 |
| 5:E:129:PRO:O | 5:E:130:ALA:C | 2.39 | 0.61 |
| 9:I:69:PRO:HG2 | 9:I:85:PHE:CD2 | 2.36 | 0.61 |
| 10:J:64:ASN:HD22 | 10:J:65:PRO:HD3 | 1.64 | 0.61 |
| 11:K:44:ASN:N | 11:K:61:TYR:CE1 | 2.68 | 0.61 |
| 1:A:18:GLN:NE2 | 1:A:228:PHE:HE1 | 1.99 | 0.61 |
| 1:A:98:LYS:HE2 | 1:A:224:PHE:CZ | 2.35 | 0.61 |
| 1:A:196:GLU:CB | 1:A:197:PRO:HD2 | 2.29 | 0.61 |
| 1:A:901:LEU:N | 1:A:926:GLN:NE2 | 2.44 | 0.61 |
| 1:A:1035:TYR:HD1 | 1:A:1037:LEU:HD23 | 1.64 | 0.61 |
| 1:A:1214:GLU:OE1 | 1:A:1214:GLU:HA | 2.01 | 0.61 |
| 1:A:1450:LEU:O | 1:A:1450:LEU:HG | 2.01 | 0.61 |
| 2:B:559:SER:CA | 2:B:563:MET:HB3 | 2.26 | 0.61 |
| 2:B:651:LEU:C | 2:B:653:VAL:H | 2.03 | 0.61 |
| 2:B:1080:LYS:HB2 | 3:C:188:HIS:HB3 | 1.80 | 0.61 |
| 2:B:1201:LYS:HE2 | 2:B:1205:GLN:NE2 | 2.15 | 0.61 |
| 7:G:112:LYS:O | 7:G:115:MET:HG2 | 2.00 | 0.61 |
| 11:K:7:PHE:HA | 11:K:10:PHE:CE2 | 2.35 | 0.61 |
| 1:A:43:GLU:HG3 | 1:A:48:ALA:HB3 | 1.82 | 0.61 |
| 1:A:225:ASN:ND2 | 1:A:227:VAL:H | 1.99 | 0.61 |
| 1:A:1154:TYR:HD1 | 1:A:1191:TRP:CZ3 | 2.19 | 0.61 |
| 2:B:944:THR:HG21 | 2:B:1122:ARG:NH2 | 2.14 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1065:GLN:HB3 | 2:B:1069:PHE:O | 2.00 | 0.61 |
| 3:C:66:ARG:HH21 | 10:J:5:VAL:H | 1.49 | 0.61 |
| 1:A:152:VAL:CG1 | 1:A:153:PRO:HD2 | 2.31 | 0.61 |
| 1:A:590:ARG:HB2 | 1:A:590:ARG:NH1 | 2.08 | 0.61 |
| 1:A:882:SER:H | 1:A:1025:ARG:NH2 | 1.98 | 0.61 |
| 1:A:1039:LYS:HE3 | 1:A:1043:ASP:OD2 | 2.01 | 0.61 |
| 1:A:1149:ALA:CB | 9:I:47:GLU:HA | 2.31 | 0.61 |
| 2:B:259:TYR:HB2 | 2:B:268:THR:HG23 | 1.83 | 0.61 |
| 2:B:261:ARG:HH11 | 2:B:262:GLU:H | 1.48 | 0.61 |
| 2:B:573:GLN:O | 2:B:575:PRO:HD3 | 2.00 | 0.61 |
| 2:B:776:GLN:OE1 | 15:P:9:C:H4' | 2.01 | 0.61 |
| 2:B:999:MET:HB3 | 2:B:1007:VAL:CG2 | 2.30 | 0.61 |
| 3:C:177:GLU:HG3 | 3:C:231:ASN:HB3 | 1.83 | 0.61 |
| 6:F:94:LEU:HD21 | 6:F:122:MET:HA | 1.81 | 0.61 |
| 1:A:382:PRO:CD | 1:A:428:TYR:HD2 | 2.09 | 0.61 |
| 1:A:403:LYS:O | 1:A:415:LEU:HB2 | 2.00 | 0.61 |
| 4:D:56:ARG:HB2 | 4:D:148:LEU:HD22 | 1.82 | 0.61 |
| 1:A:573:SER:O | 1:A:576:GLN:HB3 | 2.01 | 0.61 |
| 1:A:665:GLY:O | 1:A:666:ILE:HD12 | 2.00 | 0.61 |
| 1:A:741:ASN:ND2 | 1:A:744:LYS:H | 1.99 | 0.61 |
| 2:B:352:ALA:HA | 2:B:355:ILE:HD12 | 1.83 | 0.61 |
| 4:D:53:SER:H | 4:D:148:LEU:CD2 | 2.13 | 0.61 |
| 6:F:130:ILE:O | 6:F:148:VAL:HG21 | 2.01 | 0.61 |
| 1:A:74:MET:H | 1:A:74:MET:CE | 2.13 | 0.60 |
| 1:A:695:LYS:HG2 | 1:A:698:GLN:OE1 | 2.01 | 0.60 |
| 2:B:680:THR:OG1 | 2:B:681:TRP:N | 2.33 | 0.60 |
| 3:C:66:ARG:NH1 | 10:J:2:ILE:HG21 | 2.16 | 0.60 |
| 7:G:17:PHE:N | 7:G:17:PHE:CD2 | 2.68 | 0.60 |
| 8:H:26:ILE:HG22 | 8:H:27:GLU:H | 1.66 | 0.60 |
| 10:J:12:LYS:O | 10:J:14:VAL:HG23 | 2.00 | 0.60 |
| 1:A:20:GLY:O | 1:A:21:LEU:HD23 | 2.01 | 0.60 |
| 1:A:1427:ASN:HD22 | 1:A:1427:ASN:H | 1.50 | 0.60 |
| 2:B:236:HIS:CE1 | 2:B:389:ALA:HA | 2.35 | 0.60 |
| 2:B:582:VAL:HB | 2:B:587:HIS:CD2 | 2.35 | 0.60 |
| 2:B:653:VAL:HA | 2:B:657:HIS:CD2 | 2.35 | 0.60 |
| 2:B:1072:MET:HG3 | 2:B:1085:ILE:HD13 | 1.81 | 0.60 |
| 2:B:1201:LYS:HE2 | 2:B:1205:GLN:CD | 2.21 | 0.60 |
| 4:D:119:ARG:HG2 | 4:D:120:GLU:H | 1.64 | 0.60 |
| 8:H:32:THR:HG22 | 8:H:33:GLN:N | 2.16 | 0.60 |
| 8:H:40:LEU:HD22 | 8:H:123:MET:CE | 2.27 | 0.60 |
| 1:A:154:SER:HB3 | 1:A:162:VAL:HG23 | 1.82 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:679:ILE:HG12 | 1:A:732:LEU:HD12 | 1.83 | 0.60 |
| 1:A:930:ASP:O | 1:A:934:LYS:HG2 | 2.01 | 0.60 |
| 1:A:1173:HIS:CD2 | 1:A:1227:ILE:HG23 | 2.36 | 0.60 |
| 2:B:327:ARG:O | 2:B:331:LEU:HD13 | 2.02 | 0.60 |
| 2:B:900:ALA:HB3 | 12:L:61:THR:OG1 | 2.02 | 0.60 |
| 5:E:154:ILE:O | 5:E:196:VAL:HA | 2.01 | 0.60 |
| 5:E:182:ASP:HB3 | 5:E:185:ALA:HB2 | 1.83 | 0.60 |
| 6:F:125:LEU:HG | 6:F:125:LEU:O | 2.01 | 0.60 |
| 7:G:56:ILE:O | 7:G:57:GLN:HB2 | 2.01 | 0.60 |
| 9:I:35:VAL:CG1 | 9:I:36:GLU:N | 2.65 | 0.60 |
| 1:A:512:VAL:HA | 1:A:519:PRO:HA | 1.83 | 0.60 |
| 1:A:857:ARG:NH2 | 6:F:139:PRO:HG3 | 2.16 | 0.60 |
| 2:B:277:LYS:CG | 2:B:338:GLY:HA2 | 2.31 | 0.60 |
| 3:C:98:VAL:O | 3:C:99:LEU:HD23 | 2.00 | 0.60 |
| 8:H:91:ASP:C | 8:H:93:TYR:H | 2.03 | 0.60 |
| 1:A:544:ASP:CG | 1:A:545:GLN:H | 2.05 | 0.60 |
| 1:A:1313:LEU:O | 1:A:1315:GLU:N | 2.34 | 0.60 |
| 2:B:20:ASP:C | 2:B:22:SER:H | 2.04 | 0.60 |
| 2:B:314:LEU:HD21 | 2:B:386:LEU:HD11 | 1.83 | 0.60 |
| 2:B:446:LEU:O | 2:B:447:ALA:HB3 | 2.02 | 0.60 |
| 2:B:579:ARG:CB | 2:B:586:TRP:HE1 | 2.13 | 0.60 |
| 2:B:611:PRO:CG | 2:B:685:LEU:HD11 | 2.31 | 0.60 |
| 5:E:4:GLU:C | 5:E:6:GLU:N | 2.55 | 0.60 |
| 5:E:46:TYR:O | 5:E:54:GLN:HG2 | 2.02 | 0.60 |
| 7:G:14:HIS:ND1 | 7:G:15:PRO:HD2 | 2.17 | 0.60 |
| 8:H:24:CYS:HB2 | 8:H:44:VAL:HG21 | 1.83 | 0.60 |
| 8:H:30:SER:CB | 8:H:36:CYS:HB3 | 2.31 | 0.60 |
| 9:I:14:LEU:HA | 9:I:28:GLU:O | 2.01 | 0.60 |
| 1:A:343:LYS:HZ2 | 2:B:1151:LEU:HD12 | 1.65 | 0.60 |
| 1:A:666:ILE:HD11 | 2:B:1067:ARG:O | 2.00 | 0.60 |
| 1:A:722:LEU:HD12 | 1:A:722:LEU:N | 2.16 | 0.60 |
| 1:A:731:ARG:O | 1:A:734:GLU:HB3 | 2.00 | 0.60 |
| 1:A:746:MET:CE | 2:B:1018:PRO:HG2 | 2.32 | 0.60 |
| 1:A:832:ALA:HA | 13:T:18:DA:N7 | 2.15 | 0.60 |
| 2:B:639:ILE:HD11 | 2:B:691:GLU:CG | 2.22 | 0.60 |
| 2:B:941:LEU:HD21 | 2:B:946:ASN:HA | 1.82 | 0.60 |
| 3:C:101:LEU:CD1 | 3:C:118:LEU:HD23 | 2.26 | 0.60 |
| 5:E:46:TYR:CD2 | 5:E:58:MET:HG2 | 2.36 | 0.60 |
| 12:L:68:GLU:OE1 | 12:L:68:GLU:N | 2.31 | 0.60 |
| 1:A:18:GLN:NE2 | 1:A:228:PHE:CE1 | 2.70 | 0.60 |
| 1:A:186:LYS:O | 1:A:194:ALA:HB1 | 2.02 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1319:VAL:O | 1:A:1322:ILE:HG12 | 2.02 | 0.60 |
| 1:A:1453:TYR:O | 1:A:1454:MET:HB3 | 2.01 | 0.60 |
| 2:B:361:LEU:HD21 | 2:B:377:PHE:CD2 | 2.36 | 0.60 |
| 2:B:723:VAL:HG12 | 2:B:724:ASP:N | 2.14 | 0.60 |
| 3:C:173:ALA:O | 3:C:174:ALA:HB3 | 2.01 | 0.60 |
| 7:G:1:MET:SD | 7:G:79:PHE:CD1 | 2.93 | 0.60 |
| 12:L:44:ASP:O | 12:L:45:ALA:HB3 | 2.02 | 0.60 |
| 1:A:91:PHE:HB3 | 1:A:96:ILE:CD1 | 2.31 | 0.60 |
| 1:A:150:THR:HG23 | 1:A:165:GLY:O | 2.01 | 0.60 |
| 1:A:154:SER:HB3 | 1:A:162:VAL:CG2 | 2.31 | 0.60 |
| 1:A:369:SER:CB | 11:K:2:ASN:HD21 | 2.15 | 0.60 |
| 1:A:420:ARG:HG2 | 1:A:423:ASP:HB3 | 1.84 | 0.60 |
| 1:A:441:PRO:CG | 1:A:498:ARG:HB2 | 2.30 | 0.60 |
| 1:A:1152:ILE:HG23 | 1:A:1193:LEU:HD13 | 1.84 | 0.60 |
| 2:B:616:ILE:HD13 | 2:B:625:LYS:HB2 | 1.83 | 0.60 |
| 4:D:195:ILE:HG22 | 4:D:198:LEU:HG | 1.83 | 0.60 |
| 5:E:55:ARG:C | 5:E:57:MET:H | 2.02 | 0.60 |
| 8:H:40:LEU:CD1 | 8:H:123:MET:HB2 | 2.32 | 0.60 |
| 10:J:7:CYS:HA | 10:J:49:MET:HE3 | 1.84 | 0.60 |
| 1:A:339:ASN:O | 1:A:343:LYS:HG2 | 2.01 | 0.60 |
| 2:B:654:ARG:N | 2:B:657:HIS:HD2 | 1.98 | 0.60 |
| 3:C:183:TRP:CZ2 | 3:C:207:CYS:HB3 | 2.37 | 0.60 |
| 9:I:2:THR:HG22 | 9:I:3:THR:H | 1.66 | 0.60 |
| 1:A:172:PRO:HG3 | 1:A:185:TRP:CZ2 | 2.37 | 0.60 |
| 1:A:946:VAL:HG22 | 5:E:201:LYS:HD2 | 1.82 | 0.60 |
| 2:B:127:GLY:C | 2:B:128:LEU:HD12 | 2.22 | 0.60 |
| 2:B:135:ARG:HB2 | 2:B:137:TYR:HE1 | 1.67 | 0.60 |
| 2:B:642:ASP:N | 2:B:649:LYS:HG3 | 2.16 | 0.60 |
| 3:C:261:ALA:HA | 3:C:264:GLN:OE1 | 2.02 | 0.60 |
| 11:K:18:LYS:HZ2 | 11:K:38:GLU:HG2 | 1.66 | 0.60 |
| 11:K:21:ILE:HG22 | 11:K:31:VAL:HG11 | 1.84 | 0.60 |
| 1:A:784:LEU:HB3 | 1:A:785:PRO:HD2 | 1.84 | 0.59 |
| 1:A:845:LEU:HD12 | 1:A:1069:ALA:HB2 | 1.84 | 0.59 |
| 1:A:1315:GLU:C | 1:A:1317:MET:N | 2.55 | 0.59 |
| 3:C:3:GLU:CB | 11:K:104:ASN:HD21 | 2.15 | 0.59 |
| 4:D:56:ARG:HA | 4:D:148:LEU:HD13 | 1.83 | 0.59 |
| 5:E:79:TRP:HE1 | 5:E:81:GLU:HB2 | 1.67 | 0.59 |
| 5:E:136:ASN:O | 5:E:140:LEU:HG | 2.01 | 0.59 |
| 7:G:132:SER:HB3 | 7:G:135:ASP:HB2 | 1.83 | 0.59 |
| 1:A:1157:ASP:C | 1:A:1159:ARG:H | 2.05 | 0.59 |
| 1:A:1187:GLN:O | 1:A:1244:ARG:HG3 | 2.02 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1193:LEU:HD12 | 1:A:1194:ARG:N | 2.17 | 0.59 |
| 2:B:35:SER:O | 2:B:39:ARG:HG3 | 2.02 | 0.59 |
| 2:B:510:LYS:CG | 2:B:511:PRO:HD3 | 2.31 | 0.59 |
| 2:B:604:ARG:C | 2:B:606:LYS:N | 2.55 | 0.59 |
| 2:B:758:PHE:CE2 | 2:B:1044:ALA:HA | 2.37 | 0.59 |
| 2:B:944:THR:HG21 | 2:B:1122:ARG:CZ | 2.32 | 0.59 |
| 2:B:1047:PHE:O | 2:B:1048:THR:HG23 | 2.01 | 0.59 |
| 4:D:50:LEU:HD11 | 7:G:4:ILE:HD11 | 1.83 | 0.59 |
| 4:D:63:LEU:HD12 | 4:D:129:LEU:HG | 1.84 | 0.59 |
| 1:A:56:PRO:O | 1:A:57:ARG:CG | 2.49 | 0.59 |
| 1:A:567:LYS:HZ3 | 8:H:95:TYR:HB2 | 1.67 | 0.59 |
| 2:B:65:GLU:HG3 | 2:B:66:ASP:OD1 | 2.03 | 0.59 |
| 2:B:67:SER:HB2 | 2:B:92:PHE:HD1 | 1.67 | 0.59 |
| 2:B:842:ASN:HD22 | 2:B:845:SER:CB | 2.15 | 0.59 |
| 3:C:18:VAL:HG23 | 3:C:240:VAL:HG12 | 1.82 | 0.59 |
| 5:E:153:HIS:C | 5:E:154:ILE:HG13 | 2.22 | 0.59 |
| 6:F:103:MET:O | 6:F:104:ASN:HB2 | 2.02 | 0.59 |
| 8:H:42:ILE:O | 8:H:44:VAL:HG23 | 2.02 | 0.59 |
| 12:L:34:CYS:O | 12:L:34:CYS:SG | 2.60 | 0.59 |
| 1:A:49:LYS:HE2 | 1:A:61:ILE:HD12 | 1.84 | 0.59 |
| 1:A:115:LEU:CG | 1:A:142:CYS:HB3 | 2.32 | 0.59 |
| 1:A:115:LEU:CD1 | 1:A:142:CYS:HB3 | 2.32 | 0.59 |
| 1:A:697:ALA:HB2 | 1:A:702:LEU:HD12 | 1.84 | 0.59 |
| 1:A:829:VAL:C | 1:A:831:THR:N | 2.56 | 0.59 |
| 1:A:986:ILE:HG22 | 1:A:987:VAL:N | 2.16 | 0.59 |
| 1:A:1277:GLU:O | 1:A:1279:ILE:N | 2.34 | 0.59 |
| 2:B:258:LEU:HB2 | 2:B:385:LEU:HD21 | 1.85 | 0.59 |
| 2:B:992:ILE:CD1 | 11:K:66:PRO:HB2 | 2.32 | 0.59 |
| 4:D:114:MET:HA | 4:D:114:MET:CE | 2.32 | 0.59 |
| 4:D:134:THR:HG22 | 4:D:135:GLY:N | 2.16 | 0.59 |
| 4:D:207:LEU:HA | 4:D:210:ILE:HD12 | 1.85 | 0.59 |
| 5:E:190:LEU:HD13 | 5:E:191:LYS:H | 1.68 | 0.59 |
| 7:G:143:ILE:HG22 | 7:G:144:ARG:N | 2.17 | 0.59 |
| 1:A:337:ARG:HD3 | 1:A:839:ARG:NH2 | 2.18 | 0.59 |
| 1:A:511:ILE:HA | 1:A:521:MET:CE | 2.32 | 0.59 |
| 1:A:564:ALA:O | 8:H:97:MET:HA | 2.02 | 0.59 |
| 1:A:590:ARG:HH11 | 1:A:590:ARG:CG | 2.15 | 0.59 |
| 1:A:756:ILE:O | 1:A:759:ALA:HB3 | 2.01 | 0.59 |
| 1:A:1121:GLU:HG2 | 1:A:1122:PRO:HD2 | 1.84 | 0.59 |
| 2:B:798:TYR:N | 2:B:798:TYR:HD2 | 2.01 | 0.59 |
| 4:D:47:LEU:HD11 | 7:G:3:PHE:CD2 | 2.38 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:G:13:LEU:CD2 | 7:G:17:PHE:HB2 | 2.32 | 0.59 |
| 11:K:7:PHE:HB2 | 11:K:11:LEU:CD2 | 2.31 | 0.59 |
| 1:A:409:SER:O | 1:A:411:ASP:N | 2.36 | 0.59 |
| 1:A:456:MET:CE | 1:A:507:VAL:HG13 | 2.32 | 0.59 |
| 1:A:537:ARG:HD2 | 8:H:20:TYR:CE1 | 2.28 | 0.59 |
| 1:A:666:ILE:CD1 | 1:A:667:GLY:H | 2.10 | 0.59 |
| 1:A:845:LEU:O | 1:A:846:GLU:C | 2.41 | 0.59 |
| 2:B:31:TRP:CE3 | 2:B:31:TRP:HA | 2.37 | 0.59 |
| 2:B:652:LYS:HD3 | 2:B:688:GLY:O | 2.01 | 0.59 |
| 2:B:830:TYR:HE2 | 2:B:1000:PRO:HD3 | 1.66 | 0.59 |
| 2:B:992:ILE:HD11 | 11:K:66:PRO:HB2 | 1.84 | 0.59 |
| 3:C:147:LEU:N | 3:C:147:LEU:HD23 | 2.17 | 0.59 |
| 7:G:30:LEU:HD13 | 7:G:72:VAL:CG1 | 2.32 | 0.59 |
| 11:K:11:LEU:HD22 | 11:K:11:LEU:N | 2.17 | 0.59 |
| 1:A:785:PRO:HG2 | 1:A:786:HIS:HD2 | 1.68 | 0.59 |
| 1:A:853:ASP:OD1 | 1:A:855:THR:HB | 2.03 | 0.59 |
| 1:A:1030:ARG:HG3 | 1:A:1034:GLU:CD | 2.23 | 0.59 |
| 2:B:172:ILE:HD13 | 2:B:178:ASN:ND2 | 2.18 | 0.59 |
| 2:B:235:SER:C | 2:B:236:HIS:HD2 | 2.06 | 0.59 |
| 2:B:331:LEU:CD2 | 2:B:353:LYS:HG2 | 2.33 | 0.59 |
| 2:B:483:LEU:HD11 | 2:B:491:THR:CG2 | 2.32 | 0.59 |
| 2:B:891:ASP:O | 2:B:893:LEU:N | 2.35 | 0.59 |
| 4:D:3:VAL:HG12 | 4:D:4:SER:N | 2.17 | 0.59 |
| 8:H:128:ASN:N | 8:H:130:ARG:NH1 | 2.45 | 0.59 |
| 12:L:27:LEU:HD23 | 12:L:27:LEU:N | 2.13 | 0.59 |
| 1:A:69:THR:C | 1:A:71:GLN:N | 2.55 | 0.59 |
| 1:A:323:LYS:H | 1:A:323:LYS:HD2 | 1.68 | 0.59 |
| 1:A:523:ILE:HB | 1:A:622:VAL:CG2 | 2.33 | 0.59 |
| 1:A:700:ASN:ND2 | 9:I:115:LYS:HD2 | 2.17 | 0.59 |
| 1:A:898:ARG:HD3 | 1:A:933:TYR:CD1 | 2.37 | 0.59 |
| 2:B:123:THR:O | 2:B:125:SER:N | 2.35 | 0.59 |
| 2:B:333:PHE:CE1 | 2:B:337:ARG:NH2 | 2.70 | 0.59 |
| 2:B:498:THR:O | 2:B:536:VAL:HA | 2.03 | 0.59 |
| 2:B:516:ASN:N | 2:B:516:ASN:ND2 | 2.49 | 0.59 |
| 6:F:82:THR:CG2 | 6:F:84:TYR:H | 2.16 | 0.59 |
| 9:I:64:SER:O | 9:I:66:PRO:HD3 | 2.01 | 0.59 |
| 12:L:49:LYS:O | 12:L:50:ASP:HB2 | 2.03 | 0.59 |
| 1:A:401:GLY:C | 1:A:435:HIS:HD2 | 2.05 | 0.59 |
| 1:A:475:THR:CG2 | 1:A:476:SER:H | 2.15 | 0.59 |
| 1:A:1130:GLN:HG3 | 1:A:1134:ILE:HD11 | 1.84 | 0.59 |
| 2:B:557:PHE:HZ | 2:B:603:LEU:HD21 | 1.67 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:563:MET:CE | 2:B:580:VAL:HB | 2.32 | 0.59 |
| 2:B:732:SER:HB2 | 2:B:734:HIS:CE1 | 2.38 | 0.59 |
| 3:C:124:LEU:HD21 | 3:C:129:ILE:O | 2.03 | 0.59 |
| 6:F:138:LEU:HB3 | 6:F:139:PRO:HD2 | 1.84 | 0.59 |
| 10:J:35:ALA:O | 10:J:38:ARG:HB3 | 2.02 | 0.59 |
| 1:A:208:LEU:HD23 | 1:A:208:LEU:C | 2.24 | 0.59 |
| 1:A:353:ILE:HG21 | 1:A:487:MET:HE3 | 1.84 | 0.59 |
| 1:A:528:LEU:O | 1:A:528:LEU:HD12 | 2.02 | 0.59 |
| 1:A:567:LYS:HD2 | 8:H:95:TYR:CG | 2.38 | 0.59 |
| 1:A:731:ARG:HG3 | 1:A:755:PHE:CE1 | 2.38 | 0.59 |
| 1:A:867:ILE:HG22 | 1:A:872:GLY:H | 1.66 | 0.59 |
| 2:B:180:TYR:H | 2:B:180:TYR:HD1 | 1.51 | 0.59 |
| 2:B:308:TRP:HA | 2:B:311:LEU:HD12 | 1.84 | 0.59 |
| 2:B:956:THR:HG22 | 2:B:957:ASN:H | 1.68 | 0.59 |
| 2:B:1215:ARG:CZ | 4:D:15:LEU:HD21 | 2.33 | 0.59 |
| 3:C:112:ASN:CB | 3:C:114:TYR:HE1 | 2.15 | 0.59 |
| 4:D:40:HIS:HB3 | 7:G:6:ASP:HB3 | 1.85 | 0.59 |
| 5:E:182:ASP:O | 5:E:185:ALA:HB3 | 2.03 | 0.59 |
| 8:H:95:TYR:O | 8:H:143:LEU:HA | 2.03 | 0.59 |
| 9:I:95:THR:HG22 | 9:I:96:SER:O | 2.03 | 0.59 |
| 1:A:340:LEU:HD21 | 2:B:1199:ALA:HB3 | 1.85 | 0.58 |
| 1:A:471:ASN:OD1 | 1:A:472:LEU:N | 2.36 | 0.58 |
| 1:A:1445:ILE:HD12 | 7:G:59:GLY:O | 2.03 | 0.58 |
| 2:B:864:LYS:HB2 | 2:B:872:GLU:HG3 | 1.85 | 0.58 |
| 8:H:64:ASN:ND2 | 8:H:88:SER:HB2 | 2.18 | 0.58 |
| 8:H:110:ASP:HB2 | 8:H:128:ASN:ND2 | 2.17 | 0.58 |
| 1:A:164:ARG:HG3 | 1:A:165:GLY:H | 1.68 | 0.58 |
| 1:A:1173:HIS:ND1 | 1:A:1173:HIS:O | 2.36 | 0.58 |
| 1:A:1224:LEU:HG | 1:A:1226:VAL:HG23 | 1.85 | 0.58 |
| 2:B:553:PRO:O | 2:B:557:PHE:HB2 | 2.03 | 0.58 |
| 2:B:797:TYR:HB3 | 2:B:798:TYR:CD2 | 2.39 | 0.58 |
| 2:B:1006:ILE:HG23 | 10:J:43:ARG:HG3 | 1.85 | 0.58 |
| 3:C:82:TYR:CE1 | 3:C:161:LYS:HG2 | 2.37 | 0.58 |
| 3:C:232:VAL:HG21 | 3:C:244:VAL:HG22 | 1.84 | 0.58 |
| 4:D:59:ILE:O | 4:D:63:LEU:HB2 | 2.03 | 0.58 |
| 5:E:67:GLU:O | 5:E:70:SER:HB2 | 2.03 | 0.58 |
| 1:A:23:SER:HA | 1:A:233:TRP:CD1 | 2.38 | 0.58 |
| 1:A:523:ILE:HB | 1:A:622:VAL:HG22 | 1.85 | 0.58 |
| 1:A:590:ARG:O | 1:A:591:PHE:HB2 | 2.03 | 0.58 |
| 2:B:25:ILE:HD11 | 2:B:653:VAL:O | 2.03 | 0.58 |
| 2:B:164:LYS:N | 2:B:164:LYS:HD3 | 2.18 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:274:PRO:CG | 2:B:359:GLU:HB3 | 2.32 | 0.58 |
| 2:B:827:ILE:O | 2:B:1085:ILE:HG23 | 2.03 | 0.58 |
| 4:D:127:ASP:OD2 | 4:D:142:LYS:HE3 | 2.02 | 0.58 |
| 5:E:85:GLU:O | 5:E:88:VAL:HG23 | 2.03 | 0.58 |
| 7:G:106:MET:HG2 | 7:G:107:LYS:N | 2.18 | 0.58 |
| 1:A:525:GLN:OE1 | 2:B:836:GLU:HG2 | 2.02 | 0.58 |
| 1:A:709:THR:HG22 | 1:A:710:LEU:N | 2.18 | 0.58 |
| 2:B:20:ASP:O | 2:B:22:SER:N | 2.35 | 0.58 |
| 2:B:56:ASP:HB2 | 2:B:57:TYR:CD1 | 2.38 | 0.58 |
| 2:B:357:GLN:HG2 | 2:B:366:GLN:O | 2.04 | 0.58 |
| 2:B:515:HIS:H | 2:B:518:HIS:HD2 | 1.49 | 0.58 |
| 2:B:1169:MET:HE3 | 2:B:1201:LYS:HG2 | 1.84 | 0.58 |
| 4:D:116:SER:O | 4:D:118:THR:HG23 | 2.03 | 0.58 |
| 5:E:22:MET:HG3 | 5:E:187:TYR:CD1 | 2.38 | 0.58 |
| 7:G:91:VAL:HG23 | 7:G:141:SER:O | 2.03 | 0.58 |
| 8:H:5:LEU:O | 8:H:133:ASN:HB3 | 2.03 | 0.58 |
| 1:A:164:ARG:HG3 | 1:A:165:GLY:N | 2.18 | 0.58 |
| 1:A:295:LEU:O | 1:A:298:PHE:HB3 | 2.03 | 0.58 |
| 1:A:853:ASP:OD1 | 1:A:855:THR:N | 2.33 | 0.58 |
| 1:A:901:LEU:HD11 | 1:A:983:ILE:HD13 | 1.85 | 0.58 |
| 1:A:901:LEU:HG | 1:A:926:GLN:HE21 | 1.67 | 0.58 |
| 1:A:1101:LEU:HD12 | 1:A:1101:LEU:C | 2.23 | 0.58 |
| 6:F:117:PRO:C | 6:F:119:ARG:H | 2.06 | 0.58 |
| 1:A:278:THR:HG23 | 1:A:282:ASN:ND2 | 2.19 | 0.58 |
| 1:A:1036:ARG:HG2 | 1:A:1036:ARG:NH1 | 2.19 | 0.58 |
| 2:B:603:LEU:HB3 | 2:B:609:ILE:HD11 | 1.86 | 0.58 |
| 2:B:615:MET:HA | 2:B:625:LYS:O | 2.04 | 0.58 |
| 2:B:811:TYR:N | 2:B:811:TYR:CD1 | 2.71 | 0.58 |
| 2:B:916:THR:HB | 2:B:935:ARG:HG3 | 1.86 | 0.58 |
| 2:B:1115:THR:HG22 | 2:B:1117:GLN:HG3 | 1.85 | 0.58 |
| 2:B:1163:CYS:HB2 | 2:B:1182:CYS:SG | 2.43 | 0.58 |
| 4:D:49:ALA:HB1 | 4:D:178:ALA:HB2 | 1.86 | 0.58 |
| 7:G:140:LYS:O | 7:G:141:SER:C | 2.42 | 0.58 |
| 9:I:50:THR:HB | 9:I:92:ARG:NH1 | 2.18 | 0.58 |
| 12:L:30:ILE:C | 12:L:56:LEU:HD23 | 2.24 | 0.58 |
| 1:A:427:GLN:HB2 | 1:A:430:TRP:CG | 2.39 | 0.58 |
| 1:A:456:MET:HE1 | 1:A:507:VAL:HG13 | 1.86 | 0.58 |
| 1:A:583:PRO:O | 1:A:610:GLY:HA3 | 2.03 | 0.58 |
| 1:A:774:ARG:O | 1:A:775:ILE:C | 2.41 | 0.58 |
| 1:A:814:PHE:CE1 | 2:B:519:TRP:HA | 2.38 | 0.58 |
| 1:A:998:LEU:H | 1:A:998:LEU:HD12 | 1.69 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:326:ASP:C | 2:B:328:GLU:H | 2.06 | 0.58 |
| 2:B:641:GLU:HB2 | 2:B:643:ASP:OD2 | 2.03 | 0.58 |
| 2:B:798:TYR:N | 2:B:798:TYR:CD2 | 2.72 | 0.58 |
| 5:E:98:ILE:HG22 | 5:E:102:GLU:HG3 | 1.86 | 0.58 |
| 10:J:39:LEU:HD12 | 10:J:39:LEU:N | 2.18 | 0.58 |
| 1:A:2:VAL:HG11 | 2:B:1157:ALA:CB | 2.33 | 0.58 |
| 1:A:335:ARG:HA | 1:A:339:ASN:HD22 | 1.69 | 0.58 |
| 1:A:860:LEU:HD11 | 1:A:1393:ASN:ND2 | 2.18 | 0.58 |
| 1:A:860:LEU:O | 2:B:1224:PHE:HE2 | 1.86 | 0.58 |
| 1:A:984:LYS:O | 1:A:988:LEU:HB2 | 2.04 | 0.58 |
| 1:A:1143:LEU:HD23 | 1:A:1267:MET:HB3 | 1.85 | 0.58 |
| 2:B:274:PRO:HG2 | 2:B:359:GLU:HB3 | 1.85 | 0.58 |
| 2:B:918:ILE:HG22 | 2:B:919:SER:N | 2.19 | 0.58 |
| 2:B:1177:HIS:CB | 2:B:1179:GLN:HE21 | 2.17 | 0.58 |
| 5:E:99:HIS:CE1 | 5:E:103:LYS:HG3 | 2.39 | 0.58 |
| 7:G:88:ASP:CB | 7:G:144:ARG:HA | 2.33 | 0.58 |
| 1:A:17:VAL:HB | 1:A:1419:ASP:HB3 | 1.84 | 0.58 |
| 1:A:180:LYS:NZ | 1:A:294:SER:HB3 | 2.16 | 0.58 |
| 1:A:317:LYS:HA | 2:B:471:LYS:HE2 | 1.86 | 0.58 |
| 1:A:568:PRO:CG | 8:H:46:LEU:HD22 | 2.29 | 0.58 |
| 2:B:345:LYS:C | 2:B:348:ARG:HG2 | 2.24 | 0.58 |
| 2:B:1006:ILE:HD13 | 10:J:44:TYR:CE2 | 2.39 | 0.58 |
| 1:A:7:SER:C | 1:A:9:ALA:H | 2.07 | 0.58 |
| 1:A:947:PHE:CE2 | 1:A:954:TRP:CE2 | 2.92 | 0.58 |
| 1:A:1197:LEU:HD11 | 1:A:1238:ILE:HD11 | 1.86 | 0.58 |
| 2:B:95:ILE:HB | 2:B:130:VAL:HG22 | 1.85 | 0.58 |
| 2:B:479:VAL:HG12 | 2:B:480:SER:H | 1.69 | 0.58 |
| 2:B:708:GLU:O | 2:B:710:LEU:N | 2.36 | 0.58 |
| 2:B:770:GLN:OE1 | 2:B:983:ARG:HA | 2.04 | 0.58 |
| 2:B:899:ILE:CG2 | 2:B:949:VAL:HG21 | 2.34 | 0.58 |
| 2:B:918:ILE:HD12 | 2:B:935:ARG:NH1 | 2.19 | 0.58 |
| 7:G:85:GLU:HB3 | 7:G:147:ILE:HD12 | 1.86 | 0.58 |
| 13:T:7:DC:H2" | 13:T:8:DT:C7 | 2.34 | 0.58 |
| 1:A:265:LYS:O | 1:A:269:ILE:HG13 | 2.04 | 0.57 |
| 1:A:302:THR:HA | 1:A:305:ASP:O | 2.04 | 0.57 |
| 1:A:353:ILE:HG21 | 1:A:487:MET:HG3 | 1.84 | 0.57 |
| 1:A:381:THR:C | 1:A:383:TYR:N | 2.56 | 0.57 |
| 1:A:825:ILE:CD1 | 2:B:512:ARG:HB3 | 2.15 | 0.57 |
| 2:B:216:GLU:OE1 | 2:B:537:LYS:HE3 | 2.04 | 0.57 |
| 2:B:615:MET:O | 2:B:697:GLU:HG3 | 2.04 | 0.57 |
| 2:B:1181:GLU:H | 2:B:1188:LYS:HG3 | 1.69 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:34:ARG:O | 3:C:38:ILE:HG13 | 2.04 | 0.57 |
| 3:C:112:ASN:CB | 3:C:114:TYR:CE1 | 2.87 | 0.57 |
| 3:C:189:THR:HG22 | 3:C:190:ASP:N | 2.19 | 0.57 |
| 4:D:25:ALA:C | 4:D:27:LEU:H | 2.08 | 0.57 |
| 6:F:85:MET:HB3 | 6:F:155:LEU:HD11 | 1.86 | 0.57 |
| 9:I:51:ASN:O | 9:I:54:GLU:HG3 | 2.03 | 0.57 |
| 10:J:44:TYR:CD2 | 10:J:44:TYR:N | 2.69 | 0.57 |
| 1:A:62:ASP:O | 1:A:63:ARG:C | 2.42 | 0.57 |
| 1:A:147:VAL:HG13 | 1:A:168:GLY:O | 2.04 | 0.57 |
| 1:A:434:ARG:HG2 | 1:A:434:ARG:HH11 | 1.69 | 0.57 |
| 1:A:1035:TYR:O | 1:A:1036:ARG:C | 2.41 | 0.57 |
| 2:B:953:LEU:HB3 | 12:L:57:LEU:HD23 | 1.86 | 0.57 |
| 1:A:469:ARG:NH1 | 1:A:469:ARG:HB3 | 2.19 | 0.57 |
| 1:A:523:ILE:CG2 | 1:A:527:THR:HB | 2.34 | 0.57 |
| 1:A:1053:PHE:O | 1:A:1056:SER:N | 2.37 | 0.57 |
| 1:A:1427:ASN:O | 1:A:1430:LEU:N | 2.37 | 0.57 |
| 2:B:1165:ILE:CD1 | 4:D:17:LYS:HD3 | 2.34 | 0.57 |
| 3:C:66:ARG:NH1 | 10:J:2:ILE:CG2 | 2.67 | 0.57 |
| 3:C:167:HIS:CD2 | 12:L:70:ARG:HB3 | 2.39 | 0.57 |
| 6:F:85:MET:HB3 | 6:F:155:LEU:CD1 | 2.34 | 0.57 |
| 1:A:826:ASP:HB2 | 1:A:830:LYS:HD3 | 1.86 | 0.57 |
| 1:A:864:ILE:HG21 | 1:A:1374:VAL:HG22 | 1.85 | 0.57 |
| 1:A:897:TYR:CD2 | 1:A:936:LEU:HD13 | 2.27 | 0.57 |
| 2:B:39:ARG:HG2 | 2:B:39:ARG:HH11 | 1.69 | 0.57 |
| 2:B:487:THR:CG2 | 2:B:488:TYR:N | 2.66 | 0.57 |
| 2:B:1178:ASN:O | 2:B:1179:GLN:C | 2.43 | 0.57 |
| 3:C:24:ASN:O | 3:C:25:VAL:HG13 | 2.04 | 0.57 |
| 3:C:100:THR:HG22 | 3:C:101:LEU:N | 2.19 | 0.57 |
| 9:I:76:PRO:HD2 | 9:I:108:HIS:CD2 | 2.36 | 0.57 |
| 11:K:49:GLU:HG3 | 11:K:94:ILE:HG12 | 1.87 | 0.57 |
| 1:A:41:MET:O | 1:A:42:ASP:O | 2.23 | 0.57 |
| 1:A:67:CYS:C | 1:A:68:GLN:HG3 | 2.23 | 0.57 |
| 1:A:618:GLU:O | 1:A:620:LYS:N | 2.38 | 0.57 |
| 1:A:701:LEU:O | 1:A:702:LEU:HG | 2.03 | 0.57 |
| 1:A:709:THR:HG21 | 9:I:93:LYS:O | 2.04 | 0.57 |
| 1:A:775:ILE:HD12 | 1:A:818:MET:SD | 2.44 | 0.57 |
| 1:A:804:TYR:HE1 | 2:B:1021:MET:HE3 | 1.69 | 0.57 |
| 1:A:896:ARG:HH21 | 1:A:1030:ARG:NE | 2.01 | 0.57 |
| 1:A:1017:LEU:HD23 | 5:E:204:THR:O | 2.05 | 0.57 |
| 1:A:1100:ARG:O | 1:A:1103:GLU:HB3 | 2.04 | 0.57 |
| 1:A:1142:THR:HB | 1:A:1271:ILE:O | 2.04 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:640:VAL:HG13 | 2:B:650:GLU:C | 2.24 | 0.57 |
| 2:B:640:VAL:CG2 | 2:B:651:LEU:HD23 | 2.32 | 0.57 |
| 2:B:642:ASP:HB3 | 2:B:649:LYS:HG3 | 1.86 | 0.57 |
| 2:B:1167:GLY:HA3 | 2:B:1216:LEU:H | 1.68 | 0.57 |
| 5:E:106:GLN:HA | 5:E:130:ALA:CB | 2.35 | 0.57 |
| 6:F:74:ILE:HD12 | 6:F:144:GLU:HG3 | 1.85 | 0.57 |
| 7:G:91:VAL:HB | 7:G:139:ILE:O | 2.05 | 0.57 |
| 10:J:23:ASN:C | 10:J:25:LEU:N | 2.58 | 0.57 |
| 1:A:189:ARG:O | 1:A:190:ALA:HB3 | 2.05 | 0.57 |
| 1:A:1445:ILE:HD12 | 1:A:1445:ILE:N | 2.09 | 0.57 |
| 2:B:204:ILE:C | 2:B:205:ILE:HD12 | 2.24 | 0.57 |
| 2:B:265:SER:O | 2:B:267:ARG:N | 2.37 | 0.57 |
| 2:B:351:TYR:CE1 | 2:B:355:ILE:HD11 | 2.40 | 0.57 |
| 2:B:1121:GLY:HA2 | 13:T:22:DC:OP2 | 2.05 | 0.57 |
| 3:C:18:VAL:HG12 | 3:C:20:PHE:HD2 | 1.70 | 0.57 |
| 4:D:60:LYS:HZ3 | 4:D:115:HIS:CE1 | 2.22 | 0.57 |
| 5:E:10:SER:O | 5:E:13:TRP:HB3 | 2.04 | 0.57 |
| 5:E:85:GLU:C | 5:E:87:SER:H | 2.08 | 0.57 |
| 5:E:178:ILE:HB | 5:E:212:ARG:HD2 | 1.86 | 0.57 |
| 6:F:132:LEU:CD2 | 7:G:61:ILE:HD11 | 2.34 | 0.57 |
| 7:G:44:TYR:HE1 | 7:G:157:ILE:H | 1.52 | 0.57 |
| 1:A:590:ARG:HG2 | 1:A:591:PHE:N | 2.19 | 0.57 |
| 1:A:1322:ILE:O | 1:A:1324:PRO:HD3 | 2.05 | 0.57 |
| 2:B:603:LEU:CD1 | 2:B:608:ASP:HB3 | 2.34 | 0.57 |
| 2:B:794:ASN:C | 2:B:795:ILE:HD12 | 2.24 | 0.57 |
| 2:B:950:ASP:O | 2:B:951:GLN:HB3 | 2.04 | 0.57 |
| 3:C:164:ALA:HA | 3:C:167:HIS:O | 2.04 | 0.57 |
| 4:D:31:GLN:O | 4:D:34:GLN:HG3 | 2.03 | 0.57 |
| 7:G:51:TYR:O | 7:G:54:ILE:HG13 | 2.04 | 0.57 |
| 7:G:146:LYS:HB2 | 7:G:168:LEU:HD11 | 1.84 | 0.57 |
| 13:T:25:DG:H2' | 13:T:26:DT:H5' | 1.86 | 0.57 |
| 1:A:11:LEU:HB2 | 2:B:1193:GLN:O | 2.04 | 0.57 |
| 1:A:356:ASP:OD2 | 11:K:65:HIS:HE1 | 1.87 | 0.57 |
| 1:A:416:ARG:HG3 | 1:A:417:TYR:CE2 | 2.39 | 0.57 |
| 1:A:470:LEU:CD1 | 1:A:487:MET:HE1 | 2.31 | 0.57 |
| 1:A:873:MET:C | 1:A:1058:VAL:HG23 | 2.24 | 0.57 |
| 3:C:82:TYR:CD1 | 3:C:161:LYS:HG2 | 2.40 | 0.57 |
| 4:D:130:LEU:C | 4:D:132:GLN:H | 2.08 | 0.57 |
| 6:F:109:VAL:HG12 | 6:F:110:ASP:H | 1.67 | 0.57 |
| 8:H:11:GLN:O | 8:H:28:ALA:HB1 | 2.05 | 0.57 |
| 8:H:26:ILE:HD13 | 8:H:49:VAL:HG11 | 1.87 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 10:J:1:MET:H1 | 10:J:56:LEU:HB2 | 1.69 | 0.57 |
| 13:T:24:DG:H2' | 13:T:25:DG:C8 | 2.40 | 0.57 |
| 1:A:860:LEU:HD11 | 1:A:1393:ASN:HD22 | 1.69 | 0.57 |
| 1:A:898:ARG:HD2 | 1:A:899:VAL:H | 1.68 | 0.57 |
| 1:A:1453:TYR:CE2 | 6:F:129:LYS:HA | 2.39 | 0.57 |
| 2:B:558:LEU:HD21 | 2:B:600:LEU:HD11 | 1.87 | 0.57 |
| 4:D:159:THR:O | 4:D:163:VAL:HG23 | 2.05 | 0.57 |
| 7:G:18:PHE:HA | 7:G:22:MET:HE3 | 1.86 | 0.57 |
| 7:G:115:MET:HB2 | 7:G:116:PRO:HD2 | 1.86 | 0.57 |
| 9:I:58:VAL:O | 9:I:58:VAL:HG12 | 2.03 | 0.57 |
| 1:A:236:LEU:N | 1:A:236:LEU:HD23 | 2.20 | 0.57 |
| 1:A:331:GLY:O | 1:A:332:LYS:HB3 | 2.05 | 0.57 |
| 1:A:336:ILE:HD13 | 1:A:340:LEU:HD12 | 1.86 | 0.57 |
| 1:A:682:THR:HG23 | 1:A:728:LYS:HE3 | 1.85 | 0.57 |
| 1:A:1106:ASN:O | 1:A:1107:VAL:HB | 2.04 | 0.57 |
| 2:B:186:GLU:CG | 10:J:62:ARG:HH22 | 2.18 | 0.57 |
| 2:B:648:HIS:CG | 2:B:649:LYS:N | 2.71 | 0.57 |
| 2:B:653:VAL:CG2 | 2:B:689:LEU:HB3 | 2.33 | 0.57 |
| 2:B:864:LYS:HG3 | 2:B:872:GLU:OE1 | 2.04 | 0.57 |
| 3:C:36:VAL:HG21 | 3:C:251:LEU:CD1 | 2.35 | 0.57 |
| 3:C:214:ASN:HB3 | 3:C:217:ASP:OD2 | 2.04 | 0.57 |
| 4:D:214:LEU:C | 4:D:216:ASN:H | 2.09 | 0.57 |
| 6:F:87:LYS:HA | 6:F:155:LEU:HD22 | 1.87 | 0.57 |
| 7:G:15:PRO:HA | 7:G:18:PHE:CE1 | 2.39 | 0.57 |
| 7:G:127:PRO:HG3 | 7:G:139:ILE:HG13 | 1.86 | 0.57 |
| 1:A:567:LYS:NZ | 8:H:47:PHE:HB2 | 2.20 | 0.56 |
| 1:A:768:GLN:CG | 1:A:816:HIS:HA | 2.17 | 0.56 |
| 1:A:1293:SER:OG | 1:A:1295:THR:HG23 | 2.05 | 0.56 |
| 2:B:126:SER:CB | 2:B:172:ILE:HD11 | 2.34 | 0.56 |
| 2:B:165:VAL:HG12 | 2:B:166:PHE:N | 2.20 | 0.56 |
| 2:B:1116:ARG:HG3 | 2:B:1198:TYR:CE2 | 2.40 | 0.56 |
| 2:B:1130:PHE:CE1 | 2:B:1134:GLU:HB3 | 2.40 | 0.56 |
| 3:C:132:PRO:O | 3:C:134:ILE:HG13 | 2.05 | 0.56 |
| 3:C:229:TYR:N | 3:C:229:TYR:CD1 | 2.72 | 0.56 |
| 5:E:22:MET:HE3 | 5:E:26:ARG:HD2 | 1.86 | 0.56 |
| 5:E:59:SER:HB3 | 5:E:81:GLU:HA | 1.85 | 0.56 |
| 5:E:180:ARG:HH21 | 5:E:192:ARG:HD2 | 1.70 | 0.56 |
| 6:F:75:PRO:O | 6:F:77:ASP:O | 2.23 | 0.56 |
| 1:A:167:CYS:HB2 | 1:A:169:ASN:ND2 | 2.20 | 0.56 |
| 1:A:542:GLU:O | 1:A:546:VAL:HG23 | 2.05 | 0.56 |
| 1:A:1161:THR:C | 1:A:1163:ILE:H | 2.07 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:750:GLY:O | 2:B:751:VAL:C | 2.42 | 0.56 |
| 3:C:212:PRO:CB | 3:C:213:PRO:HD2 | 2.35 | 0.56 |
| 9:I:4:PHE:CE1 | 9:I:6:PHE:HE2 | 2.23 | 0.56 |
| 1:A:37:PHE:HB2 | 1:A:52:GLY:HA3 | 1.86 | 0.56 |
| 1:A:134:ARG:HG2 | 1:A:138:ILE:CD1 | 2.31 | 0.56 |
| 1:A:388:LEU:O | 1:A:392:VAL:HG23 | 2.05 | 0.56 |
| 1:A:503:GLN:HE21 | 6:F:90:ARG:HH21 | 1.54 | 0.56 |
| 1:A:584:ASN:C | 1:A:586:ILE:H | 2.07 | 0.56 |
| 1:A:639:PRO:HG2 | 1:A:640:GLN:N | 2.20 | 0.56 |
| 1:A:794:PRO:HG2 | 1:A:795:GLU:OE2 | 2.06 | 0.56 |
| 1:A:798:GLY:HA2 | 1:A:815:PHE:HD1 | 1.69 | 0.56 |
| 1:A:828:ALA:CB | 2:B:530:GLY:HA2 | 2.36 | 0.56 |
| 1:A:865:GLN:HE21 | 1:A:1370:LEU:HA | 1.71 | 0.56 |
| 1:A:881:GLN:NE2 | 1:A:958:VAL:O | 2.39 | 0.56 |
| 1:A:1226:VAL:HG22 | 1:A:1240:CYS:HB3 | 1.87 | 0.56 |
| 2:B:299:GLU:CB | 2:B:571:PRO:HG3 | 2.32 | 0.56 |
| 2:B:343:ILE:HD12 | 2:B:347:LYS:NZ | 2.21 | 0.56 |
| 2:B:465:ASN:HB3 | 2:B:475:SER:OG | 2.05 | 0.56 |
| 2:B:604:ARG:NH2 | 2:B:613:VAL:O | 2.35 | 0.56 |
| 2:B:839:MET:HG3 | 2:B:1010:LEU:HD11 | 1.87 | 0.56 |
| 2:B:997:GLU:CD | 2:B:997:GLU:H | 2.06 | 0.56 |
| 2:B:1017:ILE:CB | 2:B:1018:PRO:HD3 | 2.33 | 0.56 |
| 3:C:61:GLU:HA | 3:C:64:ALA:HB3 | 1.86 | 0.56 |
| 4:D:3:VAL:CG2 | 7:G:10:ASN:HB2 | 2.32 | 0.56 |
| 5:E:9:ILE:HD11 | 5:E:53:PRO:HD3 | 1.88 | 0.56 |
| 5:E:156:LEU:HD12 | 5:E:195:VAL:CB | 2.31 | 0.56 |
| 7:G:34:VAL:HG12 | 7:G:45:ILE:HG21 | 1.85 | 0.56 |
| 7:G:35:GLU:HG2 | 7:G:48:VAL:HG23 | 1.88 | 0.56 |
| 7:G:127:PRO:HG3 | 7:G:139:ILE:HD11 | 1.85 | 0.56 |
| 8:H:118:PHE:C | 8:H:120:GLY:H | 2.07 | 0.56 |
| 8:H:127:GLY:O | 8:H:128:ASN:HB2 | 2.05 | 0.56 |
| 9:I:71:SER:HG | 9:I:101:PHE:HD2 | 1.53 | 0.56 |
| 9:I:106:CYS:O | 9:I:107:SER:HB2 | 2.05 | 0.56 |
| 10:J:36:LEU:HD12 | 10:J:47:ARG:NH1 | 2.20 | 0.56 |
| 12:L:60:ARG:NH2 | 12:L:65:VAL:HG21 | 2.20 | 0.56 |
| 13:T:21:DC:H2'' | 13:T:22:DC:C5' | 2.35 | 0.56 |
| 1:A:35:ILE:HA | 1:A:52:GLY:O | 2.06 | 0.56 |
| 1:A:69:THR:C | 1:A:71:GLN:H | 2.07 | 0.56 |
| 1:A:108:MET:N | 1:A:108:MET:SD | 2.78 | 0.56 |
| 1:A:140:THR:HA | 1:A:143:LYS:HE2 | 1.87 | 0.56 |
| 1:A:477:PRO:CG | 1:A:521:MET:HG2 | 2.35 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:503:GLN:HE21 | 6:F:90:ARG:NH2 | 2.04 | 0.56 |
| 1:A:711:ARG:O | 1:A:714:PHE:HB3 | 2.05 | 0.56 |
| 2:B:879:ARG:O | 2:B:934:LYS:HE2 | 2.05 | 0.56 |
| 2:B:957:ASN:O | 2:B:957:ASN:CG | 2.42 | 0.56 |
| 4:D:155:ARG:HD3 | 4:D:221:TYR:CE1 | 2.40 | 0.56 |
| 5:E:17:ARG:HH11 | 5:E:17:ARG:CB | 2.14 | 0.56 |
| 9:I:101:PHE:N | 9:I:101:PHE:CD1 | 2.73 | 0.56 |
| 1:A:1313:LEU:HD11 | 1:A:1317:MET:HE2 | 1.87 | 0.56 |
| 2:B:616:ILE:HG12 | 2:B:697:GLU:HA | 1.85 | 0.56 |
| 3:C:243:VAL:O | 3:C:243:VAL:HG12 | 2.05 | 0.56 |
| 1:A:993:LEU:HD22 | 1:A:1046:LEU:HD22 | 1.86 | 0.56 |
| 1:A:1050:GLU:O | 1:A:1053:PHE:HB3 | 2.05 | 0.56 |
| 1:A:1322:ILE:O | 1:A:1322:ILE:HG13 | 2.06 | 0.56 |
| 2:B:235:SER:HB3 | 2:B:258:LEU:HG | 1.88 | 0.56 |
| 2:B:603:LEU:HB3 | 2:B:609:ILE:CD1 | 2.35 | 0.56 |
| 2:B:792:MET:HA | 2:B:856:PHE:O | 2.05 | 0.56 |
| 3:C:89:GLU:O | 3:C:90:ASP:CB | 2.54 | 0.56 |
| 3:C:169:LYS:HE3 | 3:C:170:TRP:CH2 | 2.40 | 0.56 |
| 4:D:217:LEU:O | 4:D:219:THR:N | 2.39 | 0.56 |
| 7:G:29:LYS:HD2 | 7:G:32:GLU:OE1 | 2.06 | 0.56 |
| 8:H:99:GLY:HA3 | 8:H:117:SER:O | 2.06 | 0.56 |
| 10:J:34:THR:O | 10:J:35:ALA:C | 2.44 | 0.56 |
| 1:A:64:ASN:H | 1:A:74:MET:CE | 2.19 | 0.56 |
| 1:A:821:ARG:HB2 | 1:A:821:ARG:NH1 | 2.20 | 0.56 |
| 3:C:2:SER:O | 3:C:3:GLU:HB2 | 2.05 | 0.56 |
| 3:C:39:ALA:HA | 3:C:164:ALA:CB | 2.31 | 0.56 |
| 9:I:50:THR:CG2 | 9:I:52:ILE:HG12 | 2.35 | 0.56 |
| 1:A:57:ARG:O | 1:A:58:LEU:O | 2.23 | 0.56 |
| 1:A:93:VAL:CG2 | 1:A:301:ALA:HA | 2.34 | 0.56 |
| 1:A:332:LYS:HG3 | 1:A:333:GLU:CD | 2.26 | 0.56 |
| 1:A:500:GLU:OE2 | 1:A:1438:THR:HG21 | 2.06 | 0.56 |
| 1:A:715:GLU:OE1 | 1:A:774:ARG:HD3 | 2.05 | 0.56 |
| 1:A:1029:ARG:HH11 | 1:A:1029:ARG:HG3 | 1.71 | 0.56 |
| 1:A:1141:THR:HA | 1:A:1205:LYS:HZ3 | 1.71 | 0.56 |
| 1:A:1356:ILE:HD12 | 1:A:1368:MET:SD | 2.46 | 0.56 |
| 2:B:613:VAL:HG13 | 2:B:627:PHE:C | 2.26 | 0.56 |
| 2:B:785:TYR:CE1 | 2:B:795:ILE:HG12 | 2.41 | 0.56 |
| 2:B:824:ILE:HG22 | 2:B:1087:PHE:HE2 | 1.71 | 0.56 |
| 3:C:138:GLU:OE1 | 3:C:138:GLU:N | 2.39 | 0.56 |
| 3:C:242:GLN:C | 3:C:244:VAL:H | 2.07 | 0.56 |
| 8:H:84:ALA:O | 8:H:89:LEU:HD21 | 2.06 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 8:H:98:TYR:HE1 | 8:H:139:ASN:HA | 1.69 | 0.56 |
| 1:A:269:ILE:CG1 | 1:A:299:HIS:HB3 | 2.31 | 0.56 |
| 1:A:1220:PHE:O | 1:A:1221:LYS:HB2 | 2.06 | 0.56 |
| 2:B:707:PRO:HA | 2:B:741:CYS:SG | 2.46 | 0.56 |
| 2:B:973:ILE:CG2 | 2:B:974:PRO:HD2 | 2.36 | 0.56 |
| 5:E:117:THR:HB | 5:E:120:ALA:HB2 | 1.86 | 0.56 |
| 6:F:86:THR:HG23 | 6:F:89:GLU:OE1 | 2.05 | 0.56 |
| 1:A:125:ALA:C | 1:A:127:ALA:H | 2.08 | 0.56 |
| 1:A:172:PRO:HB3 | 1:A:185:TRP:CE3 | 2.41 | 0.56 |
| 1:A:340:LEU:CD2 | 2:B:1199:ALA:HB3 | 2.36 | 0.56 |
| 1:A:899:VAL:HG13 | 1:A:908:LEU:CD2 | 2.32 | 0.56 |
| 1:A:1289:ARG:HD2 | 1:A:1303:GLU:OE2 | 2.06 | 0.56 |
| 1:A:1437:GLY:O | 1:A:1439:GLY:N | 2.39 | 0.56 |
| 2:B:562:GLY:HA3 | 2:B:590:HIS:ND1 | 2.21 | 0.56 |
| 2:B:834:ASN:CA | 2:B:838:SER:O | 2.54 | 0.56 |
| 2:B:1147:LEU:C | 2:B:1147:LEU:HD23 | 2.26 | 0.56 |
| 2:B:1169:MET:HE1 | 2:B:1201:LYS:HA | 1.88 | 0.56 |
| 3:C:18:VAL:HG12 | 3:C:18:VAL:O | 2.05 | 0.56 |
| 10:J:1:MET:H1 | 10:J:56:LEU:N | 2.02 | 0.56 |
| 10:J:24:LEU:O | 10:J:30:LEU:HB2 | 2.06 | 0.56 |
| 11:K:68:PHE:HB3 | 11:K:70:ARG:HH11 | 1.70 | 0.56 |
| 1:A:61:ILE:HG22 | 1:A:62:ASP:N | 2.21 | 0.55 |
| 1:A:567:LYS:HB3 | 1:A:568:PRO:CD | 2.36 | 0.55 |
| 1:A:919:ILE:HG21 | 1:A:983:ILE:HD11 | 1.88 | 0.55 |
| 2:B:402:GLY:HA2 | 2:B:695:ALA:HB3 | 1.87 | 0.55 |
| 2:B:467:GLY:O | 2:B:469:GLN:N | 2.39 | 0.55 |
| 3:C:58:LEU:HD22 | 3:C:58:LEU:N | 2.21 | 0.55 |
| 3:C:77:ILE:HG23 | 3:C:161:LYS:NZ | 2.21 | 0.55 |
| 5:E:114:ASN:O | 5:E:115:ASN:CB | 2.47 | 0.55 |
| 5:E:128:PRO:HA | 5:E:129:PRO:C | 2.25 | 0.55 |
| 5:E:136:ASN:OD1 | 5:E:137:GLU:N | 2.38 | 0.55 |
| 8:H:100:THR:CG2 | 8:H:101:ALA:N | 2.70 | 0.55 |
| 1:A:150:THR:HG22 | 1:A:150:THR:O | 2.05 | 0.55 |
| 1:A:818:MET:HG2 | 2:B:514:LEU:HG | 1.87 | 0.55 |
| 1:A:849:MET:HB2 | 1:A:1062:GLU:O | 2.05 | 0.55 |
| 1:A:1317:MET:O | 1:A:1322:ILE:HD11 | 2.06 | 0.55 |
| 2:B:662:MET:HA | 2:B:665:GLU:HB2 | 1.88 | 0.55 |
| 2:B:855:PHE:CD1 | 2:B:856:PHE:N | 2.73 | 0.55 |
| 2:B:1109:GLY:O | 2:B:1111:MET:HG2 | 2.06 | 0.55 |
| 4:D:137:ASN:HD22 | 4:D:137:ASN:N | 2.03 | 0.55 |
| 8:H:104:PHE:CE2 | 8:H:136:LYS:HG2 | 2.41 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 8:H:129:TYR:HA | 8:H:131:ASN:ND2 | 2.21 | 0.55 |
| 11:K:44:ASN:N | 11:K:61:TYR:HE1 | 2.03 | 0.55 |
| 11:K:65:HIS:CD2 | 11:K:67:PHE:HB2 | 2.41 | 0.55 |
| 12:L:27:LEU:HB3 | 12:L:37:LYS:HB3 | 1.88 | 0.55 |
| 1:A:107:CYS:SG | 1:A:148:CYS:HB2 | 2.47 | 0.55 |
| 1:A:903:ASN:ND2 | 1:A:903:ASN:C | 2.58 | 0.55 |
| 1:A:913:LEU:HD12 | 1:A:914:GLU:N | 2.18 | 0.55 |
| 5:E:173:SER:C | 5:E:175:LEU:H | 2.09 | 0.55 |
| 7:G:51:TYR:C | 7:G:51:TYR:CD2 | 2.80 | 0.55 |
| 10:J:64:ASN:CB | 10:J:65:PRO:CD | 2.80 | 0.55 |
| 1:A:915:SER:O | 1:A:919:ILE:HG13 | 2.07 | 0.55 |
| 1:A:1155:ASP:OD2 | 1:A:1161:THR:HG23 | 2.06 | 0.55 |
| 1:A:1262:LYS:C | 1:A:1264:GLU:N | 2.59 | 0.55 |
| 2:B:344:LYS:O | 2:B:345:LYS:C | 2.44 | 0.55 |
| 2:B:594:ALA:HB2 | 9:I:61:ASP:OD1 | 2.06 | 0.55 |
| 3:C:176:ILE:HG22 | 3:C:177:GLU:N | 2.22 | 0.55 |
| 4:D:53:SER:HA | 4:D:56:ARG:HB3 | 1.88 | 0.55 |
| 5:E:4:GLU:C | 5:E:6:GLU:H | 2.08 | 0.55 |
| 5:E:154:ILE:HG22 | 5:E:155:ARG:O | 2.05 | 0.55 |
| 8:H:108:SER:O | 8:H:110:ASP:N | 2.39 | 0.55 |
| 9:I:50:THR:HB | 9:I:92:ARG:HH12 | 1.71 | 0.55 |
| 1:A:21:LEU:HD12 | 1:A:229:SER:HB2 | 1.89 | 0.55 |
| 1:A:104:GLU:HG3 | 1:A:174:ILE:HD12 | 1.88 | 0.55 |
| 1:A:639:PRO:HG2 | 1:A:640:GLN:H | 1.72 | 0.55 |
| 1:A:886:ILE:HG23 | 1:A:887:GLY:N | 2.21 | 0.55 |
| 3:C:252:GLN:HG3 | 11:K:95:ILE:HG23 | 1.87 | 0.55 |
| 4:D:40:HIS:HD2 | 7:G:73:LYS:CG | 2.19 | 0.55 |
| 5:E:109:ILE:CG2 | 5:E:110:PHE:H | 2.16 | 0.55 |
| 9:I:34:TYR:CD2 | 9:I:35:VAL:N | 2.75 | 0.55 |
| 1:A:35:ILE:HG13 | 1:A:241:VAL:HG21 | 1.88 | 0.55 |
| 2:B:243:ALA:HB2 | 2:B:251:ILE:HG12 | 1.89 | 0.55 |
| 2:B:244:LEU:HD12 | 2:B:250:PHE:H | 1.71 | 0.55 |
| 2:B:284:ILE:HG23 | 2:B:324:ILE:HD13 | 1.89 | 0.55 |
| 2:B:549:THR:HG22 | 2:B:550:ASP:N | 2.22 | 0.55 |
| 3:C:196:ASP:HB3 | 3:C:199:LYS:HB2 | 1.87 | 0.55 |
| 5:E:55:ARG:C | 5:E:57:MET:N | 2.60 | 0.55 |
| 9:I:52:ILE:HG13 | 9:I:52:ILE:O | 2.05 | 0.55 |
| 9:I:73:ARG:HH12 | 9:I:112:SER:CB | 2.19 | 0.55 |
| 10:J:6:ARG:HB3 | 10:J:11:GLY:O | 2.07 | 0.55 |
| 1:A:535:THR:HG21 | 1:A:616:VAL:CA | 2.28 | 0.55 |
| 1:A:935:GLN:HE22 | 1:A:938:LYS:HD2 | 1.71 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1284:MET:HA | 1:A:1306:LEU:HD23 | 1.89 | 0.55 |
| 1:A:1342:GLU:CD | 5:E:198:ILE:HG21 | 2.26 | 0.55 |
| 1:A:1373:ASP:O | 1:A:1377:THR:HG23 | 2.07 | 0.55 |
| 1:A:1423:GLY:HA3 | 1:A:1426:GLU:HG2 | 1.88 | 0.55 |
| 3:C:6:PRO:HB2 | 11:K:101:LEU:HD12 | 1.89 | 0.55 |
| 4:D:40:HIS:HB2 | 7:G:73:LYS:HD3 | 1.88 | 0.55 |
| 5:E:38:PRO:HG2 | 5:E:41:ASP:HB2 | 1.87 | 0.55 |
| 5:E:133:GLU:HG2 | 5:E:135:PHE:HE1 | 1.70 | 0.55 |
| 9:I:99:LEU:O | 9:I:111:THR:HG23 | 2.07 | 0.55 |
| 1:A:98:LYS:O | 1:A:102:VAL:HG23 | 2.06 | 0.55 |
| 1:A:224:PHE:CD2 | 1:A:231:PRO:HG3 | 2.42 | 0.55 |
| 2:B:526:GLU:OE1 | 2:B:752:ALA:HB3 | 2.07 | 0.55 |
| 2:B:579:ARG:HD2 | 2:B:586:TRP:CZ2 | 2.42 | 0.55 |
| 2:B:1115:THR:O | 2:B:1116:ARG:HB2 | 2.06 | 0.55 |
| 4:D:163:VAL:O | 4:D:166:LEU:HB3 | 2.06 | 0.55 |
| 5:E:52:ARG:HB3 | 5:E:53:PRO:CD | 2.35 | 0.55 |
| 5:E:90:VAL:CA | 5:E:120:ALA:HB2 | 2.37 | 0.55 |
| 5:E:153:HIS:HB3 | 5:E:196:VAL:HG11 | 1.87 | 0.55 |
| 5:E:206:GLY:O | 5:E:207:ARG:HG2 | 2.07 | 0.55 |
| 6:F:116:ASP:O | 6:F:120:ILE:HG13 | 2.06 | 0.55 |
| 8:H:10:PHE:N | 8:H:10:PHE:CD1 | 2.75 | 0.55 |
| 1:A:849:MET:CE | 1:A:1061:GLY:HA2 | 2.35 | 0.55 |
| 1:A:929:LEU:O | 1:A:929:LEU:HD13 | 2.06 | 0.55 |
| 1:A:1318:THR:HB | 5:E:141:VAL:HG11 | 1.87 | 0.55 |
| 1:A:1341:ILE:HG23 | 1:A:1342:GLU:H | 1.70 | 0.55 |
| 2:B:69:LEU:CD1 | 2:B:429:PHE:HD1 | 1.89 | 0.55 |
| 2:B:842:ASN:HD22 | 2:B:845:SER:HB3 | 1.71 | 0.55 |
| 2:B:873:THR:O | 2:B:914:LYS:HA | 2.07 | 0.55 |
| 4:D:8:PHE:CE1 | 4:D:37:GLN:HB2 | 2.41 | 0.55 |
| 5:E:177:ARG:C | 5:E:212:ARG:HD3 | 2.27 | 0.55 |
| 6:F:99:LEU:O | 6:F:103:MET:CG | 2.55 | 0.55 |
| 8:H:5:LEU:O | 8:H:6:PHE:HB2 | 2.06 | 0.55 |
| 1:A:154:SER:C | 1:A:156:ASP:H | 2.10 | 0.55 |
| 1:A:590:ARG:CD | 1:A:604:GLY:HA2 | 2.37 | 0.55 |
| 1:A:1141:THR:OG1 | 1:A:1205:LYS:HD3 | 2.07 | 0.55 |
| 2:B:278:GLN:CG | 2:B:279:ASP:H | 2.13 | 0.55 |
| 2:B:620:ARG:NH1 | 9:I:68:LEU:HD21 | 2.23 | 0.55 |
| 2:B:696:GLU:O | 2:B:699:GLU:HB2 | 2.07 | 0.55 |
| 2:B:708:GLU:HG3 | 2:B:709:ASP:N | 2.22 | 0.55 |
| 7:G:7:LEU:O | 7:G:73:LYS:HE2 | 2.07 | 0.55 |
| 1:A:55:ASP:C | 1:A:57:ARG:N | 2.58 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:134:ARG:O | 1:A:138:ILE:HG13 | 2.07 | 0.54 |
| 1:A:1074:GLU:HB3 | 1:A:1075:PRO:CD | 2.36 | 0.54 |
| 1:A:1152:ILE:HG22 | 1:A:1192:LEU:O | 2.06 | 0.54 |
| 1:A:1330:ASN:O | 1:A:1332:PHE:N | 2.40 | 0.54 |
| 2:B:390:LEU:O | 2:B:392:ARG:N | 2.40 | 0.54 |
| 2:B:613:VAL:CG2 | 2:B:628:THR:HA | 2.35 | 0.54 |
| 2:B:807:ARG:NH1 | 2:B:807:ARG:HB3 | 2.22 | 0.54 |
| 2:B:893:LEU:HD22 | 2:B:897:GLY:C | 2.27 | 0.54 |
| 4:D:14:ARG:O | 4:D:16:LYS:HG2 | 2.07 | 0.54 |
| 7:G:22:MET:O | 7:G:23:LYS:C | 2.46 | 0.54 |
| 9:I:35:VAL:CG1 | 9:I:36:GLU:H | 2.18 | 0.54 |
| 11:K:31:VAL:CG1 | 11:K:32:VAL:H | 2.18 | 0.54 |
| 1:A:41:MET:CB | 1:A:50:ILE:H | 2.19 | 0.54 |
| 1:A:1308:THR:CG2 | 1:A:1309:ASP:N | 2.57 | 0.54 |
| 2:B:788:ARG:NH1 | 2:B:790:ASP:OD1 | 2.41 | 0.54 |
| 2:B:847:ASP:C | 2:B:849:GLY:N | 2.59 | 0.54 |
| 5:E:39:LEU:O | 5:E:42:PHE:HB3 | 2.07 | 0.54 |
| 5:E:124:VAL:N | 5:E:125:PRO:CD | 2.70 | 0.54 |
| 9:I:55:THR:HG21 | 9:I:109:ILE:HD13 | 1.88 | 0.54 |
| 1:A:9:ALA:HB3 | 2:B:1193:GLN:HB2 | 1.88 | 0.54 |
| 1:A:658:LEU:HD23 | 1:A:659:HIS:HE1 | 1.69 | 0.54 |
| 1:A:1001:ARG:O | 1:A:1002:GLY:O | 2.25 | 0.54 |
| 1:A:1081:LEU:HD12 | 1:A:1098:VAL:HG23 | 1.89 | 0.54 |
| 2:B:205:ILE:HD12 | 2:B:205:ILE:N | 2.23 | 0.54 |
| 2:B:305:VAL:O | 2:B:305:VAL:HG12 | 2.07 | 0.54 |
| 3:C:148:ARG:HG2 | 3:C:149:LYS:N | 2.23 | 0.54 |
| 4:D:203:SER:OG | 4:D:206:GLU:HB2 | 2.08 | 0.54 |
| 5:E:185:ALA:O | 5:E:190:LEU:HB2 | 2.08 | 0.54 |
| 9:I:59:VAL:HG12 | 9:I:60:GLN:H | 1.72 | 0.54 |
| 1:A:427:GLN:HB2 | 1:A:430:TRP:CE2 | 2.42 | 0.54 |
| 1:A:427:GLN:HG3 | 1:A:430:TRP:CE2 | 2.42 | 0.54 |
| 1:A:746:MET:HE3 | 2:B:1018:PRO:HG2 | 1.90 | 0.54 |
| 1:A:967:ALA:CA | 1:A:1044:TRP:HZ3 | 2.21 | 0.54 |
| 1:A:1114:PRO:O | 1:A:1115:SER:O | 2.24 | 0.54 |
| 1:A:1161:THR:C | 1:A:1163:ILE:N | 2.61 | 0.54 |
| 2:B:360:PHE:O | 2:B:361:LEU:C | 2.46 | 0.54 |
| 2:B:936:ASP:OD1 | 2:B:937:ALA:N | 2.40 | 0.54 |
| 3:C:7:GLN:HG2 | 11:K:104:ASN:ND2 | 2.23 | 0.54 |
| 5:E:89:GLY:C | 5:E:91:LYS:H | 2.10 | 0.54 |
| 7:G:96:GLN:HA | 7:G:121:PHE:CZ | 2.41 | 0.54 |
| 1:A:185:TRP:CZ3 | 1:A:200:ARG:HB3 | 2.43 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:316:GLN:O | 1:A:317:LYS:C | 2.45 | 0.54 |
| 1:A:728:LYS:CA | 1:A:731:ARG:HH21 | 2.20 | 0.54 |
| 1:A:1019:CYS:O | 1:A:1022:LEU:HB3 | 2.07 | 0.54 |
| 1:A:1223:ASP:HA | 1:A:1243:VAL:HG11 | 1.88 | 0.54 |
| 2:B:68:THR:HG23 | 2:B:91:SER:HB3 | 1.88 | 0.54 |
| 2:B:455:SER:O | 2:B:456:GLY:C | 2.46 | 0.54 |
| 2:B:707:PRO:HG2 | 2:B:708:GLU:H | 1.72 | 0.54 |
| 5:E:153:HIS:O | 5:E:154:ILE:CG1 | 2.48 | 0.54 |
| 8:H:76:THR:O | 8:H:77:ARG:HB2 | 2.08 | 0.54 |
| 9:I:7:CYS:HB3 | 9:I:14:LEU:CD2 | 2.38 | 0.54 |
| 9:I:12:ASN:OD1 | 9:I:31:THR:HG21 | 2.08 | 0.54 |
| 10:J:60:PHE:O | 10:J:63:TYR:HD1 | 1.90 | 0.54 |
| 12:L:55:ILE:CG1 | 12:L:56:LEU:H | 2.21 | 0.54 |
| 1:A:254:GLU:HB2 | 2:B:935:ARG:NH2 | 2.23 | 0.54 |
| 1:A:343:LYS:HZ3 | 2:B:1151:LEU:HD12 | 1.69 | 0.54 |
| 1:A:688:LYS:HA | 1:A:691:LEU:HB3 | 1.88 | 0.54 |
| 1:A:831:THR:HG23 | 1:A:832:ALA:N | 2.23 | 0.54 |
| 3:C:91:HIS:ND1 | 3:C:158:VAL:HG11 | 2.22 | 0.54 |
| 3:C:184:ASN:HD21 | 3:C:187:LYS:HA | 1.72 | 0.54 |
| 4:D:170:THR:C | 4:D:172:LEU:N | 2.61 | 0.54 |
| 5:E:85:GLU:HB2 | 5:E:88:VAL:CG2 | 2.35 | 0.54 |
| 5:E:93:MET:O | 5:E:95:THR:N | 2.41 | 0.54 |
| 7:G:34:VAL:HG11 | 7:G:74:TYR:HE1 | 1.72 | 0.54 |
| 8:H:62:SER:OG | 8:H:63:LEU:N | 2.41 | 0.54 |
| 1:A:111:GLY:O | 1:A:214:ILE:HA | 2.07 | 0.54 |
| 1:A:578:LEU:HD23 | 1:A:612:ILE:CD1 | 2.38 | 0.54 |
| 1:A:602:ASP:HB3 | 1:A:616:VAL:HG23 | 1.88 | 0.54 |
| 1:A:852:TYR:CD2 | 1:A:1060:PRO:CB | 2.89 | 0.54 |
| 1:A:898:ARG:HA | 1:A:933:TYR:CD1 | 2.42 | 0.54 |
| 1:A:1254:ALA:O | 1:A:1255:GLU:CB | 2.54 | 0.54 |
| 2:B:68:THR:HG22 | 2:B:69:LEU:H | 1.71 | 0.54 |
| 2:B:170:LEU:C | 2:B:170:LEU:HD12 | 2.27 | 0.54 |
| 2:B:616:ILE:CG2 | 2:B:700:SER:OG | 2.56 | 0.54 |
| 2:B:711:GLU:HB2 | 2:B:712:PRO:CD | 2.38 | 0.54 |
| 3:C:177:GLU:CG | 3:C:231:ASN:HB3 | 2.37 | 0.54 |
| 4:D:66:ARG:HD2 | 4:D:133:THR:HB | 1.90 | 0.54 |
| 4:D:207:LEU:C | 4:D:207:LEU:HD23 | 2.28 | 0.54 |
| 8:H:19:ARG:O | 8:H:20:TYR:HD2 | 1.91 | 0.54 |
| 8:H:38:LEU:HD12 | 8:H:39:THR:H | 1.73 | 0.54 |
| 9:I:4:PHE:HD1 | 9:I:4:PHE:C | 2.11 | 0.54 |
| 1:A:105:CYS:SG | 1:A:139:TRP:HA | 2.48 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:152:VAL:HG12 | 1:A:153:PRO:HD2 | 1.90 | 0.54 |
| 1:A:193:ASP:O | 1:A:194:ALA:HB3 | 2.08 | 0.54 |
| 1:A:1418:LEU:HB3 | 2:B:1222:ARG:NH1 | 2.23 | 0.54 |
| 2:B:63:ILE:HA | 2:B:421:PHE:CE2 | 2.43 | 0.54 |
| 2:B:658:ILE:HG22 | 2:B:662:MET:HE2 | 1.89 | 0.54 |
| 2:B:802:PRO:HG2 | 2:B:805:THR:HG22 | 1.89 | 0.54 |
| 3:C:14:SER:HA | 11:K:114:LEU:HD22 | 1.89 | 0.54 |
| 8:H:145:ARG:O | 8:H:146:ARG:HB2 | 2.08 | 0.54 |
| 1:A:407:ARG:HG2 | 1:A:430:TRP:CH2 | 2.42 | 0.54 |
| 1:A:556:TRP:CE3 | 1:A:558:GLY:HA2 | 2.42 | 0.54 |
| 1:A:590:ARG:HH21 | 1:A:620:LYS:CB | 2.19 | 0.54 |
| 1:A:729:ALA:HA | 1:A:732:LEU:HD12 | 1.88 | 0.54 |
| 1:A:738:LYS:H | 1:A:738:LYS:CD | 2.15 | 0.54 |
| 1:A:874:ASP:N | 1:A:1058:VAL:HG23 | 2.23 | 0.54 |
| 1:A:968:GLN:HE22 | 1:A:1035:TYR:HB2 | 1.72 | 0.54 |
| 1:A:1156:PRO:HA | 1:A:1190:PRO:CB | 2.38 | 0.54 |
| 2:B:38:PHE:CD1 | 2:B:811:TYR:CD2 | 2.96 | 0.54 |
| 2:B:230:ALA:N | 2:B:231:PRO:CD | 2.70 | 0.54 |
| 2:B:326:ASP:O | 2:B:328:GLU:N | 2.41 | 0.54 |
| 3:C:213:PRO:O | 3:C:214:ASN:CB | 2.55 | 0.54 |
| 8:H:81:PRO:CB | 8:H:82:PRO:CD | 2.74 | 0.54 |
| 1:A:18:GLN:HG2 | 1:A:1418:LEU:CD1 | 2.34 | 0.54 |
| 1:A:551:TYR:CZ | 11:K:62:LYS:HE2 | 2.43 | 0.54 |
| 1:A:974:ASP:OD2 | 1:A:976:THR:OG1 | 2.26 | 0.54 |
| 1:A:1063:MET:CG | 1:A:1436:ILE:HG23 | 2.38 | 0.54 |
| 1:A:1153:TYR:CD2 | 1:A:1163:ILE:HD11 | 2.43 | 0.54 |
| 1:A:1386:ARG:HB2 | 1:A:1403:GLU:OE1 | 2.08 | 0.54 |
| 1:A:1446:ASP:O | 1:A:1447:GLU:C | 2.45 | 0.54 |
| 2:B:60:GLN:NE2 | 2:B:94:LYS:HA | 2.23 | 0.54 |
| 2:B:95:ILE:CG1 | 2:B:130:VAL:HG22 | 2.38 | 0.54 |
| 2:B:124:TYR:HH | 2:B:179:CYS:HG | 1.55 | 0.54 |
| 2:B:850:LEU:CD2 | 2:B:1009:ASP:HB3 | 2.38 | 0.54 |
| 3:C:34:ARG:HA | 3:C:37:MET:HE2 | 1.89 | 0.54 |
| 5:E:13:TRP:CZ3 | 5:E:39:LEU:HB2 | 2.43 | 0.54 |
| 10:J:27:GLU:O | 10:J:29:GLU:HG3 | 2.07 | 0.54 |
| 11:K:31:VAL:CG1 | 11:K:32:VAL:N | 2.69 | 0.54 |
| 1:A:262:LEU:HD12 | 1:A:328:ARG:NH2 | 2.23 | 0.53 |
| 1:A:269:ILE:HD13 | 1:A:300:VAL:HG22 | 1.89 | 0.53 |
| 1:A:444:PHE:HB3 | 1:A:458:HIS:HD2 | 1.73 | 0.53 |
| 1:A:567:LYS:CB | 1:A:568:PRO:CD | 2.86 | 0.53 |
| 1:A:583:PRO:HG2 | 1:A:586:ILE:CG1 | 2.38 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:884:ASP:O | 1:A:886:ILE:N | 2.41 | 0.53 |
| 2:B:97:VAL:CG2 | 2:B:128:LEU:HG | 2.38 | 0.53 |
| 2:B:1098:MET:HE3 | 2:B:1098:MET:H | 1.73 | 0.53 |
| 2:B:1171:VAL:HA | 2:B:1182:CYS:HB2 | 1.90 | 0.53 |
| 3:C:102:GLN:HG2 | 3:C:154:LYS:HG2 | 1.90 | 0.53 |
| 3:C:165:LYS:O | 11:K:6:ARG:NH1 | 2.39 | 0.53 |
| 4:D:24:ALA:C | 4:D:26:THR:N | 2.60 | 0.53 |
| 6:F:119:ARG:HH11 | 6:F:119:ARG:HG3 | 1.72 | 0.53 |
| 7:G:51:TYR:C | 7:G:51:TYR:HD2 | 2.12 | 0.53 |
| 11:K:23:PRO:HA | 11:K:31:VAL:HG13 | 1.90 | 0.53 |
| 13:T:22:DC:H2' | 13:T:23:BRU:H6 | 1.90 | 0.53 |
| 1:A:64:ASN:O | 1:A:65:LEU:C | 2.46 | 0.53 |
| 1:A:371:ALA:HB2 | 1:A:462:VAL:HG13 | 1.90 | 0.53 |
| 1:A:396:PRO:HB3 | 1:A:403:LYS:HA | 1.90 | 0.53 |
| 1:A:1120:LEU:HD22 | 1:A:1124:HIS:O | 2.09 | 0.53 |
| 1:A:1230:GLU:C | 1:A:1232:ASN:H | 2.11 | 0.53 |
| 2:B:57:TYR:CD1 | 2:B:57:TYR:N | 2.76 | 0.53 |
| 3:C:235:VAL:HG12 | 10:J:13:VAL:CG2 | 2.37 | 0.53 |
| 4:D:40:HIS:CD2 | 7:G:73:LYS:HZ3 | 2.26 | 0.53 |
| 4:D:126:ILE:HD13 | 4:D:145:MET:HE2 | 1.91 | 0.53 |
| 4:D:139:LYS:HG3 | 4:D:143:ASN:ND2 | 2.23 | 0.53 |
| 7:G:99:PHE:HZ | 7:G:163:ILE:HD13 | 1.73 | 0.53 |
| 8:H:42:ILE:HG12 | 8:H:97:MET:HE1 | 1.90 | 0.53 |
| 10:J:7:CYS:SG | 10:J:49:MET:HE3 | 2.48 | 0.53 |
| 11:K:7:PHE:C | 11:K:9:LEU:N | 2.62 | 0.53 |
| 1:A:233:TRP:C | 1:A:235:ILE:N | 2.61 | 0.53 |
| 1:A:384:ASN:OD1 | 1:A:388:LEU:HD12 | 2.07 | 0.53 |
| 1:A:825:ILE:HG22 | 1:A:826:ASP:N | 2.22 | 0.53 |
| 1:A:1103:GLU:O | 1:A:1108:ALA:HB2 | 2.08 | 0.53 |
| 2:B:563:MET:HE3 | 2:B:580:VAL:HB | 1.91 | 0.53 |
| 2:B:685:LEU:HG | 2:B:686:ASN:N | 2.24 | 0.53 |
| 2:B:899:ILE:HG23 | 2:B:903:VAL:HG21 | 1.89 | 0.53 |
| 2:B:1073:TYR:CE2 | 2:B:1080:LYS:HG2 | 2.43 | 0.53 |
| 3:C:74:SER:OG | 3:C:237:SER:HB2 | 2.07 | 0.53 |
| 5:E:121:MET:O | 5:E:124:VAL:HG23 | 2.09 | 0.53 |
| 1:A:340:LEU:HD21 | 2:B:1200:ALA:N | 2.23 | 0.53 |
| 1:A:353:ILE:CD1 | 1:A:487:MET:HE2 | 2.36 | 0.53 |
| 1:A:463:ILE:HD11 | 1:A:469:ARG:HG3 | 1.89 | 0.53 |
| 1:A:525:GLN:O | 1:A:528:LEU:N | 2.42 | 0.53 |
| 1:A:591:PHE:HA | 1:A:595:THR:CG2 | 2.37 | 0.53 |
| 1:A:1008:GLN:O | 1:A:1011:GLN:HB3 | 2.09 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:39:ARG:HH21 | 2:B:665:GLU:CD | 2.11 | 0.53 |
| 2:B:377:PHE:O | 2:B:380:TYR:N | 2.42 | 0.53 |
| 2:B:465:ASN:N | 2:B:465:ASN:ND2 | 2.55 | 0.53 |
| 2:B:616:ILE:HG23 | 2:B:700:SER:OG | 2.08 | 0.53 |
| 2:B:753:ALA:HA | 2:B:756:ILE:CD1 | 2.39 | 0.53 |
| 2:B:880:THR:HB | 2:B:934:LYS:HE2 | 1.88 | 0.53 |
| 2:B:900:ALA:CB | 12:L:61:THR:OG1 | 2.56 | 0.53 |
| 2:B:1106:ARG:HH12 | 2:B:1110:PRO:HG2 | 1.72 | 0.53 |
| 3:C:193:TYR:HD1 | 3:C:193:TYR:O | 1.91 | 0.53 |
| 3:C:245:VAL:O | 3:C:249:ASP:N | 2.40 | 0.53 |
| 4:D:52:LEU:O | 4:D:54:GLU:N | 2.39 | 0.53 |
| 4:D:60:LYS:O | 4:D:64:VAL:HG23 | 2.08 | 0.53 |
| 8:H:64:ASN:ND2 | 8:H:88:SER:C | 2.61 | 0.53 |
| 1:A:70:CYS:O | 1:A:72:GLU:HG2 | 2.08 | 0.53 |
| 1:A:92:HIS:O | 1:A:94:GLY:N | 2.42 | 0.53 |
| 1:A:676:MET:O | 1:A:679:ILE:HB | 2.08 | 0.53 |
| 1:A:913:LEU:HG | 1:A:914:GLU:N | 2.23 | 0.53 |
| 1:A:1397:LEU:O | 1:A:1400:CYS:HB3 | 2.09 | 0.53 |
| 2:B:284:ILE:HG23 | 2:B:324:ILE:CD1 | 2.38 | 0.53 |
| 2:B:469:GLN:CG | 2:B:470:LYS:H | 2.22 | 0.53 |
| 2:B:637:LEU:CD1 | 2:B:693:ILE:HD12 | 2.22 | 0.53 |
| 2:B:659:ALA:HA | 2:B:662:MET:HE2 | 1.91 | 0.53 |
| 2:B:899:ILE:O | 2:B:952:VAL:HG21 | 2.09 | 0.53 |
| 2:B:984:HIS:NE2 | 2:B:1025:HIS:HA | 2.23 | 0.53 |
| 5:E:178:ILE:HG13 | 5:E:182:ASP:OD2 | 2.08 | 0.53 |
| 12:L:24:THR:O | 12:L:25:ALA:HB3 | 2.08 | 0.53 |
| 1:A:182:VAL:CG2 | 1:A:201:VAL:HA | 2.32 | 0.53 |
| 1:A:311:GLN:O | 1:A:312:PRO:C | 2.46 | 0.53 |
| 1:A:473:SER:HG | 1:A:646:PHE:HD2 | 1.56 | 0.53 |
| 1:A:613:ILE:O | 1:A:614:PHE:HB3 | 2.08 | 0.53 |
| 1:A:682:THR:HG22 | 1:A:728:LYS:HE3 | 1.91 | 0.53 |
| 1:A:687:LYS:O | 1:A:690:VAL:HB | 2.08 | 0.53 |
| 1:A:896:ARG:NH2 | 1:A:1030:ARG:NH2 | 2.56 | 0.53 |
| 1:A:963:ILE:HD11 | 1:A:1048:ASN:HB3 | 1.89 | 0.53 |
| 1:A:997:LEU:HD13 | 1:A:1018:PHE:CE2 | 2.43 | 0.53 |
| 2:B:802:PRO:HG2 | 2:B:805:THR:CG2 | 2.39 | 0.53 |
| 2:B:955:THR:HG23 | 2:B:956:THR:H | 1.74 | 0.53 |
| 2:B:1058:LEU:N | 2:B:1058:LEU:HD23 | 2.23 | 0.53 |
| 2:B:1178:ASN:O | 2:B:1180:PHE:CD1 | 2.61 | 0.53 |
| 3:C:209:TYR:CD1 | 3:C:209:TYR:N | 2.76 | 0.53 |
| 5:E:212:ARG:HH11 | 5:E:212:ARG:CG | 2.20 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:H:89:LEU:C | 8:H:91:ASP:N | 2.62 | 0.53 |
| 1:A:178:GLY:C | 1:A:179:LEU:HD23 | 2.28 | 0.53 |
| 1:A:408:ASP:O | 1:A:410:GLY:N | 2.42 | 0.53 |
| 1:A:740:LEU:HD12 | 1:A:741:ASN:N | 2.24 | 0.53 |
| 1:A:940:ARG:HG2 | 1:A:940:ARG:NH1 | 2.20 | 0.53 |
| 1:A:947:PHE:N | 1:A:947:PHE:CD1 | 2.76 | 0.53 |
| 1:A:1163:ILE:HG22 | 1:A:1165:GLU:HG2 | 1.91 | 0.53 |
| 1:A:1187:GLN:HA | 1:A:1244:ARG:HD2 | 1.91 | 0.53 |
| 2:B:222:ILE:O | 2:B:240:ILE:HA | 2.08 | 0.53 |
| 2:B:265:SER:O | 2:B:266:ALA:C | 2.47 | 0.53 |
| 4:D:66:ARG:HG3 | 7:G:51:TYR:CD1 | 2.43 | 0.53 |
| 4:D:126:ILE:HD13 | 4:D:145:MET:CE | 2.39 | 0.53 |
| 5:E:110:PHE:HE2 | 5:E:112:TYR:HB3 | 1.72 | 0.53 |
| 7:G:13:LEU:HD22 | 7:G:17:PHE:HB2 | 1.90 | 0.53 |
| 9:I:44:TYR:CD1 | 9:I:45:ARG:N | 2.77 | 0.53 |
| 10:J:31:ASP:O | 10:J:32:GLU:C | 2.47 | 0.53 |
| 1:A:343:LYS:HD3 | 2:B:1155:SER:OG | 2.09 | 0.53 |
| 1:A:704:ALA:O | 1:A:705:LYS:C | 2.46 | 0.53 |
| 1:A:798:GLY:HA2 | 1:A:815:PHE:CD1 | 2.44 | 0.53 |
| 1:A:1015:VAL:CG1 | 1:A:1019:CYS:SG | 2.96 | 0.53 |
| 2:B:294:ASP:HB2 | 9:I:12:ASN:HA | 1.91 | 0.53 |
| 2:B:309:GLN:CD | 9:I:52:ILE:HD11 | 2.29 | 0.53 |
| 2:B:506:GLY:CA | 2:B:512:ARG:HH21 | 2.07 | 0.53 |
| 2:B:896:ASP:OD2 | 12:L:58:LYS:HE3 | 2.09 | 0.53 |
| 4:D:51:ASN:O | 4:D:52:LEU:O | 2.27 | 0.53 |
| 4:D:137:ASN:ND2 | 4:D:137:ASN:H | 2.06 | 0.53 |
| 5:E:112:TYR:CZ | 5:E:136:ASN:HB2 | 2.44 | 0.53 |
| 1:A:135:PHE:HD1 | 1:A:222:LEU:HD22 | 1.74 | 0.53 |
| 1:A:224:PHE:CG | 1:A:231:PRO:HG3 | 2.43 | 0.53 |
| 1:A:278:THR:CG2 | 1:A:282:ASN:HD22 | 2.21 | 0.53 |
| 1:A:675:THR:O | 1:A:679:ILE:HG13 | 2.09 | 0.53 |
| 1:A:734:GLU:C | 1:A:736:ASN:H | 2.10 | 0.53 |
| 1:A:858:ASN:C | 1:A:858:ASN:ND2 | 2.62 | 0.53 |
| 1:A:1100:ARG:O | 1:A:1104:ILE:HG13 | 2.08 | 0.53 |
| 1:A:1446:ASP:HB2 | 6:F:133:VAL:CG2 | 2.38 | 0.53 |
| 2:B:62:ILE:HG23 | 2:B:418:LYS:HG3 | 1.91 | 0.53 |
| 2:B:63:ILE:HD12 | 2:B:421:PHE:CE2 | 2.43 | 0.53 |
| 2:B:215:GLN:HA | 2:B:215:GLN:NE2 | 2.24 | 0.53 |
| 2:B:273:LEU:HD12 | 2:B:276:ILE:CD1 | 2.37 | 0.53 |
| 2:B:745:PRO:C | 2:B:747:MET:H | 2.13 | 0.53 |
| 2:B:882:THR:HG21 | 2:B:934:LYS:O | 2.09 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:174:ALA:O | 3:C:175:ALA:HB2 | 2.08 | 0.53 |
| 3:C:181:ASP:OD2 | 3:C:184:ASN:HA | 2.08 | 0.53 |
| 4:D:7:THR:HB | 7:G:42:PHE:CZ | 2.43 | 0.53 |
| 4:D:50:LEU:HD11 | 7:G:4:ILE:CD1 | 2.38 | 0.53 |
| 5:E:9:ILE:CD1 | 5:E:53:PRO:HD3 | 2.38 | 0.53 |
| 5:E:14:ARG:HA | 5:E:17:ARG:HG2 | 1.91 | 0.53 |
| 5:E:22:MET:O | 5:E:26:ARG:HB2 | 2.09 | 0.53 |
| 6:F:85:MET:O | 6:F:155:LEU:HD21 | 2.08 | 0.53 |
| 7:G:17:PHE:N | 7:G:17:PHE:HD2 | 2.07 | 0.53 |
| 10:J:16:ASP:OD1 | 10:J:17:LYS:HD2 | 2.09 | 0.53 |
| 1:A:75:ASN:O | 1:A:76:GLU:CB | 2.56 | 0.53 |
| 1:A:308:ILE:HG22 | 1:A:309:ALA:N | 2.12 | 0.53 |
| 1:A:401:GLY:C | 1:A:435:HIS:CD2 | 2.82 | 0.53 |
| 1:A:598:LEU:O | 1:A:599:SER:C | 2.47 | 0.53 |
| 1:A:1206:ASP:HB3 | 1:A:1274:ARG:NH1 | 2.19 | 0.53 |
| 1:A:1272:THR:C | 1:A:1273:LEU:HD12 | 2.30 | 0.53 |
| 1:A:1276:VAL:HG12 | 1:A:1277:GLU:N | 2.23 | 0.53 |
| 1:A:1351:GLU:O | 1:A:1355:VAL:HG23 | 2.09 | 0.53 |
| 2:B:133:LYS:HG3 | 2:B:135:ARG:HE | 1.73 | 0.53 |
| 2:B:221:ASN:OD1 | 2:B:242:SER:HA | 2.09 | 0.53 |
| 2:B:272:THR:O | 2:B:273:LEU:HD23 | 2.09 | 0.53 |
| 2:B:589:VAL:HG12 | 2:B:590:HIS:H | 1.73 | 0.53 |
| 2:B:710:LEU:HA | 2:B:733:HIS:HB3 | 1.90 | 0.53 |
| 2:B:879:ARG:CZ | 2:B:883:LEU:HD22 | 2.38 | 0.53 |
| 2:B:955:THR:OG1 | 12:L:55:ILE:HA | 2.09 | 0.53 |
| 2:B:1159:ARG:HD2 | 2:B:1159:ARG:C | 2.29 | 0.53 |
| 3:C:123:ASN:CG | 3:C:125:MET:H | 2.11 | 0.53 |
| 3:C:148:ARG:HG2 | 3:C:149:LYS:H | 1.74 | 0.53 |
| 4:D:60:LYS:NZ | 4:D:115:HIS:CE1 | 2.76 | 0.53 |
| 5:E:63:ASN:HB3 | 5:E:64:PRO:CD | 2.38 | 0.53 |
| 5:E:86:PRO:HA | 5:E:113:GLN:HB2 | 1.90 | 0.53 |
| 8:H:100:THR:CG2 | 8:H:101:ALA:H | 2.22 | 0.53 |
| 8:H:135:LEU:HD13 | 8:H:137:GLN:HE21 | 1.73 | 0.53 |
| 1:A:107:CYS:N | 1:A:114:LEU:HD21 | 2.24 | 0.52 |
| 1:A:168:GLY:O | 1:A:169:ASN:C | 2.46 | 0.52 |
| 1:A:867:ILE:HG13 | 1:A:1000:LEU:HD21 | 1.91 | 0.52 |
| 2:B:318:VAL:C | 2:B:320:ASP:N | 2.62 | 0.52 |
| 2:B:605:ARG:CZ | 2:B:639:ILE:HD13 | 2.38 | 0.52 |
| 2:B:687:GLU:HB3 | 2:B:689:LEU:HG | 1.90 | 0.52 |
| 2:B:1065:GLN:NE2 | 2:B:1066:SER:N | 2.57 | 0.52 |
| 2:B:1085:ILE:N | 2:B:1085:ILE:HD12 | 2.23 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:22:LEU:HD13 | 3:C:230:MET:HE1 | 1.90 | 0.52 |
| 3:C:69:LEU:N | 3:C:69:LEU:HD12 | 2.24 | 0.52 |
| 4:D:64:VAL:C | 4:D:66:ARG:N | 2.62 | 0.52 |
| 5:E:94:LYS:HG3 | 5:E:98:ILE:CD1 | 2.39 | 0.52 |
| 8:H:80:ARG:NH1 | 11:K:57:LEU:HD21 | 2.20 | 0.52 |
| 1:A:21:LEU:HG | 1:A:1413:GLY:O | 2.09 | 0.52 |
| 1:A:23:SER:HB3 | 1:A:233:TRP:CZ2 | 2.45 | 0.52 |
| 1:A:523:ILE:HD12 | 1:A:622:VAL:HG21 | 1.91 | 0.52 |
| 2:B:273:LEU:CD1 | 2:B:276:ILE:HD12 | 2.39 | 0.52 |
| 2:B:313:MET:CE | 2:B:390:LEU:HD21 | 2.39 | 0.52 |
| 2:B:859:TYR:HD1 | 2:B:859:TYR:H | 1.57 | 0.52 |
| 5:E:162:ARG:CZ | 5:E:162:ARG:HB3 | 2.39 | 0.52 |
| 7:G:112:LYS:HA | 7:G:115:MET:CE | 2.40 | 0.52 |
| 14:N:3:DT:H3' | 14:N:3:DT:OP2 | 2.09 | 0.52 |
| 1:A:322:VAL:O | 1:A:322:VAL:CG1 | 2.58 | 0.52 |
| 1:A:334:GLY:O | 1:A:335:ARG:C | 2.48 | 0.52 |
| 1:A:452:LYS:HG3 | 2:B:1140:ALA:HB1 | 1.90 | 0.52 |
| 1:A:618:GLU:OE2 | 1:A:620:LYS:HB2 | 2.09 | 0.52 |
| 1:A:677:ARG:HD2 | 1:A:678:GLU:N | 2.25 | 0.52 |
| 1:A:825:ILE:HG22 | 1:A:826:ASP:H | 1.73 | 0.52 |
| 1:A:954:TRP:CZ3 | 5:E:203:GLU:HB2 | 2.43 | 0.52 |
| 2:B:192:LEU:O | 2:B:193:LYS:HB2 | 2.09 | 0.52 |
| 2:B:460:ALA:HB1 | 2:B:466:TRP:CZ3 | 2.44 | 0.52 |
| 2:B:597:MET:HA | 2:B:597:MET:HE2 | 1.90 | 0.52 |
| 2:B:955:THR:HG23 | 2:B:956:THR:N | 2.24 | 0.52 |
| 2:B:1167:GLY:O | 2:B:1215:ARG:HA | 2.10 | 0.52 |
| 3:C:189:THR:HG22 | 3:C:190:ASP:H | 1.73 | 0.52 |
| 9:I:7:CYS:SG | 9:I:8:ARG:O | 2.67 | 0.52 |
| 1:A:507:VAL:N | 1:A:508:PRO:CD | 2.72 | 0.52 |
| 1:A:884:ASP:HB3 | 1:A:896:ARG:HH12 | 1.74 | 0.52 |
| 1:A:1074:GLU:HB3 | 1:A:1075:PRO:HD3 | 1.90 | 0.52 |
| 1:A:1394:THR:CG2 | 1:A:1398:MET:SD | 2.97 | 0.52 |
| 2:B:175:ARG:HG2 | 2:B:175:ARG:NH1 | 2.23 | 0.52 |
| 2:B:260:GLY:O | 2:B:267:ARG:NH1 | 2.43 | 0.52 |
| 2:B:368:GLU:O | 2:B:370:PHE:N | 2.38 | 0.52 |
| 2:B:542:MET:HG2 | 2:B:747:MET:HB3 | 1.91 | 0.52 |
| 2:B:613:VAL:CG1 | 2:B:628:THR:HA | 2.39 | 0.52 |
| 2:B:805:THR:HB | 2:B:809:MET:SD | 2.49 | 0.52 |
| 2:B:952:VAL:HG12 | 2:B:953:LEU:N | 2.24 | 0.52 |
| 2:B:956:THR:HG22 | 2:B:960:GLY:HA2 | 1.91 | 0.52 |
| 2:B:1030:LEU:HD11 | 2:B:1059:LEU:HD22 | 1.92 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1053:GLU:HB3 | 2:B:1057:LYS:HE3 | 1.90 | 0.52 |
| 4:D:34:GLN:O | 4:D:47:LEU:HD23 | 2.09 | 0.52 |
| 5:E:134:THR:C | 5:E:135:PHE:HD1 | 2.13 | 0.52 |
| 6:F:90:ARG:HB2 | 6:F:90:ARG:HH11 | 1.73 | 0.52 |
| 7:G:34:VAL:HG11 | 7:G:74:TYR:CE1 | 2.45 | 0.52 |
| 12:L:33:GLU:C | 12:L:35:SER:H | 2.13 | 0.52 |
| 1:A:63:ARG:HG3 | 1:A:63:ARG:O | 2.09 | 0.52 |
| 1:A:64:ASN:H | 1:A:74:MET:HE1 | 1.74 | 0.52 |
| 1:A:179:LEU:O | 1:A:180:LYS:HG3 | 2.09 | 0.52 |
| 1:A:219:PHE:CE2 | 1:A:231:PRO:HD2 | 2.45 | 0.52 |
| 1:A:555:ASP:O | 1:A:556:TRP:O | 2.27 | 0.52 |
| 1:A:575:LYS:HB3 | 1:A:612:ILE:HG21 | 1.92 | 0.52 |
| 1:A:853:ASP:OD1 | 1:A:855:THR:CB | 2.58 | 0.52 |
| 1:A:913:LEU:CG | 1:A:914:GLU:N | 2.72 | 0.52 |
| 1:A:1063:MET:HG3 | 1:A:1436:ILE:HG23 | 1.92 | 0.52 |
| 1:A:1313:LEU:C | 1:A:1315:GLU:H | 2.13 | 0.52 |
| 2:B:376:PHE:O | 2:B:586:TRP:HZ3 | 1.93 | 0.52 |
| 2:B:485:ARG:CZ | 2:B:782:LEU:HD11 | 2.40 | 0.52 |
| 2:B:648:HIS:CD2 | 2:B:649:LYS:H | 2.28 | 0.52 |
| 2:B:745:PRO:O | 2:B:747:MET:N | 2.43 | 0.52 |
| 2:B:763:GLN:HG2 | 2:B:765:PRO:HD2 | 1.92 | 0.52 |
| 3:C:132:PRO:O | 3:C:133:ILE:C | 2.47 | 0.52 |
| 4:D:179:GLN:O | 4:D:183:LEU:HB2 | 2.10 | 0.52 |
| 5:E:22:MET:HE1 | 5:E:26:ARG:HH11 | 1.71 | 0.52 |
| 5:E:91:LYS:C | 5:E:93:MET:H | 2.11 | 0.52 |
| 5:E:178:ILE:HG23 | 5:E:178:ILE:O | 2.08 | 0.52 |
| 8:H:64:ASN:OD1 | 8:H:90:ALA:CB | 2.58 | 0.52 |
| 8:H:135:LEU:HD13 | 8:H:137:GLN:NE2 | 2.24 | 0.52 |
| 1:A:333:GLU:OE2 | 1:A:333:GLU:N | 2.43 | 0.52 |
| 1:A:808:LEU:HD23 | 1:A:813:PHE:HA | 1.90 | 0.52 |
| 1:A:919:ILE:HG21 | 1:A:983:ILE:CD1 | 2.39 | 0.52 |
| 1:A:1225:PHE:HZ | 1:A:1227:ILE:HD11 | 1.73 | 0.52 |
| 1:A:1299:VAL:HG12 | 1:A:1300:LYS:N | 2.23 | 0.52 |
| 2:B:724:ASP:HB3 | 2:B:727:LYS:HG3 | 1.91 | 0.52 |
| 2:B:755:ILE:O | 2:B:755:ILE:HG22 | 2.09 | 0.52 |
| 2:B:1150:ARG:NH1 | 2:B:1150:ARG:HB3 | 2.25 | 0.52 |
| 3:C:154:LYS:O | 3:C:155:LEU:HD23 | 2.10 | 0.52 |
| 4:D:159:THR:O | 4:D:162:ALA:HB3 | 2.09 | 0.52 |
| 6:F:103:MET:HE3 | 7:G:66:GLY:H | 1.74 | 0.52 |
| 9:I:82:GLU:O | 9:I:104:LEU:HG | 2.09 | 0.52 |
| 9:I:85:PHE:N | 9:I:85:PHE:CD2 | 2.57 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:I:95:THR:HG22 | 9:I:96:SER:N | 2.25 | 0.52 |
| 1:A:567:LYS:HG3 | 8:H:94:ASP:O | 2.10 | 0.52 |
| 1:A:606:LEU:HG | 1:A:613:ILE:HD12 | 1.90 | 0.52 |
| 1:A:919:ILE:HG23 | 1:A:925:LEU:HD12 | 1.91 | 0.52 |
| 1:A:1224:LEU:HD12 | 1:A:1225:PHE:N | 2.25 | 0.52 |
| 1:A:1316:VAL:O | 1:A:1316:VAL:HG12 | 2.10 | 0.52 |
| 1:A:1438:THR:O | 1:A:1438:THR:HG22 | 2.10 | 0.52 |
| 2:B:120:ARG:HE | 2:B:955:THR:HG21 | 1.73 | 0.52 |
| 2:B:1106:ARG:HD3 | 2:B:1127:GLY:CA | 2.40 | 0.52 |
| 3:C:136:ASP:CB | 3:C:141:GLY:H | 2.23 | 0.52 |
| 5:E:65:THR:O | 5:E:68:SER:N | 2.42 | 0.52 |
| 6:F:71:GLU:O | 6:F:72:LYS:C | 2.48 | 0.52 |
| 8:H:15:VAL:HG21 | 8:H:49:VAL:HG12 | 1.91 | 0.52 |
| 13:T:11:DA:H2'' | 13:T:12:DG:C8 | 2.45 | 0.52 |
| 14:N:6:DT:H2'' | 14:N:7:DT:OP2 | 2.10 | 0.52 |
| 1:A:157:ASP:C | 1:A:159:THR:H | 2.13 | 0.52 |
| 1:A:244:PRO:HB2 | 1:A:245:PRO:HD3 | 1.92 | 0.52 |
| 1:A:298:PHE:O | 1:A:301:ALA:HB3 | 2.10 | 0.52 |
| 1:A:1263:ILE:O | 1:A:1263:ILE:HG22 | 2.09 | 0.52 |
| 1:A:1434:ALA:O | 1:A:1436:ILE:N | 2.42 | 0.52 |
| 2:B:203:PHE:HB3 | 2:B:205:ILE:CD1 | 2.39 | 0.52 |
| 2:B:309:GLN:O | 2:B:310:MET:C | 2.47 | 0.52 |
| 2:B:496:ARG:HD2 | 2:B:751:VAL:CG2 | 2.40 | 0.52 |
| 2:B:995:ARG:NH1 | 3:C:165:LYS:HA | 2.25 | 0.52 |
| 3:C:123:ASN:ND2 | 3:C:125:MET:HA | 2.25 | 0.52 |
| 5:E:85:GLU:O | 5:E:87:SER:N | 2.43 | 0.52 |
| 7:G:1:MET:HE1 | 7:G:80:LYS:O | 2.09 | 0.52 |
| 9:I:82:GLU:HB3 | 9:I:104:LEU:CD1 | 2.37 | 0.52 |
| 12:L:29:TYR:HA | 12:L:57:LEU:O | 2.10 | 0.52 |
| 1:A:41:MET:HE1 | 1:A:42:ASP:HB2 | 1.90 | 0.52 |
| 1:A:369:SER:HB3 | 11:K:2:ASN:HD21 | 1.75 | 0.52 |
| 1:A:1001:ARG:HG2 | 1:A:1001:ARG:HH11 | 1.73 | 0.52 |
| 1:A:1038:THR:HG23 | 1:A:1041:ALA:HB2 | 1.92 | 0.52 |
| 1:A:1389:PHE:CD1 | 1:A:1390:ASN:N | 2.78 | 0.52 |
| 1:A:1423:GLY:CA | 1:A:1426:GLU:HG2 | 2.39 | 0.52 |
| 2:B:31:TRP:CZ3 | 2:B:34:ILE:HD12 | 2.45 | 0.52 |
| 2:B:616:ILE:CG1 | 2:B:697:GLU:HA | 2.40 | 0.52 |
| 3:C:11:ARG:NH2 | 3:C:229:TYR:HD2 | 2.08 | 0.52 |
| 3:C:66:ARG:NH2 | 10:J:5:VAL:HG23 | 2.24 | 0.52 |
| 3:C:73:GLN:HG3 | 3:C:74:SER:N | 2.25 | 0.52 |
| 3:C:136:ASP:HB2 | 3:C:141:GLY:H | 1.74 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:E:124:VAL:H | 5:E:125:PRO:HD2 | 1.74 | 0.52 |
| 6:F:70:LYS:C | 6:F:72:LYS:H | 2.13 | 0.52 |
| 6:F:140:ASP:OD1 | 6:F:141:GLY:N | 2.43 | 0.52 |
| 9:I:40:SER:OG | 9:I:41:PRO:HD2 | 2.10 | 0.52 |
| 10:J:48:ARG:HD2 | 10:J:48:ARG:C | 2.30 | 0.52 |
| 14:N:5:DC:H2'' | 14:N:6:DT:O5' | 2.10 | 0.52 |
| 1:A:61:ILE:HG22 | 1:A:62:ASP:H | 1.74 | 0.52 |
| 1:A:593:GLU:C | 1:A:595:THR:H | 2.14 | 0.52 |
| 1:A:865:GLN:NE2 | 1:A:1370:LEU:HA | 2.24 | 0.52 |
| 1:A:942:PHE:HZ | 5:E:207:ARG:CG | 2.23 | 0.52 |
| 1:A:1100:ARG:HH22 | 1:A:1111:MET:HE1 | 1.74 | 0.52 |
| 1:A:1121:GLU:HB3 | 1:A:1124:HIS:NE2 | 2.24 | 0.52 |
| 1:A:1402:PHE:O | 1:A:1403:GLU:HB2 | 2.09 | 0.52 |
| 2:B:990:ILE:HG22 | 2:B:991:GLY:N | 2.25 | 0.52 |
| 7:G:125:SER:C | 7:G:126:ASN:HD22 | 2.13 | 0.52 |
| 8:H:63:LEU:HD13 | 8:H:64:ASN:H | 1.74 | 0.52 |
| 8:H:80:ARG:NH1 | 11:K:57:LEU:HD11 | 2.25 | 0.52 |
| 10:J:8:PHE:H | 10:J:49:MET:CE | 2.23 | 0.52 |
| 10:J:53:HIS:CD2 | 10:J:54:VAL:N | 2.78 | 0.52 |
| 1:A:445:ASN:CB | 1:A:455:MET:HG2 | 2.29 | 0.51 |
| 1:A:481:ASP:CG | 1:A:485:ASP:OD2 | 2.49 | 0.51 |
| 1:A:698:GLN:O | 9:I:98:VAL:HG13 | 2.10 | 0.51 |
| 1:A:700:ASN:HB2 | 9:I:98:VAL:HG21 | 1.92 | 0.51 |
| 1:A:947:PHE:N | 1:A:947:PHE:HD1 | 2.08 | 0.51 |
| 2:B:60:GLN:HE22 | 2:B:94:LYS:HA | 1.75 | 0.51 |
| 2:B:68:THR:HG22 | 2:B:69:LEU:N | 2.25 | 0.51 |
| 2:B:331:LEU:HD23 | 2:B:353:LYS:HG2 | 1.91 | 0.51 |
| 2:B:1039:GLY:HA2 | 10:J:51:LEU:HD21 | 1.92 | 0.51 |
| 3:C:242:GLN:C | 3:C:244:VAL:N | 2.63 | 0.51 |
| 4:D:206:GLU:O | 4:D:210:ILE:HG13 | 2.11 | 0.51 |
| 5:E:65:THR:O | 5:E:66:GLU:C | 2.48 | 0.51 |
| 9:I:58:VAL:CG1 | 9:I:62:ILE:HD12 | 2.29 | 0.51 |
| 1:A:40:THR:HB | 1:A:41:MET:CE | 2.40 | 0.51 |
| 1:A:343:LYS:HZ2 | 2:B:1151:LEU:CD1 | 2.23 | 0.51 |
| 1:A:630:ILE:CG2 | 1:A:631:HIS:N | 2.72 | 0.51 |
| 1:A:722:LEU:H | 1:A:722:LEU:CD1 | 2.22 | 0.51 |
| 1:A:743:VAL:O | 1:A:747:VAL:HG23 | 2.10 | 0.51 |
| 1:A:767:GLN:HA | 1:A:799:PHE:HA | 1.92 | 0.51 |
| 2:B:120:ARG:NH1 | 12:L:54:ARG:HH11 | 2.08 | 0.51 |
| 2:B:298:LEU:HD22 | 2:B:298:LEU:N | 2.26 | 0.51 |
| 2:B:638:PHE:HB3 | 2:B:651:LEU:HD22 | 1.90 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:952:VAL:HG13 | 2:B:966:VAL:HG22 | 1.92 | 0.51 |
| 2:B:1002:THR:HG21 | 2:B:1006:ILE:CD1 | 2.40 | 0.51 |
| 2:B:1102:LYS:O | 2:B:1103:ILE:C | 2.48 | 0.51 |
| 3:C:31:ASN:OD1 | 3:C:34:ARG:HD3 | 2.10 | 0.51 |
| 3:C:77:ILE:O | 3:C:79:GLN:N | 2.43 | 0.51 |
| 3:C:204:SER:H | 3:C:207:CYS:HG | 1.56 | 0.51 |
| 4:D:56:ARG:HD3 | 4:D:149:THR:HA | 1.92 | 0.51 |
| 4:D:118:THR:OG1 | 4:D:121:LYS:HB2 | 2.10 | 0.51 |
| 8:H:14:GLU:O | 8:H:26:ILE:HG23 | 2.10 | 0.51 |
| 8:H:110:ASP:HB2 | 8:H:128:ASN:HD22 | 1.76 | 0.51 |
| 9:I:4:PHE:C | 9:I:4:PHE:CD1 | 2.82 | 0.51 |
| 11:K:109:TRP:C | 11:K:111:LEU:H | 2.13 | 0.51 |
| 1:A:450:LEU:HB2 | 1:A:838:GLN:HE21 | 1.74 | 0.51 |
| 1:A:544:ASP:CG | 1:A:545:GLN:N | 2.62 | 0.51 |
| 1:A:817:ALA:O | 1:A:820:GLY:N | 2.43 | 0.51 |
| 1:A:1017:LEU:HD12 | 1:A:1017:LEU:O | 2.10 | 0.51 |
| 1:A:1098:VAL:HB | 1:A:1099:PRO:CD | 2.40 | 0.51 |
| 2:B:100:PRO:HD2 | 2:B:180:TYR:HE1 | 1.72 | 0.51 |
| 2:B:120:ARG:NH1 | 12:L:54:ARG:NH1 | 2.58 | 0.51 |
| 2:B:244:LEU:O | 2:B:249:ARG:HG2 | 2.10 | 0.51 |
| 2:B:508:LEU:O | 2:B:509:ALA:CB | 2.57 | 0.51 |
| 2:B:942:ARG:O | 2:B:943:SER:C | 2.48 | 0.51 |
| 3:C:3:GLU:HG3 | 11:K:104:ASN:CG | 2.31 | 0.51 |
| 4:D:63:LEU:HD23 | 7:G:47:CYS:SG | 2.50 | 0.51 |
| 6:F:103:MET:CE | 7:G:66:GLY:N | 2.68 | 0.51 |
| 9:I:82:GLU:HB3 | 9:I:104:LEU:HB2 | 1.91 | 0.51 |
| 10:J:27:GLU:O | 10:J:29:GLU:N | 2.43 | 0.51 |
| 10:J:36:LEU:HB2 | 10:J:47:ARG:NH1 | 2.24 | 0.51 |
| 11:K:78:THR:O | 11:K:81:TYR:HB3 | 2.10 | 0.51 |
| 1:A:284:ALA:O | 1:A:286:HIS:N | 2.41 | 0.51 |
| 1:A:306:ASN:ND2 | 1:A:322:VAL:HG12 | 2.26 | 0.51 |
| 1:A:343:LYS:NZ | 2:B:1151:LEU:CD1 | 2.70 | 0.51 |
| 1:A:463:ILE:HB | 1:A:464:PRO:CD | 2.40 | 0.51 |
| 1:A:466:SER:HB2 | 2:B:1099:VAL:HG22 | 1.91 | 0.51 |
| 1:A:567:LYS:CG | 1:A:568:PRO:CD | 2.87 | 0.51 |
| 1:A:877:HIS:N | 1:A:877:HIS:CD2 | 2.78 | 0.51 |
| 1:A:896:ARG:HH21 | 1:A:1030:ARG:HE | 1.53 | 0.51 |
| 1:A:1102:LYS:O | 1:A:1106:ASN:ND2 | 2.43 | 0.51 |
| 1:A:1167:GLU:HA | 1:A:1170:ILE:HD12 | 1.92 | 0.51 |
| 2:B:562:GLY:O | 2:B:590:HIS:ND1 | 2.43 | 0.51 |
| 2:B:746:SER:CB | 2:B:1046:PRO:HG2 | 2.39 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:C:31:ASN:ND2 | 3:C:35:ARG:HD2 | 2.26 | 0.51 |
| 3:C:124:LEU:O | 3:C:126:GLY:N | 2.44 | 0.51 |
| 4:D:145:MET:O | 4:D:149:THR:HB | 2.11 | 0.51 |
| 5:E:5:ASN:O | 5:E:9:ILE:HG13 | 2.10 | 0.51 |
| 9:I:62:ILE:HD13 | 9:I:102:VAL:HG11 | 1.93 | 0.51 |
| 13:T:12:DG:H2'' | 13:T:13:DT:O5' | 2.09 | 0.51 |
| 1:A:74:MET:H | 1:A:74:MET:HE2 | 1.75 | 0.51 |
| 1:A:104:GLU:CG | 1:A:174:ILE:HD12 | 2.41 | 0.51 |
| 1:A:284:ALA:HB1 | 1:A:289:ILE:HD11 | 1.91 | 0.51 |
| 1:A:477:PRO:HG2 | 1:A:521:MET:CG | 2.40 | 0.51 |
| 1:A:543:LEU:O | 1:A:546:VAL:N | 2.44 | 0.51 |
| 1:A:562:THR:HG21 | 8:H:98:TYR:CD2 | 2.46 | 0.51 |
| 1:A:591:PHE:HA | 1:A:595:THR:CB | 2.41 | 0.51 |
| 1:A:725:ALA:HA | 1:A:728:LYS:HE2 | 1.93 | 0.51 |
| 1:A:767:GLN:NE2 | 1:A:797:LYS:O | 2.42 | 0.51 |
| 1:A:901:LEU:HD13 | 1:A:919:ILE:CG2 | 2.41 | 0.51 |
| 1:A:1102:LYS:HG2 | 1:A:1106:ASN:HD21 | 1.75 | 0.51 |
| 1:A:1118:VAL:CG2 | 1:A:1306:LEU:HB2 | 2.41 | 0.51 |
| 1:A:1120:LEU:H | 1:A:1120:LEU:HD12 | 1.75 | 0.51 |
| 2:B:730:ARG:NH2 | 2:B:1047:PHE:HB3 | 2.26 | 0.51 |
| 2:B:737:THR:HG21 | 9:I:66:PRO:HA | 1.91 | 0.51 |
| 2:B:781:PHE:O | 2:B:782:LEU:HG | 2.10 | 0.51 |
| 2:B:866:TYR:O | 2:B:868:MET:N | 2.41 | 0.51 |
| 2:B:884:ARG:O | 2:B:936:ASP:HB2 | 2.10 | 0.51 |
| 2:B:899:ILE:HG21 | 2:B:949:VAL:HG21 | 1.92 | 0.51 |
| 3:C:82:TYR:CZ | 3:C:161:LYS:HG2 | 2.45 | 0.51 |
| 5:E:117:THR:HG22 | 5:E:120:ALA:H | 1.74 | 0.51 |
| 7:G:119:LEU:HA | 7:G:131:GLN:O | 2.09 | 0.51 |
| 8:H:10:PHE:O | 8:H:54:SER:HA | 2.09 | 0.51 |
| 9:I:6:PHE:HA | 9:I:14:LEU:HG | 1.93 | 0.51 |
| 10:J:1:MET:H1 | 10:J:57:ILE:N | 2.05 | 0.51 |
| 13:T:8:DT:H2'' | 13:T:9:DC:OP2 | 2.10 | 0.51 |
| 1:A:230:ARG:O | 1:A:231:PRO:C | 2.49 | 0.51 |
| 1:A:556:TRP:CZ3 | 1:A:558:GLY:HA2 | 2.45 | 0.51 |
| 1:A:598:LEU:O | 1:A:598:LEU:HD23 | 2.11 | 0.51 |
| 1:A:765:VAL:HG23 | 1:A:802:ASN:O | 2.11 | 0.51 |
| 1:A:830:LYS:HG3 | 1:A:1098:VAL:HG11 | 1.91 | 0.51 |
| 1:A:1446:ASP:HB2 | 6:F:133:VAL:HG21 | 1.91 | 0.51 |
| 2:B:186:GLU:HG3 | 10:J:62:ARG:NH2 | 2.26 | 0.51 |
| 2:B:391:ASP:HB2 | 9:I:92:ARG:HG3 | 1.91 | 0.51 |
| 2:B:510:LYS:HB2 | 2:B:511:PRO:HD3 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:582:VAL:HG22 | 2:B:626:ILE:HG21 | 1.92 | 0.51 |
| 2:B:797:TYR:HB3 | 2:B:798:TYR:HD2 | 1.76 | 0.51 |
| 2:B:882:THR:HG22 | 2:B:884:ARG:CB | 2.35 | 0.51 |
| 2:B:1044:ALA:O | 2:B:1045:SER:O | 2.29 | 0.51 |
| 3:C:168:ALA:O | 3:C:171:GLY:N | 2.43 | 0.51 |
| 10:J:23:ASN:O | 10:J:25:LEU:N | 2.43 | 0.51 |
| 1:A:76:GLU:O | 1:A:78:PRO:HD3 | 2.11 | 0.51 |
| 1:A:387:ARG:O | 1:A:390:GLN:HB3 | 2.10 | 0.51 |
| 1:A:432:VAL:O | 1:A:433:GLU:C | 2.47 | 0.51 |
| 1:A:498:ARG:HG3 | 1:A:499:ALA:N | 2.26 | 0.51 |
| 1:A:535:THR:CG2 | 1:A:575:LYS:HE2 | 2.39 | 0.51 |
| 1:A:574:GLY:O | 1:A:575:LYS:C | 2.49 | 0.51 |
| 1:A:637:LYS:HB3 | 1:A:641:VAL:HG11 | 1.93 | 0.51 |
| 1:A:843:LYS:HD3 | 1:A:846:GLU:OE2 | 2.11 | 0.51 |
| 1:A:898:ARG:O | 1:A:1029:ARG:NH1 | 2.44 | 0.51 |
| 1:A:1001:ARG:HH11 | 1:A:1001:ARG:CG | 2.24 | 0.51 |
| 1:A:1345:ARG:NH1 | 1:A:1373:ASP:OD1 | 2.44 | 0.51 |
| 2:B:69:LEU:CD1 | 2:B:429:PHE:HE1 | 2.19 | 0.51 |
| 2:B:515:HIS:O | 2:B:518:HIS:HB2 | 2.11 | 0.51 |
| 2:B:798:TYR:CE1 | 10:J:4:PRO:HA | 2.46 | 0.51 |
| 4:D:137:ASN:N | 4:D:137:ASN:ND2 | 2.58 | 0.51 |
| 6:F:93:ILE:HD13 | 6:F:148:VAL:HG12 | 1.93 | 0.51 |
| 9:I:6:PHE:N | 9:I:6:PHE:CD2 | 2.75 | 0.51 |
| 9:I:61:ASP:C | 9:I:63:GLY:H | 2.13 | 0.51 |
| 1:A:284:ALA:C | 1:A:286:HIS:N | 2.59 | 0.51 |
| 1:A:427:GLN:HB2 | 1:A:430:TRP:CD2 | 2.46 | 0.51 |
| 1:A:524:VAL:CG1 | 1:A:525:GLN:N | 2.73 | 0.51 |
| 1:A:677:ARG:HD2 | 1:A:677:ARG:C | 2.31 | 0.51 |
| 1:A:832:ALA:HA | 13:T:18:DA:C8 | 2.45 | 0.51 |
| 1:A:1048:ASN:O | 1:A:1052:GLN:HB2 | 2.11 | 0.51 |
| 1:A:1425:SER:HA | 1:A:1428:VAL:CG2 | 2.40 | 0.51 |
| 2:B:842:ASN:O | 2:B:846:ILE:HG13 | 2.11 | 0.51 |
| 2:B:857:ARG:HH21 | 2:B:942:ARG:NH2 | 2.09 | 0.51 |
| 3:C:36:VAL:CG2 | 3:C:251:LEU:HD13 | 2.41 | 0.51 |
| 3:C:51:VAL:HB | 12:L:65:VAL:HG23 | 1.93 | 0.51 |
| 4:D:8:PHE:CD2 | 7:G:6:ASP:O | 2.64 | 0.51 |
| 5:E:153:HIS:HB3 | 5:E:196:VAL:HG13 | 1.93 | 0.51 |
| 7:G:55:ASP:OD1 | 7:G:57:GLN:HG3 | 2.10 | 0.51 |
| 8:H:101:ALA:HB2 | 8:H:116:TYR:CE1 | 2.46 | 0.51 |
| 9:I:50:THR:HG22 | 9:I:51:ASN:N | 2.26 | 0.51 |
| 9:I:69:PRO:HB2 | 9:I:85:PHE:CE2 | 2.46 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:I:74:GLU:O | 9:I:74:GLU:HG3 | 2.10 | 0.51 |
| 10:J:25:LEU:O | 10:J:29:GLU:HA | 2.10 | 0.51 |
| 12:L:36:SER:O | 12:L:37:LYS:C | 2.48 | 0.51 |
| 1:A:42:ASP:OD1 | 1:A:47:ARG:HA | 2.10 | 0.51 |
| 1:A:130:ASP:O | 1:A:132:LYS:N | 2.44 | 0.51 |
| 1:A:391:LEU:HD22 | 1:A:401:GLY:O | 2.10 | 0.51 |
| 1:A:900:ASP:HA | 1:A:926:GLN:HE22 | 1.75 | 0.51 |
| 1:A:1015:VAL:O | 1:A:1017:LEU:N | 2.44 | 0.51 |
| 1:A:1151:GLU:HG2 | 9:I:45:ARG:HB2 | 1.93 | 0.51 |
| 2:B:95:ILE:CB | 2:B:130:VAL:HG22 | 2.40 | 0.51 |
| 2:B:114:PRO:O | 2:B:116:GLU:N | 2.44 | 0.51 |
| 2:B:521:LEU:HD22 | 2:B:633:VAL:CG1 | 2.27 | 0.51 |
| 2:B:601:ARG:HH11 | 2:B:605:ARG:NH2 | 2.08 | 0.51 |
| 2:B:797:TYR:C | 2:B:798:TYR:HD2 | 2.15 | 0.51 |
| 2:B:912:ILE:O | 2:B:938:SER:HA | 2.10 | 0.51 |
| 2:B:1166:CYS:O | 2:B:1168:LEU:N | 2.33 | 0.51 |
| 5:E:98:ILE:HA | 5:E:101:GLN:HB3 | 1.93 | 0.51 |
| 5:E:124:VAL:HA | 5:E:132:ILE:CD1 | 2.40 | 0.51 |
| 5:E:181:ALA:O | 5:E:182:ASP:C | 2.49 | 0.51 |
| 6:F:114:GLU:HA | 6:F:114:GLU:OE2 | 2.11 | 0.51 |
| 7:G:48:VAL:HA | 7:G:76:ALA:CB | 2.40 | 0.51 |
| 7:G:112:LYS:HA | 7:G:115:MET:HE3 | 1.93 | 0.51 |
| 1:A:19:PHE:O | 1:A:1416:ALA:HA | 2.11 | 0.51 |
| 1:A:172:PRO:HD3 | 1:A:185:TRP:CE2 | 2.45 | 0.51 |
| 1:A:1272:THR:HG22 | 1:A:1273:LEU:N | 2.26 | 0.51 |
| 1:A:1388:GLY:O | 1:A:1391:ARG:HG3 | 2.11 | 0.51 |
| 1:A:1445:ILE:HD13 | 7:G:70:PHE:CZ | 2.46 | 0.51 |
| 2:B:95:ILE:HG13 | 2:B:129:PHE:O | 2.11 | 0.51 |
| 2:B:190:TYR:HD2 | 10:J:62:ARG:O | 1.92 | 0.51 |
| 2:B:276:ILE:O | 2:B:278:GLN:N | 2.37 | 0.51 |
| 2:B:293:PRO:O | 2:B:297:ILE:HG13 | 2.11 | 0.51 |
| 2:B:969:ARG:HG2 | 2:B:970:THR:N | 2.25 | 0.51 |
| 2:B:992:ILE:HG12 | 2:B:993:THR:N | 2.26 | 0.51 |
| 5:E:16:PHE:HE2 | 5:E:37:LEU:HD23 | 1.76 | 0.51 |
| 13:T:11:DA:H2" | 13:T:12:DG:H8 | 1.76 | 0.51 |
| 1:A:531:ILE:HD11 | 1:A:578:LEU:HD21 | 1.93 | 0.50 |
| 1:A:787:PHE:CE1 | 1:A:796:SER:HA | 2.46 | 0.50 |
| 1:A:896:ARG:HH22 | 1:A:1030:ARG:HH21 | 1.57 | 0.50 |
| 2:B:229:ALA:CB | 2:B:231:PRO:HD2 | 2.39 | 0.50 |
| 2:B:606:LYS:HD3 | 2:B:608:ASP:HB2 | 1.93 | 0.50 |
| 2:B:685:LEU:C | 2:B:685:LEU:HD12 | 2.31 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:891:ASP:C | 2:B:893:LEU:N | 2.64 | 0.50 |
| 2:B:1158:PHE:CG | 2:B:1159:ARG:N | 2.79 | 0.50 |
| 2:B:1182:CYS:O | 2:B:1183:LYS:O | 2.29 | 0.50 |
| 3:C:168:ALA:O | 3:C:170:TRP:N | 2.44 | 0.50 |
| 5:E:116:ILE:CG2 | 5:E:117:THR:N | 2.74 | 0.50 |
| 7:G:39:THR:O | 7:G:43:GLY:HA2 | 2.11 | 0.50 |
| 7:G:127:PRO:HG3 | 7:G:139:ILE:CG1 | 2.40 | 0.50 |
| 7:G:142:ARG:CB | 7:G:171:ILE:HD11 | 2.41 | 0.50 |
| 7:G:143:ILE:CG2 | 7:G:144:ARG:N | 2.74 | 0.50 |
| 12:L:38:LEU:O | 12:L:39:SER:CB | 2.60 | 0.50 |
| 12:L:68:GLU:H | 12:L:68:GLU:CD | 2.15 | 0.50 |
| 1:A:37:PHE:CD2 | 1:A:50:ILE:HG21 | 2.46 | 0.50 |
| 1:A:1187:GLN:CD | 1:A:1188:GLN:HE21 | 2.15 | 0.50 |
| 2:B:189:LEU:O | 2:B:192:LEU:N | 2.45 | 0.50 |
| 2:B:258:LEU:O | 2:B:258:LEU:CG | 2.59 | 0.50 |
| 2:B:307:ASP:O | 2:B:309:GLN:N | 2.44 | 0.50 |
| 2:B:464:GLY:C | 2:B:465:ASN:ND2 | 2.63 | 0.50 |
| 2:B:469:GLN:HG3 | 2:B:470:LYS:H | 1.74 | 0.50 |
| 2:B:619:ILE:O | 2:B:622:LYS:N | 2.44 | 0.50 |
| 2:B:644:GLU:OE2 | 2:B:646:LEU:HB2 | 2.11 | 0.50 |
| 2:B:778:MET:HE2 | 2:B:1094:ARG:HG2 | 1.93 | 0.50 |
| 2:B:785:TYR:N | 2:B:785:TYR:HD2 | 2.09 | 0.50 |
| 2:B:1115:THR:HG22 | 2:B:1117:GLN:CG | 2.41 | 0.50 |
| 3:C:248:ILE:HD13 | 11:K:102:LYS:HA | 1.94 | 0.50 |
| 8:H:84:ALA:HA | 8:H:87:ARG:HG3 | 1.92 | 0.50 |
| 1:A:125:ALA:O | 1:A:127:ALA:N | 2.45 | 0.50 |
| 1:A:286:HIS:C | 1:A:288:ALA:H | 2.15 | 0.50 |
| 1:A:699:ALA:HB3 | 1:A:701:LEU:HG | 1.92 | 0.50 |
| 1:A:1191:TRP:CB | 1:A:1260:LEU:HD23 | 2.40 | 0.50 |
| 2:B:542:MET:SD | 2:B:747:MET:HE2 | 2.52 | 0.50 |
| 2:B:811:TYR:H | 2:B:811:TYR:HD1 | 1.58 | 0.50 |
| 2:B:864:LYS:O | 2:B:871:THR:HG23 | 2.11 | 0.50 |
| 2:B:877:PRO:C | 2:B:878:GLN:HG3 | 2.31 | 0.50 |
| 3:C:8:VAL:HG12 | 3:C:9:LYS:N | 2.22 | 0.50 |
| 7:G:88:ASP:HB3 | 7:G:144:ARG:CA | 2.40 | 0.50 |
| 1:A:25:GLU:OE1 | 1:A:25:GLU:N | 2.20 | 0.50 |
| 1:A:58:LEU:HA | 1:A:80:HIS:HB2 | 1.93 | 0.50 |
| 1:A:282:ASN:O | 1:A:284:ALA:N | 2.44 | 0.50 |
| 1:A:506:ALA:CB | 1:A:508:PRO:HD2 | 2.39 | 0.50 |
| 1:A:590:ARG:NH1 | 1:A:590:ARG:CG | 2.74 | 0.50 |
| 2:B:593:PRO:O | 2:B:596:LEU:N | 2.44 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:654:ARG:O | 2:B:656:GLY:N | 2.45 | 0.50 |
| 2:B:706:GLN:NE2 | 2:B:730:ARG:HH11 | 2.09 | 0.50 |
| 2:B:847:ASP:O | 2:B:849:GLY:N | 2.44 | 0.50 |
| 2:B:969:ARG:HD3 | 3:C:61:GLU:OE2 | 2.11 | 0.50 |
| 2:B:983:ARG:HD2 | 2:B:1091:TYR:HB3 | 1.92 | 0.50 |
| 3:C:169:LYS:HE3 | 3:C:170:TRP:CZ2 | 2.47 | 0.50 |
| 4:D:14:ARG:O | 4:D:16:LYS:N | 2.42 | 0.50 |
| 4:D:54:GLU:O | 4:D:58:VAL:HG23 | 2.11 | 0.50 |
| 7:G:45:ILE:HD13 | 7:G:78:VAL:CG1 | 2.41 | 0.50 |
| 8:H:44:VAL:CG1 | 8:H:48:PRO:HA | 2.38 | 0.50 |
| 9:I:111:THR:HG22 | 9:I:113:ASP:H | 1.76 | 0.50 |
| 10:J:16:ASP:O | 10:J:18:TRP:N | 2.45 | 0.50 |
| 1:A:40:THR:HB | 1:A:41:MET:HE2 | 1.93 | 0.50 |
| 1:A:345:VAL:HG21 | 2:B:1150:ARG:NH2 | 2.24 | 0.50 |
| 1:A:402:ALA:HB2 | 1:A:434:ARG:HA | 1.94 | 0.50 |
| 1:A:461:LYS:O | 1:A:463:ILE:HG23 | 2.12 | 0.50 |
| 1:A:767:GLN:OE1 | 1:A:799:PHE:HB2 | 2.12 | 0.50 |
| 1:A:909:ASP:O | 1:A:911:SER:N | 2.42 | 0.50 |
| 1:A:1396:ALA:HA | 1:A:1399:ARG:NH2 | 2.27 | 0.50 |
| 2:B:54:PHE:O | 2:B:58:THR:HB | 2.11 | 0.50 |
| 2:B:57:TYR:HD1 | 2:B:57:TYR:N | 2.10 | 0.50 |
| 2:B:278:GLN:HG2 | 2:B:279:ASP:N | 2.18 | 0.50 |
| 2:B:331:LEU:HD12 | 2:B:331:LEU:N | 2.26 | 0.50 |
| 2:B:660:LYS:HB3 | 2:B:679:TYR:CE2 | 2.46 | 0.50 |
| 2:B:785:TYR:N | 2:B:785:TYR:CD2 | 2.80 | 0.50 |
| 2:B:860:MET:CG | 2:B:965:LYS:HG2 | 2.41 | 0.50 |
| 2:B:1050:ILE:HD12 | 2:B:1050:ILE:N | 2.26 | 0.50 |
| 3:C:88:CYS:SG | 3:C:91:HIS:C | 2.90 | 0.50 |
| 3:C:174:ALA:O | 10:J:10:CYS:O | 2.29 | 0.50 |
| 5:E:186:LEU:O | 5:E:189:GLY:N | 2.41 | 0.50 |
| 9:I:33:SER:O | 9:I:35:VAL:HG23 | 2.11 | 0.50 |
| 11:K:7:PHE:O | 11:K:11:LEU:HD23 | 2.11 | 0.50 |
| 1:A:87:ALA:CB | 1:A:276:LEU:HD23 | 2.42 | 0.50 |
| 1:A:125:ALA:HA | 1:A:128:ILE:HG13 | 1.93 | 0.50 |
| 1:A:418:SER:C | 1:A:420:ARG:H | 2.14 | 0.50 |
| 1:A:699:ALA:O | 1:A:700:ASN:HB3 | 2.11 | 0.50 |
| 1:A:1138:ILE:C | 1:A:1275:GLY:HA2 | 2.32 | 0.50 |
| 1:A:1453:TYR:O | 1:A:1454:MET:CB | 2.59 | 0.50 |
| 2:B:68:THR:CG2 | 2:B:91:SER:HB3 | 2.41 | 0.50 |
| 2:B:914:LYS:HD3 | 2:B:937:ALA:O | 2.11 | 0.50 |
| 3:C:146:LYS:C | 3:C:147:LEU:HD23 | 2.32 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:59:ILE:HG21 | 4:D:145:MET:SD | 2.52 | 0.50 |
| 5:E:42:PHE:HZ | 5:E:58:MET:HE1 | 1.77 | 0.50 |
| 10:J:5:VAL:HG12 | 10:J:6:ARG:CG | 2.29 | 0.50 |
| 1:A:244:PRO:HG2 | 1:A:245:PRO:HD3 | 1.94 | 0.50 |
| 1:A:441:PRO:HD2 | 1:A:498:ARG:CZ | 2.41 | 0.50 |
| 1:A:523:ILE:CD1 | 1:A:649:ILE:HG21 | 2.41 | 0.50 |
| 1:A:575:LYS:HB3 | 1:A:612:ILE:CG2 | 2.42 | 0.50 |
| 1:A:728:LYS:HB3 | 1:A:731:ARG:HH21 | 1.77 | 0.50 |
| 1:A:929:LEU:HD23 | 1:A:983:ILE:HG21 | 1.94 | 0.50 |
| 1:A:1218:GLN:O | 1:A:1221:LYS:HE3 | 2.12 | 0.50 |
| 1:A:1259:MET:C | 1:A:1261:LYS:H | 2.15 | 0.50 |
| 1:A:1443:VAL:CG1 | 6:F:132:LEU:HD13 | 2.42 | 0.50 |
| 2:B:34:ILE:HG12 | 2:B:542:MET:HE1 | 1.94 | 0.50 |
| 2:B:170:LEU:O | 2:B:172:ILE:HG13 | 2.11 | 0.50 |
| 2:B:193:LYS:HD3 | 2:B:787:VAL:HG11 | 1.93 | 0.50 |
| 2:B:313:MET:O | 2:B:316:PRO:HD2 | 2.11 | 0.50 |
| 2:B:637:LEU:HD22 | 2:B:741:CYS:O | 2.12 | 0.50 |
| 2:B:800:GLN:CB | 10:J:52:THR:HG22 | 2.39 | 0.50 |
| 2:B:839:MET:HG3 | 2:B:1010:LEU:CD1 | 2.41 | 0.50 |
| 2:B:1069:PHE:HA | 2:B:1085:ILE:O | 2.11 | 0.50 |
| 3:C:82:TYR:O | 3:C:83:SER:C | 2.49 | 0.50 |
| 3:C:101:LEU:O | 3:C:102:GLN:HG3 | 2.11 | 0.50 |
| 3:C:166:GLU:O | 3:C:167:HIS:HB2 | 2.12 | 0.50 |
| 3:C:268:ASP:O | 3:C:269:LYS:HB2 | 2.11 | 0.50 |
| 4:D:153:ARG:NH2 | 4:D:184:ALA:HA | 2.27 | 0.50 |
| 7:G:153:GLN:O | 7:G:154:VAL:C | 2.50 | 0.50 |
| 8:H:26:ILE:O | 8:H:27:GLU:HG3 | 2.12 | 0.50 |
| 14:N:4:DA:H2'' | 14:N:5:DC:C5 | 2.46 | 0.50 |
| 1:A:65:LEU:O | 1:A:66:LYS:C | 2.49 | 0.50 |
| 1:A:219:PHE:CD2 | 1:A:231:PRO:HD2 | 2.47 | 0.50 |
| 1:A:262:LEU:HD22 | 1:A:303:TYR:HE1 | 1.77 | 0.50 |
| 1:A:265:LYS:HG2 | 1:A:303:TYR:HA | 1.94 | 0.50 |
| 1:A:741:ASN:HD22 | 1:A:744:LYS:HB2 | 1.75 | 0.50 |
| 1:A:960:ILE:HA | 1:A:963:ILE:HG22 | 1.91 | 0.50 |
| 1:A:1141:THR:CG2 | 1:A:1205:LYS:HD3 | 2.42 | 0.50 |
| 2:B:390:LEU:O | 2:B:392:ARG:HG3 | 2.12 | 0.50 |
| 2:B:547:VAL:N | 2:B:612:GLU:OE2 | 2.38 | 0.50 |
| 2:B:744:HIS:CG | 2:B:745:PRO:HD2 | 2.47 | 0.50 |
| 2:B:810:GLU:CA | 2:B:815:ARG:NH2 | 2.66 | 0.50 |
| 2:B:826:ALA:HB2 | 2:B:1008:PRO:HB3 | 1.92 | 0.50 |
| 3:C:112:ASN:HB2 | 3:C:114:TYR:HE1 | 1.76 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:C:249:ASP:O | 3:C:250:THR:C | 2.48 | 0.50 |
| 4:D:3:VAL:HG12 | 4:D:4:SER:H | 1.77 | 0.50 |
| 5:E:121:MET:C | 5:E:123:LEU:H | 2.15 | 0.50 |
| 6:F:70:LYS:O | 6:F:72:LYS:NZ | 2.42 | 0.50 |
| 8:H:89:LEU:O | 8:H:91:ASP:N | 2.45 | 0.50 |
| 8:H:101:ALA:HA | 8:H:116:TYR:HA | 1.94 | 0.50 |
| 1:A:220:THR:O | 1:A:221:SER:C | 2.50 | 0.50 |
| 1:A:347:PHE:CE2 | 1:A:493:GLN:OE1 | 2.65 | 0.50 |
| 1:A:491:VAL:HG12 | 1:A:492:PRO:O | 2.12 | 0.50 |
| 1:A:548:ASN:HA | 11:K:60:ALA:HB1 | 1.92 | 0.50 |
| 1:A:870:GLU:HB2 | 5:E:204:THR:HG21 | 1.94 | 0.50 |
| 2:B:244:LEU:HB2 | 2:B:249:ARG:HA | 1.93 | 0.50 |
| 2:B:558:LEU:O | 2:B:560:GLU:N | 2.30 | 0.50 |
| 2:B:731:VAL:HG12 | 2:B:732:SER:N | 2.27 | 0.50 |
| 2:B:785:TYR:CD1 | 2:B:795:ILE:HG12 | 2.47 | 0.50 |
| 2:B:1178:ASN:N | 2:B:1178:ASN:ND2 | 2.59 | 0.50 |
| 4:D:57:LEU:O | 4:D:61:GLU:HB2 | 2.11 | 0.50 |
| 4:D:153:ARG:HB3 | 4:D:154:PHE:CE1 | 2.47 | 0.50 |
| 4:D:153:ARG:HB3 | 4:D:154:PHE:CD1 | 2.46 | 0.50 |
| 4:D:155:ARG:HH11 | 4:D:155:ARG:HG3 | 1.77 | 0.50 |
| 5:E:197:LYS:HE2 | 5:E:199:ILE:HD11 | 1.94 | 0.50 |
| 9:I:5:ARG:HG3 | 9:I:14:LEU:HD12 | 1.92 | 0.50 |
| 12:L:61:THR:HG22 | 12:L:63:ARG:N | 2.24 | 0.50 |
| 1:A:95:PHE:O | 1:A:96:ILE:C | 2.51 | 0.49 |
| 1:A:786:HIS:NE2 | 2:B:742:GLU:OE1 | 2.45 | 0.49 |
| 1:A:1111:MET:HB2 | 1:A:1113:THR:O | 2.12 | 0.49 |
| 1:A:1114:PRO:HB2 | 1:A:1311:VAL:HG23 | 1.93 | 0.49 |
| 1:A:1341:ILE:O | 1:A:1344:GLY:N | 2.45 | 0.49 |
| 1:A:1402:PHE:CD1 | 1:A:1403:GLU:HG3 | 2.47 | 0.49 |
| 2:B:49:ASP:HA | 2:B:52:ASN:HD22 | 1.77 | 0.49 |
| 2:B:243:ALA:HB1 | 2:B:251:ILE:HG12 | 1.92 | 0.49 |
| 2:B:298:LEU:N | 2:B:298:LEU:CD2 | 2.75 | 0.49 |
| 2:B:661:LEU:HD11 | 2:B:684:LEU:HD11 | 1.93 | 0.49 |
| 2:B:863:GLU:OE1 | 2:B:962:LYS:HB2 | 2.11 | 0.49 |
| 3:C:76:ASP:OD2 | 3:C:127:ARG:HB2 | 2.11 | 0.49 |
| 3:C:105:GLY:HA3 | 3:C:149:LYS:O | 2.12 | 0.49 |
| 3:C:114:TYR:HB2 | 3:C:116:LYS:HG2 | 1.94 | 0.49 |
| 4:D:40:HIS:HB2 | 7:G:73:LYS:NZ | 2.27 | 0.49 |
| 4:D:47:LEU:CD1 | 4:D:48:ILE:H | 2.20 | 0.49 |
| 4:D:138:ASN:HD21 | 7:G:35:GLU:HB3 | 1.76 | 0.49 |
| 10:J:27:GLU:C | 10:J:29:GLU:H | 2.15 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:452:LYS:HG3 | 2:B:1140:ALA:CB | 2.42 | 0.49 |
| 1:A:679:ILE:HG23 | 1:A:729:ALA:HB1 | 1.94 | 0.49 |
| 2:B:49:ASP:HA | 2:B:52:ASN:ND2 | 2.27 | 0.49 |
| 2:B:118:ARG:HH22 | 2:B:194:GLU:CD | 2.16 | 0.49 |
| 2:B:405:ARG:CZ | 2:B:632:ARG:HG2 | 2.41 | 0.49 |
| 2:B:455:SER:O | 2:B:458:LYS:N | 2.44 | 0.49 |
| 2:B:821:GLN:HE22 | 2:B:851:PHE:N | 2.06 | 0.49 |
| 3:C:236:GLY:O | 3:C:237:SER:C | 2.51 | 0.49 |
| 5:E:26:ARG:HA | 5:E:188:LEU:HD23 | 1.93 | 0.49 |
| 9:I:28:GLU:HG3 | 9:I:29:CYS:N | 2.27 | 0.49 |
| 9:I:73:ARG:NH1 | 9:I:112:SER:HB3 | 2.27 | 0.49 |
| 1:A:345:VAL:HG23 | 1:A:346:ASP:O | 2.13 | 0.49 |
| 1:A:402:ALA:HB1 | 1:A:433:GLU:O | 2.12 | 0.49 |
| 1:A:543:LEU:O | 1:A:544:ASP:C | 2.50 | 0.49 |
| 1:A:741:ASN:ND2 | 1:A:744:LYS:N | 2.60 | 0.49 |
| 1:A:866:PHE:O | 1:A:867:ILE:HD12 | 2.10 | 0.49 |
| 1:A:889:SER:HA | 1:A:1297:GLU:N | 2.27 | 0.49 |
| 1:A:1273:LEU:HD12 | 1:A:1273:LEU:N | 2.27 | 0.49 |
| 1:A:1291:VAL:HG13 | 1:A:1292:PRO:CD | 2.40 | 0.49 |
| 2:B:235:SER:C | 2:B:236:HIS:CD2 | 2.86 | 0.49 |
| 2:B:291:ILE:HG22 | 2:B:291:ILE:O | 2.11 | 0.49 |
| 2:B:609:ILE:HG13 | 2:B:609:ILE:O | 2.12 | 0.49 |
| 2:B:654:ARG:O | 2:B:657:HIS:N | 2.45 | 0.49 |
| 2:B:661:LEU:C | 2:B:663:ALA:N | 2.66 | 0.49 |
| 2:B:958:GLN:C | 2:B:960:GLY:H | 2.15 | 0.49 |
| 2:B:1215:ARG:C | 2:B:1216:LEU:HD23 | 2.31 | 0.49 |
| 3:C:124:LEU:C | 3:C:126:GLY:H | 2.14 | 0.49 |
| 5:E:161:LYS:HG3 | 5:E:195:VAL:HG21 | 1.94 | 0.49 |
| 7:G:138:THR:HG22 | 7:G:139:ILE:HG13 | 1.95 | 0.49 |
| 8:H:82:PRO:HG3 | 11:K:54:ARG:NH1 | 2.26 | 0.49 |
| 8:H:84:ALA:CB | 8:H:87:ARG:HD2 | 2.42 | 0.49 |
| 1:A:334:GLY:O | 1:A:336:ILE:N | 2.46 | 0.49 |
| 1:A:511:ILE:HD11 | 1:A:646:PHE:HE1 | 1.76 | 0.49 |
| 1:A:655:PHE:O | 1:A:658:LEU:HB3 | 2.12 | 0.49 |
| 1:A:741:ASN:HD22 | 1:A:744:LYS:CB | 2.26 | 0.49 |
| 1:A:761:MET:HA | 1:A:804:TYR:HB2 | 1.94 | 0.49 |
| 1:A:836:TYR:HB2 | 13:T:18:DA:H5' | 1.93 | 0.49 |
| 1:A:884:ASP:C | 1:A:886:ILE:H | 2.16 | 0.49 |
| 1:A:1120:LEU:O | 1:A:1323:ASP:HB2 | 2.12 | 0.49 |
| 1:A:1313:LEU:HD11 | 1:A:1317:MET:CE | 2.43 | 0.49 |
| 2:B:65:GLU:HG3 | 2:B:66:ASP:N | 2.19 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:102:VAL:N | 2:B:110:HIS:O | 2.45 | 0.49 |
| 2:B:205:ILE:O | 2:B:207:GLY:N | 2.44 | 0.49 |
| 2:B:542:MET:HB3 | 2:B:636:PRO:CD | 2.42 | 0.49 |
| 2:B:579:ARG:N | 2:B:589:VAL:HG13 | 2.27 | 0.49 |
| 2:B:1156:ASP:OD2 | 2:B:1199:ALA:HB2 | 2.12 | 0.49 |
| 3:C:124:LEU:O | 3:C:127:ARG:HG2 | 2.12 | 0.49 |
| 5:E:190:LEU:CD1 | 5:E:214:CYS:HB2 | 2.42 | 0.49 |
| 8:H:62:SER:OG | 8:H:63:LEU:HD12 | 2.13 | 0.49 |
| 9:I:10:CYS:O | 9:I:10:CYS:SG | 2.70 | 0.49 |
| 1:A:11:LEU:C | 1:A:11:LEU:CD1 | 2.75 | 0.49 |
| 1:A:344:ARG:HA | 2:B:1129:ARG:HA | 1.94 | 0.49 |
| 1:A:416:ARG:NH1 | 1:A:417:TYR:CE2 | 2.76 | 0.49 |
| 1:A:492:PRO:HB3 | 1:A:501:LEU:CD1 | 2.42 | 0.49 |
| 1:A:608:ILE:C | 1:A:610:GLY:N | 2.66 | 0.49 |
| 1:A:731:ARG:HA | 1:A:734:GLU:HB3 | 1.95 | 0.49 |
| 1:A:795:GLU:CD | 1:A:795:GLU:H | 2.15 | 0.49 |
| 1:A:1118:VAL:HG23 | 1:A:1306:LEU:HB2 | 1.95 | 0.49 |
| 2:B:102:VAL:CG2 | 2:B:112:LEU:HB2 | 2.43 | 0.49 |
| 2:B:240:ILE:CG2 | 2:B:254:LEU:HB3 | 2.42 | 0.49 |
| 2:B:281:PRO:O | 2:B:283:VAL:N | 2.46 | 0.49 |
| 2:B:485:ARG:NH1 | 2:B:782:LEU:HD11 | 2.28 | 0.49 |
| 2:B:1084:GLN:NE2 | 2:B:1084:GLN:H | 1.91 | 0.49 |
| 5:E:31:THR:HG23 | 5:E:34:GLU:HB2 | 1.94 | 0.49 |
| 5:E:61:GLN:NE2 | 5:E:105:PHE:CZ | 2.79 | 0.49 |
| 8:H:17:PRO:HB3 | 8:H:24:CYS:SG | 2.52 | 0.49 |
| 8:H:144:ILE:HG22 | 8:H:145:ARG:H | 1.77 | 0.49 |
| 9:I:61:ASP:O | 9:I:63:GLY:N | 2.45 | 0.49 |
| 1:A:189:ARG:O | 1:A:190:ALA:CB | 2.61 | 0.49 |
| 1:A:412:ARG:HH22 | 2:B:1108:ARG:NH2 | 2.10 | 0.49 |
| 1:A:681:GLU:C | 1:A:683:ILE:N | 2.65 | 0.49 |
| 1:A:780:VAL:O | 1:A:780:VAL:HG12 | 2.12 | 0.49 |
| 1:A:1054:LEU:O | 1:A:1057:VAL:HG23 | 2.12 | 0.49 |
| 2:B:37:PHE:CE1 | 2:B:41:LYS:HG3 | 2.47 | 0.49 |
| 2:B:244:LEU:HD13 | 2:B:247:GLY:O | 2.13 | 0.49 |
| 2:B:343:ILE:HG23 | 2:B:347:LYS:CD | 2.42 | 0.49 |
| 2:B:348:ARG:HG3 | 2:B:349:ILE:N | 2.28 | 0.49 |
| 2:B:372:SER:O | 2:B:376:PHE:HB2 | 2.13 | 0.49 |
| 2:B:614:SER:HB3 | 2:B:694:ASP:CB | 2.42 | 0.49 |
| 2:B:1096:ARG:O | 2:B:1097:HIS:CG | 2.66 | 0.49 |
| 5:E:109:ILE:CG2 | 5:E:110:PHE:N | 2.69 | 0.49 |
| 9:I:61:ASP:O | 9:I:64:SER:N | 2.43 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 10:J:64:ASN:HB3 | 10:J:65:PRO:HD3 | 1.92 | 0.49 |
| 15:P:5:C:O2' | 15:P:6:A:H5' | 2.12 | 0.49 |
| 1:A:23:SER:O | 1:A:24:PRO:C | 2.49 | 0.49 |
| 1:A:208:LEU:HD23 | 1:A:209:ASN:N | 2.28 | 0.49 |
| 1:A:270:LEU:O | 1:A:273:ASN:HB3 | 2.13 | 0.49 |
| 1:A:412:ARG:NH2 | 2:B:1108:ARG:NH2 | 2.60 | 0.49 |
| 1:A:639:PRO:CG | 1:A:640:GLN:N | 2.76 | 0.49 |
| 1:A:1148:ILE:HG12 | 1:A:1198:ASP:HB2 | 1.95 | 0.49 |
| 2:B:203:PHE:HB3 | 2:B:205:ILE:HD11 | 1.94 | 0.49 |
| 2:B:210:LYS:HG3 | 2:B:461:LEU:O | 2.12 | 0.49 |
| 2:B:531:GLN:HG3 | 2:B:532:ALA:H | 1.77 | 0.49 |
| 2:B:558:LEU:C | 2:B:560:GLU:H | 2.12 | 0.49 |
| 2:B:952:VAL:HG22 | 2:B:966:VAL:HG13 | 1.94 | 0.49 |
| 2:B:1221:SER:HB3 | 4:D:12:ARG:HE | 1.77 | 0.49 |
| 4:D:204:ASP:O | 4:D:208:GLU:HB2 | 2.12 | 0.49 |
| 5:E:89:GLY:CA | 5:E:117:THR:OG1 | 2.60 | 0.49 |
| 7:G:1:MET:HE1 | 7:G:3:PHE:HE1 | 1.77 | 0.49 |
| 11:K:45:LEU:HG | 11:K:94:ILE:CD1 | 2.41 | 0.49 |
| 13:T:7:DC:H2'' | 13:T:8:DT:H71 | 1.94 | 0.49 |
| 1:A:6:TYR:CD1 | 1:A:7:SER:N | 2.81 | 0.49 |
| 1:A:49:LYS:HD2 | 1:A:55:ASP:HB3 | 1.94 | 0.49 |
| 1:A:374:LEU:O | 1:A:436:ILE:HG12 | 2.13 | 0.49 |
| 1:A:381:THR:CG2 | 1:A:382:PRO:HD2 | 2.42 | 0.49 |
| 1:A:730:GLY:O | 1:A:731:ARG:C | 2.50 | 0.49 |
| 1:A:1125:ALA:C | 1:A:1127:ASP:H | 2.14 | 0.49 |
| 2:B:22:SER:HA | 2:B:654:ARG:CB | 2.43 | 0.49 |
| 2:B:95:ILE:HG13 | 2:B:130:VAL:HG22 | 1.95 | 0.49 |
| 2:B:529:GLU:OE1 | 2:B:769:TYR:HE1 | 1.96 | 0.49 |
| 2:B:579:ARG:HG2 | 2:B:579:ARG:HH11 | 1.77 | 0.49 |
| 2:B:882:THR:HG22 | 2:B:884:ARG:N | 2.23 | 0.49 |
| 2:B:1072:MET:HE3 | 2:B:1085:ILE:CB | 2.42 | 0.49 |
| 4:D:52:LEU:O | 4:D:53:SER:OG | 2.28 | 0.49 |
| 5:E:100:ILE:HG22 | 5:E:100:ILE:O | 2.13 | 0.49 |
| 5:E:156:LEU:HA | 5:E:160:GLU:OE1 | 2.13 | 0.49 |
| 7:G:50:ASP:OD1 | 7:G:50:ASP:O | 2.30 | 0.49 |
| 7:G:117:GLN:OE1 | 7:G:117:GLN:N | 2.46 | 0.49 |
| 8:H:143:LEU:HD12 | 8:H:143:LEU:N | 2.27 | 0.49 |
| 10:J:14:VAL:CG1 | 10:J:50:ILE:HD11 | 2.42 | 0.49 |
| 12:L:53:HIS:HB3 | 12:L:55:ILE:HD12 | 1.92 | 0.49 |
| 1:A:670:ILE:HA | 1:A:805:LEU:HD22 | 1.94 | 0.49 |
| 1:A:774:ARG:CZ | 1:A:797:LYS:HG3 | 2.42 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1053:PHE:O | 1:A:1055:ARG:N | 2.46 | 0.49 |
| 2:B:115:GLN:HG2 | 2:B:193:LYS:CB | 2.33 | 0.49 |
| 2:B:190:TYR:CD2 | 10:J:62:ARG:HB3 | 2.48 | 0.49 |
| 2:B:259:TYR:HD1 | 2:B:259:TYR:H | 1.61 | 0.49 |
| 2:B:592:ASN:HD21 | 2:B:595:ARG:NH1 | 2.11 | 0.49 |
| 2:B:601:ARG:NH1 | 2:B:605:ARG:NH2 | 2.61 | 0.49 |
| 2:B:880:THR:HG22 | 2:B:880:THR:O | 2.13 | 0.49 |
| 3:C:101:LEU:C | 3:C:102:GLN:HG3 | 2.33 | 0.49 |
| 3:C:124:LEU:C | 3:C:126:GLY:N | 2.66 | 0.49 |
| 6:F:120:ILE:O | 6:F:124:GLU:HG3 | 2.13 | 0.49 |
| 6:F:138:LEU:CB | 6:F:139:PRO:HD2 | 2.43 | 0.49 |
| 8:H:102:TYR:N | 8:H:102:TYR:CD2 | 2.63 | 0.49 |
| 9:I:25:LEU:HB3 | 9:I:38:ALA:HB2 | 1.93 | 0.49 |
| 1:A:391:LEU:O | 1:A:394:ASN:HB3 | 2.13 | 0.49 |
| 1:A:528:LEU:HA | 1:A:531:ILE:HG22 | 1.94 | 0.49 |
| 1:A:535:THR:HG22 | 1:A:536:LEU:N | 2.28 | 0.49 |
| 1:A:1348:LEU:HG | 1:A:1372:VAL:HG23 | 1.95 | 0.49 |
| 2:B:276:ILE:HG22 | 2:B:278:GLN:O | 2.13 | 0.49 |
| 2:B:361:LEU:N | 2:B:362:PRO:CD | 2.75 | 0.49 |
| 2:B:792:MET:O | 2:B:793:ALA:HB2 | 2.13 | 0.49 |
| 3:C:38:ILE:HA | 3:C:173:ALA:CB | 2.40 | 0.49 |
| 3:C:83:SER:HA | 3:C:95:CYS:CB | 2.43 | 0.49 |
| 5:E:11:ARG:C | 5:E:13:TRP:N | 2.66 | 0.49 |
| 5:E:161:LYS:HD2 | 5:E:195:VAL:HG23 | 1.95 | 0.49 |
| 6:F:85:MET:C | 6:F:155:LEU:HD11 | 2.32 | 0.49 |
| 7:G:37:SER:OG | 7:G:45:ILE:HG13 | 2.12 | 0.49 |
| 7:G:138:THR:CG2 | 7:G:139:ILE:N | 2.53 | 0.49 |
| 9:I:111:THR:CG2 | 9:I:112:SER:H | 2.25 | 0.49 |
| 13:T:18:DA:H8 | 13:T:18:DA:O5' | 1.95 | 0.49 |
| 1:A:55:ASP:N | 1:A:56:PRO:HD3 | 2.28 | 0.48 |
| 1:A:605:MET:HG2 | 1:A:621:THR:CG2 | 2.43 | 0.48 |
| 1:A:728:LYS:HG3 | 1:A:729:ALA:N | 2.28 | 0.48 |
| 1:A:868:TYR:CZ | 1:A:1064:VAL:HG11 | 2.48 | 0.48 |
| 1:A:1074:GLU:C | 1:A:1076:ALA:H | 2.16 | 0.48 |
| 1:A:1120:LEU:HD12 | 1:A:1120:LEU:N | 2.27 | 0.48 |
| 1:A:1134:ILE:O | 1:A:1138:ILE:HG12 | 2.13 | 0.48 |
| 1:A:1197:LEU:O | 1:A:1236:LEU:HD12 | 2.12 | 0.48 |
| 1:A:1211:GLN:O | 1:A:1212:VAL:C | 2.52 | 0.48 |
| 1:A:1237:ILE:CG2 | 1:A:1238:ILE:N | 2.75 | 0.48 |
| 1:A:1389:PHE:CG | 1:A:1390:ASN:N | 2.80 | 0.48 |
| 1:A:1450:LEU:HD11 | 6:F:108:PHE:CZ | 2.48 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:44:VAL:O | 2:B:45:SER:C | 2.51 | 0.48 |
| 2:B:46:GLN:HG3 | 2:B:47:GLN:H | 1.78 | 0.48 |
| 2:B:225:VAL:HA | 2:B:237:VAL:O | 2.13 | 0.48 |
| 2:B:295:GLY:N | 2:B:298:LEU:HD23 | 2.28 | 0.48 |
| 2:B:865:LYS:HE3 | 2:B:961:LEU:HD21 | 1.94 | 0.48 |
| 2:B:956:THR:CG2 | 2:B:960:GLY:HA2 | 2.43 | 0.48 |
| 2:B:1097:HIS:H | 2:B:1098:MET:CE | 2.09 | 0.48 |
| 3:C:76:ASP:OD2 | 3:C:128:ASN:N | 2.46 | 0.48 |
| 4:D:7:THR:HB | 7:G:42:PHE:CE2 | 2.48 | 0.48 |
| 6:F:130:ILE:O | 6:F:148:VAL:CG2 | 2.61 | 0.48 |
| 7:G:1:MET:HE2 | 7:G:1:MET:HA | 1.94 | 0.48 |
| 7:G:44:TYR:OH | 7:G:156:SER:HA | 2.12 | 0.48 |
| 10:J:9:SER:OG | 10:J:48:ARG:NH2 | 2.46 | 0.48 |
| 11:K:48:ALA:O | 11:K:51:LEU:N | 2.45 | 0.48 |
| 1:A:114:LEU:N | 1:A:114:LEU:HD23 | 2.28 | 0.48 |
| 1:A:187:LYS:O | 1:A:194:ALA:HB3 | 2.13 | 0.48 |
| 1:A:543:LEU:O | 1:A:545:GLN:N | 2.46 | 0.48 |
| 1:A:560:ILE:HG13 | 8:H:79:TRP:H | 1.78 | 0.48 |
| 2:B:120:ARG:NE | 2:B:955:THR:HG21 | 2.28 | 0.48 |
| 2:B:326:ASP:C | 2:B:328:GLU:N | 2.66 | 0.48 |
| 2:B:343:ILE:CG2 | 2:B:347:LYS:HG3 | 2.43 | 0.48 |
| 2:B:451:LYS:O | 2:B:455:SER:OG | 2.30 | 0.48 |
| 2:B:751:VAL:O | 2:B:752:ALA:C | 2.52 | 0.48 |
| 2:B:802:PRO:HA | 2:B:822:ASN:OD1 | 2.13 | 0.48 |
| 2:B:873:THR:CG2 | 2:B:874:PHE:N | 2.76 | 0.48 |
| 2:B:1007:VAL:HG22 | 2:B:1008:PRO:CD | 2.43 | 0.48 |
| 2:B:1077:THR:HG22 | 11:K:44:ASN:ND2 | 2.28 | 0.48 |
| 2:B:1082:MET:HA | 3:C:189:THR:HA | 1.95 | 0.48 |
| 2:B:1215:ARG:NH1 | 4:D:15:LEU:HD21 | 2.28 | 0.48 |
| 3:C:238:ILE:HG22 | 3:C:243:VAL:CG2 | 2.40 | 0.48 |
| 4:D:53:SER:H | 4:D:148:LEU:HD22 | 1.78 | 0.48 |
| 4:D:214:LEU:C | 4:D:216:ASN:N | 2.64 | 0.48 |
| 5:E:33:GLU:OE1 | 5:E:33:GLU:N | 2.41 | 0.48 |
| 6:F:71:GLU:OE1 | 6:F:71:GLU:N | 2.46 | 0.48 |
| 8:H:58:THR:C | 8:H:59:ILE:HG13 | 2.34 | 0.48 |
| 8:H:91:ASP:C | 8:H:93:TYR:N | 2.66 | 0.48 |
| 1:A:55:ASP:O | 1:A:55:ASP:OD2 | 2.31 | 0.48 |
| 1:A:57:ARG:O | 1:A:68:GLN:HG2 | 2.13 | 0.48 |
| 1:A:380:VAL:HG21 | 1:A:430:TRP:HB2 | 1.94 | 0.48 |
| 1:A:384:ASN:O | 1:A:385:ILE:C | 2.52 | 0.48 |
| 1:A:556:TRP:C | 1:A:558:GLY:H | 2.15 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1191:TRP:HA | 1:A:1191:TRP:HE3 | 1.76 | 0.48 |
| 1:A:1271:ILE:O | 1:A:1271:ILE:HG22 | 2.13 | 0.48 |
| 2:B:34:ILE:O | 2:B:37:PHE:HB3 | 2.14 | 0.48 |
| 2:B:798:TYR:HD1 | 10:J:4:PRO:HB3 | 1.78 | 0.48 |
| 2:B:890:TYR:CE2 | 2:B:910:VAL:HG21 | 2.49 | 0.48 |
| 2:B:1055:ILE:O | 2:B:1058:LEU:N | 2.46 | 0.48 |
| 4:D:22:GLU:CD | 4:D:22:GLU:N | 2.65 | 0.48 |
| 5:E:168:TYR:CB | 5:E:170:LEU:HG | 2.42 | 0.48 |
| 5:E:173:SER:OG | 5:E:174:GLN:N | 2.46 | 0.48 |
| 9:I:90:GLN:HE21 | 9:I:92:ARG:HB2 | 1.77 | 0.48 |
| 1:A:121:LEU:O | 1:A:124:GLN:HB2 | 2.14 | 0.48 |
| 1:A:247:ARG:HH11 | 1:A:263:THR:HG23 | 1.77 | 0.48 |
| 1:A:310:GLY:C | 1:A:312:PRO:HD2 | 2.34 | 0.48 |
| 1:A:639:PRO:CG | 1:A:640:GLN:H | 2.26 | 0.48 |
| 1:A:679:ILE:HG12 | 1:A:732:LEU:CD1 | 2.43 | 0.48 |
| 1:A:730:GLY:O | 1:A:732:LEU:N | 2.46 | 0.48 |
| 1:A:1105:LEU:HD22 | 1:A:1384:VAL:HG21 | 1.96 | 0.48 |
| 1:A:1115:SER:O | 1:A:1311:VAL:HG22 | 2.13 | 0.48 |
| 1:A:1187:GLN:HA | 1:A:1244:ARG:CD | 2.44 | 0.48 |
| 2:B:909:ASP:OD1 | 2:B:909:ASP:N | 2.47 | 0.48 |
| 3:C:168:ALA:O | 3:C:169:LYS:C | 2.50 | 0.48 |
| 3:C:260:LEU:O | 3:C:264:GLN:HG3 | 2.13 | 0.48 |
| 8:H:84:ALA:HA | 8:H:87:ARG:CG | 2.43 | 0.48 |
| 10:J:7:CYS:CA | 10:J:49:MET:HE3 | 2.42 | 0.48 |
| 11:K:63:VAL:O | 11:K:63:VAL:CG2 | 2.61 | 0.48 |
| 13:T:10:DA:H2'' | 13:T:11:DA:C8 | 2.47 | 0.48 |
| 1:A:41:MET:N | 1:A:41:MET:HE3 | 2.28 | 0.48 |
| 1:A:88:LYS:HD2 | 1:A:293:GLU:OE2 | 2.13 | 0.48 |
| 1:A:244:PRO:CB | 1:A:245:PRO:HD3 | 2.43 | 0.48 |
| 1:A:266:LEU:HD21 | 1:A:303:TYR:CZ | 2.48 | 0.48 |
| 1:A:358:ASN:ND2 | 2:B:833:TYR:OH | 2.46 | 0.48 |
| 1:A:481:ASP:OD2 | 1:A:481:ASP:N | 2.45 | 0.48 |
| 1:A:666:ILE:CD1 | 1:A:667:GLY:N | 2.75 | 0.48 |
| 1:A:710:LEU:N | 1:A:710:LEU:HD12 | 2.28 | 0.48 |
| 1:A:843:LYS:HZ3 | 2:B:1135:ARG:HH12 | 1.61 | 0.48 |
| 2:B:50:SER:OG | 2:B:411:PRO:HD3 | 2.13 | 0.48 |
| 2:B:319:GLU:HA | 2:B:322:PHE:HB2 | 1.96 | 0.48 |
| 2:B:797:TYR:O | 10:J:1:MET:HG2 | 2.12 | 0.48 |
| 2:B:1030:LEU:CD1 | 2:B:1059:LEU:HD22 | 2.44 | 0.48 |
| 2:B:1177:HIS:HB2 | 2:B:1179:GLN:HE21 | 1.77 | 0.48 |
| 3:C:79:GLN:HG3 | 3:C:127:ARG:HD2 | 1.94 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:H:43:ASN:OD1 | 8:H:46:LEU:N | 2.45 | 0.48 |
| 10:J:1:MET:H1 | 10:J:56:LEU:CA | 2.27 | 0.48 |
| 10:J:2:ILE:HG12 | 10:J:57:ILE:HD12 | 1.95 | 0.48 |
| 10:J:24:LEU:CD1 | 10:J:38:ARG:HG2 | 2.44 | 0.48 |
| 1:A:79:GLY:CA | 1:A:243:PRO:HG3 | 2.44 | 0.48 |
| 1:A:427:GLN:O | 1:A:428:TYR:C | 2.51 | 0.48 |
| 1:A:444:PHE:HB3 | 1:A:458:HIS:CD2 | 2.48 | 0.48 |
| 1:A:587:HIS:CE1 | 1:A:609:ASP:H | 2.31 | 0.48 |
| 1:A:785:PRO:O | 2:B:702:LEU:HD12 | 2.14 | 0.48 |
| 1:A:1057:VAL:CG1 | 1:A:1058:VAL:N | 2.76 | 0.48 |
| 1:A:1329:THR:HG23 | 1:A:1335:ILE:HG13 | 1.95 | 0.48 |
| 2:B:39:ARG:NH2 | 2:B:665:GLU:HG2 | 2.27 | 0.48 |
| 2:B:450:ALA:O | 2:B:451:LYS:C | 2.51 | 0.48 |
| 2:B:653:VAL:O | 2:B:654:ARG:HD3 | 2.14 | 0.48 |
| 2:B:731:VAL:HG12 | 2:B:732:SER:H | 1.79 | 0.48 |
| 2:B:864:LYS:HD2 | 2:B:872:GLU:OE2 | 2.14 | 0.48 |
| 2:B:1072:MET:CG | 2:B:1085:ILE:HD13 | 2.43 | 0.48 |
| 2:B:1166:CYS:O | 2:B:1166:CYS:SG | 2.71 | 0.48 |
| 4:D:134:THR:CG2 | 4:D:135:GLY:N | 2.75 | 0.48 |
| 7:G:144:ARG:HG2 | 7:G:168:LEU:HD23 | 1.96 | 0.48 |
| 10:J:36:LEU:HD11 | 10:J:51:LEU:HB2 | 1.95 | 0.48 |
| 14:N:4:DA:H2'' | 14:N:5:DC:C6 | 2.48 | 0.48 |
| 1:A:29:ALA:HB1 | 2:B:1184:GLY:CA | 2.43 | 0.48 |
| 1:A:356:ASP:OD1 | 1:A:358:ASN:N | 2.35 | 0.48 |
| 1:A:567:LYS:HZ1 | 8:H:47:PHE:HB2 | 1.78 | 0.48 |
| 1:A:586:ILE:HD11 | 1:A:633:VAL:HA | 1.95 | 0.48 |
| 1:A:993:LEU:HD23 | 1:A:1022:LEU:HD11 | 1.94 | 0.48 |
| 2:B:35:SER:HA | 2:B:811:TYR:CE2 | 2.38 | 0.48 |
| 2:B:595:ARG:HG3 | 2:B:595:ARG:HH11 | 1.78 | 0.48 |
| 2:B:687:GLU:CB | 2:B:689:LEU:HG | 2.43 | 0.48 |
| 2:B:707:PRO:O | 2:B:708:GLU:O | 2.32 | 0.48 |
| 3:C:62:PHE:HD2 | 3:C:62:PHE:C | 2.17 | 0.48 |
| 5:E:198:ILE:H | 5:E:198:ILE:CD1 | 2.27 | 0.48 |
| 8:H:139:ASN:O | 8:H:140:ALA:CB | 2.61 | 0.48 |
| 11:K:42:LEU:HD21 | 11:K:46:ILE:HD12 | 1.94 | 0.48 |
| 12:L:43:THR:C | 12:L:45:ALA:H | 2.16 | 0.48 |
| 12:L:61:THR:CG2 | 12:L:63:ARG:HB2 | 2.44 | 0.48 |
| 1:A:40:THR:CG2 | 1:A:41:MET:HE2 | 2.44 | 0.48 |
| 1:A:334:GLY:C | 1:A:336:ILE:N | 2.64 | 0.48 |
| 1:A:466:SER:CB | 2:B:1103:ILE:HG12 | 2.35 | 0.48 |
| 1:A:866:PHE:N | 5:E:208:TYR:OH | 2.43 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1067:LEU:O | 1:A:1068:ALA:C | 2.51 | 0.48 |
| 2:B:373:ARG:HG2 | 2:B:566:LEU:HD23 | 1.96 | 0.48 |
| 2:B:502:ILE:HD12 | 2:B:502:ILE:N | 2.26 | 0.48 |
| 2:B:597:MET:O | 2:B:599:THR:N | 2.46 | 0.48 |
| 2:B:705:MET:N | 2:B:710:LEU:HD12 | 2.28 | 0.48 |
| 3:C:88:CYS:O | 3:C:90:ASP:N | 2.47 | 0.48 |
| 5:E:4:GLU:HA | 5:E:4:GLU:OE1 | 2.14 | 0.48 |
| 9:I:102:VAL:HA | 9:I:108:HIS:O | 2.14 | 0.48 |
| 1:A:514:PRO:C | 1:A:516:SER:H | 2.16 | 0.48 |
| 1:A:787:PHE:CZ | 1:A:796:SER:HA | 2.49 | 0.48 |
| 1:A:859:SER:HB2 | 1:A:1422:ARG:HB2 | 1.96 | 0.48 |
| 1:A:865:GLN:NE2 | 1:A:1370:LEU:HD13 | 2.29 | 0.48 |
| 1:A:1123:GLY:O | 1:A:1125:ALA:N | 2.47 | 0.48 |
| 1:A:1130:GLN:HE21 | 1:A:1134:ILE:CD1 | 2.21 | 0.48 |
| 1:A:1224:LEU:HD12 | 1:A:1241:ARG:O | 2.13 | 0.48 |
| 2:B:123:THR:CB | 2:B:458:LYS:HE2 | 2.44 | 0.48 |
| 2:B:262:GLU:HA | 2:B:267:ARG:NH2 | 2.29 | 0.48 |
| 2:B:345:LYS:O | 2:B:346:GLU:C | 2.51 | 0.48 |
| 2:B:895:ASP:C | 2:B:897:GLY:H | 2.16 | 0.48 |
| 2:B:1016:ALA:HA | 2:B:1020:ARG:NH1 | 2.29 | 0.48 |
| 3:C:6:PRO:CB | 11:K:101:LEU:HD12 | 2.44 | 0.48 |
| 3:C:15:LYS:HG2 | 3:C:15:LYS:O | 2.14 | 0.48 |
| 3:C:66:ARG:HH21 | 10:J:5:VAL:HG23 | 1.77 | 0.48 |
| 4:D:47:LEU:HD13 | 4:D:48:ILE:N | 2.22 | 0.48 |
| 4:D:151:PHE:HZ | 7:G:90:THR:HG1 | 1.60 | 0.48 |
| 5:E:90:VAL:O | 5:E:90:VAL:HG22 | 2.14 | 0.48 |
| 1:A:150:THR:OG1 | 1:A:166:GLY:HA2 | 2.13 | 0.48 |
| 1:A:341:MET:CE | 2:B:1135:ARG:NH1 | 2.77 | 0.48 |
| 1:A:441:PRO:HD2 | 1:A:498:ARG:NH2 | 2.29 | 0.48 |
| 1:A:509:LEU:O | 1:A:511:ILE:N | 2.47 | 0.48 |
| 1:A:509:LEU:C | 1:A:511:ILE:H | 2.17 | 0.48 |
| 1:A:668:ASP:CG | 1:A:742:ASN:HD22 | 2.18 | 0.48 |
| 1:A:1161:THR:HG22 | 1:A:1163:ILE:HG13 | 1.95 | 0.48 |
| 1:A:1193:LEU:HD12 | 1:A:1193:LEU:C | 2.34 | 0.48 |
| 1:A:1230:GLU:C | 1:A:1232:ASN:N | 2.67 | 0.48 |
| 1:A:1290:LYS:O | 1:A:1291:VAL:HG23 | 2.14 | 0.48 |
| 1:A:1376:THR:O | 1:A:1377:THR:C | 2.52 | 0.48 |
| 1:A:1450:LEU:HD13 | 6:F:131:PRO:HG3 | 1.95 | 0.48 |
| 2:B:358:LYS:HA | 2:B:366:GLN:HB3 | 1.96 | 0.48 |
| 2:B:430:ARG:O | 2:B:434:ARG:CD | 2.62 | 0.48 |
| 2:B:539:LEU:H | 2:B:539:LEU:CD1 | 2.17 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:542:MET:HG2 | 2:B:747:MET:HE3 | 1.95 | 0.48 |
| 2:B:745:PRO:C | 2:B:747:MET:N | 2.67 | 0.48 |
| 2:B:899:ILE:HD11 | 2:B:910:VAL:O | 2.14 | 0.48 |
| 2:B:1084:GLN:OE1 | 3:C:189:THR:CG2 | 2.61 | 0.48 |
| 2:B:1156:ASP:O | 2:B:1157:ALA:O | 2.32 | 0.48 |
| 2:B:1163:CYS:SG | 2:B:1165:ILE:HB | 2.54 | 0.48 |
| 4:D:164:ILE:CG2 | 4:D:168:LYS:HD2 | 2.38 | 0.48 |
| 1:A:107:CYS:HB2 | 1:A:171:GLN:NE2 | 2.29 | 0.47 |
| 1:A:331:GLY:O | 1:A:332:LYS:O | 2.31 | 0.47 |
| 1:A:341:MET:HE1 | 2:B:1135:ARG:NH1 | 2.29 | 0.47 |
| 1:A:392:VAL:HG21 | 1:A:426:LEU:HD11 | 1.96 | 0.47 |
| 1:A:549:MET:HE2 | 1:A:656:TRP:HD1 | 1.78 | 0.47 |
| 1:A:1422:ARG:HH12 | 2:B:1224:PHE:HD2 | 1.62 | 0.47 |
| 1:A:1424:VAL:HG13 | 1:A:1436:ILE:CD1 | 2.35 | 0.47 |
| 2:B:174:LEU:HD22 | 2:B:202:TYR:CE1 | 2.49 | 0.47 |
| 2:B:345:LYS:O | 2:B:347:LYS:N | 2.47 | 0.47 |
| 2:B:405:ARG:HA | 2:B:631:GLY:O | 2.14 | 0.47 |
| 2:B:519:TRP:NE1 | 2:B:635:ARG:NH2 | 2.61 | 0.47 |
| 2:B:578:THR:C | 2:B:589:VAL:HG13 | 2.34 | 0.47 |
| 2:B:603:LEU:HD12 | 2:B:609:ILE:HG12 | 1.96 | 0.47 |
| 2:B:708:GLU:CG | 2:B:709:ASP:H | 2.19 | 0.47 |
| 2:B:976:ILE:O | 2:B:990:ILE:HB | 2.13 | 0.47 |
| 3:C:8:VAL:HG21 | 11:K:105:PHE:HA | 1.96 | 0.47 |
| 3:C:91:HIS:C | 3:C:91:HIS:CD2 | 2.86 | 0.47 |
| 4:D:10:THR:HG23 | 4:D:10:THR:O | 2.13 | 0.47 |
| 4:D:198:LEU:HA | 4:D:201:LYS:HD2 | 1.95 | 0.47 |
| 7:G:115:MET:SD | 7:G:119:LEU:HD23 | 2.53 | 0.47 |
| 11:K:46:ILE:O | 11:K:46:ILE:HG22 | 2.14 | 0.47 |
| 1:A:592:ASP:N | 1:A:595:THR:OG1 | 2.46 | 0.47 |
| 1:A:596:THR:C | 1:A:598:LEU:N | 2.62 | 0.47 |
| 1:A:1038:THR:HG23 | 1:A:1041:ALA:CB | 2.44 | 0.47 |
| 1:A:1198:ASP:HB3 | 1:A:1201:ALA:CB | 2.43 | 0.47 |
| 1:A:1313:LEU:CD1 | 1:A:1327:ILE:HD13 | 2.44 | 0.47 |
| 2:B:52:ASN:O | 2:B:55:VAL:N | 2.44 | 0.47 |
| 2:B:128:LEU:HD12 | 2:B:128:LEU:N | 2.29 | 0.47 |
| 2:B:186:GLU:HG3 | 10:J:62:ARG:NH1 | 2.29 | 0.47 |
| 2:B:324:ILE:HD11 | 2:B:329:THR:O | 2.14 | 0.47 |
| 2:B:613:VAL:HG13 | 2:B:628:THR:CA | 2.43 | 0.47 |
| 2:B:642:ASP:CB | 2:B:649:LYS:HG3 | 2.43 | 0.47 |
| 2:B:1058:LEU:O | 2:B:1061:GLU:HB2 | 2.14 | 0.47 |
| 5:E:33:GLU:O | 5:E:36:GLU:N | 2.47 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 7:G:62:LEU:CB | 7:G:63:PRO:HD2 | 2.33 | 0.47 |
| 10:J:16:ASP:CG | 10:J:17:LYS:HD2 | 2.34 | 0.47 |
| 12:L:43:THR:HG22 | 12:L:43:THR:O | 2.13 | 0.47 |
| 1:A:44:THR:O | 1:A:45:GLN:HB2 | 2.15 | 0.47 |
| 1:A:90:VAL:CG1 | 1:A:297:GLN:HA | 2.43 | 0.47 |
| 1:A:185:TRP:CE3 | 1:A:185:TRP:N | 2.82 | 0.47 |
| 1:A:322:VAL:O | 1:A:322:VAL:HG13 | 2.13 | 0.47 |
| 1:A:518:LYS:HE2 | 1:A:624:SER:O | 2.14 | 0.47 |
| 1:A:600:PRO:CG | 1:A:601:LYS:H | 2.20 | 0.47 |
| 1:A:853:ASP:OD1 | 1:A:853:ASP:C | 2.52 | 0.47 |
| 1:A:1054:LEU:HD13 | 6:F:84:TYR:OH | 2.13 | 0.47 |
| 1:A:1159:ARG:HD3 | 1:A:1174:PHE:CZ | 2.49 | 0.47 |
| 1:A:1199:ARG:HH21 | 1:A:1234:GLU:HA | 1.78 | 0.47 |
| 2:B:239:GLU:HA | 2:B:254:LEU:O | 2.14 | 0.47 |
| 2:B:306:ASN:C | 2:B:308:TRP:H | 2.17 | 0.47 |
| 2:B:605:ARG:HB3 | 2:B:688:GLY:CA | 2.45 | 0.47 |
| 2:B:762:ASN:HD21 | 2:B:1024:ALA:HB3 | 1.79 | 0.47 |
| 2:B:1033:LYS:NZ | 2:B:1068:GLY:O | 2.47 | 0.47 |
| 2:B:1167:GLY:HA3 | 2:B:1215:ARG:HB3 | 1.95 | 0.47 |
| 3:C:76:ASP:O | 3:C:78:GLU:N | 2.44 | 0.47 |
| 5:E:117:THR:CG2 | 5:E:119:SER:HB2 | 2.43 | 0.47 |
| 5:E:173:SER:C | 5:E:175:LEU:N | 2.67 | 0.47 |
| 7:G:8:SER:O | 7:G:9:LEU:HB2 | 2.14 | 0.47 |
| 7:G:96:GLN:HA | 7:G:121:PHE:CE2 | 2.49 | 0.47 |
| 8:H:36:CYS:HB2 | 8:H:130:ARG:HH22 | 1.79 | 0.47 |
| 8:H:130:ARG:N | 8:H:130:ARG:CD | 2.73 | 0.47 |
| 1:A:447:GLN:HE22 | 13:T:20:DG:H4' | 1.79 | 0.47 |
| 1:A:506:ALA:O | 1:A:509:LEU:HB2 | 2.14 | 0.47 |
| 1:A:628:GLY:O | 1:A:632:VAL:HG23 | 2.14 | 0.47 |
| 1:A:645:LEU:HG | 1:A:649:ILE:HD11 | 1.95 | 0.47 |
| 1:A:725:ALA:O | 1:A:728:LYS:HG2 | 2.14 | 0.47 |
| 1:A:958:VAL:CG2 | 1:A:1053:PHE:HA | 2.44 | 0.47 |
| 1:A:1273:LEU:N | 1:A:1273:LEU:CD1 | 2.76 | 0.47 |
| 1:A:1430:LEU:HB3 | 1:A:1432:GLN:HG3 | 1.95 | 0.47 |
| 2:B:39:ARG:HG2 | 2:B:39:ARG:NH1 | 2.29 | 0.47 |
| 2:B:226:PHE:HA | 2:B:395:GLN:HG3 | 1.97 | 0.47 |
| 2:B:635:ARG:HB2 | 2:B:636:PRO:HD2 | 1.96 | 0.47 |
| 2:B:766:ARG:HG3 | 2:B:1022:THR:CG2 | 2.41 | 0.47 |
| 2:B:911:ILE:O | 2:B:911:ILE:HG22 | 2.14 | 0.47 |
| 2:B:1081:LEU:O | 2:B:1083:ALA:N | 2.48 | 0.47 |
| 3:C:86:CYS:SG | 3:C:87:PHE:N | 2.87 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:C:183:TRP:O | 3:C:184:ASN:HB3 | 2.14 | 0.47 |
| 3:C:190:ASP:O | 3:C:191:TYR:C | 2.52 | 0.47 |
| 4:D:47:LEU:HD11 | 7:G:3:PHE:HD2 | 1.78 | 0.47 |
| 4:D:68:ARG:O | 4:D:72:ARG:HG3 | 2.14 | 0.47 |
| 5:E:138:ALA:HA | 5:E:141:VAL:HG23 | 1.96 | 0.47 |
| 5:E:157:SER:C | 5:E:159:ASP:N | 2.67 | 0.47 |
| 6:F:109:VAL:CG1 | 6:F:110:ASP:N | 2.76 | 0.47 |
| 9:I:25:LEU:CB | 9:I:38:ALA:HB2 | 2.45 | 0.47 |
| 10:J:27:GLU:C | 10:J:29:GLU:N | 2.67 | 0.47 |
| 1:A:381:THR:HG22 | 1:A:383:TYR:CD2 | 2.49 | 0.47 |
| 1:A:728:LYS:O | 1:A:732:LEU:HG | 2.14 | 0.47 |
| 1:A:1243:VAL:HG22 | 1:A:1244:ARG:H | 1.80 | 0.47 |
| 1:A:1243:VAL:HG22 | 1:A:1244:ARG:N | 2.28 | 0.47 |
| 1:A:1332:PHE:N | 1:A:1332:PHE:CD2 | 2.83 | 0.47 |
| 1:A:1443:VAL:HG11 | 6:F:132:LEU:HD13 | 1.96 | 0.47 |
| 2:B:261:ARG:NH1 | 2:B:262:GLU:H | 2.13 | 0.47 |
| 2:B:288:ALA:N | 2:B:330:ALA:HB1 | 2.29 | 0.47 |
| 2:B:370:PHE:HD2 | 2:B:373:ARG:HD2 | 1.79 | 0.47 |
| 2:B:412:LEU:HD13 | 2:B:479:VAL:HG11 | 1.96 | 0.47 |
| 2:B:604:ARG:O | 2:B:606:LYS:N | 2.47 | 0.47 |
| 2:B:686:ASN:C | 2:B:688:GLY:N | 2.68 | 0.47 |
| 2:B:867:GLY:C | 2:B:869:SER:N | 2.67 | 0.47 |
| 5:E:30:ILE:HG23 | 5:E:34:GLU:OE1 | 2.15 | 0.47 |
| 5:E:90:VAL:HB | 5:E:120:ALA:HB2 | 1.96 | 0.47 |
| 6:F:135:ARG:HG2 | 6:F:137:TYR:CE1 | 2.48 | 0.47 |
| 7:G:139:ILE:HG22 | 7:G:140:LYS:N | 2.29 | 0.47 |
| 9:I:111:THR:CG2 | 9:I:112:SER:N | 2.76 | 0.47 |
| 1:A:230:ARG:HG3 | 1:A:233:TRP:CZ3 | 2.49 | 0.47 |
| 1:A:280:GLU:C | 1:A:282:ASN:H | 2.16 | 0.47 |
| 1:A:399:HIS:CB | 1:A:400:PRO:CD | 2.84 | 0.47 |
| 1:A:605:MET:HG2 | 1:A:621:THR:HG23 | 1.97 | 0.47 |
| 1:A:777:PHE:C | 1:A:779:PHE:H | 2.17 | 0.47 |
| 1:A:852:TYR:HD2 | 1:A:1060:PRO:CB | 2.27 | 0.47 |
| 1:A:1129:GLU:O | 1:A:1130:GLN:C | 2.51 | 0.47 |
| 2:B:1104:HIS:CG | 2:B:1122:ARG:HB2 | 2.50 | 0.47 |
| 4:D:40:HIS:HB2 | 7:G:73:LYS:CD | 2.44 | 0.47 |
| 5:E:45:LYS:HB3 | 5:E:46:TYR:CD1 | 2.49 | 0.47 |
| 5:E:73:PRO:HB2 | 5:E:74:ASP:OD1 | 2.15 | 0.47 |
| 5:E:164:LEU:C | 5:E:165:LEU:HD23 | 2.34 | 0.47 |
| 8:H:26:ILE:HG22 | 8:H:27:GLU:N | 2.28 | 0.47 |
| 1:A:134:ARG:C | 1:A:136:ALA:N | 2.68 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:233:TRP:O | 1:A:235:ILE:N | 2.47 | 0.47 |
| 1:A:572:TRP:HA | 1:A:576:GLN:OE1 | 2.14 | 0.47 |
| 1:A:822:GLU:O | 1:A:825:ILE:HG22 | 2.15 | 0.47 |
| 1:A:890:ASP:OD2 | 1:A:1296:GLY:HA2 | 2.14 | 0.47 |
| 1:A:1037:LEU:HD13 | 1:A:1041:ALA:CB | 2.43 | 0.47 |
| 1:A:1378:GLN:OE1 | 1:A:1378:GLN:HA | 2.15 | 0.47 |
| 1:A:1389:PHE:O | 1:A:1391:ARG:N | 2.44 | 0.47 |
| 1:A:1448:GLU:O | 1:A:1449:SER:C | 2.51 | 0.47 |
| 2:B:54:PHE:HE1 | 2:B:414:ALA:HA | 1.79 | 0.47 |
| 2:B:114:PRO:O | 2:B:115:GLN:C | 2.53 | 0.47 |
| 2:B:336:ARG:NE | 2:B:348:ARG:HH12 | 2.03 | 0.47 |
| 2:B:496:ARG:HD2 | 2:B:751:VAL:HG23 | 1.97 | 0.47 |
| 2:B:515:HIS:CD2 | 2:B:517:THR:HG23 | 2.49 | 0.47 |
| 2:B:539:LEU:HD12 | 2:B:539:LEU:N | 2.17 | 0.47 |
| 2:B:557:PHE:CZ | 2:B:603:LEU:HD21 | 2.49 | 0.47 |
| 2:B:591:ARG:O | 2:B:593:PRO:HD3 | 2.15 | 0.47 |
| 2:B:618:ASP:O | 2:B:622:LYS:N | 2.47 | 0.47 |
| 2:B:898:LEU:HD13 | 2:B:952:VAL:CG1 | 2.44 | 0.47 |
| 2:B:955:THR:HG22 | 2:B:956:THR:N | 2.30 | 0.47 |
| 2:B:1053:GLU:O | 2:B:1057:LYS:HG3 | 2.15 | 0.47 |
| 4:D:12:ARG:HG3 | 4:D:14:ARG:NH2 | 2.30 | 0.47 |
| 4:D:157:GLN:O | 4:D:158:GLU:C | 2.53 | 0.47 |
| 5:E:78:LEU:HD23 | 5:E:79:TRP:N | 2.29 | 0.47 |
| 8:H:11:GLN:O | 8:H:28:ALA:CB | 2.63 | 0.47 |
| 1:A:7:SER:O | 1:A:9:ALA:N | 2.48 | 0.47 |
| 1:A:38:PRO:HG2 | 1:A:39:GLU:N | 2.30 | 0.47 |
| 1:A:635:ARG:HA | 1:A:635:ARG:NH1 | 2.24 | 0.47 |
| 1:A:755:PHE:O | 1:A:758:ILE:HG13 | 2.15 | 0.47 |
| 1:A:933:TYR:O | 1:A:937:VAL:HG23 | 2.15 | 0.47 |
| 1:A:1063:MET:SD | 1:A:1436:ILE:HG12 | 2.55 | 0.47 |
| 1:A:1209:MET:SD | 1:A:1236:LEU:HB3 | 2.55 | 0.47 |
| 1:A:1362:TYR:CD1 | 1:A:1363:VAL:N | 2.83 | 0.47 |
| 1:A:1399:ARG:HB3 | 1:A:1408:ILE:CD1 | 2.44 | 0.47 |
| 1:A:1399:ARG:HB3 | 1:A:1408:ILE:HD13 | 1.97 | 0.47 |
| 2:B:130:VAL:HG23 | 2:B:167:ILE:HD13 | 1.95 | 0.47 |
| 2:B:203:PHE:N | 2:B:203:PHE:CD1 | 2.83 | 0.47 |
| 3:C:107:SER:C | 3:C:109:SER:N | 2.65 | 0.47 |
| 3:C:238:ILE:CD1 | 3:C:246:ARG:HD2 | 2.44 | 0.47 |
| 5:E:138:ALA:HA | 5:E:141:VAL:CG2 | 2.45 | 0.47 |
| 8:H:84:ALA:C | 8:H:86:ASP:N | 2.68 | 0.47 |
| 9:I:14:LEU:HD22 | 9:I:28:GLU:O | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:9:ALA:CB | 2:B:1193:GLN:HB2 | 2.44 | 0.47 |
| 1:A:352:VAL:O | 1:A:467:THR:HG22 | 2.15 | 0.47 |
| 1:A:489:LEU:C | 1:A:489:LEU:HD12 | 2.35 | 0.47 |
| 1:A:531:ILE:HD11 | 1:A:578:LEU:CD2 | 2.44 | 0.47 |
| 1:A:783:THR:HB | 1:A:787:PHE:CD1 | 2.50 | 0.47 |
| 1:A:829:VAL:O | 1:A:831:THR:N | 2.48 | 0.47 |
| 1:A:1035:TYR:CD1 | 1:A:1037:LEU:HD23 | 2.47 | 0.47 |
| 1:A:1366:ARG:HG2 | 1:A:1366:ARG:HH11 | 1.79 | 0.47 |
| 2:B:294:ASP:C | 2:B:296:GLU:N | 2.62 | 0.47 |
| 2:B:318:VAL:C | 2:B:320:ASP:H | 2.18 | 0.47 |
| 2:B:373:ARG:HA | 2:B:566:LEU:HD23 | 1.97 | 0.47 |
| 3:C:62:PHE:C | 3:C:62:PHE:CD2 | 2.88 | 0.47 |
| 3:C:105:GLY:HA3 | 3:C:148:ARG:O | 2.15 | 0.47 |
| 6:F:82:THR:HG23 | 6:F:84:TYR:H | 1.79 | 0.47 |
| 9:I:101:PHE:N | 9:I:101:PHE:HD1 | 2.13 | 0.47 |
| 1:A:108:MET:HB3 | 1:A:210:ILE:CD1 | 2.45 | 0.47 |
| 1:A:146:MET:HB3 | 1:A:171:GLN:O | 2.15 | 0.47 |
| 1:A:162:VAL:HG12 | 1:A:163:SER:N | 2.29 | 0.47 |
| 1:A:191:THR:HG22 | 1:A:192:GLY:N | 2.30 | 0.47 |
| 1:A:929:LEU:CD1 | 1:A:929:LEU:O | 2.63 | 0.47 |
| 1:A:953:ASN:C | 1:A:954:TRP:CD1 | 2.89 | 0.47 |
| 1:A:1345:ARG:HD2 | 1:A:1373:ASP:OD1 | 2.14 | 0.47 |
| 2:B:540:SER:HB3 | 2:B:747:MET:O | 2.15 | 0.47 |
| 2:B:705:MET:H | 2:B:710:LEU:CD1 | 2.27 | 0.47 |
| 2:B:973:ILE:HG23 | 2:B:974:PRO:HD2 | 1.96 | 0.47 |
| 3:C:29:MET:HA | 11:K:45:LEU:HD13 | 1.96 | 0.47 |
| 3:C:258:ILE:O | 3:C:262:LEU:HG | 2.14 | 0.47 |
| 5:E:47:CYS:HA | 5:E:52:ARG:O | 2.15 | 0.47 |
| 5:E:108:GLY:HA3 | 5:E:132:ILE:HG22 | 1.96 | 0.47 |
| 5:E:169:ARG:HB3 | 6:F:140:ASP:OD2 | 2.14 | 0.47 |
| 8:H:103:LYS:HG2 | 8:H:104:PHE:N | 2.29 | 0.47 |
| 8:H:113:ALA:HB1 | 8:H:125:LEU:O | 2.14 | 0.47 |
| 9:I:16:PRO:HB2 | 9:I:25:LEU:HD11 | 1.97 | 0.47 |
| 10:J:56:LEU:O | 10:J:59:LYS:N | 2.48 | 0.47 |
| 11:K:89:ASN:C | 11:K:91:CYS:N | 2.68 | 0.47 |
| 1:A:342:GLY:HA3 | 2:B:1131:GLY:HA2 | 1.97 | 0.46 |
| 1:A:606:LEU:CG | 1:A:613:ILE:HD12 | 2.44 | 0.46 |
| 1:A:896:ARG:HD3 | 1:A:897:TYR:HE1 | 1.79 | 0.46 |
| 1:A:1030:ARG:O | 1:A:1034:GLU:HB2 | 2.15 | 0.46 |
| 1:A:1140:HIS:HA | 1:A:1275:GLY:HA3 | 1.97 | 0.46 |
| 1:A:1236:LEU:C | 1:A:1237:ILE:HG13 | 2.36 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1259:MET:O | 1:A:1263:ILE:HD12 | 2.14 | 0.46 |
| 2:B:185:THR:O | 2:B:186:GLU:C | 2.53 | 0.46 |
| 2:B:453:ILE:O | 2:B:454:THR:C | 2.53 | 0.46 |
| 2:B:563:MET:HE1 | 2:B:580:VAL:HB | 1.97 | 0.46 |
| 2:B:810:GLU:CB | 2:B:815:ARG:NH2 | 2.77 | 0.46 |
| 2:B:1055:ILE:O | 2:B:1057:LYS:N | 2.48 | 0.46 |
| 3:C:104:PHE:HB3 | 3:C:106:GLU:OE1 | 2.14 | 0.46 |
| 3:C:125:MET:HG3 | 3:C:127:ARG:NH2 | 2.30 | 0.46 |
| 4:D:29:LEU:HD22 | 7:G:82:PHE:CE2 | 2.50 | 0.46 |
| 5:E:4:GLU:HB3 | 5:E:7:ARG:HE | 1.80 | 0.46 |
| 6:F:89:GLU:HB3 | 6:F:134:ILE:CD1 | 2.45 | 0.46 |
| 8:H:82:PRO:HG2 | 8:H:83:GLN:N | 2.30 | 0.46 |
| 11:K:65:HIS:HD2 | 11:K:67:PHE:N | 2.07 | 0.46 |
| 11:K:110:ASN:O | 11:K:111:LEU:HD23 | 2.15 | 0.46 |
| 12:L:55:ILE:H | 12:L:55:ILE:CD1 | 2.19 | 0.46 |
| 12:L:60:ARG:HG2 | 12:L:61:THR:H | 1.80 | 0.46 |
| 1:A:84:ILE:O | 1:A:84:ILE:CG2 | 2.63 | 0.46 |
| 1:A:695:LYS:HA | 1:A:698:GLN:HB2 | 1.97 | 0.46 |
| 1:A:993:LEU:CD2 | 1:A:1022:LEU:HD11 | 2.45 | 0.46 |
| 1:A:1011:GLN:NE2 | 1:A:1015:VAL:HG21 | 2.31 | 0.46 |
| 1:A:1143:LEU:O | 1:A:1146:VAL:HG23 | 2.15 | 0.46 |
| 1:A:1265:ASN:C | 1:A:1267:MET:N | 2.68 | 0.46 |
| 1:A:1451:VAL:C | 1:A:1453:TYR:H | 2.17 | 0.46 |
| 2:B:235:SER:HB2 | 2:B:267:ARG:HH12 | 1.80 | 0.46 |
| 2:B:309:GLN:HG3 | 9:I:52:ILE:CD1 | 2.44 | 0.46 |
| 2:B:311:LEU:O | 2:B:312:GLU:C | 2.53 | 0.46 |
| 2:B:483:LEU:CD1 | 2:B:491:THR:HG23 | 2.45 | 0.46 |
| 2:B:611:PRO:O | 2:B:692:TYR:HB2 | 2.16 | 0.46 |
| 2:B:871:THR:HG22 | 2:B:872:GLU:O | 2.15 | 0.46 |
| 2:B:1065:GLN:NE2 | 2:B:1067:ARG:N | 2.43 | 0.46 |
| 2:B:1068:GLY:O | 2:B:1069:PHE:O | 2.33 | 0.46 |
| 3:C:115:SER:HB3 | 3:C:142:VAL:HB | 1.96 | 0.46 |
| 5:E:178:ILE:HG22 | 5:E:213:ILE:O | 2.15 | 0.46 |
| 7:G:13:LEU:HD21 | 7:G:17:PHE:HB2 | 1.97 | 0.46 |
| 7:G:88:ASP:HA | 7:G:144:ARG:HA | 1.97 | 0.46 |
| 9:I:100:PHE:N | 9:I:100:PHE:CD1 | 2.83 | 0.46 |
| 1:A:289:ILE:O | 1:A:292:ALA:N | 2.32 | 0.46 |
| 1:A:332:LYS:C | 1:A:334:GLY:N | 2.69 | 0.46 |
| 1:A:575:LYS:HD2 | 8:H:120:GLY:HA2 | 1.95 | 0.46 |
| 1:A:623:GLY:C | 1:A:625:SER:H | 2.17 | 0.46 |
| 1:A:670:ILE:HG22 | 1:A:676:MET:HE2 | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1040:GLN:O | 1:A:1041:ALA:C | 2.54 | 0.46 |
| 1:A:1441:PHE:CE1 | 6:F:92:ARG:HG2 | 2.50 | 0.46 |
| 1:A:1445:ILE:HD11 | 7:G:68:ALA:HB1 | 1.96 | 0.46 |
| 2:B:53:GLN:HG2 | 2:B:547:VAL:CG2 | 2.46 | 0.46 |
| 2:B:126:SER:HB3 | 2:B:172:ILE:HD11 | 1.98 | 0.46 |
| 2:B:397:ASP:OD1 | 2:B:399:ASP:N | 2.38 | 0.46 |
| 2:B:458:LYS:O | 2:B:459:TYR:C | 2.53 | 0.46 |
| 2:B:498:THR:N | 2:B:537:LYS:O | 2.49 | 0.46 |
| 2:B:547:VAL:HG13 | 2:B:548:GLY:N | 2.30 | 0.46 |
| 2:B:806:THR:HB | 2:B:809:MET:HG3 | 1.98 | 0.46 |
| 2:B:934:LYS:O | 2:B:934:LYS:HG2 | 2.14 | 0.46 |
| 2:B:1060:ARG:HA | 2:B:1060:ARG:HD2 | 1.68 | 0.46 |
| 2:B:1125:ASP:O | 2:B:1125:ASP:OD1 | 2.34 | 0.46 |
| 3:C:228:PHE:CD1 | 3:C:228:PHE:N | 2.83 | 0.46 |
| 4:D:46:GLU:HG2 | 4:D:47:LEU:N | 2.31 | 0.46 |
| 11:K:77:THR:HG21 | 11:K:83:PRO:HA | 1.97 | 0.46 |
| 1:A:40:THR:C | 1:A:41:MET:HG3 | 2.34 | 0.46 |
| 1:A:144:THR:O | 1:A:146:MET:CE | 2.63 | 0.46 |
| 1:A:874:ASP:CA | 1:A:1058:VAL:HG23 | 2.46 | 0.46 |
| 1:A:889:SER:CB | 1:A:1297:GLU:HG3 | 2.44 | 0.46 |
| 1:A:949:ASP:OD2 | 1:A:951:GLU:HB2 | 2.15 | 0.46 |
| 1:A:1152:ILE:HD11 | 9:I:44:TYR:CE2 | 2.50 | 0.46 |
| 2:B:261:ARG:O | 2:B:263:GLY:N | 2.48 | 0.46 |
| 2:B:287:ARG:HH11 | 2:B:324:ILE:HG22 | 1.81 | 0.46 |
| 2:B:435:THR:CG2 | 2:B:437:GLU:HB2 | 2.45 | 0.46 |
| 2:B:509:ALA:O | 2:B:510:LYS:C | 2.54 | 0.46 |
| 2:B:581:PHE:O | 2:B:626:ILE:HB | 2.16 | 0.46 |
| 2:B:1001:PHE:CE2 | 3:C:34:ARG:CZ | 2.99 | 0.46 |
| 2:B:1065:GLN:HB2 | 3:C:201:TRP:CZ3 | 2.50 | 0.46 |
| 4:D:4:SER:O | 7:G:9:LEU:HD13 | 2.15 | 0.46 |
| 4:D:119:ARG:HD3 | 4:D:221:TYR:HE2 | 1.80 | 0.46 |
| 6:F:82:THR:HG22 | 6:F:84:TYR:H | 1.80 | 0.46 |
| 1:A:159:THR:O | 1:A:159:THR:HG22 | 2.16 | 0.46 |
| 1:A:203:SER:O | 1:A:206:GLU:HB3 | 2.16 | 0.46 |
| 1:A:226:GLU:O | 1:A:226:GLU:HG2 | 2.14 | 0.46 |
| 1:A:369:SER:HB2 | 11:K:2:ASN:HD21 | 1.81 | 0.46 |
| 1:A:427:GLN:HB2 | 1:A:430:TRP:NE1 | 2.31 | 0.46 |
| 1:A:608:ILE:CB | 1:A:613:ILE:HD11 | 2.42 | 0.46 |
| 1:A:802:ASN:HD21 | 2:B:728:ARG:HB2 | 1.76 | 0.46 |
| 1:A:857:ARG:CZ | 6:F:139:PRO:CB | 2.93 | 0.46 |
| 1:A:1284:MET:O | 1:A:1285:MET:HG2 | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1341:ILE:CG2 | 1:A:1342:GLU:N | 2.76 | 0.46 |
| 2:B:307:ASP:C | 2:B:309:GLN:N | 2.69 | 0.46 |
| 2:B:326:ASP:CG | 2:B:328:GLU:HB3 | 2.36 | 0.46 |
| 4:D:8:PHE:HZ | 4:D:37:GLN:HB2 | 1.79 | 0.46 |
| 5:E:29:PHE:N | 5:E:65:THR:HG22 | 2.31 | 0.46 |
| 6:F:111:LEU:HD12 | 6:F:111:LEU:N | 2.10 | 0.46 |
| 6:F:117:PRO:C | 6:F:119:ARG:N | 2.69 | 0.46 |
| 7:G:18:PHE:HZ | 7:G:68:ALA:HB2 | 1.80 | 0.46 |
| 9:I:25:LEU:CG | 9:I:38:ALA:HB2 | 2.46 | 0.46 |
| 9:I:61:ASP:C | 9:I:63:GLY:N | 2.68 | 0.46 |
| 1:A:83:HIS:CD2 | 1:A:83:HIS:C | 2.89 | 0.46 |
| 1:A:218:ASP:O | 1:A:219:PHE:C | 2.54 | 0.46 |
| 1:A:280:GLU:C | 1:A:282:ASN:N | 2.69 | 0.46 |
| 1:A:393:ARG:CB | 1:A:393:ARG:HH11 | 2.27 | 0.46 |
| 1:A:642:CYS:O | 1:A:645:LEU:HB3 | 2.16 | 0.46 |
| 1:A:751:SER:O | 1:A:752:LYS:HG2 | 2.15 | 0.46 |
| 1:A:870:GLU:O | 1:A:871:ASP:HB3 | 2.15 | 0.46 |
| 2:B:205:ILE:N | 2:B:205:ILE:CD1 | 2.79 | 0.46 |
| 2:B:529:GLU:OE2 | 2:B:769:TYR:CE1 | 2.68 | 0.46 |
| 2:B:753:ALA:O | 2:B:756:ILE:HG13 | 2.15 | 0.46 |
| 2:B:762:ASN:OD1 | 2:B:1022:THR:HA | 2.14 | 0.46 |
| 3:C:13:ALA:O | 11:K:114:LEU:HD22 | 2.14 | 0.46 |
| 3:C:82:TYR:CG | 3:C:161:LYS:HG2 | 2.51 | 0.46 |
| 5:E:17:ARG:HG3 | 5:E:18:THR:N | 2.31 | 0.46 |
| 5:E:145:THR:HG21 | 5:E:187:TYR:CD2 | 2.50 | 0.46 |
| 6:F:114:GLU:OE2 | 6:F:119:ARG:HG2 | 2.15 | 0.46 |
| 7:G:59:GLY:CA | 7:G:70:PHE:CD2 | 2.97 | 0.46 |
| 7:G:145:VAL:HG12 | 7:G:146:LYS:H | 1.80 | 0.46 |
| 9:I:25:LEU:HG | 9:I:38:ALA:HB2 | 1.97 | 0.46 |
| 9:I:62:ILE:O | 9:I:62:ILE:HG12 | 2.15 | 0.46 |
| 10:J:14:VAL:O | 10:J:14:VAL:CG1 | 2.63 | 0.46 |
| 1:A:79:GLY:H | 2:B:1205:GLN:HE22 | 1.64 | 0.46 |
| 1:A:184:SER:HB3 | 1:A:199:LEU:CD2 | 2.44 | 0.46 |
| 1:A:372:LYS:HA | 1:A:435:HIS:CE1 | 2.50 | 0.46 |
| 1:A:516:SER:O | 1:A:518:LYS:HB3 | 2.16 | 0.46 |
| 1:A:672:ASP:OD2 | 1:A:674:PRO:HG2 | 2.16 | 0.46 |
| 1:A:720:ARG:HB3 | 1:A:720:ARG:CZ | 2.46 | 0.46 |
| 1:A:852:TYR:CE1 | 6:F:136:ARG:HG2 | 2.51 | 0.46 |
| 1:A:1067:LEU:HD13 | 1:A:1067:LEU:C | 2.36 | 0.46 |
| 1:A:1140:HIS:HB2 | 1:A:1276:VAL:O | 2.16 | 0.46 |
| 1:A:1340:GLY:O | 1:A:1342:GLU:N | 2.48 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1438:THR:O | 6:F:92:ARG:NH1 | 2.49 | 0.46 |
| 1:A:1444:MET:HG3 | 7:G:59:GLY:O | 2.16 | 0.46 |
| 2:B:641:GLU:C | 2:B:643:ASP:H | 2.18 | 0.46 |
| 2:B:827:ILE:HD12 | 2:B:1086:PHE:CD2 | 2.51 | 0.46 |
| 2:B:844:SER:O | 2:B:847:ASP:HB2 | 2.16 | 0.46 |
| 2:B:860:MET:HG2 | 2:B:861:ASP:H | 1.80 | 0.46 |
| 2:B:895:ASP:C | 2:B:897:GLY:N | 2.69 | 0.46 |
| 3:C:58:LEU:N | 3:C:58:LEU:CD2 | 2.79 | 0.46 |
| 3:C:99:LEU:HD23 | 3:C:99:LEU:N | 2.30 | 0.46 |
| 5:E:35:VAL:C | 5:E:37:LEU:H | 2.19 | 0.46 |
| 5:E:186:LEU:O | 5:E:187:TYR:C | 2.53 | 0.46 |
| 11:K:61:TYR:HD2 | 11:K:61:TYR:O | 1.98 | 0.46 |
| 1:A:718:VAL:O | 1:A:721:PHE:HB2 | 2.16 | 0.46 |
| 1:A:826:ASP:C | 1:A:828:ALA:N | 2.68 | 0.46 |
| 1:A:875:ALA:HA | 1:A:878:ILE:CD1 | 2.45 | 0.46 |
| 1:A:897:TYR:N | 1:A:897:TYR:CD1 | 2.83 | 0.46 |
| 1:A:932:GLU:O | 1:A:936:LEU:HG | 2.16 | 0.46 |
| 1:A:1258:HIS:HB3 | 1:A:1259:MET:CE | 2.46 | 0.46 |
| 1:A:1345:ARG:NH1 | 5:E:200:ARG:NH2 | 2.64 | 0.46 |
| 2:B:100:PRO:HD3 | 2:B:172:ILE:HD13 | 1.98 | 0.46 |
| 2:B:240:ILE:HG23 | 2:B:240:ILE:O | 2.15 | 0.46 |
| 2:B:292:ILE:HG23 | 2:B:326:ASP:HA | 1.98 | 0.46 |
| 2:B:333:PHE:CD2 | 2:B:333:PHE:O | 2.69 | 0.46 |
| 2:B:834:ASN:O | 2:B:838:SER:O | 2.32 | 0.46 |
| 2:B:890:TYR:O | 2:B:893:LEU:HB2 | 2.16 | 0.46 |
| 3:C:35:ARG:HH11 | 11:K:41:THR:CA | 2.29 | 0.46 |
| 3:C:226:ASP:O | 3:C:227:THR:HB | 2.16 | 0.46 |
| 4:D:29:LEU:HD22 | 7:G:82:PHE:CD2 | 2.51 | 0.46 |
| 4:D:155:ARG:HB2 | 4:D:155:ARG:CZ | 2.45 | 0.46 |
| 4:D:185:CYS:HB2 | 4:D:211:LEU:HD21 | 1.96 | 0.46 |
| 5:E:82:PHE:CD1 | 5:E:82:PHE:N | 2.83 | 0.46 |
| 9:I:55:THR:HG22 | 9:I:55:THR:O | 2.16 | 0.46 |
| 10:J:64:ASN:ND2 | 10:J:65:PRO:HD3 | 2.31 | 0.46 |
| 11:K:89:ASN:O | 11:K:91:CYS:N | 2.49 | 0.46 |
| 1:A:377:PRO:HG3 | 1:A:493:GLN:HG3 | 1.98 | 0.46 |
| 1:A:407:ARG:HA | 1:A:430:TRP:CD2 | 2.51 | 0.46 |
| 1:A:896:ARG:HH21 | 1:A:1030:ARG:CZ | 2.29 | 0.46 |
| 2:B:291:ILE:HD13 | 2:B:300:HIS:CD2 | 2.51 | 0.46 |
| 2:B:552:MET:N | 2:B:553:PRO:HD2 | 2.30 | 0.46 |
| 2:B:579:ARG:HA | 2:B:589:VAL:HG22 | 1.98 | 0.46 |
| 2:B:654:ARG:C | 2:B:656:GLY:N | 2.68 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1020:ARG:HH11 | 2:B:1020:ARG:HG3 | 1.80 | 0.46 |
| 2:B:1106:ARG:HD3 | 2:B:1127:GLY:N | 2.31 | 0.46 |
| 3:C:10:ILE:HG13 | 11:K:108:GLU:HB3 | 1.98 | 0.46 |
| 3:C:245:VAL:HA | 3:C:248:ILE:HD12 | 1.98 | 0.46 |
| 5:E:22:MET:CE | 5:E:26:ARG:HD2 | 2.46 | 0.46 |
| 6:F:116:ASP:C | 6:F:116:ASP:OD1 | 2.54 | 0.46 |
| 6:F:148:VAL:HA | 6:F:151:LEU:HD12 | 1.96 | 0.46 |
| 8:H:25:ARG:HB2 | 8:H:41:ASP:OD1 | 2.15 | 0.46 |
| 11:K:82:ASP:OD1 | 11:K:84:LYS:N | 2.46 | 0.46 |
| 12:L:39:SER:O | 12:L:40:LEU:HG | 2.15 | 0.46 |
| 1:A:616:VAL:CG1 | 1:A:617:VAL:H | 2.19 | 0.46 |
| 1:A:619:LYS:O | 1:A:623:GLY:HA3 | 2.16 | 0.46 |
| 1:A:1018:PHE:O | 1:A:1021:LEU:N | 2.49 | 0.46 |
| 1:A:1111:MET:CE | 1:A:1331:SER:HA | 2.31 | 0.46 |
| 1:A:1118:VAL:O | 1:A:1305:VAL:HG13 | 2.16 | 0.46 |
| 1:A:1261:LYS:HE3 | 9:I:44:TYR:CE2 | 2.51 | 0.46 |
| 1:A:1372:VAL:O | 1:A:1376:THR:HG23 | 2.16 | 0.46 |
| 1:A:1402:PHE:O | 1:A:1402:PHE:CG | 2.67 | 0.46 |
| 1:A:1418:LEU:HB3 | 2:B:1222:ARG:HH11 | 1.79 | 0.46 |
| 2:B:334:ILE:C | 2:B:336:ARG:H | 2.20 | 0.46 |
| 2:B:591:ARG:O | 2:B:592:ASN:C | 2.55 | 0.46 |
| 2:B:756:ILE:O | 2:B:759:PRO:HD3 | 2.16 | 0.46 |
| 2:B:1065:GLN:HG3 | 2:B:1067:ARG:H | 1.80 | 0.46 |
| 2:B:1081:LEU:C | 2:B:1083:ALA:N | 2.69 | 0.46 |
| 2:B:1221:SER:HB3 | 4:D:12:ARG:NE | 2.30 | 0.46 |
| 3:C:46:ILE:HD12 | 3:C:67:LEU:O | 2.16 | 0.46 |
| 3:C:215:GLU:O | 3:C:216:GLY:C | 2.54 | 0.46 |
| 4:D:119:ARG:HD3 | 4:D:221:TYR:HD2 | 1.76 | 0.46 |
| 5:E:167:ARG:HA | 5:E:167:ARG:HD3 | 1.66 | 0.46 |
| 5:E:190:LEU:HD12 | 5:E:214:CYS:CB | 2.45 | 0.46 |
| 5:E:195:VAL:CG1 | 5:E:196:VAL:N | 2.78 | 0.46 |
| 7:G:34:VAL:HG13 | 7:G:45:ILE:HG21 | 1.98 | 0.46 |
| 7:G:51:TYR:O | 7:G:51:TYR:HD2 | 1.98 | 0.46 |
| 7:G:127:PRO:HG2 | 7:G:138:THR:CG2 | 2.34 | 0.46 |
| 8:H:15:VAL:HG22 | 8:H:26:ILE:CG2 | 2.45 | 0.46 |
| 8:H:37:LYS:HD2 | 8:H:126:GLU:OE1 | 2.16 | 0.46 |
| 11:K:68:PHE:N | 11:K:68:PHE:CD2 | 2.84 | 0.46 |
| 12:L:30:ILE:HG22 | 12:L:31:CYS:N | 2.31 | 0.46 |
| 1:A:42:ASP:C | 1:A:44:THR:N | 2.69 | 0.45 |
| 1:A:503:GLN:NE2 | 6:F:90:ARG:HH21 | 2.12 | 0.45 |
| 1:A:560:ILE:CG1 | 8:H:79:TRP:H | 2.29 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:584:ASN:C | 1:A:586:ILE:N | 2.69 | 0.45 |
| 1:A:590:ARG:HD3 | 1:A:592:ASP:OD2 | 2.16 | 0.45 |
| 1:A:699:ALA:O | 1:A:700:ASN:CB | 2.64 | 0.45 |
| 1:A:944:ARG:NE | 1:A:1298:TYR:HE1 | 2.14 | 0.45 |
| 1:A:1239:ARG:NH1 | 1:A:1239:ARG:HB3 | 2.30 | 0.45 |
| 1:A:1427:ASN:H | 1:A:1427:ASN:ND2 | 2.14 | 0.45 |
| 2:B:25:ILE:HG23 | 2:B:658:ILE:CD1 | 2.43 | 0.45 |
| 2:B:128:LEU:O | 2:B:167:ILE:HD12 | 2.16 | 0.45 |
| 2:B:235:SER:OG | 2:B:236:HIS:CD2 | 2.69 | 0.45 |
| 2:B:286:PHE:HE1 | 2:B:382:ILE:HD12 | 1.81 | 0.45 |
| 2:B:459:TYR:C | 2:B:459:TYR:CD2 | 2.88 | 0.45 |
| 2:B:479:VAL:HG12 | 2:B:480:SER:N | 2.31 | 0.45 |
| 2:B:601:ARG:NH1 | 2:B:605:ARG:HH22 | 2.14 | 0.45 |
| 2:B:601:ARG:O | 2:B:605:ARG:HG3 | 2.16 | 0.45 |
| 2:B:680:THR:HG23 | 2:B:683:SER:H | 1.81 | 0.45 |
| 2:B:693:ILE:HD13 | 2:B:701:ILE:HD13 | 1.97 | 0.45 |
| 2:B:1007:VAL:HG23 | 2:B:1008:PRO:HD2 | 1.97 | 0.45 |
| 3:C:35:ARG:NH1 | 11:K:41:THR:CA | 2.79 | 0.45 |
| 4:D:51:ASN:O | 4:D:52:LEU:C | 2.54 | 0.45 |
| 5:E:164:LEU:HD11 | 5:E:211:TYR:CE1 | 2.51 | 0.45 |
| 6:F:77:ASP:O | 6:F:78:GLN:CB | 2.55 | 0.45 |
| 6:F:103:MET:CE | 7:G:65:ASP:HB2 | 2.45 | 0.45 |
| 7:G:13:LEU:HD23 | 7:G:14:HIS:N | 2.27 | 0.45 |
| 8:H:4:THR:HG22 | 8:H:6:PHE:H | 1.81 | 0.45 |
| 11:K:100:ALA:O | 11:K:103:THR:HB | 2.17 | 0.45 |
| 12:L:34:CYS:O | 12:L:35:SER:C | 2.52 | 0.45 |
| 1:A:88:LYS:HG3 | 1:A:276:LEU:HD21 | 1.98 | 0.45 |
| 1:A:150:THR:O | 1:A:163:SER:HA | 2.16 | 0.45 |
| 1:A:239:LEU:HA | 1:A:240:PRO:HD2 | 1.81 | 0.45 |
| 1:A:728:LYS:HA | 1:A:731:ARG:HH21 | 1.80 | 0.45 |
| 1:A:896:ARG:HH21 | 1:A:1030:ARG:NH2 | 2.14 | 0.45 |
| 1:A:1051:ALA:O | 1:A:1055:ARG:HG3 | 2.16 | 0.45 |
| 1:A:1110:ASN:CG | 1:A:1110:ASN:O | 2.55 | 0.45 |
| 1:A:1262:LYS:O | 1:A:1264:GLU:N | 2.49 | 0.45 |
| 2:B:59:LEU:HD12 | 2:B:417:PHE:CD2 | 2.51 | 0.45 |
| 2:B:102:VAL:HG23 | 2:B:110:HIS:O | 2.16 | 0.45 |
| 2:B:656:GLY:O | 2:B:657:HIS:C | 2.53 | 0.45 |
| 2:B:1181:GLU:HG2 | 2:B:1188:LYS:HD2 | 1.98 | 0.45 |
| 3:C:133:ILE:HG13 | 3:C:237:SER:H | 1.80 | 0.45 |
| 7:G:50:ASP:O | 7:G:51:TYR:C | 2.53 | 0.45 |
| 8:H:93:TYR:CD1 | 8:H:143:LEU:HD23 | 2.51 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:J:56:LEU:O | 10:J:57:ILE:C | 2.55 | 0.45 |
| 11:K:107:THR:HG22 | 11:K:108:GLU:N | 2.30 | 0.45 |
| 11:K:110:ASN:C | 11:K:111:LEU:HD23 | 2.36 | 0.45 |
| 1:A:7:SER:C | 1:A:9:ALA:N | 2.70 | 0.45 |
| 1:A:54:ASN:HA | 1:A:247:ARG:HH22 | 1.82 | 0.45 |
| 1:A:332:LYS:H | 1:A:337:ARG:HB3 | 1.81 | 0.45 |
| 1:A:509:LEU:C | 1:A:511:ILE:N | 2.70 | 0.45 |
| 1:A:684:ALA:O | 1:A:687:LYS:HB2 | 2.16 | 0.45 |
| 1:A:1332:PHE:H | 1:A:1332:PHE:HD2 | 1.61 | 0.45 |
| 2:B:128:LEU:HD11 | 2:B:170:LEU:HB3 | 1.98 | 0.45 |
| 2:B:469:GLN:O | 2:B:470:LYS:HB2 | 2.16 | 0.45 |
| 2:B:570:VAL:HB | 2:B:573:GLN:HB3 | 1.99 | 0.45 |
| 2:B:834:ASN:ND2 | 2:B:1013:ASN:HA | 2.31 | 0.45 |
| 2:B:882:THR:C | 2:B:884:ARG:H | 2.20 | 0.45 |
| 2:B:1039:GLY:HA2 | 10:J:51:LEU:CD2 | 2.47 | 0.45 |
| 3:C:56:THR:CG2 | 3:C:58:LEU:HD23 | 2.46 | 0.45 |
| 7:G:1:MET:CE | 7:G:80:LYS:O | 2.64 | 0.45 |
| 1:A:524:VAL:CG1 | 1:A:525:GLN:H | 2.28 | 0.45 |
| 1:A:821:ARG:HB2 | 1:A:821:ARG:HH11 | 1.81 | 0.45 |
| 1:A:964:ILE:O | 1:A:967:ALA:N | 2.48 | 0.45 |
| 1:A:1166:ASP:OD2 | 1:A:1239:ARG:NE | 2.40 | 0.45 |
| 1:A:1191:TRP:HD1 | 1:A:1256:GLU:HB3 | 1.80 | 0.45 |
| 1:A:1402:PHE:O | 1:A:1403:GLU:CB | 2.64 | 0.45 |
| 2:B:324:ILE:HG23 | 2:B:325:GLN:N | 2.30 | 0.45 |
| 2:B:487:THR:H | 2:B:490:SER:HB3 | 1.79 | 0.45 |
| 2:B:558:LEU:C | 2:B:560:GLU:N | 2.70 | 0.45 |
| 2:B:782:LEU:HB3 | 2:B:784:ASN:OD1 | 2.16 | 0.45 |
| 2:B:1149:GLU:HA | 2:B:1153:GLU:OE1 | 2.16 | 0.45 |
| 3:C:91:HIS:HA | 3:C:95:CYS:SG | 2.56 | 0.45 |
| 4:D:191:ALA:O | 4:D:193:THR:N | 2.49 | 0.45 |
| 4:D:208:GLU:O | 4:D:212:LYS:HG3 | 2.16 | 0.45 |
| 5:E:11:ARG:O | 5:E:13:TRP:N | 2.49 | 0.45 |
| 5:E:50:MET:HB3 | 5:E:52:ARG:NH1 | 2.32 | 0.45 |
| 9:I:15:TYR:CD1 | 9:I:15:TYR:N | 2.83 | 0.45 |
| 9:I:82:GLU:C | 9:I:104:LEU:HG | 2.37 | 0.45 |
| 11:K:40:HIS:O | 11:K:41:THR:C | 2.55 | 0.45 |
| 13:T:10:DA:H2" | 13:T:11:DA:OP2 | 2.16 | 0.45 |
| 1:A:108:MET:SD | 1:A:210:ILE:HD13 | 2.56 | 0.45 |
| 1:A:424:ILE:C | 1:A:425:GLN:OE1 | 2.55 | 0.45 |
| 1:A:600:PRO:C | 1:A:602:ASP:H | 2.20 | 0.45 |
| 1:A:663:SER:OG | 1:A:664:THR:N | 2.48 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:896:ARG:NH2 | 1:A:1030:ARG:NE | 2.55 | 0.45 |
| 1:A:996:ASN:HB3 | 1:A:1050:GLU:OE2 | 2.17 | 0.45 |
| 1:A:1012:ARG:O | 1:A:1013:ASP:C | 2.54 | 0.45 |
| 1:A:1100:ARG:NH2 | 1:A:1351:GLU:CG | 2.72 | 0.45 |
| 1:A:1131:ALA:O | 1:A:1132:LYS:C | 2.54 | 0.45 |
| 1:A:1313:LEU:CD2 | 1:A:1338:VAL:HG21 | 2.43 | 0.45 |
| 2:B:131:ASP:HA | 2:B:164:LYS:N | 2.32 | 0.45 |
| 2:B:180:TYR:CD1 | 2:B:180:TYR:N | 2.78 | 0.45 |
| 2:B:383:ASN:ND2 | 2:B:387:LEU:HD11 | 2.32 | 0.45 |
| 2:B:498:THR:O | 2:B:498:THR:HG22 | 2.15 | 0.45 |
| 2:B:502:ILE:HG22 | 2:B:507:LYS:CG | 2.47 | 0.45 |
| 2:B:503:GLY:HA3 | 2:B:507:LYS:CE | 2.32 | 0.45 |
| 2:B:529:GLU:CD | 2:B:769:TYR:HE1 | 2.18 | 0.45 |
| 2:B:766:ARG:HG2 | 2:B:766:ARG:NH1 | 2.30 | 0.45 |
| 2:B:880:THR:HB | 2:B:934:LYS:HE3 | 1.95 | 0.45 |
| 6:F:116:ASP:OD1 | 6:F:119:ARG:HB2 | 2.17 | 0.45 |
| 7:G:94:CYS:HA | 7:G:99:PHE:HA | 1.98 | 0.45 |
| 8:H:58:THR:HG22 | 8:H:59:ILE:N | 2.31 | 0.45 |
| 15:P:6:A:H2' | 15:P:7:G:C8 | 2.51 | 0.45 |
| 15:P:6:A:H2' | 15:P:7:G:H8 | 1.82 | 0.45 |
| 1:A:254:GLU:O | 1:A:255:SER:OG | 2.32 | 0.45 |
| 1:A:402:ALA:HB1 | 1:A:434:ARG:HA | 1.96 | 0.45 |
| 1:A:531:ILE:HG23 | 1:A:532:ARG:N | 2.32 | 0.45 |
| 1:A:767:GLN:HE22 | 1:A:797:LYS:C | 2.20 | 0.45 |
| 1:A:867:ILE:CG2 | 1:A:872:GLY:H | 2.30 | 0.45 |
| 1:A:877:HIS:C | 1:A:878:ILE:HG13 | 2.37 | 0.45 |
| 1:A:982:THR:C | 1:A:984:LYS:N | 2.66 | 0.45 |
| 1:A:1176:LEU:O | 1:A:1176:LEU:HD23 | 2.17 | 0.45 |
| 1:A:1441:PHE:HE1 | 6:F:92:ARG:HG2 | 1.81 | 0.45 |
| 2:B:20:ASP:C | 2:B:22:SER:N | 2.70 | 0.45 |
| 2:B:186:GLU:HG3 | 10:J:62:ARG:HH22 | 1.80 | 0.45 |
| 2:B:361:LEU:O | 2:B:363:HIS:O | 2.35 | 0.45 |
| 2:B:408:LEU:HD12 | 2:B:408:LEU:HA | 1.74 | 0.45 |
| 2:B:975:GLN:HG2 | 2:B:976:ILE:H | 1.82 | 0.45 |
| 3:C:6:PRO:HB3 | 3:C:25:VAL:HG12 | 1.98 | 0.45 |
| 3:C:77:ILE:C | 3:C:79:GLN:H | 2.20 | 0.45 |
| 4:D:136:GLY:C | 4:D:138:ASN:H | 2.20 | 0.45 |
| 4:D:210:ILE:HG13 | 4:D:210:ILE:H | 1.42 | 0.45 |
| 5:E:22:MET:CE | 5:E:26:ARG:NH1 | 2.64 | 0.45 |
| 6:F:93:ILE:CD1 | 6:F:148:VAL:HG12 | 2.47 | 0.45 |
| 7:G:92:VAL:CG2 | 7:G:102:GLN:HB2 | 2.46 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 9:I:50:THR:HG22 | 9:I:52:ILE:H | 1.81 | 0.45 |
| 9:I:90:GLN:NE2 | 9:I:92:ARG:HD2 | 2.31 | 0.45 |
| 1:A:7:SER:O | 4:D:1:MET:HG3 | 2.17 | 0.45 |
| 1:A:11:LEU:HD22 | 2:B:1195:HIS:CD2 | 2.52 | 0.45 |
| 1:A:418:SER:O | 1:A:420:ARG:N | 2.45 | 0.45 |
| 1:A:700:ASN:HD22 | 9:I:115:LYS:HD2 | 1.81 | 0.45 |
| 1:A:1140:HIS:N | 1:A:1275:GLY:HA3 | 2.32 | 0.45 |
| 1:A:1427:ASN:O | 1:A:1431:GLY:N | 2.47 | 0.45 |
| 2:B:38:PHE:HD1 | 2:B:811:TYR:HD2 | 1.60 | 0.45 |
| 2:B:199:MET:SD | 2:B:199:MET:N | 2.88 | 0.45 |
| 2:B:290:GLY:HA2 | 2:B:327:ARG:HD2 | 1.98 | 0.45 |
| 2:B:806:THR:HG22 | 2:B:807:ARG:N | 2.32 | 0.45 |
| 2:B:806:THR:HG21 | 2:B:808:ALA:HB3 | 1.99 | 0.45 |
| 2:B:876:LYS:HD2 | 2:B:893:LEU:O | 2.17 | 0.45 |
| 2:B:1081:LEU:O | 2:B:1083:ALA:O | 2.34 | 0.45 |
| 3:C:64:ALA:HA | 3:C:67:LEU:HD12 | 1.97 | 0.45 |
| 4:D:8:PHE:HD2 | 7:G:6:ASP:O | 1.99 | 0.45 |
| 5:E:45:LYS:HD3 | 5:E:46:TYR:HE1 | 1.81 | 0.45 |
| 6:F:116:ASP:OD1 | 6:F:119:ARG:N | 2.50 | 0.45 |
| 7:G:27:LYS:HG2 | 7:G:54:ILE:HD12 | 1.98 | 0.45 |
| 7:G:111:THR:O | 7:G:112:LYS:C | 2.55 | 0.45 |
| 9:I:34:TYR:CD2 | 9:I:34:TYR:C | 2.89 | 0.45 |
| 1:A:345:VAL:CG2 | 2:B:1150:ARG:HH22 | 2.29 | 0.45 |
| 1:A:350:ARG:O | 1:A:351:THR:HG22 | 2.17 | 0.45 |
| 1:A:786:HIS:CE1 | 2:B:705:MET:SD | 3.10 | 0.45 |
| 1:A:794:PRO:C | 1:A:796:SER:H | 2.20 | 0.45 |
| 1:A:1194:ARG:HG3 | 1:A:1237:ILE:CG2 | 2.46 | 0.45 |
| 1:A:1350:LYS:O | 1:A:1354:ASN:ND2 | 2.50 | 0.45 |
| 1:A:1436:ILE:O | 1:A:1439:GLY:N | 2.39 | 0.45 |
| 1:A:1444:MET:HG3 | 7:G:60:ARG:CA | 2.41 | 0.45 |
| 2:B:541:LEU:HB2 | 2:B:747:MET:HE3 | 1.99 | 0.45 |
| 2:B:638:PHE:HB2 | 2:B:741:CYS:HB3 | 1.99 | 0.45 |
| 2:B:785:TYR:HE2 | 10:J:60:PHE:CE1 | 2.35 | 0.45 |
| 2:B:906:SER:O | 2:B:907:GLY:O | 2.33 | 0.45 |
| 3:C:241:ASP:O | 3:C:245:VAL:HG22 | 2.16 | 0.45 |
| 5:E:78:LEU:HD23 | 5:E:78:LEU:C | 2.37 | 0.45 |
| 6:F:82:THR:HA | 6:F:83:PRO:HD3 | 1.71 | 0.45 |
| 12:L:60:ARG:HG2 | 12:L:61:THR:N | 2.32 | 0.45 |
| 1:A:41:MET:HB2 | 1:A:50:ILE:H | 1.82 | 0.45 |
| 1:A:134:ARG:C | 1:A:136:ALA:H | 2.20 | 0.45 |
| 1:A:323:LYS:HD2 | 1:A:323:LYS:N | 2.30 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:369:SER:HB2 | 11:K:2:ASN:OD1 | 2.17 | 0.45 |
| 1:A:665:GLY:C | 1:A:666:ILE:HD12 | 2.37 | 0.45 |
| 2:B:29:ASP:HB3 | 2:B:658:ILE:CD1 | 2.46 | 0.45 |
| 2:B:100:PRO:CG | 2:B:180:TYR:HE1 | 2.30 | 0.45 |
| 2:B:383:ASN:O | 2:B:385:LEU:N | 2.49 | 0.45 |
| 2:B:529:GLU:CD | 2:B:769:TYR:CE1 | 2.91 | 0.45 |
| 2:B:547:VAL:HG13 | 2:B:548:GLY:H | 1.82 | 0.45 |
| 2:B:1159:ARG:HD3 | 2:B:1193:GLN:HG3 | 1.97 | 0.45 |
| 3:C:33:LEU:O | 3:C:34:ARG:C | 2.54 | 0.45 |
| 5:E:74:ASP:OD1 | 5:E:74:ASP:N | 2.49 | 0.45 |
| 5:E:180:ARG:HB2 | 5:E:215:MET:OXT | 2.16 | 0.45 |
| 7:G:14:HIS:ND1 | 7:G:15:PRO:CD | 2.80 | 0.45 |
| 7:G:27:LYS:HD3 | 7:G:51:TYR:CE2 | 2.52 | 0.45 |
| 8:H:98:TYR:CE1 | 8:H:139:ASN:HA | 2.51 | 0.45 |
| 11:K:10:PHE:N | 11:K:10:PHE:CD2 | 2.84 | 0.45 |
| 11:K:49:GLU:HA | 11:K:52:ASN:ND2 | 2.31 | 0.45 |
| 1:A:21:LEU:CD1 | 1:A:229:SER:HB2 | 2.47 | 0.45 |
| 1:A:29:ALA:HB1 | 2:B:1184:GLY:HA3 | 1.98 | 0.45 |
| 1:A:306:ASN:HB2 | 1:A:324:SER:HB3 | 1.98 | 0.45 |
| 1:A:608:ILE:HD12 | 1:A:613:ILE:CD1 | 2.47 | 0.45 |
| 1:A:645:LEU:CG | 1:A:649:ILE:HD11 | 2.47 | 0.45 |
| 1:A:647:GLY:O | 1:A:651:LYS:HG3 | 2.17 | 0.45 |
| 1:A:675:THR:O | 1:A:675:THR:HG22 | 2.17 | 0.45 |
| 1:A:1161:THR:OG1 | 1:A:1239:ARG:NH2 | 2.50 | 0.45 |
| 1:A:1167:GLU:O | 1:A:1170:ILE:HG13 | 2.17 | 0.45 |
| 1:A:1175:SER:O | 1:A:1176:LEU:CB | 2.59 | 0.45 |
| 1:A:1437:GLY:C | 1:A:1439:GLY:H | 2.21 | 0.45 |
| 2:B:266:ALA:C | 2:B:268:THR:H | 2.20 | 0.45 |
| 2:B:274:PRO:C | 2:B:276:ILE:H | 2.20 | 0.45 |
| 2:B:304:ASP:OD1 | 2:B:306:ASN:N | 2.51 | 0.45 |
| 2:B:570:VAL:HA | 2:B:571:PRO:HD2 | 1.85 | 0.45 |
| 2:B:593:PRO:CA | 2:B:596:LEU:HB3 | 2.46 | 0.45 |
| 2:B:641:GLU:HB2 | 2:B:643:ASP:CG | 2.37 | 0.45 |
| 2:B:826:ALA:O | 2:B:1011:ILE:HA | 2.17 | 0.45 |
| 2:B:1034:VAL:O | 2:B:1037:LEU:N | 2.36 | 0.45 |
| 3:C:80:LEU:O | 3:C:80:LEU:HG | 2.16 | 0.45 |
| 4:D:124:GLU:O | 4:D:128:VAL:HG23 | 2.17 | 0.45 |
| 7:G:39:THR:HG22 | 7:G:40:GLY:H | 1.82 | 0.45 |
| 9:I:68:LEU:HB3 | 9:I:84:VAL:HG23 | 1.99 | 0.45 |
| 11:K:49:GLU:HG3 | 11:K:94:ILE:CG1 | 2.47 | 0.45 |
| 12:L:26:THR:HG23 | 12:L:62:LYS:HZ1 | 1.82 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 12:L:44:ASP:O | 12:L:45:ALA:CB | 2.65 | 0.45 |
| 13:T:12:DG:N2 | 14:N:6:DT:C2 | 2.85 | 0.45 |
| 13:T:25:DG:H2'' | 13:T:26:DT:C5' | 2.47 | 0.45 |
| 1:A:41:MET:CE | 1:A:42:ASP:HB2 | 2.47 | 0.44 |
| 1:A:288:ALA:HA | 1:A:291:GLU:CD | 2.37 | 0.44 |
| 1:A:364:VAL:O | 1:A:364:VAL:HG13 | 2.17 | 0.44 |
| 1:A:567:LYS:CB | 8:H:96:VAL:H | 2.26 | 0.44 |
| 1:A:608:ILE:C | 1:A:610:GLY:H | 2.19 | 0.44 |
| 1:A:661:GLY:O | 1:A:662:PHE:HB2 | 2.16 | 0.44 |
| 1:A:871:ASP:O | 1:A:873:MET:N | 2.50 | 0.44 |
| 1:A:1151:GLU:HG2 | 9:I:45:ARG:CB | 2.47 | 0.44 |
| 1:A:1341:ILE:CG2 | 1:A:1342:GLU:H | 2.29 | 0.44 |
| 1:A:1447:GLU:O | 1:A:1448:GLU:C | 2.56 | 0.44 |
| 2:B:451:LYS:O | 2:B:452:THR:C | 2.55 | 0.44 |
| 2:B:789:MET:HE2 | 2:B:953:LEU:HD21 | 1.98 | 0.44 |
| 2:B:814:PHE:C | 2:B:816:GLU:N | 2.68 | 0.44 |
| 2:B:834:ASN:HB3 | 2:B:840:ILE:HG13 | 1.99 | 0.44 |
| 3:C:114:TYR:OH | 10:J:19:GLU:OE1 | 2.34 | 0.44 |
| 3:C:220:ASP:OD1 | 3:C:223:ALA:N | 2.50 | 0.44 |
| 3:C:239:PRO:O | 3:C:241:ASP:N | 2.50 | 0.44 |
| 4:D:185:CYS:CB | 4:D:211:LEU:HD21 | 2.47 | 0.44 |
| 5:E:11:ARG:C | 5:E:13:TRP:H | 2.20 | 0.44 |
| 5:E:84:ASP:O | 5:E:86:PRO:HD3 | 2.17 | 0.44 |
| 5:E:92:THR:O | 5:E:92:THR:HG22 | 2.17 | 0.44 |
| 8:H:128:ASN:OD1 | 8:H:128:ASN:O | 2.35 | 0.44 |
| 10:J:3:VAL:HG21 | 10:J:18:TRP:CB | 2.47 | 0.44 |
| 12:L:40:LEU:HB3 | 12:L:41:SER:H | 1.56 | 0.44 |
| 1:A:186:LYS:O | 1:A:187:LYS:HB3 | 2.16 | 0.44 |
| 1:A:618:GLU:O | 1:A:621:THR:N | 2.44 | 0.44 |
| 1:A:722:LEU:HB3 | 1:A:799:PHE:CE1 | 2.52 | 0.44 |
| 1:A:853:ASP:OD1 | 1:A:855:THR:HG22 | 2.17 | 0.44 |
| 1:A:968:GLN:O | 1:A:970:THR:N | 2.51 | 0.44 |
| 1:A:1383:SER:O | 1:A:1388:GLY:HA3 | 2.17 | 0.44 |
| 2:B:318:VAL:O | 2:B:320:ASP:N | 2.50 | 0.44 |
| 2:B:335:GLY:HA3 | 2:B:348:ARG:HB2 | 1.99 | 0.44 |
| 2:B:693:ILE:HD11 | 2:B:740:HIS:CD2 | 2.52 | 0.44 |
| 2:B:701:ILE:HB | 2:B:739:THR:OG1 | 2.17 | 0.44 |
| 2:B:980:PHE:HE1 | 2:B:990:ILE:HD11 | 1.82 | 0.44 |
| 2:B:986:GLN:OE1 | 2:B:986:GLN:HA | 2.18 | 0.44 |
| 2:B:1201:LYS:HE2 | 2:B:1205:GLN:HE22 | 1.80 | 0.44 |
| 3:C:6:PRO:HB3 | 3:C:25:VAL:CG1 | 2.47 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:173:ALA:O | 3:C:174:ALA:CB | 2.65 | 0.44 |
| 5:E:13:TRP:CH2 | 5:E:39:LEU:HB2 | 2.52 | 0.44 |
| 6:F:69:LEU:C | 6:F:71:GLU:H | 2.21 | 0.44 |
| 6:F:97:ARG:HG3 | 6:F:124:GLU:OE1 | 2.17 | 0.44 |
| 9:I:33:SER:O | 9:I:34:TYR:C | 2.55 | 0.44 |
| 10:J:2:ILE:HG23 | 10:J:3:VAL:O | 2.18 | 0.44 |
| 11:K:29:ASN:O | 11:K:76:GLN:HG3 | 2.16 | 0.44 |
| 1:A:47:ARG:O | 1:A:48:ALA:HB2 | 2.17 | 0.44 |
| 1:A:666:ILE:HD11 | 2:B:1086:PHE:HE1 | 1.83 | 0.44 |
| 1:A:683:ILE:O | 1:A:686:ALA:N | 2.44 | 0.44 |
| 1:A:700:ASN:HB2 | 9:I:98:VAL:CG2 | 2.48 | 0.44 |
| 1:A:770:VAL:O | 1:A:771:GLU:HB2 | 2.16 | 0.44 |
| 1:A:858:ASN:ND2 | 1:A:860:LEU:H | 2.15 | 0.44 |
| 1:A:1220:PHE:O | 1:A:1221:LYS:CB | 2.65 | 0.44 |
| 1:A:1404:GLU:HB2 | 1:A:1408:ILE:CD1 | 2.40 | 0.44 |
| 1:A:1409:LEU:O | 1:A:1412:ALA:HB3 | 2.17 | 0.44 |
| 2:B:172:ILE:HG22 | 2:B:173:MET:O | 2.17 | 0.44 |
| 2:B:516:ASN:C | 2:B:518:HIS:H | 2.20 | 0.44 |
| 2:B:827:ILE:O | 2:B:828:ALA:CB | 2.61 | 0.44 |
| 3:C:181:ASP:OD2 | 3:C:185:LYS:N | 2.50 | 0.44 |
| 3:C:258:ILE:HD12 | 3:C:258:ILE:N | 2.32 | 0.44 |
| 4:D:22:GLU:N | 4:D:22:GLU:OE1 | 2.38 | 0.44 |
| 5:E:26:ARG:HG2 | 5:E:28:TYR:HE1 | 1.82 | 0.44 |
| 5:E:212:ARG:CG | 5:E:212:ARG:NH1 | 2.78 | 0.44 |
| 6:F:85:MET:CB | 6:F:155:LEU:HD11 | 2.46 | 0.44 |
| 7:G:138:THR:O | 7:G:139:ILE:C | 2.56 | 0.44 |
| 7:G:163:ILE:HA | 7:G:168:LEU:HD13 | 2.00 | 0.44 |
| 11:K:21:ILE:HG22 | 11:K:31:VAL:HG12 | 1.98 | 0.44 |
| 12:L:47:ARG:HG2 | 12:L:54:ARG:HG2 | 1.99 | 0.44 |
| 14:N:5:DC:H2' | 14:N:6:DT:H72 | 1.98 | 0.44 |
| 1:A:6:TYR:CE1 | 4:D:1:MET:HG3 | 2.52 | 0.44 |
| 1:A:16:GLU:CD | 2:B:1220:ARG:HA | 2.37 | 0.44 |
| 1:A:75:ASN:O | 1:A:76:GLU:HB2 | 2.18 | 0.44 |
| 1:A:116:ASP:C | 1:A:118:HIS:N | 2.68 | 0.44 |
| 1:A:119:ASN:O | 1:A:122:MET:HB3 | 2.17 | 0.44 |
| 1:A:315:LEU:HD13 | 2:B:471:LYS:O | 2.18 | 0.44 |
| 1:A:843:LYS:HD3 | 1:A:843:LYS:HA | 1.82 | 0.44 |
| 1:A:879:GLU:OE2 | 1:A:959:ASN:ND2 | 2.48 | 0.44 |
| 1:A:1159:ARG:HD3 | 1:A:1174:PHE:HZ | 1.81 | 0.44 |
| 1:A:1392:SER:C | 1:A:1394:THR:H | 2.21 | 0.44 |
| 2:B:312:GLU:O | 2:B:315:LYS:HB2 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:425:THR:O | 2:B:428:ILE:HD12 | 2.17 | 0.44 |
| 2:B:953:LEU:HB3 | 12:L:57:LEU:CD2 | 2.47 | 0.44 |
| 2:B:1001:PHE:CD2 | 3:C:34:ARG:NH2 | 2.85 | 0.44 |
| 3:C:143:LEU:HD21 | 3:C:146:LYS:HE3 | 1.99 | 0.44 |
| 4:D:167:LEU:O | 4:D:169:SER:N | 2.50 | 0.44 |
| 4:D:176:GLU:C | 4:D:178:ALA:N | 2.71 | 0.44 |
| 5:E:49:SER:C | 5:E:50:MET:HE2 | 2.38 | 0.44 |
| 7:G:63:PRO:HG2 | 7:G:64:THR:H | 1.82 | 0.44 |
| 9:I:22:ASN:O | 9:I:23:ASN:HB2 | 2.15 | 0.44 |
| 12:L:40:LEU:CD1 | 12:L:44:ASP:HB3 | 2.28 | 0.44 |
| 1:A:34:LYS:HD3 | 1:A:34:LYS:N | 2.33 | 0.44 |
| 1:A:106:VAL:HG21 | 1:A:214:ILE:HD13 | 2.00 | 0.44 |
| 1:A:130:ASP:C | 1:A:132:LYS:H | 2.21 | 0.44 |
| 1:A:134:ARG:CG | 1:A:138:ILE:HD11 | 2.37 | 0.44 |
| 1:A:280:GLU:O | 1:A:282:ASN:N | 2.50 | 0.44 |
| 1:A:734:GLU:C | 1:A:736:ASN:N | 2.70 | 0.44 |
| 1:A:914:GLU:C | 1:A:916:GLY:H | 2.21 | 0.44 |
| 1:A:1107:VAL:O | 1:A:1107:VAL:CG1 | 2.63 | 0.44 |
| 1:A:1120:LEU:H | 1:A:1120:LEU:CD1 | 2.29 | 0.44 |
| 1:A:1125:ALA:C | 1:A:1127:ASP:N | 2.70 | 0.44 |
| 2:B:401:PHE:HB2 | 2:B:517:THR:OG1 | 2.17 | 0.44 |
| 2:B:615:MET:O | 2:B:615:MET:CE | 2.66 | 0.44 |
| 2:B:784:ASN:O | 2:B:788:ARG:HG3 | 2.17 | 0.44 |
| 2:B:827:ILE:HD12 | 2:B:1086:PHE:HD2 | 1.83 | 0.44 |
| 2:B:1107:ALA:O | 2:B:1108:ARG:O | 2.36 | 0.44 |
| 2:B:1200:ALA:HA | 2:B:1203:LEU:HB3 | 1.99 | 0.44 |
| 3:C:77:ILE:HG23 | 3:C:161:LYS:HZ2 | 1.81 | 0.44 |
| 3:C:83:SER:OG | 3:C:160:LYS:HD3 | 2.18 | 0.44 |
| 3:C:268:ASP:O | 3:C:269:LYS:CB | 2.65 | 0.44 |
| 5:E:55:ARG:O | 5:E:57:MET:N | 2.51 | 0.44 |
| 7:G:26:LEU:HD23 | 7:G:26:LEU:HA | 1.85 | 0.44 |
| 7:G:39:THR:HB | 7:G:42:PHE:H | 1.83 | 0.44 |
| 7:G:41:LYS:HD3 | 7:G:42:PHE:CE1 | 2.52 | 0.44 |
| 7:G:91:VAL:HA | 7:G:101:VAL:HA | 2.00 | 0.44 |
| 8:H:77:ARG:O | 8:H:78:SER:O | 2.34 | 0.44 |
| 9:I:83:ASN:OD1 | 9:I:103:CYS:HA | 2.17 | 0.44 |
| 9:I:100:PHE:N | 9:I:100:PHE:HD1 | 2.15 | 0.44 |
| 1:A:7:SER:OG | 2:B:1193:GLN:NE2 | 2.51 | 0.44 |
| 1:A:472:LEU:HD11 | 2:B:835:GLN:NE2 | 2.33 | 0.44 |
| 1:A:500:GLU:OE1 | 2:B:1143:ALA:C | 2.56 | 0.44 |
| 1:A:608:ILE:CG1 | 1:A:613:ILE:HD11 | 2.47 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:811:GLN:O | 1:A:812:GLU:C | 2.55 | 0.44 |
| 1:A:1217:LYS:O | 1:A:1221:LYS:N | 2.50 | 0.44 |
| 2:B:129:PHE:CE2 | 2:B:166:PHE:HD1 | 2.36 | 0.44 |
| 2:B:304:ASP:OD1 | 2:B:306:ASN:HB2 | 2.17 | 0.44 |
| 2:B:426:LYS:O | 2:B:429:PHE:HB2 | 2.18 | 0.44 |
| 2:B:516:ASN:C | 2:B:518:HIS:N | 2.71 | 0.44 |
| 2:B:522:VAL:HG12 | 2:B:523:CYS:N | 2.33 | 0.44 |
| 2:B:797:TYR:HE2 | 3:C:62:PHE:HA | 1.82 | 0.44 |
| 2:B:797:TYR:CE1 | 2:B:971:THR:HG23 | 2.48 | 0.44 |
| 2:B:798:TYR:HE1 | 10:J:4:PRO:HA | 1.83 | 0.44 |
| 2:B:1142:GLY:HA3 | 6:F:88:TYR:CE2 | 2.46 | 0.44 |
| 3:C:181:ASP:OD2 | 3:C:186:LEU:HD13 | 2.18 | 0.44 |
| 4:D:115:HIS:H | 4:D:115:HIS:CD2 | 2.36 | 0.44 |
| 5:E:83:CYS:C | 5:E:85:GLU:N | 2.70 | 0.44 |
| 5:E:159:ASP:HA | 5:E:162:ARG:HH22 | 1.80 | 0.44 |
| 5:E:202:SER:C | 5:E:204:THR:H | 2.19 | 0.44 |
| 10:J:20:SER:O | 10:J:24:LEU:HG | 2.18 | 0.44 |
| 10:J:24:LEU:HD12 | 10:J:39:LEU:CD1 | 2.44 | 0.44 |
| 10:J:24:LEU:CD1 | 10:J:39:LEU:HD11 | 2.45 | 0.44 |
| 12:L:40:LEU:HD11 | 12:L:49:LYS:NZ | 2.32 | 0.44 |
| 1:A:49:LYS:HZ2 | 1:A:60:SER:HA | 1.82 | 0.44 |
| 1:A:79:GLY:HA3 | 1:A:243:PRO:HG2 | 1.96 | 0.44 |
| 1:A:108:MET:CE | 1:A:210:ILE:HD13 | 2.48 | 0.44 |
| 1:A:447:GLN:H | 1:A:447:GLN:HG3 | 1.55 | 0.44 |
| 1:A:492:PRO:HB3 | 1:A:501:LEU:HD11 | 1.99 | 0.44 |
| 1:A:693:VAL:HG21 | 1:A:721:PHE:HE1 | 1.83 | 0.44 |
| 1:A:857:ARG:CZ | 6:F:139:PRO:HB2 | 2.47 | 0.44 |
| 1:A:1100:ARG:HH12 | 1:A:1111:MET:CE | 2.30 | 0.44 |
| 1:A:1141:THR:CB | 1:A:1205:LYS:HZ3 | 2.31 | 0.44 |
| 1:A:1329:THR:HG22 | 1:A:1335:ILE:HG13 | 2.00 | 0.44 |
| 1:A:1381:LEU:HA | 1:A:1381:LEU:HD23 | 1.71 | 0.44 |
| 2:B:53:GLN:HG2 | 2:B:547:VAL:HG23 | 2.00 | 0.44 |
| 2:B:276:ILE:O | 2:B:276:ILE:HG22 | 2.18 | 0.44 |
| 2:B:541:LEU:HB2 | 2:B:747:MET:CE | 2.48 | 0.44 |
| 2:B:650:GLU:HG3 | 2:B:651:LEU:N | 2.32 | 0.44 |
| 2:B:791:THR:O | 2:B:792:MET:CB | 2.66 | 0.44 |
| 2:B:825:VAL:HG21 | 2:B:1092:TYR:CE1 | 2.53 | 0.44 |
| 2:B:871:THR:HG22 | 2:B:872:GLU:N | 2.32 | 0.44 |
| 2:B:903:VAL:CG1 | 2:B:904:ARG:N | 2.79 | 0.44 |
| 2:B:1080:LYS:HD2 | 3:C:188:HIS:CB | 2.46 | 0.44 |
| 2:B:1167:GLY:CA | 2:B:1216:LEU:H | 2.30 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:22:LEU:HD23 | 3:C:22:LEU:C | 2.38 | 0.44 |
| 3:C:72:LEU:O | 3:C:237:SER:HB3 | 2.17 | 0.44 |
| 4:D:40:HIS:HD2 | 7:G:73:LYS:HG3 | 1.81 | 0.44 |
| 4:D:56:ARG:HH21 | 4:D:155:ARG:HA | 1.79 | 0.44 |
| 4:D:130:LEU:C | 4:D:132:GLN:N | 2.71 | 0.44 |
| 5:E:137:GLU:C | 5:E:139:ALA:H | 2.21 | 0.44 |
| 7:G:92:VAL:HG21 | 7:G:102:GLN:HB2 | 1.99 | 0.44 |
| 8:H:64:ASN:ND2 | 8:H:88:SER:O | 2.50 | 0.44 |
| 8:H:82:PRO:HG2 | 8:H:83:GLN:H | 1.82 | 0.44 |
| 1:A:203:SER:OG | 1:A:206:GLU:HB2 | 2.18 | 0.44 |
| 1:A:258:GLY:O | 1:A:259:GLU:O | 2.36 | 0.44 |
| 1:A:446:ARG:HB3 | 1:A:478:TYR:HB3 | 1.99 | 0.44 |
| 1:A:532:ARG:NH1 | 1:A:532:ARG:HG2 | 2.33 | 0.44 |
| 1:A:910:PRO:HB3 | 1:A:917:SER:N | 2.33 | 0.44 |
| 1:A:982:THR:HB | 1:A:985:ASP:H | 1.83 | 0.44 |
| 1:A:1208:THR:HG22 | 1:A:1210:GLY:N | 2.32 | 0.44 |
| 1:A:1220:PHE:CD1 | 1:A:1224:LEU:HD23 | 2.53 | 0.44 |
| 1:A:1244:ARG:CB | 1:A:1245:PRO:CA | 2.89 | 0.44 |
| 1:A:1293:SER:O | 1:A:1294:PRO:C | 2.54 | 0.44 |
| 2:B:40:GLU:OE1 | 2:B:682:SER:HB2 | 2.17 | 0.44 |
| 2:B:132:VAL:H | 2:B:164:LYS:N | 2.16 | 0.44 |
| 2:B:620:ARG:HD2 | 9:I:68:LEU:HD11 | 1.99 | 0.44 |
| 2:B:758:PHE:HB3 | 2:B:761:HIS:HD2 | 1.82 | 0.44 |
| 2:B:846:ILE:HG23 | 2:B:974:PRO:HG2 | 2.00 | 0.44 |
| 4:D:166:LEU:HG | 4:D:167:LEU:HD23 | 2.00 | 0.44 |
| 5:E:93:MET:C | 5:E:95:THR:N | 2.71 | 0.44 |
| 6:F:94:LEU:CD2 | 6:F:122:MET:HA | 2.46 | 0.44 |
| 9:I:76:PRO:HG2 | 9:I:110:PHE:HB3 | 1.99 | 0.44 |
| 9:I:86:PHE:HE1 | 9:I:100:PHE:HB2 | 1.80 | 0.44 |
| 1:A:320:ARG:HG2 | 1:A:322:VAL:H | 1.83 | 0.44 |
| 1:A:332:LYS:HG3 | 1:A:333:GLU:HG2 | 2.00 | 0.44 |
| 1:A:496:GLU:O | 1:A:499:ALA:HB3 | 2.18 | 0.44 |
| 1:A:994:GLN:HG2 | 1:A:1022:LEU:HD23 | 2.00 | 0.44 |
| 1:A:1265:ASN:O | 1:A:1267:MET:N | 2.51 | 0.44 |
| 2:B:188:ASP:O | 2:B:192:LEU:HD12 | 2.18 | 0.44 |
| 2:B:210:LYS:HE2 | 2:B:461:LEU:O | 2.17 | 0.44 |
| 2:B:346:GLU:HG2 | 2:B:347:LYS:N | 2.32 | 0.44 |
| 2:B:410:GLY:O | 2:B:411:PRO:C | 2.56 | 0.44 |
| 2:B:616:ILE:CD1 | 2:B:625:LYS:HB2 | 2.48 | 0.44 |
| 2:B:766:ARG:HH21 | 2:B:1020:ARG:HG2 | 1.83 | 0.44 |
| 2:B:1064:TYR:O | 2:B:1065:GLN:C | 2.56 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:C:88:CYS:SG | 3:C:91:HIS:CA | 3.06 | 0.44 |
| 4:D:64:VAL:C | 4:D:66:ARG:H | 2.21 | 0.44 |
| 5:E:42:PHE:O | 5:E:43:LYS:C | 2.56 | 0.44 |
| 5:E:90:VAL:HA | 5:E:93:MET:HB2 | 1.99 | 0.44 |
| 5:E:108:GLY:O | 5:E:132:ILE:HG22 | 2.18 | 0.44 |
| 8:H:40:LEU:CD2 | 8:H:123:MET:HE3 | 2.31 | 0.44 |
| 1:A:15:LYS:O | 1:A:1420:ASP:O | 2.35 | 0.43 |
| 1:A:71:GLN:CG | 1:A:72:GLU:N | 2.80 | 0.43 |
| 1:A:262:LEU:CD2 | 1:A:303:TYR:CE1 | 3.01 | 0.43 |
| 1:A:543:LEU:CD1 | 1:A:547:LEU:HG | 2.48 | 0.43 |
| 1:A:1377:THR:OG1 | 1:A:1378:GLN:N | 2.51 | 0.43 |
| 2:B:224:GLN:HA | 2:B:396:ASP:OD2 | 2.18 | 0.43 |
| 2:B:257:LYS:N | 2:B:270:LYS:O | 2.51 | 0.43 |
| 3:C:20:PHE:CE1 | 3:C:230:MET:HB2 | 2.52 | 0.43 |
| 1:A:71:GLN:HG3 | 1:A:72:GLU:N | 2.32 | 0.43 |
| 1:A:276:LEU:HD11 | 1:A:293:GLU:HB2 | 2.00 | 0.43 |
| 1:A:377:PRO:HD3 | 1:A:493:GLN:OE1 | 2.18 | 0.43 |
| 1:A:384:ASN:HB3 | 1:A:387:ARG:HH21 | 1.82 | 0.43 |
| 1:A:595:THR:C | 1:A:596:THR:HG23 | 2.38 | 0.43 |
| 1:A:658:LEU:HD12 | 2:B:830:TYR:CD1 | 2.53 | 0.43 |
| 1:A:784:LEU:HD11 | 1:A:815:PHE:CE2 | 2.53 | 0.43 |
| 1:A:883:LEU:CD2 | 1:A:1021:LEU:HB2 | 2.48 | 0.43 |
| 1:A:943:LEU:C | 1:A:945:GLU:H | 2.20 | 0.43 |
| 1:A:1157:ASP:O | 1:A:1159:ARG:N | 2.51 | 0.43 |
| 1:A:1194:ARG:HG3 | 1:A:1237:ILE:HG23 | 2.00 | 0.43 |
| 2:B:205:ILE:HG12 | 2:B:461:LEU:HB3 | 2.00 | 0.43 |
| 2:B:258:LEU:O | 2:B:259:TYR:O | 2.36 | 0.43 |
| 2:B:446:LEU:O | 2:B:447:ALA:CB | 2.66 | 0.43 |
| 2:B:562:GLY:HA3 | 2:B:590:HIS:CE1 | 2.53 | 0.43 |
| 2:B:570:VAL:CG2 | 2:B:573:GLN:HB3 | 2.48 | 0.43 |
| 2:B:615:MET:HE2 | 2:B:697:GLU:CD | 2.38 | 0.43 |
| 2:B:825:VAL:CG2 | 2:B:1010:LEU:HD23 | 2.48 | 0.43 |
| 2:B:865:LYS:CG | 2:B:961:LEU:HD21 | 2.46 | 0.43 |
| 2:B:1063:GLY:O | 3:C:202:PRO:HG2 | 2.18 | 0.43 |
| 2:B:1098:MET:O | 2:B:1099:VAL:C | 2.55 | 0.43 |
| 2:B:1202:LEU:C | 2:B:1206:GLU:HG3 | 2.37 | 0.43 |
| 5:E:204:THR:CG2 | 5:E:205:SER:N | 2.79 | 0.43 |
| 7:G:112:LYS:HE3 | 7:G:113:HIS:CE1 | 2.53 | 0.43 |
| 8:H:56:THR:HB | 8:H:145:ARG:HG2 | 2.00 | 0.43 |
| 8:H:129:TYR:C | 8:H:130:ARG:HD2 | 2.38 | 0.43 |
| 1:A:106:VAL:C | 1:A:114:LEU:HD21 | 2.38 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:353:ILE:HD13 | 1:A:487:MET:CE | 2.45 | 0.43 |
| 1:A:481:ASP:OD1 | 1:A:485:ASP:OD2 | 2.37 | 0.43 |
| 1:A:1005:GLU:O | 1:A:1009:ASN:HB2 | 2.18 | 0.43 |
| 2:B:46:GLN:CG | 2:B:47:GLN:H | 2.31 | 0.43 |
| 2:B:827:ILE:O | 2:B:1085:ILE:CG2 | 2.66 | 0.43 |
| 2:B:843:GLN:NE2 | 2:B:847:ASP:OD1 | 2.43 | 0.43 |
| 2:B:865:LYS:HE3 | 2:B:961:LEU:CD2 | 2.49 | 0.43 |
| 2:B:1084:GLN:OE1 | 3:C:189:THR:HG22 | 2.18 | 0.43 |
| 2:B:1116:ARG:HD2 | 2:B:1198:TYR:CD1 | 2.53 | 0.43 |
| 3:C:77:ILE:C | 3:C:79:GLN:N | 2.72 | 0.43 |
| 4:D:9:GLN:HE22 | 4:D:31:GLN:HG2 | 1.83 | 0.43 |
| 6:F:119:ARG:HG3 | 6:F:119:ARG:NH1 | 2.33 | 0.43 |
| 8:H:24:CYS:HB2 | 8:H:44:VAL:CG2 | 2.46 | 0.43 |
| 8:H:144:ILE:CG2 | 8:H:145:ARG:N | 2.81 | 0.43 |
| 9:I:7:CYS:HB2 | 9:I:34:TYR:CD2 | 2.53 | 0.43 |
| 11:K:22:ASP:O | 11:K:31:VAL:HG13 | 2.18 | 0.43 |
| 1:A:17:VAL:HG23 | 1:A:1421:CYS:SG | 2.58 | 0.43 |
| 1:A:877:HIS:O | 1:A:878:ILE:HG12 | 2.17 | 0.43 |
| 1:A:877:HIS:O | 1:A:878:ILE:CG1 | 2.66 | 0.43 |
| 1:A:1011:GLN:HE21 | 1:A:1015:VAL:HG21 | 1.82 | 0.43 |
| 1:A:1258:HIS:O | 1:A:1262:LYS:HG3 | 2.18 | 0.43 |
| 1:A:1308:THR:CG2 | 1:A:1310:GLY:O | 2.65 | 0.43 |
| 1:A:1450:LEU:CD1 | 6:F:108:PHE:CZ | 3.01 | 0.43 |
| 2:B:38:PHE:O | 2:B:39:ARG:C | 2.56 | 0.43 |
| 2:B:510:LYS:CB | 2:B:511:PRO:CD | 2.96 | 0.43 |
| 2:B:660:LYS:C | 2:B:679:TYR:HD2 | 2.22 | 0.43 |
| 2:B:766:ARG:NH1 | 2:B:769:TYR:HE2 | 2.16 | 0.43 |
| 2:B:766:ARG:HD2 | 2:B:984:HIS:O | 2.18 | 0.43 |
| 2:B:890:TYR:CZ | 2:B:910:VAL:HG21 | 2.54 | 0.43 |
| 2:B:1040:ASN:O | 2:B:1041:GLU:C | 2.57 | 0.43 |
| 2:B:1106:ARG:HD2 | 2:B:1125:ASP:O | 2.17 | 0.43 |
| 2:B:1150:ARG:CG | 2:B:1150:ARG:NH1 | 2.70 | 0.43 |
| 3:C:66:ARG:NH1 | 3:C:144:ILE:O | 2.51 | 0.43 |
| 4:D:52:LEU:N | 4:D:182:SER:HB3 | 2.34 | 0.43 |
| 5:E:93:MET:HG3 | 5:E:94:LYS:N | 2.33 | 0.43 |
| 8:H:15:VAL:HG22 | 8:H:26:ILE:HG21 | 1.99 | 0.43 |
| 8:H:109:LYS:HD2 | 8:H:111:LEU:CD1 | 2.45 | 0.43 |
| 12:L:52:GLY:O | 12:L:54:ARG:N | 2.51 | 0.43 |
| 1:A:299:HIS:HA | 1:A:302:THR:HG22 | 2.00 | 0.43 |
| 1:A:353:ILE:O | 1:A:353:ILE:HG13 | 2.17 | 0.43 |
| 1:A:573:SER:O | 1:A:574:GLY:C | 2.57 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------------|-------------------|--------------------------|-------------------|
| 1:A:715:GLU:OE2 | 1:A:774:ARG:NH1 | 2.51 | 0.43 |
| 1:A:777:PHE:C | 1:A:779:PHE:N | 2.71 | 0.43 |
| 1:A:779:PHE:CE1 | 1:A:785:PRO:HD3 | 2.37 | 0.43 |
| 1:A:783:THR:HB | 1:A:787:PHE:HD1 | 1.84 | 0.43 |
| 1:A:885:THR:O | 1:A:885:THR:CG2 | 2.60 | 0.43 |
| 1:A:923:LEU:O | 1:A:927:VAL:HG23 | 2.18 | 0.43 |
| 1:A:999:VAL:HG12 | 1:A:1000:LEU:HG | 1.99 | 0.43 |
| 1:A:1105:LEU:CD2 | 1:A:1384:VAL:HG21 | 2.48 | 0.43 |
| 1:A:1124:HIS:ND1 | 1:A:1124:HIS:N | 2.51 | 0.43 |
| 1:A:1225:PHE:O | 1:A:1240:CYS:CB | 2.67 | 0.43 |
| 2:B:23:ALA:O | 2:B:654:ARG:HD2 | 2.19 | 0.43 |
| 2:B:526:GLU:CD | 2:B:752:ALA:HB3 | 2.39 | 0.43 |
| 2:B:595:ARG:NH1 | 2:B:595:ARG:HG3 | 2.33 | 0.43 |
| 2:B:658:ILE:HG22 | 2:B:659:ALA:N | 2.33 | 0.43 |
| 2:B:705:MET:HA | 2:B:705:MET:CE | 2.49 | 0.43 |
| 2:B:846:ILE:CG2 | 2:B:974:PRO:HG2 | 2.49 | 0.43 |
| 2:B:1174:LYS:O | 2:B:1175:LEU:C | 2.56 | 0.43 |
| 3:C:143:LEU:HD21 | 3:C:146:LYS:CE | 2.48 | 0.43 |
| 4:D:138:ASN:ND2 | 7:G:35:GLU:HB3 | 2.33 | 0.43 |
| 4:D:202:ILE:HD11 | 4:D:206:GLU:OE1 | 2.19 | 0.43 |
| 7:G:51:TYR:O | 7:G:51:TYR:CD2 | 2.71 | 0.43 |
| 7:G:122:ASN:HB3 | 7:G:129:SER:OG | 2.18 | 0.43 |
| 9:I:2:THR:CG2 | 9:I:3:THR:N | 2.80 | 0.43 |
| 9:I:7:CYS:CB | 9:I:14:LEU:HD21 | 2.41 | 0.43 |
| 14:N:10:DG:H2 [?] | 14:N:11:DC:OP2 | 2.18 | 0.43 |
| 1:A:49:LYS:CD | 1:A:55:ASP:HB3 | 2.48 | 0.43 |
| 1:A:115:LEU:CD1 | 1:A:141:LEU:HB3 | 2.49 | 0.43 |
| 1:A:125:ALA:C | 1:A:127:ALA:N | 2.72 | 0.43 |
| 1:A:172:PRO:HB2 | 1:A:183:GLY:HA3 | 2.00 | 0.43 |
| 1:A:909:ASP:C | 1:A:911:SER:H | 2.21 | 0.43 |
| 1:A:961:ARG:NH1 | 1:A:961:ARG:HG3 | 2.34 | 0.43 |
| 1:A:1154:TYR:CE2 | 1:A:1156:PRO:HD3 | 2.53 | 0.43 |
| 1:A:1223:ASP:HA | 1:A:1243:VAL:CG1 | 2.47 | 0.43 |
| 2:B:192:LEU:C | 2:B:194:GLU:H | 2.22 | 0.43 |
| 2:B:785:TYR:HD2 | 2:B:785:TYR:H | 1.66 | 0.43 |
| 2:B:800:GLN:HB2 | 2:B:821:GLN:HA | 2.01 | 0.43 |
| 2:B:867:GLY:O | 2:B:869:SER:N | 2.46 | 0.43 |
| 2:B:1116:ARG:HG3 | 2:B:1198:TYR:CD2 | 2.54 | 0.43 |
| 3:C:41:ILE:CG2 | 3:C:172:PRO:HG3 | 2.49 | 0.43 |
| 3:C:55:THR:O | 3:C:55:THR:HG22 | 2.17 | 0.43 |
| 3:C:186:LEU:O | 3:C:187:LYS:HB2 | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:E:73:PRO:HB2 | 5:E:74:ASP:H | 1.66 | 0.43 |
| 7:G:111:THR:HG22 | 7:G:112:LYS:N | 2.33 | 0.43 |
| 7:G:119:LEU:HD11 | 7:G:137:ILE:HD11 | 2.00 | 0.43 |
| 9:I:111:THR:HG22 | 9:I:113:ASP:N | 2.32 | 0.43 |
| 12:L:48:CYS:O | 12:L:50:ASP:N | 2.44 | 0.43 |
| 1:A:66:LYS:O | 1:A:67:CYS:HB2 | 2.19 | 0.43 |
| 1:A:289:ILE:C | 1:A:291:GLU:N | 2.71 | 0.43 |
| 1:A:342:GLY:O | 2:B:1129:ARG:NH1 | 2.52 | 0.43 |
| 1:A:725:ALA:O | 1:A:726:ARG:C | 2.56 | 0.43 |
| 1:A:966:ASN:O | 1:A:967:ALA:C | 2.57 | 0.43 |
| 1:A:1037:LEU:HD12 | 1:A:1042:PHE:CA | 2.48 | 0.43 |
| 1:A:1425:SER:O | 1:A:1426:GLU:C | 2.57 | 0.43 |
| 2:B:23:ALA:O | 2:B:654:ARG:HB3 | 2.18 | 0.43 |
| 2:B:29:ASP:OD1 | 2:B:658:ILE:HD13 | 2.17 | 0.43 |
| 2:B:37:PHE:CZ | 2:B:41:LYS:HG3 | 2.54 | 0.43 |
| 2:B:99:LYS:HA | 2:B:178:ASN:ND2 | 2.32 | 0.43 |
| 2:B:100:PRO:CD | 2:B:180:TYR:HE1 | 2.31 | 0.43 |
| 2:B:261:ARG:NH1 | 2:B:261:ARG:HG3 | 2.33 | 0.43 |
| 2:B:328:GLU:C | 2:B:330:ALA:N | 2.71 | 0.43 |
| 2:B:784:ASN:ND2 | 2:B:788:ARG:HD2 | 2.33 | 0.43 |
| 2:B:996:ARG:HH21 | 3:C:175:ALA:HA | 1.84 | 0.43 |
| 3:C:146:LYS:HD2 | 10:J:57:ILE:HD13 | 2.00 | 0.43 |
| 3:C:148:ARG:CG | 3:C:149:LYS:H | 2.31 | 0.43 |
| 6:F:106:PRO:HG2 | 7:G:18:PHE:C | 2.38 | 0.43 |
| 6:F:113:GLY:O | 6:F:114:GLU:C | 2.57 | 0.43 |
| 7:G:18:PHE:HA | 7:G:22:MET:HE2 | 2.00 | 0.43 |
| 8:H:36:CYS:HB2 | 8:H:130:ARG:NH2 | 2.33 | 0.43 |
| 9:I:55:THR:HG1 | 9:I:100:PHE:HD2 | 1.62 | 0.43 |
| 10:J:35:ALA:O | 10:J:39:LEU:CD1 | 2.67 | 0.43 |
| 12:L:39:SER:OG | 12:L:40:LEU:N | 2.51 | 0.43 |
| 1:A:101:LYS:HE2 | 1:A:139:TRP:CZ2 | 2.54 | 0.43 |
| 1:A:332:LYS:C | 1:A:333:GLU:HG2 | 2.39 | 0.43 |
| 1:A:435:HIS:O | 1:A:437:MET:HG3 | 2.19 | 0.43 |
| 1:A:458:HIS:CE1 | 1:A:507:VAL:HG21 | 2.53 | 0.43 |
| 1:A:541:ILE:HG21 | 1:A:549:MET:HE1 | 2.01 | 0.43 |
| 1:A:774:ARG:NH2 | 1:A:797:LYS:HB2 | 2.33 | 0.43 |
| 1:A:779:PHE:HD1 | 1:A:784:LEU:HA | 1.82 | 0.43 |
| 1:A:855:THR:HG23 | 1:A:857:ARG:HG3 | 2.00 | 0.43 |
| 1:A:875:ALA:HA | 1:A:878:ILE:HD12 | 2.01 | 0.43 |
| 1:A:997:LEU:HD13 | 1:A:1018:PHE:HE2 | 1.82 | 0.43 |
| 1:A:1029:ARG:HG3 | 1:A:1029:ARG:NH1 | 2.34 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1213:GLY:O | 1:A:1216:ILE:N | 2.51 | 0.43 |
| 1:A:1279:ILE:O | 1:A:1280:GLU:HG3 | 2.19 | 0.43 |
| 1:A:1418:LEU:HD23 | 2:B:1222:ARG:HD2 | 2.01 | 0.43 |
| 2:B:277:LYS:HE3 | 2:B:338:GLY:O | 2.18 | 0.43 |
| 2:B:290:GLY:CA | 2:B:327:ARG:HD2 | 2.48 | 0.43 |
| 2:B:340:ALA:C | 2:B:342:GLY:H | 2.21 | 0.43 |
| 2:B:361:LEU:HD21 | 2:B:364:ILE:HD12 | 1.99 | 0.43 |
| 2:B:492:LEU:O | 2:B:495:LEU:N | 2.51 | 0.43 |
| 2:B:642:ASP:C | 2:B:644:GLU:H | 2.22 | 0.43 |
| 2:B:872:GLU:HA | 2:B:917:PRO:HD3 | 2.00 | 0.43 |
| 2:B:952:VAL:HG12 | 2:B:953:LEU:H | 1.83 | 0.43 |
| 2:B:1122:ARG:HB3 | 13:T:22:DC:OP1 | 2.18 | 0.43 |
| 2:B:1167:GLY:HA3 | 2:B:1216:LEU:N | 2.32 | 0.43 |
| 2:B:1178:ASN:HD22 | 2:B:1178:ASN:N | 2.15 | 0.43 |
| 2:B:1197:PRO:C | 2:B:1199:ALA:N | 2.71 | 0.43 |
| 5:E:85:GLU:C | 5:E:87:SER:N | 2.71 | 0.43 |
| 5:E:135:PHE:HD2 | 5:E:140:LEU:HD21 | 1.83 | 0.43 |
| 5:E:161:LYS:O | 5:E:164:LEU:N | 2.52 | 0.43 |
| 8:H:4:THR:HA | 8:H:60:ALA:CB | 2.49 | 0.43 |
| 11:K:17:SER:O | 11:K:18:LYS:C | 2.56 | 0.43 |
| 1:A:279:LEU:O | 1:A:289:ILE:HD11 | 2.19 | 0.43 |
| 1:A:409:SER:O | 1:A:410:GLY:C | 2.56 | 0.43 |
| 1:A:626:ASN:O | 1:A:631:HIS:CD2 | 2.72 | 0.43 |
| 1:A:700:ASN:C | 1:A:701:LEU:HD23 | 2.39 | 0.43 |
| 1:A:825:ILE:HD12 | 1:A:825:ILE:HA | 1.70 | 0.43 |
| 1:A:1299:VAL:CG1 | 1:A:1300:LYS:N | 2.82 | 0.43 |
| 1:A:1330:ASN:OD1 | 1:A:1331:SER:N | 2.52 | 0.43 |
| 1:A:1343:ALA:HB2 | 5:E:150:VAL:CG2 | 2.41 | 0.43 |
| 2:B:186:GLU:HB3 | 2:B:187:SER:H | 1.49 | 0.43 |
| 2:B:355:ILE:HG13 | 2:B:355:ILE:H | 1.68 | 0.43 |
| 2:B:402:GLY:CA | 2:B:695:ALA:HB3 | 2.49 | 0.43 |
| 2:B:476:ARG:O | 2:B:477:ALA:C | 2.57 | 0.43 |
| 2:B:660:LYS:HB3 | 2:B:679:TYR:CD2 | 2.54 | 0.43 |
| 2:B:681:TRP:O | 2:B:684:LEU:N | 2.52 | 0.43 |
| 2:B:1177:HIS:HB3 | 2:B:1179:GLN:HE21 | 1.83 | 0.43 |
| 4:D:64:VAL:HG22 | 4:D:129:LEU:CD2 | 2.49 | 0.43 |
| 5:E:15:ALA:HA | 5:E:140:LEU:O | 2.18 | 0.43 |
| 5:E:137:GLU:C | 5:E:139:ALA:N | 2.72 | 0.43 |
| 5:E:204:THR:CG2 | 5:E:205:SER:H | 2.28 | 0.43 |
| 7:G:114:LEU:HD12 | 7:G:114:LEU:HA | 1.89 | 0.43 |
| 8:H:40:LEU:HD13 | 8:H:123:MET:HE3 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:142:CYS:C | 1:A:144:THR:H | 2.22 | 0.43 |
| 1:A:275:SER:O | 1:A:279:LEU:HG | 2.18 | 0.43 |
| 1:A:286:HIS:O | 1:A:288:ALA:N | 2.52 | 0.43 |
| 1:A:350:ARG:HB2 | 1:A:488:ASN:OD1 | 2.18 | 0.43 |
| 1:A:515:GLN:HB2 | 1:A:1071:SER:HB3 | 2.00 | 0.43 |
| 1:A:526:ASP:HB2 | 2:B:835:GLN:OE1 | 2.18 | 0.43 |
| 1:A:645:LEU:HG | 1:A:649:ILE:CD1 | 2.48 | 0.43 |
| 1:A:826:ASP:O | 1:A:830:LYS:N | 2.37 | 0.43 |
| 1:A:899:VAL:O | 1:A:929:LEU:HD12 | 2.19 | 0.43 |
| 2:B:165:VAL:CG1 | 2:B:166:PHE:N | 2.82 | 0.43 |
| 2:B:426:LYS:HG2 | 2:B:426:LYS:H | 1.51 | 0.43 |
| 2:B:484:ASN:O | 2:B:485:ARG:HD2 | 2.19 | 0.43 |
| 2:B:619:ILE:O | 2:B:622:LYS:HG3 | 2.19 | 0.43 |
| 2:B:651:LEU:C | 2:B:653:VAL:N | 2.71 | 0.43 |
| 2:B:708:GLU:O | 2:B:709:ASP:C | 2.57 | 0.43 |
| 2:B:879:ARG:HD3 | 2:B:879:ARG:HA | 1.46 | 0.43 |
| 2:B:1050:ILE:HG22 | 2:B:1051:THR:N | 2.34 | 0.43 |
| 3:C:3:GLU:HG3 | 11:K:104:ASN:ND2 | 2.34 | 0.43 |
| 3:C:17:ASN:H | 3:C:240:VAL:HG21 | 1.84 | 0.43 |
| 3:C:35:ARG:HH11 | 11:K:41:THR:HA | 1.83 | 0.43 |
| 3:C:136:ASP:OD1 | 3:C:137:LYS:N | 2.52 | 0.43 |
| 4:D:13:ARG:O | 4:D:13:ARG:CD | 2.67 | 0.43 |
| 4:D:214:LEU:O | 4:D:216:ASN:N | 2.51 | 0.43 |
| 5:E:94:LYS:HE2 | 5:E:98:ILE:HD11 | 2.01 | 0.43 |
| 6:F:105:ALA:HB1 | 6:F:106:PRO:CD | 2.49 | 0.43 |
| 7:G:44:TYR:HE1 | 7:G:157:ILE:N | 2.16 | 0.43 |
| 9:I:13:MET:HE3 | 9:I:14:LEU:H | 1.84 | 0.43 |
| 11:K:18:LYS:NZ | 11:K:37:LYS:O | 2.51 | 0.43 |
| 13:T:15:DC:C6 | 13:T:16:DT:H72 | 2.53 | 0.43 |
| 1:A:460:VAL:HG12 | 1:A:461:LYS:N | 2.34 | 0.42 |
| 1:A:536:LEU:O | 1:A:537:ARG:C | 2.58 | 0.42 |
| 1:A:555:ASP:O | 1:A:556:TRP:C | 2.56 | 0.42 |
| 1:A:596:THR:C | 1:A:597:LEU:HD12 | 2.38 | 0.42 |
| 1:A:728:LYS:HA | 1:A:731:ARG:HE | 1.84 | 0.42 |
| 1:A:869:GLY:O | 1:A:870:GLU:HB2 | 2.19 | 0.42 |
| 1:A:998:LEU:H | 1:A:998:LEU:CD1 | 2.29 | 0.42 |
| 1:A:1451:VAL:O | 1:A:1454:MET:HG2 | 2.19 | 0.42 |
| 2:B:61:ASP:O | 2:B:64:CYS:O | 2.36 | 0.42 |
| 2:B:65:GLU:CG | 2:B:66:ASP:H | 2.25 | 0.42 |
| 2:B:282:ILE:CD1 | 2:B:382:ILE:HD13 | 2.48 | 0.42 |
| 2:B:637:LEU:CD1 | 2:B:703:ILE:HD13 | 2.48 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:773:MET:HE2 | 2:B:985:GLY:HA2 | 2.00 | 0.42 |
| 2:B:860:MET:HG2 | 2:B:861:ASP:N | 2.33 | 0.42 |
| 2:B:871:THR:CG2 | 2:B:872:GLU:N | 2.81 | 0.42 |
| 2:B:1020:ARG:NH1 | 2:B:1020:ARG:HG3 | 2.32 | 0.42 |
| 2:B:1146:PHE:CE1 | 2:B:1150:ARG:HD3 | 2.54 | 0.42 |
| 4:D:39:ASN:HB3 | 4:D:43:GLU:O | 2.19 | 0.42 |
| 4:D:52:LEU:H | 4:D:182:SER:HB3 | 1.84 | 0.42 |
| 6:F:85:MET:CE | 6:F:93:ILE:HD12 | 2.49 | 0.42 |
| 7:G:84:GLY:N | 7:G:147:ILE:O | 2.47 | 0.42 |
| 7:G:116:PRO:HB2 | 7:G:118:ASP:OD1 | 2.19 | 0.42 |
| 10:J:2:ILE:HG12 | 10:J:57:ILE:CD1 | 2.48 | 0.42 |
| 12:L:36:SER:O | 12:L:37:LYS:O | 2.37 | 0.42 |
| 1:A:15:LYS:O | 1:A:1421:CYS:HB2 | 2.19 | 0.42 |
| 1:A:103:CYS:HB3 | 1:A:174:ILE:CD1 | 2.49 | 0.42 |
| 1:A:185:TRP:CH2 | 1:A:200:ARG:HB3 | 2.54 | 0.42 |
| 1:A:384:ASN:O | 1:A:386:ASP:N | 2.52 | 0.42 |
| 1:A:387:ARG:HH11 | 1:A:437:MET:HE1 | 1.84 | 0.42 |
| 1:A:522:GLY:HA2 | 1:A:646:PHE:HE2 | 1.84 | 0.42 |
| 1:A:556:TRP:C | 1:A:558:GLY:N | 2.73 | 0.42 |
| 1:A:681:GLU:O | 1:A:685:GLU:HG3 | 2.18 | 0.42 |
| 1:A:831:THR:CG2 | 1:A:832:ALA:N | 2.82 | 0.42 |
| 1:A:882:SER:H | 1:A:1025:ARG:HH21 | 1.67 | 0.42 |
| 1:A:910:PRO:HB3 | 1:A:917:SER:H | 1.84 | 0.42 |
| 2:B:27:ALA:O | 2:B:29:ASP:N | 2.52 | 0.42 |
| 2:B:284:ILE:HD13 | 2:B:333:PHE:HD2 | 1.82 | 0.42 |
| 2:B:465:ASN:HD22 | 2:B:465:ASN:N | 2.13 | 0.42 |
| 2:B:831:SER:CB | 2:B:994:TYR:OH | 2.67 | 0.42 |
| 5:E:31:THR:CG2 | 5:E:34:GLU:HB2 | 2.49 | 0.42 |
| 8:H:41:ASP:HB2 | 8:H:121:LEU:HB3 | 1.99 | 0.42 |
| 8:H:63:LEU:CD1 | 8:H:64:ASN:H | 2.32 | 0.42 |
| 9:I:54:GLU:HB3 | 9:I:100:PHE:CE2 | 2.54 | 0.42 |
| 12:L:27:LEU:CB | 12:L:37:LYS:HB3 | 2.48 | 0.42 |
| 1:A:69:THR:O | 1:A:70:CYS:C | 2.58 | 0.42 |
| 1:A:108:MET:O | 1:A:109:HIS:HB2 | 2.19 | 0.42 |
| 1:A:117:GLU:CD | 1:A:117:GLU:N | 2.69 | 0.42 |
| 1:A:262:LEU:CD2 | 1:A:303:TYR:HE1 | 2.32 | 0.42 |
| 1:A:352:VAL:HG23 | 1:A:467:THR:HG22 | 1.99 | 0.42 |
| 1:A:600:PRO:HG2 | 1:A:601:LYS:HG3 | 2.00 | 0.42 |
| 1:A:711:ARG:NH2 | 9:I:87:GLN:OE1 | 2.51 | 0.42 |
| 1:A:728:LYS:CB | 1:A:731:ARG:HH21 | 2.32 | 0.42 |
| 1:A:733:ALA:O | 1:A:736:ASN:HB3 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:894:GLU:O | 1:A:896:ARG:N | 2.52 | 0.42 |
| 1:A:1242:VAL:CG1 | 1:A:1243:VAL:H | 2.13 | 0.42 |
| 1:A:1424:VAL:O | 1:A:1428:VAL:HG23 | 2.18 | 0.42 |
| 1:A:1450:LEU:HD11 | 6:F:108:PHE:HZ | 1.84 | 0.42 |
| 2:B:170:LEU:O | 2:B:170:LEU:HG | 2.20 | 0.42 |
| 2:B:186:GLU:HG3 | 10:J:62:ARG:HH12 | 1.84 | 0.42 |
| 2:B:589:VAL:CG1 | 2:B:590:HIS:N | 2.80 | 0.42 |
| 2:B:711:GLU:CB | 2:B:712:PRO:CD | 2.98 | 0.42 |
| 2:B:714:GLU:OE1 | 2:B:714:GLU:N | 2.52 | 0.42 |
| 2:B:744:HIS:CD2 | 2:B:746:SER:OG | 2.67 | 0.42 |
| 2:B:1162:ILE:HG22 | 2:B:1163:CYS:O | 2.19 | 0.42 |
| 3:C:50:GLU:HB3 | 3:C:156:THR:HB | 2.01 | 0.42 |
| 4:D:116:SER:O | 4:D:117:GLU:C | 2.57 | 0.42 |
| 4:D:186:ASP:O | 4:D:211:LEU:HD13 | 2.18 | 0.42 |
| 6:F:75:PRO:C | 6:F:77:ASP:N | 2.70 | 0.42 |
| 6:F:103:MET:HE3 | 7:G:66:GLY:N | 2.33 | 0.42 |
| 6:F:108:PHE:HE1 | 6:F:131:PRO:HG3 | 1.85 | 0.42 |
| 8:H:9:ILE:HG21 | 8:H:54:SER:HB2 | 2.01 | 0.42 |
| 8:H:79:TRP:O | 8:H:80:ARG:C | 2.57 | 0.42 |
| 9:I:61:ASP:HB3 | 9:I:64:SER:OG | 2.19 | 0.42 |
| 12:L:27:LEU:H | 12:L:27:LEU:CD2 | 2.14 | 0.42 |
| 1:A:107:CYS:HB2 | 1:A:171:GLN:HE22 | 1.83 | 0.42 |
| 1:A:167:CYS:HB2 | 1:A:169:ASN:HD22 | 1.84 | 0.42 |
| 1:A:207:ILE:O | 1:A:208:LEU:C | 2.58 | 0.42 |
| 1:A:383:TYR:N | 1:A:383:TYR:CD2 | 2.87 | 0.42 |
| 1:A:475:THR:HG23 | 1:A:476:SER:H | 1.79 | 0.42 |
| 1:A:537:ARG:NH1 | 8:H:120:GLY:O | 2.52 | 0.42 |
| 1:A:579:SER:HB3 | 1:A:611:GLN:HA | 2.00 | 0.42 |
| 1:A:591:PHE:HD2 | 1:A:595:THR:HB | 1.84 | 0.42 |
| 1:A:726:ARG:NH2 | 1:A:727:ASP:OD1 | 2.51 | 0.42 |
| 1:A:926:GLN:O | 1:A:930:ASP:HB2 | 2.19 | 0.42 |
| 1:A:1215:ARG:NH1 | 1:A:1272:THR:O | 2.52 | 0.42 |
| 1:A:1423:GLY:O | 1:A:1424:VAL:C | 2.57 | 0.42 |
| 2:B:69:LEU:O | 2:B:70:ILE:CG1 | 2.58 | 0.42 |
| 2:B:120:ARG:HH12 | 12:L:54:ARG:NH1 | 2.16 | 0.42 |
| 2:B:121:ASN:HA | 2:B:207:GLY:CA | 2.41 | 0.42 |
| 2:B:278:GLN:CG | 2:B:279:ASP:N | 2.80 | 0.42 |
| 2:B:327:ARG:O | 2:B:327:ARG:HG2 | 2.19 | 0.42 |
| 2:B:348:ARG:O | 2:B:351:TYR:HB3 | 2.19 | 0.42 |
| 2:B:388:CYS:C | 2:B:390:LEU:N | 2.72 | 0.42 |
| 2:B:436:VAL:O | 2:B:436:VAL:HG12 | 2.18 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:572:HIS:O | 2:B:573:GLN:C | 2.58 | 0.42 |
| 2:B:822:ASN:HD21 | 10:J:52:THR:CG2 | 2.30 | 0.42 |
| 2:B:847:ASP:OD2 | 3:C:167:HIS:HA | 2.20 | 0.42 |
| 2:B:952:VAL:O | 12:L:57:LEU:HD22 | 2.20 | 0.42 |
| 2:B:1029:CYS:HB3 | 2:B:1086:PHE:CE2 | 2.55 | 0.42 |
| 3:C:91:HIS:HD2 | 3:C:91:HIS:O | 2.02 | 0.42 |
| 4:D:63:LEU:CD1 | 4:D:133:THR:OG1 | 2.65 | 0.42 |
| 4:D:141:LEU:O | 4:D:145:MET:HG2 | 2.19 | 0.42 |
| 4:D:196:PRO:O | 4:D:197:SER:C | 2.57 | 0.42 |
| 5:E:12:LEU:HD22 | 5:E:55:ARG:CZ | 2.49 | 0.42 |
| 5:E:195:VAL:CG1 | 5:E:196:VAL:H | 2.27 | 0.42 |
| 7:G:1:MET:O | 7:G:2:PHE:C | 2.58 | 0.42 |
| 7:G:62:LEU:HB3 | 7:G:63:PRO:CD | 2.42 | 0.42 |
| 1:A:276:LEU:HD13 | 1:A:293:GLU:CA | 2.47 | 0.42 |
| 1:A:317:LYS:HG3 | 2:B:471:LYS:NZ | 2.34 | 0.42 |
| 1:A:392:VAL:C | 1:A:394:ASN:N | 2.73 | 0.42 |
| 1:A:526:ASP:HB2 | 2:B:835:GLN:CD | 2.40 | 0.42 |
| 1:A:568:PRO:CB | 3:C:221:TYR:CZ | 3.03 | 0.42 |
| 1:A:601:LYS:HB2 | 1:A:603:ASN:OD1 | 2.19 | 0.42 |
| 1:A:786:HIS:CE1 | 2:B:519:TRP:CZ2 | 3.08 | 0.42 |
| 1:A:1001:ARG:CG | 1:A:1001:ARG:NH1 | 2.82 | 0.42 |
| 1:A:1157:ASP:C | 1:A:1159:ARG:N | 2.70 | 0.42 |
| 1:A:1157:ASP:OD1 | 1:A:1159:ARG:HB2 | 2.19 | 0.42 |
| 2:B:365:THR:O | 2:B:374:LYS:HE3 | 2.19 | 0.42 |
| 2:B:557:PHE:CE1 | 2:B:603:LEU:HD11 | 2.53 | 0.42 |
| 2:B:615:MET:O | 2:B:615:MET:HE2 | 2.19 | 0.42 |
| 2:B:825:VAL:HG21 | 2:B:1092:TYR:HE1 | 1.85 | 0.42 |
| 2:B:1109:GLY:HA3 | 2:B:1110:PRO:HD2 | 1.75 | 0.42 |
| 2:B:1203:LEU:O | 2:B:1207:LEU:HG | 2.20 | 0.42 |
| 3:C:27:LEU:O | 3:C:28:ALA:C | 2.56 | 0.42 |
| 3:C:133:ILE:HG13 | 3:C:237:SER:N | 2.34 | 0.42 |
| 3:C:187:LYS:C | 3:C:189:THR:H | 2.22 | 0.42 |
| 3:C:234:SER:OG | 3:C:235:VAL:N | 2.52 | 0.42 |
| 6:F:138:LEU:O | 6:F:140:ASP:N | 2.53 | 0.42 |
| 7:G:14:HIS:CE1 | 7:G:15:PRO:HD2 | 2.54 | 0.42 |
| 11:K:20:LYS:O | 11:K:33:ILE:HA | 2.20 | 0.42 |
| 1:A:90:VAL:HG11 | 1:A:297:GLN:HA | 2.01 | 0.42 |
| 1:A:102:VAL:O | 1:A:105:CYS:HB2 | 2.19 | 0.42 |
| 1:A:514:PRO:C | 1:A:516:SER:N | 2.72 | 0.42 |
| 1:A:556:TRP:CD2 | 1:A:558:GLY:HA2 | 2.55 | 0.42 |
| 1:A:1037:LEU:HD13 | 1:A:1041:ALA:HB3 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1431:GLY:HA3 | 2:B:1197:PRO:HD3 | 2.00 | 0.42 |
| 1:A:1446:ASP:HB3 | 1:A:1449:SER:OG | 2.20 | 0.42 |
| 2:B:32:ALA:O | 2:B:35:SER:HB2 | 2.20 | 0.42 |
| 2:B:60:GLN:HE22 | 2:B:95:ILE:HG22 | 1.80 | 0.42 |
| 2:B:98:THR:O | 2:B:126:SER:CB | 2.64 | 0.42 |
| 2:B:104:GLU:OE1 | 12:L:54:ARG:CZ | 2.67 | 0.42 |
| 2:B:190:TYR:CE1 | 2:B:196:PRO:HG3 | 2.54 | 0.42 |
| 2:B:367:LEU:O | 2:B:368:GLU:HB2 | 2.20 | 0.42 |
| 2:B:604:ARG:HA | 2:B:609:ILE:HG13 | 2.01 | 0.42 |
| 2:B:801:LYS:HD2 | 2:B:815:ARG:HB3 | 2.01 | 0.42 |
| 2:B:996:ARG:NH2 | 3:C:175:ALA:HA | 2.34 | 0.42 |
| 2:B:1071:VAL:HG12 | 2:B:1072:MET:N | 2.33 | 0.42 |
| 2:B:1192:TYR:CD2 | 2:B:1218:THR:HG21 | 2.55 | 0.42 |
| 3:C:46:ILE:HD13 | 3:C:157:CYS:SG | 2.60 | 0.42 |
| 3:C:138:GLU:HB2 | 3:C:140:ASN:ND2 | 2.35 | 0.42 |
| 3:C:166:GLU:HG3 | 11:K:10:PHE:CZ | 2.46 | 0.42 |
| 4:D:166:LEU:O | 4:D:169:SER:OG | 2.38 | 0.42 |
| 5:E:87:SER:O | 5:E:88:VAL:C | 2.58 | 0.42 |
| 5:E:117:THR:HB | 5:E:120:ALA:HB3 | 2.00 | 0.42 |
| 5:E:156:LEU:HD12 | 5:E:195:VAL:CG1 | 2.50 | 0.42 |
| 6:F:74:ILE:H | 6:F:74:ILE:HG13 | 1.64 | 0.42 |
| 8:H:109:LYS:HB3 | 8:H:110:ASP:OD1 | 2.20 | 0.42 |
| 9:I:49:ILE:HG22 | 9:I:49:ILE:O | 2.20 | 0.42 |
| 10:J:1:MET:HG3 | 10:J:1:MET:O | 2.19 | 0.42 |
| 11:K:65:HIS:HD2 | 11:K:67:PHE:HB2 | 1.84 | 0.42 |
| 1:A:47:ARG:NH1 | 1:A:254:GLU:OE1 | 2.51 | 0.42 |
| 1:A:355:GLY:HA3 | 1:A:482:PHE:CZ | 2.55 | 0.42 |
| 1:A:524:VAL:HG12 | 1:A:525:GLN:CG | 2.50 | 0.42 |
| 1:A:584:ASN:O | 1:A:586:ILE:N | 2.53 | 0.42 |
| 1:A:701:LEU:HD21 | 9:I:114:GLN:HB2 | 2.02 | 0.42 |
| 1:A:802:ASN:CG | 2:B:728:ARG:HB2 | 2.39 | 0.42 |
| 1:A:1329:THR:HG23 | 1:A:1329:THR:O | 2.19 | 0.42 |
| 1:A:1409:LEU:O | 1:A:1410:PHE:C | 2.58 | 0.42 |
| 2:B:126:SER:O | 2:B:169:ARG:HA | 2.20 | 0.42 |
| 2:B:205:ILE:C | 2:B:207:GLY:N | 2.73 | 0.42 |
| 2:B:428:ILE:H | 2:B:428:ILE:HG13 | 1.72 | 0.42 |
| 2:B:806:THR:CG2 | 2:B:808:ALA:HB3 | 2.49 | 0.42 |
| 2:B:840:ILE:CG2 | 2:B:994:TYR:HD1 | 2.33 | 0.42 |
| 2:B:857:ARG:NH2 | 2:B:942:ARG:CZ | 2.83 | 0.42 |
| 2:B:859:TYR:OH | 2:B:941:LEU:HD12 | 2.18 | 0.42 |
| 2:B:860:MET:HG3 | 2:B:965:LYS:HE2 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:1115:THR:HG22 | 2:B:1117:GLN:CB | 2.50 | 0.42 |
| 3:C:56:THR:CG2 | 3:C:145:CYS:SG | 3.07 | 0.42 |
| 3:C:73:GLN:NE2 | 3:C:75:MET:H | 2.14 | 0.42 |
| 3:C:174:ALA:O | 10:J:10:CYS:HB2 | 2.20 | 0.42 |
| 7:G:88:ASP:OD2 | 7:G:88:ASP:N | 2.47 | 0.42 |
| 8:H:32:THR:CG2 | 8:H:33:GLN:H | 2.27 | 0.42 |
| 11:K:24:ASP:H | 11:K:31:VAL:HA | 1.85 | 0.42 |
| 1:A:57:ARG:HG2 | 1:A:57:ARG:NH1 | 2.32 | 0.42 |
| 1:A:332:LYS:O | 1:A:333:GLU:HG2 | 2.19 | 0.42 |
| 1:A:556:TRP:O | 1:A:558:GLY:N | 2.53 | 0.42 |
| 1:A:637:LYS:HA | 1:A:637:LYS:HD3 | 1.89 | 0.42 |
| 1:A:712:GLU:O | 1:A:714:PHE:N | 2.53 | 0.42 |
| 1:A:733:ALA:HA | 1:A:736:ASN:HB3 | 2.01 | 0.42 |
| 1:A:781:ASP:O | 1:A:790:ASP:N | 2.52 | 0.42 |
| 1:A:839:ARG:CG | 1:A:840:ARG:N | 2.83 | 0.42 |
| 1:A:846:GLU:OE1 | 1:A:1425:SER:OG | 2.34 | 0.42 |
| 1:A:919:ILE:HD13 | 1:A:983:ILE:CD1 | 2.49 | 0.42 |
| 1:A:1011:GLN:NE2 | 1:A:1015:VAL:CG2 | 2.82 | 0.42 |
| 1:A:1297:GLU:N | 1:A:1297:GLU:OE1 | 2.52 | 0.42 |
| 1:A:1422:ARG:NH1 | 2:B:1224:PHE:HD2 | 2.18 | 0.42 |
| 2:B:25:ILE:CD1 | 2:B:653:VAL:O | 2.68 | 0.42 |
| 2:B:247:GLY:O | 2:B:248:SER:HB3 | 2.20 | 0.42 |
| 2:B:309:GLN:O | 2:B:312:GLU:N | 2.52 | 0.42 |
| 2:B:384:ARG:HD2 | 2:B:387:LEU:HD22 | 2.01 | 0.42 |
| 2:B:1156:ASP:O | 2:B:1157:ALA:C | 2.58 | 0.42 |
| 2:B:1197:PRO:O | 2:B:1199:ALA:N | 2.53 | 0.42 |
| 3:C:82:TYR:CE2 | 3:C:161:LYS:HG2 | 2.55 | 0.42 |
| 3:C:118:LEU:HD12 | 3:C:132:PRO:HG3 | 2.02 | 0.42 |
| 4:D:119:ARG:CG | 4:D:221:TYR:HE2 | 2.33 | 0.42 |
| 4:D:175:PHE:CZ | 7:G:85:GLU:HG3 | 2.55 | 0.42 |
| 5:E:164:LEU:HD11 | 5:E:211:TYR:CD1 | 2.54 | 0.42 |
| 8:H:100:THR:HG23 | 8:H:138:GLU:CB | 2.49 | 0.42 |
| 8:H:145:ARG:O | 8:H:146:ARG:CB | 2.68 | 0.42 |
| 11:K:41:THR:CG2 | 11:K:42:LEU:N | 2.83 | 0.42 |
| 1:A:53:LEU:CD2 | 1:A:54:ASN:N | 2.61 | 0.42 |
| 1:A:120:GLU:O | 1:A:121:LEU:C | 2.58 | 0.42 |
| 1:A:690:VAL:O | 1:A:691:LEU:C | 2.59 | 0.42 |
| 1:A:818:MET:HA | 2:B:514:LEU:HB3 | 2.01 | 0.42 |
| 1:A:1059:HIS:ND1 | 6:F:86:THR:HA | 2.35 | 0.42 |
| 1:A:1138:ILE:CA | 1:A:1275:GLY:HA2 | 2.50 | 0.42 |
| 1:A:1150:SER:HA | 1:A:1195:LEU:HA | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1449:SER:C | 1:A:1451:VAL:H | 2.23 | 0.42 |
| 2:B:505:ASP:O | 2:B:506:GLY:C | 2.57 | 0.42 |
| 2:B:529:GLU:OE1 | 2:B:769:TYR:CE1 | 2.72 | 0.42 |
| 2:B:661:LEU:HD23 | 2:B:679:TYR:O | 2.20 | 0.42 |
| 2:B:789:MET:CE | 2:B:967:ARG:HB2 | 2.50 | 0.42 |
| 2:B:843:GLN:O | 2:B:844:SER:C | 2.57 | 0.42 |
| 2:B:995:ARG:HH11 | 3:C:165:LYS:HA | 1.84 | 0.42 |
| 2:B:1002:THR:O | 2:B:1004:GLU:N | 2.52 | 0.42 |
| 3:C:88:CYS:SG | 3:C:91:HIS:HA | 2.60 | 0.42 |
| 4:D:26:THR:O | 4:D:26:THR:HG22 | 2.20 | 0.42 |
| 4:D:47:LEU:CD1 | 7:G:3:PHE:HD2 | 2.31 | 0.42 |
| 4:D:64:VAL:CG2 | 4:D:129:LEU:HD21 | 2.50 | 0.42 |
| 6:F:70:LYS:O | 6:F:72:LYS:N | 2.43 | 0.42 |
| 7:G:45:ILE:HD13 | 7:G:78:VAL:HG11 | 2.01 | 0.42 |
| 9:I:82:GLU:CB | 9:I:104:LEU:HD12 | 2.40 | 0.42 |
| 1:A:179:LEU:HD23 | 1:A:179:LEU:N | 2.35 | 0.42 |
| 1:A:452:LYS:HE3 | 2:B:1141:HIS:CE1 | 2.55 | 0.42 |
| 1:A:595:THR:O | 1:A:596:THR:HG23 | 2.20 | 0.42 |
| 1:A:597:LEU:HD12 | 1:A:597:LEU:N | 2.35 | 0.42 |
| 1:A:728:LYS:O | 1:A:729:ALA:C | 2.58 | 0.42 |
| 1:A:752:LYS:HD3 | 1:A:752:LYS:HA | 1.87 | 0.42 |
| 1:A:826:ASP:O | 1:A:827:THR:C | 2.57 | 0.42 |
| 1:A:965:GLN:O | 1:A:968:GLN:HB2 | 2.20 | 0.42 |
| 1:A:1100:ARG:HH12 | 1:A:1111:MET:HE1 | 1.85 | 0.42 |
| 1:A:1277:GLU:OE1 | 1:A:1277:GLU:HA | 2.19 | 0.42 |
| 2:B:36:ALA:O | 2:B:39:ARG:HB2 | 2.20 | 0.42 |
| 2:B:195:CYS:SG | 2:B:196:PRO:HD2 | 2.60 | 0.42 |
| 2:B:566:LEU:O | 2:B:567:GLU:C | 2.58 | 0.42 |
| 3:C:73:GLN:CG | 3:C:74:SER:N | 2.82 | 0.42 |
| 3:C:100:THR:HG22 | 3:C:102:GLN:NE2 | 2.35 | 0.42 |
| 5:E:105:PHE:O | 5:E:106:GLN:HB2 | 2.18 | 0.42 |
| 6:F:125:LEU:HB2 | 6:F:130:ILE:HD11 | 2.02 | 0.42 |
| 1:A:41:MET:HE3 | 1:A:41:MET:H | 1.85 | 0.41 |
| 1:A:52:GLY:O | 1:A:56:PRO:HG2 | 2.20 | 0.41 |
| 1:A:65:LEU:O | 1:A:71:GLN:HA | 2.20 | 0.41 |
| 1:A:790:ASP:OD2 | 9:I:87:GLN:HG3 | 2.20 | 0.41 |
| 1:A:877:HIS:C | 1:A:878:ILE:CG1 | 2.89 | 0.41 |
| 1:A:1192:LEU:HD13 | 1:A:1239:ARG:NH1 | 2.35 | 0.41 |
| 1:A:1230:GLU:O | 1:A:1232:ASN:N | 2.53 | 0.41 |
| 1:A:1425:SER:HA | 1:A:1428:VAL:HG23 | 2.02 | 0.41 |
| 2:B:210:LYS:HE2 | 2:B:462:ALA:HA | 2.01 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:287:ARG:NH1 | 2:B:324:ILE:O | 2.52 | 0.41 |
| 2:B:654:ARG:C | 2:B:656:GLY:H | 2.23 | 0.41 |
| 2:B:810:GLU:HB3 | 2:B:811:TYR:CD1 | 2.54 | 0.41 |
| 2:B:818:PRO:HB2 | 2:B:1091:TYR:OH | 2.20 | 0.41 |
| 2:B:830:TYR:HB3 | 2:B:831:SER:H | 1.68 | 0.41 |
| 2:B:879:ARG:NH1 | 2:B:883:LEU:CD2 | 2.81 | 0.41 |
| 3:C:11:ARG:H | 3:C:20:PHE:HA | 1.85 | 0.41 |
| 4:D:168:LYS:O | 4:D:169:SER:HB3 | 2.20 | 0.41 |
| 6:F:127:GLU:O | 6:F:129:LYS:N | 2.53 | 0.41 |
| 11:K:30:ALA:HB2 | 11:K:76:GLN:CG | 2.41 | 0.41 |
| 1:A:164:ARG:CG | 1:A:165:GLY:N | 2.82 | 0.41 |
| 1:A:562:THR:HA | 1:A:563:PRO:HD3 | 1.87 | 0.41 |
| 1:A:602:ASP:C | 1:A:603:ASN:O | 2.57 | 0.41 |
| 1:A:685:GLU:OE2 | 1:A:686:ALA:HB2 | 2.20 | 0.41 |
| 1:A:705:LYS:O | 1:A:706:HIS:C | 2.58 | 0.41 |
| 1:A:733:ALA:O | 1:A:737:LEU:HG | 2.20 | 0.41 |
| 1:A:767:GLN:NE2 | 1:A:774:ARG:CB | 2.83 | 0.41 |
| 1:A:841:LEU:HD22 | 1:A:1371:LEU:HD13 | 2.01 | 0.41 |
| 1:A:1101:LEU:CD1 | 1:A:1105:LEU:HD11 | 2.46 | 0.41 |
| 1:A:1400:CYS:O | 1:A:1405:THR:HA | 2.20 | 0.41 |
| 2:B:236:HIS:CD2 | 2:B:236:HIS:N | 2.87 | 0.41 |
| 2:B:435:THR:C | 2:B:437:GLU:H | 2.22 | 0.41 |
| 2:B:467:GLY:O | 2:B:468:GLU:C | 2.58 | 0.41 |
| 2:B:503:GLY:CA | 2:B:507:LYS:HE2 | 2.31 | 0.41 |
| 2:B:601:ARG:HH11 | 2:B:605:ARG:HH22 | 1.66 | 0.41 |
| 2:B:831:SER:HB3 | 2:B:994:TYR:OH | 2.20 | 0.41 |
| 3:C:47:ASP:HA | 3:C:169:LYS:NZ | 2.35 | 0.41 |
| 4:D:178:ALA:O | 4:D:181:GLY:N | 2.53 | 0.41 |
| 4:D:205:ASP:O | 4:D:209:ARG:HG3 | 2.20 | 0.41 |
| 5:E:91:LYS:C | 5:E:93:MET:N | 2.72 | 0.41 |
| 8:H:55:LEU:HB3 | 8:H:144:ILE:CG2 | 2.48 | 0.41 |
| 10:J:18:TRP:CH2 | 10:J:22:LEU:HD11 | 2.55 | 0.41 |
| 1:A:54:ASN:HD21 | 1:A:61:ILE:HD11 | 1.85 | 0.41 |
| 1:A:108:MET:O | 1:A:109:HIS:CB | 2.69 | 0.41 |
| 1:A:360:GLU:O | 1:A:361:LEU:C | 2.59 | 0.41 |
| 1:A:451:HIS:NE2 | 1:A:1074:GLU:HG3 | 2.35 | 0.41 |
| 1:A:469:ARG:NH2 | 2:B:991:GLY:O | 2.46 | 0.41 |
| 1:A:516:SER:O | 1:A:517:ASN:C | 2.58 | 0.41 |
| 1:A:789:LYS:HE3 | 9:I:67:THR:OG1 | 2.21 | 0.41 |
| 1:A:958:VAL:HG13 | 1:A:1052:GLN:HB3 | 2.02 | 0.41 |
| 1:A:1038:THR:OG1 | 1:A:1039:LYS:N | 2.54 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1239:ARG:C | 1:A:1240:CYS:SG | 2.98 | 0.41 |
| 1:A:1305:VAL:HG12 | 1:A:1306:LEU:N | 2.34 | 0.41 |
| 1:A:1425:SER:HA | 1:A:1428:VAL:HG21 | 2.02 | 0.41 |
| 2:B:261:ARG:HH11 | 2:B:261:ARG:HG3 | 1.85 | 0.41 |
| 2:B:373:ARG:HD2 | 2:B:567:GLU:OE2 | 2.19 | 0.41 |
| 2:B:416:LEU:O | 2:B:420:LEU:HG | 2.20 | 0.41 |
| 2:B:529:GLU:OE2 | 2:B:769:TYR:HE1 | 2.03 | 0.41 |
| 2:B:736:THR:O | 2:B:736:THR:HG22 | 2.21 | 0.41 |
| 2:B:828:ALA:HB2 | 2:B:1085:ILE:HG23 | 2.02 | 0.41 |
| 2:B:879:ARG:O | 2:B:934:LYS:CE | 2.69 | 0.41 |
| 2:B:1162:ILE:HG22 | 2:B:1163:CYS:N | 2.35 | 0.41 |
| 2:B:1214:PRO:O | 2:B:1214:PRO:HG2 | 2.19 | 0.41 |
| 3:C:176:ILE:HG22 | 3:C:177:GLU:O | 2.20 | 0.41 |
| 3:C:254:LYS:O | 3:C:256:ALA:N | 2.53 | 0.41 |
| 5:E:89:GLY:C | 5:E:91:LYS:N | 2.72 | 0.41 |
| 6:F:135:ARG:NH2 | 6:F:145:ASP:OD2 | 2.52 | 0.41 |
| 7:G:137:ILE:HG21 | 7:G:143:ILE:HD11 | 2.03 | 0.41 |
| 8:H:64:ASN:ND2 | 8:H:88:SER:CB | 2.68 | 0.41 |
| 9:I:50:THR:CG2 | 9:I:51:ASN:N | 2.83 | 0.41 |
| 13:T:7:DC:H2'' | 13:T:8:DT:C6 | 2.54 | 0.41 |
| 1:A:23:SER:CA | 1:A:233:TRP:NE1 | 2.76 | 0.41 |
| 1:A:24:PRO:O | 1:A:27:VAL:HB | 2.20 | 0.41 |
| 1:A:50:ILE:C | 1:A:52:GLY:N | 2.73 | 0.41 |
| 1:A:269:ILE:CD1 | 1:A:300:VAL:HA | 2.49 | 0.41 |
| 1:A:567:LYS:HG2 | 1:A:568:PRO:CD | 2.49 | 0.41 |
| 1:A:598:LEU:HA | 8:H:122:LEU:HD13 | 2.03 | 0.41 |
| 1:A:1002:GLY:HA3 | 1:A:1007:ILE:CG2 | 2.42 | 0.41 |
| 1:A:1390:ASN:OD1 | 1:A:1399:ARG:HA | 2.20 | 0.41 |
| 2:B:186:GLU:HG2 | 10:J:62:ARG:HH22 | 1.85 | 0.41 |
| 2:B:311:LEU:O | 2:B:314:LEU:N | 2.53 | 0.41 |
| 2:B:312:GLU:O | 2:B:315:LYS:N | 2.45 | 0.41 |
| 2:B:424:LEU:HD23 | 2:B:453:ILE:HD11 | 2.03 | 0.41 |
| 2:B:555:ILE:HG22 | 2:B:556:THR:N | 2.35 | 0.41 |
| 2:B:593:PRO:CG | 2:B:617:ARG:CZ | 2.91 | 0.41 |
| 2:B:597:MET:O | 2:B:598:GLU:C | 2.58 | 0.41 |
| 2:B:687:GLU:O | 2:B:689:LEU:HD23 | 2.20 | 0.41 |
| 2:B:834:ASN:ND2 | 2:B:1013:ASN:CA | 2.83 | 0.41 |
| 7:G:15:PRO:HG3 | 7:G:66:GLY:C | 2.40 | 0.41 |
| 10:J:44:TYR:HD2 | 10:J:44:TYR:N | 2.05 | 0.41 |
| 1:A:102:VAL:HG11 | 1:A:211:PHE:CE2 | 2.55 | 0.41 |
| 1:A:211:PHE:HA | 1:A:214:ILE:HG13 | 2.01 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:309:ALA:O | 1:A:311:GLN:N | 2.49 | 0.41 |
| 1:A:563:PRO:HG2 | 8:H:79:TRP:CZ2 | 2.55 | 0.41 |
| 1:A:590:ARG:O | 1:A:591:PHE:CB | 2.69 | 0.41 |
| 1:A:860:LEU:O | 2:B:1224:PHE:CE2 | 2.70 | 0.41 |
| 1:A:939:ASP:O | 1:A:940:ARG:C | 2.59 | 0.41 |
| 1:A:1072:ILE:HD11 | 1:A:1368:MET:HA | 2.01 | 0.41 |
| 1:A:1104:ILE:HD12 | 1:A:1355:VAL:HG21 | 2.02 | 0.41 |
| 1:A:1142:THR:CA | 1:A:1273:LEU:HD13 | 2.48 | 0.41 |
| 1:A:1146:VAL:HG11 | 1:A:1207:LEU:HD12 | 2.02 | 0.41 |
| 1:A:1151:GLU:HB2 | 1:A:1153:TYR:HE1 | 1.86 | 0.41 |
| 1:A:1176:LEU:HD23 | 1:A:1176:LEU:C | 2.41 | 0.41 |
| 1:A:1384:VAL:C | 1:A:1385:THR:CG2 | 2.89 | 0.41 |
| 2:B:184:ALA:HB1 | 2:B:188:ASP:HB2 | 2.03 | 0.41 |
| 2:B:361:LEU:CD2 | 2:B:364:ILE:HD12 | 2.51 | 0.41 |
| 2:B:577:ALA:HB1 | 2:B:589:VAL:CG1 | 2.18 | 0.41 |
| 2:B:582:VAL:HG23 | 2:B:626:ILE:HD12 | 2.02 | 0.41 |
| 2:B:610:ASN:C | 2:B:612:GLU:H | 2.23 | 0.41 |
| 2:B:620:ARG:H | 2:B:620:ARG:HG3 | 1.70 | 0.41 |
| 2:B:637:LEU:CD2 | 2:B:742:GLU:HA | 2.51 | 0.41 |
| 2:B:825:VAL:HG22 | 2:B:1010:LEU:HB3 | 2.02 | 0.41 |
| 2:B:864:LYS:HD2 | 2:B:872:GLU:CD | 2.40 | 0.41 |
| 2:B:969:ARG:CD | 3:C:61:GLU:OE2 | 2.69 | 0.41 |
| 2:B:1001:PHE:CD1 | 2:B:1001:PHE:C | 2.93 | 0.41 |
| 3:C:66:ARG:NH1 | 10:J:2:ILE:HG23 | 2.35 | 0.41 |
| 4:D:39:ASN:C | 4:D:41:GLN:H | 2.23 | 0.41 |
| 5:E:45:LYS:HD3 | 5:E:46:TYR:CE1 | 2.55 | 0.41 |
| 5:E:52:ARG:CB | 5:E:53:PRO:HD2 | 2.45 | 0.41 |
| 5:E:114:ASN:HD22 | 5:E:114:ASN:HA | 1.58 | 0.41 |
| 6:F:90:ARG:HG3 | 6:F:91:ALA:N | 2.34 | 0.41 |
| 6:F:148:VAL:HG23 | 6:F:149:GLU:N | 2.34 | 0.41 |
| 7:G:122:ASN:HB2 | 7:G:131:GLN:NE2 | 2.17 | 0.41 |
| 7:G:145:VAL:CG1 | 7:G:146:LYS:N | 2.83 | 0.41 |
| 9:I:68:LEU:HB3 | 9:I:84:VAL:CG2 | 2.50 | 0.41 |
| 10:J:14:VAL:HG12 | 10:J:50:ILE:HD11 | 2.01 | 0.41 |
| 10:J:32:GLU:CD | 10:J:32:GLU:H | 2.24 | 0.41 |
| 1:A:38:PRO:CG | 1:A:39:GLU:N | 2.83 | 0.41 |
| 1:A:346:ASP:OD1 | 2:B:1108:ARG:HA | 2.20 | 0.41 |
| 1:A:440:ASP:O | 1:A:460:VAL:HG23 | 2.20 | 0.41 |
| 1:A:531:ILE:HD13 | 1:A:653:VAL:HG21 | 2.01 | 0.41 |
| 1:A:841:LEU:HD23 | 1:A:841:LEU:HA | 1.93 | 0.41 |
| 1:A:964:ILE:O | 1:A:967:ALA:HB3 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1074:GLU:N | 1:A:1075:PRO:HD2 | 2.35 | 0.41 |
| 1:A:1409:LEU:O | 1:A:1412:ALA:N | 2.51 | 0.41 |
| 1:A:1449:SER:O | 1:A:1453:TYR:CD1 | 2.73 | 0.41 |
| 1:A:1451:VAL:C | 1:A:1453:TYR:N | 2.73 | 0.41 |
| 2:B:22:SER:HA | 2:B:654:ARG:HB2 | 2.01 | 0.41 |
| 2:B:43:LEU:HD23 | 2:B:43:LEU:HA | 1.90 | 0.41 |
| 2:B:190:TYR:CE2 | 10:J:62:ARG:HD3 | 2.55 | 0.41 |
| 2:B:344:LYS:O | 2:B:347:LYS:HG2 | 2.20 | 0.41 |
| 2:B:390:LEU:O | 2:B:391:ASP:C | 2.58 | 0.41 |
| 2:B:435:THR:C | 2:B:437:GLU:N | 2.73 | 0.41 |
| 2:B:654:ARG:HH11 | 2:B:654:ARG:HG3 | 1.84 | 0.41 |
| 2:B:799:PRO:HD3 | 10:J:1:MET:HG2 | 2.02 | 0.41 |
| 2:B:900:ALA:HA | 2:B:901:PRO:HD3 | 1.90 | 0.41 |
| 3:C:77:ILE:CA | 3:C:129:ILE:HD11 | 2.50 | 0.41 |
| 4:D:52:LEU:HA | 4:D:148:LEU:HD21 | 2.03 | 0.41 |
| 5:E:13:TRP:O | 5:E:16:PHE:HB3 | 2.21 | 0.41 |
| 5:E:64:PRO:O | 5:E:65:THR:C | 2.59 | 0.41 |
| 6:F:70:LYS:HA | 6:F:72:LYS:HZ1 | 1.85 | 0.41 |
| 6:F:72:LYS:HB3 | 6:F:73:ALA:H | 1.64 | 0.41 |
| 6:F:109:VAL:CG2 | 6:F:124:GLU:HA | 2.51 | 0.41 |
| 7:G:121:PHE:HA | 7:G:130:TYR:HA | 2.02 | 0.41 |
| 8:H:83:GLN:C | 8:H:85:GLY:H | 2.23 | 0.41 |
| 10:J:1:MET:H3 | 10:J:56:LEU:N | 2.18 | 0.41 |
| 10:J:57:ILE:HG23 | 10:J:58:GLU:N | 2.35 | 0.41 |
| 12:L:49:LYS:O | 12:L:50:ASP:CB | 2.69 | 0.41 |
| 1:A:101:LYS:HE2 | 1:A:139:TRP:CH2 | 2.55 | 0.41 |
| 1:A:456:MET:HE2 | 1:A:507:VAL:HG22 | 2.02 | 0.41 |
| 1:A:532:ARG:HG2 | 1:A:532:ARG:HH11 | 1.86 | 0.41 |
| 1:A:637:LYS:HB3 | 1:A:641:VAL:CG2 | 2.47 | 0.41 |
| 1:A:710:LEU:HD12 | 1:A:710:LEU:H | 1.84 | 0.41 |
| 1:A:722:LEU:HD23 | 1:A:799:PHE:CG | 2.55 | 0.41 |
| 1:A:779:PHE:HD2 | 1:A:779:PHE:HA | 1.71 | 0.41 |
| 1:A:947:PHE:CE2 | 1:A:954:TRP:CD2 | 3.09 | 0.41 |
| 1:A:947:PHE:C | 1:A:949:ASP:N | 2.74 | 0.41 |
| 2:B:287:ARG:O | 2:B:327:ARG:HA | 2.21 | 0.41 |
| 2:B:324:ILE:HG12 | 2:B:329:THR:HB | 2.03 | 0.41 |
| 2:B:798:TYR:CE2 | 3:C:62:PHE:CE2 | 3.07 | 0.41 |
| 2:B:865:LYS:CD | 2:B:961:LEU:HD21 | 2.51 | 0.41 |
| 2:B:981:ALA:HB3 | 2:B:1095:LEU:HD11 | 2.03 | 0.41 |
| 2:B:1055:ILE:C | 2:B:1057:LYS:N | 2.74 | 0.41 |
| 2:B:1106:ARG:HD3 | 2:B:1126:GLY:C | 2.41 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:C:42:PRO:HA | 3:C:163:ILE:HG22 | 2.02 | 0.41 |
| 3:C:43:THR:CG2 | 3:C:44:LEU:N | 2.57 | 0.41 |
| 3:C:183:TRP:CH2 | 3:C:203:GLN:NE2 | 2.88 | 0.41 |
| 4:D:153:ARG:CZ | 4:D:184:ALA:HA | 2.50 | 0.41 |
| 5:E:2:ASP:O | 5:E:3:GLN:C | 2.59 | 0.41 |
| 6:F:70:LYS:HA | 6:F:72:LYS:NZ | 2.35 | 0.41 |
| 6:F:96:THR:O | 6:F:100:GLN:HG3 | 2.20 | 0.41 |
| 7:G:8:SER:O | 7:G:9:LEU:CB | 2.68 | 0.41 |
| 7:G:125:SER:HB2 | 7:G:127:PRO:O | 2.21 | 0.41 |
| 8:H:64:ASN:CG | 8:H:90:ALA:H | 2.14 | 0.41 |
| 9:I:35:VAL:O | 9:I:36:GLU:HB3 | 2.21 | 0.41 |
| 10:J:1:MET:H2 | 10:J:57:ILE:H | 1.65 | 0.41 |
| 11:K:55:LYS:HB3 | 11:K:81:TYR:CE1 | 2.55 | 0.41 |
| 1:A:37:PHE:HD1 | 1:A:37:PHE:H | 1.63 | 0.41 |
| 1:A:630:ILE:CG2 | 1:A:631:HIS:H | 2.34 | 0.41 |
| 1:A:683:ILE:HG22 | 1:A:684:ALA:N | 2.35 | 0.41 |
| 1:A:1141:THR:CA | 1:A:1205:LYS:HZ3 | 2.32 | 0.41 |
| 1:A:1227:ILE:CG2 | 1:A:1228:TRP:H | 2.20 | 0.41 |
| 2:B:63:ILE:HA | 2:B:63:ILE:HD12 | 1.89 | 0.41 |
| 2:B:487:THR:CG2 | 2:B:488:TYR:H | 2.33 | 0.41 |
| 2:B:581:PHE:O | 2:B:626:ILE:N | 2.53 | 0.41 |
| 2:B:605:ARG:HB3 | 2:B:688:GLY:HA3 | 2.02 | 0.41 |
| 2:B:693:ILE:HD13 | 2:B:701:ILE:CD1 | 2.50 | 0.41 |
| 2:B:859:TYR:CD1 | 2:B:859:TYR:N | 2.88 | 0.41 |
| 2:B:996:ARG:HH12 | 3:C:38:ILE:HG23 | 1.86 | 0.41 |
| 3:C:77:ILE:HD13 | 3:C:77:ILE:HA | 1.89 | 0.41 |
| 3:C:104:PHE:HD2 | 3:C:105:GLY:H | 1.68 | 0.41 |
| 3:C:131:HIS:O | 3:C:133:ILE:N | 2.53 | 0.41 |
| 4:D:3:VAL:CG1 | 4:D:4:SER:N | 2.83 | 0.41 |
| 5:E:93:MET:O | 5:E:94:LYS:C | 2.59 | 0.41 |
| 7:G:26:LEU:O | 7:G:27:LYS:C | 2.59 | 0.41 |
| 8:H:118:PHE:C | 8:H:120:GLY:N | 2.67 | 0.41 |
| 9:I:2:THR:O | 9:I:3:THR:C | 2.59 | 0.41 |
| 1:A:12:ARG:HD2 | 2:B:1218:THR:CB | 2.43 | 0.41 |
| 1:A:15:LYS:HB2 | 2:B:1219:ASP:O | 2.21 | 0.41 |
| 1:A:16:GLU:HB3 | 1:A:1418:LEU:HD11 | 2.03 | 0.41 |
| 1:A:34:LYS:HZ3 | 1:A:34:LYS:HG2 | 1.77 | 0.41 |
| 1:A:38:PRO:HG2 | 1:A:39:GLU:H | 1.86 | 0.41 |
| 1:A:244:PRO:HG2 | 1:A:245:PRO:CD | 2.50 | 0.41 |
| 1:A:265:LYS:O | 1:A:265:LYS:HG3 | 2.21 | 0.41 |
| 1:A:376:TYR:HB3 | 1:A:434:ARG:NH1 | 2.36 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:445:ASN:ND2 | 1:A:446:ARG:N | 2.68 | 0.41 |
| 1:A:746:MET:HE1 | 2:B:1018:PRO:HG2 | 2.03 | 0.41 |
| 1:A:800:VAL:HG13 | 1:A:812:GLU:OE2 | 2.21 | 0.41 |
| 1:A:868:TYR:CZ | 1:A:1366:ARG:HD3 | 2.56 | 0.41 |
| 1:A:1037:LEU:HD12 | 1:A:1042:PHE:N | 2.36 | 0.41 |
| 1:A:1098:VAL:HB | 1:A:1099:PRO:HD3 | 2.03 | 0.41 |
| 1:A:1144:LYS:HD2 | 1:A:1269:GLU:HG3 | 2.02 | 0.41 |
| 1:A:1239:ARG:HB3 | 1:A:1239:ARG:HH11 | 1.86 | 0.41 |
| 1:A:1343:ALA:CB | 5:E:150:VAL:HG22 | 2.43 | 0.41 |
| 2:B:112:LEU:HD12 | 2:B:113:TYR:N | 2.32 | 0.41 |
| 2:B:186:GLU:HG3 | 10:J:62:ARG:CZ | 2.51 | 0.41 |
| 2:B:227:LYS:HB2 | 2:B:395:GLN:OE1 | 2.21 | 0.41 |
| 2:B:265:SER:C | 2:B:267:ARG:N | 2.74 | 0.41 |
| 2:B:273:LEU:HD12 | 2:B:280:ILE:HD12 | 2.03 | 0.41 |
| 2:B:275:TYR:HB3 | 2:B:351:TYR:OH | 2.21 | 0.41 |
| 2:B:368:GLU:O | 2:B:371:GLU:OE1 | 2.38 | 0.41 |
| 2:B:457:LEU:O | 2:B:458:LYS:C | 2.58 | 0.41 |
| 2:B:1110:PRO:O | 2:B:1119:VAL:HG22 | 2.21 | 0.41 |
| 3:C:56:THR:HG22 | 3:C:58:LEU:HD23 | 2.02 | 0.41 |
| 3:C:77:ILE:CG2 | 3:C:78:GLU:N | 2.76 | 0.41 |
| 3:C:82:TYR:CD2 | 3:C:161:LYS:HG2 | 2.56 | 0.41 |
| 3:C:102:GLN:HA | 3:C:153:LEU:O | 2.21 | 0.41 |
| 3:C:183:TRP:O | 3:C:184:ASN:CB | 2.69 | 0.41 |
| 3:C:254:LYS:C | 3:C:256:ALA:N | 2.74 | 0.41 |
| 4:D:60:LYS:HE2 | 4:D:126:ILE:HD11 | 2.03 | 0.41 |
| 4:D:155:ARG:O | 4:D:156:ASP:HB2 | 2.20 | 0.41 |
| 4:D:175:PHE:O | 4:D:179:GLN:HG2 | 2.21 | 0.41 |
| 8:H:82:PRO:O | 8:H:84:ALA:N | 2.41 | 0.41 |
| 8:H:100:THR:N | 8:H:117:SER:O | 2.45 | 0.41 |
| 9:I:55:THR:O | 9:I:56:ALA:C | 2.59 | 0.41 |
| 10:J:3:VAL:HA | 10:J:4:PRO:HD3 | 1.87 | 0.41 |
| 11:K:14:GLU:O | 11:K:15:GLY:O | 2.39 | 0.41 |
| 1:A:49:LYS:NZ | 1:A:61:ILE:CG1 | 2.72 | 0.41 |
| 1:A:152:VAL:HG12 | 1:A:153:PRO:CD | 2.51 | 0.41 |
| 1:A:390:GLN:O | 1:A:394:ASN:N | 2.54 | 0.41 |
| 1:A:553:VAL:HA | 1:A:554:PRO:HD2 | 1.89 | 0.41 |
| 1:A:568:PRO:HB2 | 3:C:221:TYR:CZ | 2.56 | 0.41 |
| 1:A:866:PHE:HB2 | 5:E:208:TYR:OH | 2.21 | 0.41 |
| 1:A:966:ASN:C | 1:A:968:GLN:N | 2.73 | 0.41 |
| 1:A:1143:LEU:CD2 | 1:A:1267:MET:HB3 | 2.48 | 0.41 |
| 1:A:1308:THR:HG23 | 1:A:1310:GLY:N | 2.28 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:133:LYS:CG | 2:B:135:ARG:HE | 2.34 | 0.41 |
| 2:B:187:SER:O | 2:B:191:LYS:HG3 | 2.21 | 0.41 |
| 2:B:343:ILE:CG2 | 2:B:347:LYS:HE2 | 2.42 | 0.41 |
| 2:B:413:LEU:O | 2:B:416:LEU:HB2 | 2.21 | 0.41 |
| 2:B:488:TYR:CE2 | 2:B:813:LYS:HB2 | 2.55 | 0.41 |
| 2:B:601:ARG:HD3 | 2:B:605:ARG:HH21 | 1.85 | 0.41 |
| 2:B:1017:ILE:CB | 2:B:1018:PRO:CD | 2.99 | 0.41 |
| 3:C:192:TRP:CZ3 | 3:C:194:GLU:HG3 | 2.56 | 0.41 |
| 3:C:204:SER:N | 3:C:207:CYS:HG | 2.17 | 0.41 |
| 4:D:33:PHE:CE1 | 7:G:80:LYS:HD3 | 2.56 | 0.41 |
| 4:D:67:ARG:HH21 | 4:D:129:LEU:HD13 | 1.86 | 0.41 |
| 5:E:89:GLY:O | 5:E:91:LYS:N | 2.54 | 0.41 |
| 5:E:116:ILE:CG2 | 5:E:117:THR:H | 2.34 | 0.41 |
| 5:E:145:THR:HG21 | 5:E:187:TYR:CZ | 2.56 | 0.41 |
| 6:F:79:ARG:HH11 | 6:F:79:ARG:CB | 2.29 | 0.41 |
| 7:G:164:LYS:O | 7:G:164:LYS:HG2 | 2.21 | 0.41 |
| 8:H:31:THR:HG22 | 8:H:31:THR:O | 2.20 | 0.41 |
| 12:L:52:GLY:O | 12:L:53:HIS:C | 2.59 | 0.41 |
| 1:A:106:VAL:CG1 | 1:A:107:CYS:N | 2.82 | 0.40 |
| 1:A:472:LEU:CD1 | 2:B:835:GLN:NE2 | 2.84 | 0.40 |
| 1:A:568:PRO:HB3 | 3:C:221:TYR:OH | 2.21 | 0.40 |
| 1:A:569:LYS:O | 1:A:571:LEU:HD13 | 2.20 | 0.40 |
| 1:A:595:THR:O | 1:A:596:THR:CG2 | 2.68 | 0.40 |
| 1:A:714:PHE:O | 1:A:715:GLU:C | 2.60 | 0.40 |
| 1:A:731:ARG:O | 1:A:732:LEU:C | 2.59 | 0.40 |
| 1:A:767:GLN:HE21 | 1:A:774:ARG:HB3 | 1.87 | 0.40 |
| 1:A:814:PHE:CD2 | 1:A:814:PHE:O | 2.74 | 0.40 |
| 1:A:1348:LEU:O | 1:A:1352:VAL:HG23 | 2.20 | 0.40 |
| 1:A:1356:ILE:O | 1:A:1356:ILE:HG22 | 2.21 | 0.40 |
| 2:B:610:ASN:HA | 2:B:611:PRO:HD3 | 1.89 | 0.40 |
| 2:B:980:PHE:CE2 | 2:B:1094:ARG:HB2 | 2.56 | 0.40 |
| 3:C:116:LYS:HD3 | 3:C:140:ASN:HA | 2.02 | 0.40 |
| 3:C:252:GLN:CG | 11:K:95:ILE:HG23 | 2.50 | 0.40 |
| 4:D:51:ASN:C | 4:D:52:LEU:O | 2.57 | 0.40 |
| 4:D:60:LYS:NZ | 4:D:122:GLU:OE2 | 2.53 | 0.40 |
| 5:E:124:VAL:HB | 5:E:125:PRO:HD3 | 2.03 | 0.40 |
| 5:E:197:LYS:HG2 | 5:E:199:ILE:CG1 | 2.50 | 0.40 |
| 6:F:82:THR:HG22 | 6:F:84:TYR:N | 2.35 | 0.40 |
| 6:F:90:ARG:CG | 6:F:91:ALA:N | 2.84 | 0.40 |
| 7:G:53:ASN:N | 7:G:53:ASN:HD22 | 2.18 | 0.40 |
| 7:G:127:PRO:CG | 7:G:139:ILE:HG13 | 2.50 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:H:4:THR:CG2 | 8:H:5:LEU:N | 2.84 | 0.40 |
| 9:I:94:ASP:O | 9:I:95:THR:O | 2.40 | 0.40 |
| 9:I:99:LEU:C | 9:I:100:PHE:HD1 | 2.24 | 0.40 |
| 10:J:47:ARG:NH1 | 10:J:47:ARG:HG2 | 2.35 | 0.40 |
| 1:A:26:GLU:O | 1:A:27:VAL:C | 2.58 | 0.40 |
| 1:A:49:LYS:HZ1 | 1:A:61:ILE:CB | 2.34 | 0.40 |
| 1:A:100:LYS:O | 1:A:104:GLU:HG3 | 2.20 | 0.40 |
| 1:A:253:ASN:ND2 | 1:A:256:GLN:NE2 | 2.67 | 0.40 |
| 1:A:606:LEU:HD11 | 1:A:608:ILE:HG13 | 2.03 | 0.40 |
| 1:A:779:PHE:CD1 | 1:A:784:LEU:HA | 2.56 | 0.40 |
| 1:A:1026:LEU:HD23 | 1:A:1026:LEU:HA | 1.89 | 0.40 |
| 1:A:1219:THR:HG21 | 1:A:1271:ILE:CD1 | 2.45 | 0.40 |
| 1:A:1342:GLU:OE2 | 5:E:212:ARG:NH1 | 2.53 | 0.40 |
| 1:A:1354:ASN:HA | 1:A:1357:ALA:HB3 | 2.03 | 0.40 |
| 1:A:1425:SER:O | 1:A:1428:VAL:HG23 | 2.22 | 0.40 |
| 2:B:26:THR:O | 2:B:29:ASP:HB2 | 2.22 | 0.40 |
| 2:B:259:TYR:N | 2:B:259:TYR:CD1 | 2.89 | 0.40 |
| 2:B:287:ARG:NH1 | 2:B:325:GLN:HA | 2.36 | 0.40 |
| 2:B:605:ARG:HB3 | 2:B:688:GLY:HA2 | 2.03 | 0.40 |
| 2:B:661:LEU:C | 2:B:663:ALA:H | 2.22 | 0.40 |
| 2:B:856:PHE:N | 2:B:856:PHE:CD1 | 2.89 | 0.40 |
| 2:B:894:ASP:HB2 | 12:L:58:LYS:HZ1 | 1.85 | 0.40 |
| 2:B:980:PHE:CD2 | 2:B:1094:ARG:HA | 2.56 | 0.40 |
| 2:B:1033:LYS:NZ | 2:B:1070:GLU:OE1 | 2.45 | 0.40 |
| 3:C:191:TYR:HD2 | 3:C:201:TRP:CD1 | 2.39 | 0.40 |
| 3:C:249:ASP:O | 3:C:252:GLN:HB3 | 2.21 | 0.40 |
| 4:D:138:ASN:OD1 | 4:D:141:LEU:HB2 | 2.21 | 0.40 |
| 5:E:28:TYR:CE2 | 5:E:78:LEU:HB2 | 2.56 | 0.40 |
| 7:G:1:MET:CE | 7:G:3:PHE:CE1 | 3.05 | 0.40 |
| 7:G:88:ASP:HB3 | 7:G:144:ARG:CB | 2.51 | 0.40 |
| 9:I:95:THR:CG2 | 9:I:96:SER:N | 2.84 | 0.40 |
| 13:T:9:DC:H2" | 13:T:10:DA:H8 | 1.78 | 0.40 |
| 1:A:241:VAL:O | 1:A:242:PRO:C | 2.58 | 0.40 |
| 1:A:265:LYS:HZ3 | 1:A:302:THR:HG21 | 1.86 | 0.40 |
| 1:A:359:LEU:HA | 1:A:359:LEU:HD23 | 1.87 | 0.40 |
| 1:A:474:VAL:O | 1:A:474:VAL:CG2 | 2.68 | 0.40 |
| 1:A:524:VAL:HG12 | 1:A:525:GLN:HG3 | 2.02 | 0.40 |
| 1:A:600:PRO:HA | 8:H:25:ARG:CZ | 2.51 | 0.40 |
| 1:A:1019:CYS:O | 1:A:1020:CYS:C | 2.59 | 0.40 |
| 1:A:1072:ILE:O | 1:A:1075:PRO:HD2 | 2.21 | 0.40 |
| 1:A:1165:GLU:OE1 | 1:A:1194:ARG:NH2 | 2.54 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:172:ILE:HG22 | 2:B:173:MET:N | 2.36 | 0.40 |
| 2:B:222:ILE:N | 2:B:240:ILE:HG13 | 2.36 | 0.40 |
| 2:B:289:LEU:O | 2:B:371:GLU:HB3 | 2.21 | 0.40 |
| 2:B:324:ILE:HD13 | 2:B:330:ALA:HA | 2.03 | 0.40 |
| 2:B:465:ASN:O | 2:B:467:GLY:N | 2.54 | 0.40 |
| 2:B:658:ILE:HG22 | 2:B:662:MET:CE | 2.51 | 0.40 |
| 2:B:790:ASP:N | 2:B:790:ASP:OD2 | 2.52 | 0.40 |
| 2:B:878:GLN:O | 2:B:934:LYS:HE2 | 2.21 | 0.40 |
| 2:B:906:SER:HA | 2:B:946:ASN:CB | 2.44 | 0.40 |
| 3:C:259:LEU:O | 3:C:262:LEU:N | 2.53 | 0.40 |
| 4:D:205:ASP:O | 4:D:208:GLU:HB3 | 2.21 | 0.40 |
| 4:D:218:GLU:O | 4:D:219:THR:C | 2.60 | 0.40 |
| 6:F:70:LYS:C | 6:F:72:LYS:HZ2 | 2.22 | 0.40 |
| 7:G:26:LEU:O | 7:G:29:LYS:N | 2.54 | 0.40 |
| 7:G:144:ARG:O | 7:G:168:LEU:HD22 | 2.22 | 0.40 |
| 8:H:87:ARG:O | 8:H:89:LEU:HG | 2.21 | 0.40 |
| 11:K:11:LEU:CD2 | 11:K:11:LEU:N | 2.82 | 0.40 |
| 11:K:83:PRO:O | 11:K:84:LYS:C | 2.60 | 0.40 |
| 1:A:129:LYS:O | 1:A:130:ASP:CB | 2.66 | 0.40 |
| 1:A:215:SER:HB3 | 1:A:218:ASP:HB2 | 2.03 | 0.40 |
| 1:A:265:LYS:HA | 1:A:265:LYS:HE3 | 2.03 | 0.40 |
| 1:A:447:GLN:HA | 1:A:448:PRO:C | 2.41 | 0.40 |
| 1:A:525:GLN:O | 1:A:526:ASP:C | 2.60 | 0.40 |
| 1:A:703:THR:C | 1:A:705:LYS:H | 2.24 | 0.40 |
| 1:A:975:HIS:HA | 1:A:1036:ARG:HG3 | 2.02 | 0.40 |
| 1:A:1006:ILE:HD12 | 5:E:163:GLU:HG3 | 2.00 | 0.40 |
| 1:A:1076:ALA:HA | 1:A:1079:MET:CE | 2.51 | 0.40 |
| 1:A:1126:ALA:O | 1:A:1128:GLN:N | 2.55 | 0.40 |
| 1:A:1349:TYR:CD2 | 1:A:1349:TYR:C | 2.94 | 0.40 |
| 1:A:1437:GLY:C | 1:A:1439:GLY:N | 2.75 | 0.40 |
| 2:B:102:VAL:HB | 2:B:110:HIS:H | 1.86 | 0.40 |
| 2:B:383:ASN:CG | 2:B:387:LEU:HD11 | 2.42 | 0.40 |
| 2:B:391:ASP:CB | 9:I:92:ARG:HG3 | 2.52 | 0.40 |
| 2:B:530:GLY:C | 2:B:531:GLN:HG2 | 2.41 | 0.40 |
| 2:B:737:THR:HG22 | 9:I:66:PRO:HA | 2.02 | 0.40 |
| 2:B:814:PHE:C | 2:B:816:GLU:H | 2.24 | 0.40 |
| 2:B:901:PRO:HD2 | 12:L:59:ALA:O | 2.22 | 0.40 |
| 4:D:39:ASN:HD21 | 4:D:41:GLN:HB2 | 1.79 | 0.40 |
| 4:D:139:LYS:HG3 | 4:D:143:ASN:HD22 | 1.87 | 0.40 |
| 4:D:175:PHE:HZ | 7:G:85:GLU:HG3 | 1.87 | 0.40 |
| 5:E:117:THR:CG2 | 5:E:120:ALA:H | 2.34 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:E:117:THR:C | 5:E:119:SER:N | 2.75 | 0.40 |
| 5:E:164:LEU:HD21 | 5:E:211:TYR:CG | 2.57 | 0.40 |
| 6:F:75:PRO:O | 6:F:77:ASP:N | 2.54 | 0.40 |
| 7:G:9:LEU:C | 7:G:9:LEU:HD12 | 2.41 | 0.40 |
| 7:G:113:HIS:O | 7:G:114:LEU:HB2 | 2.21 | 0.40 |
| 9:I:2:THR:CG2 | 9:I:3:THR:H | 2.31 | 0.40 |
| 9:I:4:PHE:HD1 | 9:I:4:PHE:O | 2.05 | 0.40 |
| 9:I:5:ARG:NE | 9:I:36:GLU:OE2 | 2.55 | 0.40 |
| 11:K:67:PHE:C | 11:K:68:PHE:CD2 | 2.87 | 0.40 |
| 12:L:27:LEU:HD13 | 12:L:37:LYS:HG2 | 2.03 | 0.40 |
| 12:L:58:LYS:O | 12:L:59:ALA:O | 2.39 | 0.40 |
| 1:A:110:CYS:SG | 1:A:111:GLY:N | 2.94 | 0.40 |
| 1:A:681:GLU:C | 1:A:683:ILE:H | 2.24 | 0.40 |
| 1:A:767:GLN:NE2 | 1:A:774:ARG:HB3 | 2.37 | 0.40 |
| 1:A:947:PHE:HE2 | 1:A:954:TRP:CD1 | 2.40 | 0.40 |
| 1:A:1208:THR:HG22 | 1:A:1210:GLY:H | 1.85 | 0.40 |
| 2:B:31:TRP:HA | 2:B:31:TRP:HE3 | 1.85 | 0.40 |
| 2:B:228:LYS:HD3 | 2:B:228:LYS:HA | 1.94 | 0.40 |
| 2:B:293:PRO:CG | 2:B:296:GLU:OE1 | 2.70 | 0.40 |
| 2:B:351:TYR:CE2 | 2:B:355:ILE:HD11 | 2.55 | 0.40 |
| 2:B:469:GLN:CG | 2:B:470:LYS:N | 2.84 | 0.40 |
| 2:B:766:ARG:HH21 | 15:P:11:U:H3 | 1.70 | 0.40 |
| 2:B:816:GLU:N | 2:B:816:GLU:OE1 | 2.55 | 0.40 |
| 2:B:1045:SER:O | 2:B:1046:PRO:O | 2.39 | 0.40 |
| 2:B:1152:MET:C | 2:B:1157:ALA:HB2 | 2.42 | 0.40 |
| 5:E:176:PRO:O | 5:E:212:ARG:HA | 2.21 | 0.40 |
| 6:F:89:GLU:HB3 | 6:F:134:ILE:HD11 | 2.03 | 0.40 |
| 6:F:138:LEU:HD23 | 6:F:138:LEU:HA | 1.99 | 0.40 |
| 7:G:12:THR:HA | 7:G:68:ALA:O | 2.22 | 0.40 |
| 7:G:14:HIS:C | 7:G:16:SER:N | 2.75 | 0.40 |
| 8:H:128:ASN:N | 8:H:130:ARG:HH11 | 2.10 | 0.40 |
| 11:K:42:LEU:HD23 | 11:K:42:LEU:C | 2.42 | 0.40 |
| 13:T:12:DG:N2 | 14:N:6:DT:O2 | 2.55 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|-----------|-------------|----|
| 1 | A | 1421/1733 (82%) | 909 (64%) | 310 (22%) | 202 (14%) | 0 | 3 |
| 2 | B | 1111/1224 (91%) | 694 (62%) | 257 (23%) | 160 (14%) | 0 | 3 |
| 3 | C | 268/324 (83%) | 164 (61%) | 66 (25%) | 38 (14%) | 0 | 3 |
| 4 | D | 183/221 (83%) | 108 (59%) | 49 (27%) | 26 (14%) | 0 | 3 |
| 5 | E | 212/215 (99%) | 134 (63%) | 49 (23%) | 29 (14%) | 0 | 3 |
| 6 | F | 86/155 (56%) | 60 (70%) | 20 (23%) | 6 (7%) | 1 | 15 |
| 7 | G | 169/171 (99%) | 127 (75%) | 32 (19%) | 10 (6%) | 1 | 18 |
| 8 | H | 133/146 (91%) | 72 (54%) | 37 (28%) | 24 (18%) | 0 | 1 |
| 9 | I | 114/122 (93%) | 73 (64%) | 26 (23%) | 15 (13%) | 0 | 4 |
| 10 | J | 63/70 (90%) | 34 (54%) | 13 (21%) | 16 (25%) | 0 | 0 |
| 11 | K | 114/120 (95%) | 79 (69%) | 26 (23%) | 9 (8%) | 1 | 12 |
| 12 | L | 45/70 (64%) | 19 (42%) | 11 (24%) | 15 (33%) | 0 | 0 |
| All | All | 3919/4571 (86%) | 2473 (63%) | 896 (23%) | 550 (14%) | 0 | 3 |

All (550) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 4 | GLN |
| 1 | A | 41 | MET |
| 1 | A | 43 | GLU |
| 1 | A | 48 | ALA |
| 1 | A | 58 | LEU |
| 1 | A | 63 | ARG |
| 1 | A | 67 | CYS |
| 1 | A | 70 | CYS |
| 1 | A | 74 | MET |
| 1 | A | 76 | GLU |
| 1 | A | 93 | VAL |
| 1 | A | 130 | ASP |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A | 154 | SER |
| 1 | A | 167 | CYS |
| 1 | A | 259 | GLU |
| 1 | A | 311 | GLN |
| 1 | A | 312 | PRO |
| 1 | A | 317 | LYS |
| 1 | A | 318 | SER |
| 1 | A | 399 | HIS |
| 1 | A | 409 | SER |
| 1 | A | 410 | GLY |
| 1 | A | 535 | THR |
| 1 | A | 536 | LEU |
| 1 | A | 543 | LEU |
| 1 | A | 544 | ASP |
| 1 | A | 556 | TRP |
| 1 | A | 567 | LYS |
| 1 | A | 583 | PRO |
| 1 | A | 619 | LYS |
| 1 | A | 666 | ILE |
| 1 | A | 705 | LYS |
| 1 | A | 846 | GLU |
| 1 | A | 871 | ASP |
| 1 | A | 885 | THR |
| 1 | A | 968 | GLN |
| 1 | A | 986 | ILE |
| 1 | A | 1002 | GLY |
| 1 | A | 1016 | THR |
| 1 | A | 1110 | ASN |
| 1 | A | 1114 | PRO |
| 1 | A | 1115 | SER |
| 1 | A | 1116 | LEU |
| 1 | A | 1122 | PRO |
| 1 | A | 1124 | HIS |
| 1 | A | 1177 | LEU |
| 1 | A | 1178 | ASP |
| 1 | A | 1206 | ASP |
| 1 | A | 1212 | VAL |
| 1 | A | 1244 | ARG |
| 1 | A | 1255 | GLU |
| 1 | A | 1314 | SER |
| 1 | A | 1341 | ILE |
| 1 | A | 1393 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A | 1448 | GLU |
| 2 | B | 21 | GLU |
| 2 | B | 41 | LYS |
| 2 | B | 65 | GLU |
| 2 | B | 108 | VAL |
| 2 | B | 124 | TYR |
| 2 | B | 134 | LYS |
| 2 | B | 184 | ALA |
| 2 | B | 206 | ASN |
| 2 | B | 259 | TYR |
| 2 | B | 262 | GLU |
| 2 | B | 265 | SER |
| 2 | B | 266 | ALA |
| 2 | B | 278 | GLN |
| 2 | B | 282 | ILE |
| 2 | B | 295 | GLY |
| 2 | B | 343 | ILE |
| 2 | B | 344 | LYS |
| 2 | B | 345 | LYS |
| 2 | B | 346 | GLU |
| 2 | B | 365 | THR |
| 2 | B | 367 | LEU |
| 2 | B | 391 | ASP |
| 2 | B | 409 | ALA |
| 2 | B | 450 | ALA |
| 2 | B | 468 | GLU |
| 2 | B | 469 | GLN |
| 2 | B | 509 | ALA |
| 2 | B | 511 | PRO |
| 2 | B | 512 | ARG |
| 2 | B | 577 | ALA |
| 2 | B | 705 | MET |
| 2 | B | 708 | GLU |
| 2 | B | 709 | ASP |
| 2 | B | 751 | VAL |
| 2 | B | 878 | GLN |
| 2 | B | 879 | ARG |
| 2 | B | 892 | LYS |
| 2 | B | 958 | GLN |
| 2 | B | 987 | LYS |
| 2 | B | 1045 | SER |
| 2 | B | 1046 | PRO |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | B | 1069 | PHE |
| 2 | B | 1097 | HIS |
| 2 | B | 1099 | VAL |
| 2 | B | 1143 | ALA |
| 2 | B | 1144 | ALA |
| 2 | B | 1157 | ALA |
| 2 | B | 1175 | LEU |
| 2 | B | 1183 | LYS |
| 3 | C | 4 | GLU |
| 3 | C | 56 | THR |
| 3 | C | 60 | ASP |
| 3 | C | 74 | SER |
| 3 | C | 90 | ASP |
| 3 | C | 141 | GLY |
| 3 | C | 149 | LYS |
| 3 | C | 161 | LYS |
| 3 | C | 213 | PRO |
| 3 | C | 214 | ASN |
| 3 | C | 237 | SER |
| 4 | D | 19 | GLU |
| 4 | D | 21 | GLU |
| 4 | D | 52 | LEU |
| 4 | D | 114 | MET |
| 4 | D | 131 | GLU |
| 4 | D | 169 | SER |
| 4 | D | 198 | LEU |
| 4 | D | 218 | GLU |
| 5 | E | 45 | LYS |
| 5 | E | 88 | VAL |
| 5 | E | 93 | MET |
| 5 | E | 97 | VAL |
| 5 | E | 106 | GLN |
| 5 | E | 115 | ASN |
| 5 | E | 129 | PRO |
| 5 | E | 174 | GLN |
| 6 | F | 72 | LYS |
| 6 | F | 81 | THR |
| 6 | F | 114 | GLU |
| 7 | G | 2 | PHE |
| 7 | G | 63 | PRO |
| 7 | G | 114 | LEU |
| 7 | G | 120 | THR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 7 | G | 139 | ILE |
| 7 | G | 141 | SER |
| 7 | G | 154 | VAL |
| 8 | H | 78 | SER |
| 8 | H | 81 | PRO |
| 8 | H | 82 | PRO |
| 8 | H | 87 | ARG |
| 8 | H | 109 | LYS |
| 8 | H | 128 | ASN |
| 8 | H | 131 | ASN |
| 8 | H | 140 | ALA |
| 9 | I | 32 | CYS |
| 9 | I | 79 | HIS |
| 9 | I | 95 | THR |
| 9 | I | 106 | CYS |
| 10 | J | 2 | ILE |
| 10 | J | 64 | ASN |
| 11 | K | 8 | GLU |
| 12 | L | 40 | LEU |
| 12 | L | 42 | ARG |
| 12 | L | 50 | ASP |
| 12 | L | 55 | ILE |
| 12 | L | 59 | ALA |
| 12 | L | 60 | ARG |
| 1 | A | 5 | GLN |
| 1 | A | 8 | SER |
| 1 | A | 42 | ASP |
| 1 | A | 57 | ARG |
| 1 | A | 84 | ILE |
| 1 | A | 96 | ILE |
| 1 | A | 126 | LEU |
| 1 | A | 131 | SER |
| 1 | A | 148 | CYS |
| 1 | A | 283 | GLY |
| 1 | A | 287 | HIS |
| 1 | A | 392 | VAL |
| 1 | A | 439 | ASN |
| 1 | A | 516 | SER |
| 1 | A | 517 | ASN |
| 1 | A | 591 | PHE |
| 1 | A | 604 | GLY |
| 1 | A | 625 | SER |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A | 706 | HIS |
| 1 | A | 726 | ARG |
| 1 | A | 775 | ILE |
| 1 | A | 852 | TYR |
| 1 | A | 872 | GLY |
| 1 | A | 958 | VAL |
| 1 | A | 969 | GLN |
| 1 | A | 1036 | ARG |
| 1 | A | 1054 | LEU |
| 1 | A | 1095 | THR |
| 1 | A | 1097 | GLY |
| 1 | A | 1123 | GLY |
| 1 | A | 1127 | ASP |
| 1 | A | 1133 | LEU |
| 1 | A | 1140 | HIS |
| 1 | A | 1167 | GLU |
| 1 | A | 1176 | LEU |
| 1 | A | 1221 | LYS |
| 1 | A | 1229 | SER |
| 1 | A | 1233 | ASP |
| 1 | A | 1278 | ASN |
| 1 | A | 1316 | VAL |
| 1 | A | 1331 | SER |
| 1 | A | 1365 | TYR |
| 1 | A | 1390 | ASN |
| 1 | A | 1405 | THR |
| 1 | A | 1438 | THR |
| 1 | A | 1450 | LEU |
| 1 | A | 1454 | MET |
| 2 | B | 46 | GLN |
| 2 | B | 115 | GLN |
| 2 | B | 168 | GLY |
| 2 | B | 229 | ALA |
| 2 | B | 257 | LYS |
| 2 | B | 258 | LEU |
| 2 | B | 260 | GLY |
| 2 | B | 277 | LYS |
| 2 | B | 294 | ASP |
| 2 | B | 308 | TRP |
| 2 | B | 312 | GLU |
| 2 | B | 327 | ARG |
| 2 | B | 368 | GLU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | B | 466 | TRP |
| 2 | B | 480 | SER |
| 2 | B | 483 | LEU |
| 2 | B | 506 | GLY |
| 2 | B | 575 | PRO |
| 2 | B | 598 | GLU |
| 2 | B | 629 | ASP |
| 2 | B | 655 | LYS |
| 2 | B | 711 | GLU |
| 2 | B | 712 | PRO |
| 2 | B | 728 | ARG |
| 2 | B | 735 | ALA |
| 2 | B | 752 | ALA |
| 2 | B | 882 | THR |
| 2 | B | 907 | GLY |
| 2 | B | 943 | SER |
| 2 | B | 951 | GLN |
| 2 | B | 1003 | ALA |
| 2 | B | 1006 | ILE |
| 2 | B | 1041 | GLU |
| 2 | B | 1075 | GLY |
| 2 | B | 1103 | ILE |
| 2 | B | 1108 | ARG |
| 2 | B | 1112 | GLN |
| 2 | B | 1155 | SER |
| 2 | B | 1167 | GLY |
| 2 | B | 1171 | VAL |
| 2 | B | 1176 | ASN |
| 2 | B | 1181 | GLU |
| 2 | B | 1186 | ASP |
| 3 | C | 17 | ASN |
| 3 | C | 78 | GLU |
| 3 | C | 89 | GLU |
| 3 | C | 110 | THR |
| 3 | C | 132 | PRO |
| 3 | C | 175 | ALA |
| 4 | D | 12 | ARG |
| 4 | D | 16 | LYS |
| 4 | D | 20 | GLU |
| 4 | D | 112 | ASP |
| 4 | D | 117 | GLU |
| 4 | D | 168 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 4 | D | 201 | LYS |
| 4 | D | 220 | LEU |
| 5 | E | 3 | GLN |
| 5 | E | 43 | LYS |
| 5 | E | 66 | GLU |
| 5 | E | 70 | SER |
| 5 | E | 73 | PRO |
| 5 | E | 76 | GLY |
| 5 | E | 94 | LYS |
| 5 | E | 130 | ALA |
| 6 | F | 128 | LYS |
| 7 | G | 9 | LEU |
| 8 | H | 2 | SER |
| 8 | H | 6 | PHE |
| 8 | H | 84 | ALA |
| 8 | H | 92 | ASP |
| 8 | H | 110 | ASP |
| 8 | H | 119 | GLY |
| 8 | H | 137 | GLN |
| 9 | I | 3 | THR |
| 9 | I | 56 | ALA |
| 10 | J | 6 | ARG |
| 10 | J | 17 | LYS |
| 10 | J | 24 | LEU |
| 10 | J | 42 | LYS |
| 11 | K | 15 | GLY |
| 12 | L | 37 | LYS |
| 12 | L | 45 | ALA |
| 12 | L | 53 | HIS |
| 12 | L | 56 | LEU |
| 1 | A | 54 | ASN |
| 1 | A | 187 | LYS |
| 1 | A | 194 | ALA |
| 1 | A | 219 | PHE |
| 1 | A | 222 | LEU |
| 1 | A | 257 | ARG |
| 1 | A | 286 | HIS |
| 1 | A | 331 | GLY |
| 1 | A | 332 | LYS |
| 1 | A | 382 | PRO |
| 1 | A | 419 | LYS |
| 1 | A | 465 | TYR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A | 483 | ASP |
| 1 | A | 510 | GLN |
| 1 | A | 538 | ASP |
| 1 | A | 557 | ASP |
| 1 | A | 568 | PRO |
| 1 | A | 597 | LEU |
| 1 | A | 600 | PRO |
| 1 | A | 731 | ARG |
| 1 | A | 734 | GLU |
| 1 | A | 789 | LYS |
| 1 | A | 875 | ALA |
| 1 | A | 895 | LYS |
| 1 | A | 910 | PRO |
| 1 | A | 979 | SER |
| 1 | A | 1098 | VAL |
| 1 | A | 1168 | GLU |
| 1 | A | 1211 | GLN |
| 1 | A | 1223 | ASP |
| 1 | A | 1270 | ASN |
| 1 | A | 1388 | GLY |
| 1 | A | 1416 | ALA |
| 1 | A | 1435 | PRO |
| 2 | B | 28 | GLU |
| 2 | B | 48 | LEU |
| 2 | B | 100 | PRO |
| 2 | B | 135 | ARG |
| 2 | B | 186 | GLU |
| 2 | B | 197 | PHE |
| 2 | B | 267 | ARG |
| 2 | B | 305 | VAL |
| 2 | B | 384 | ARG |
| 2 | B | 385 | LEU |
| 2 | B | 394 | ASP |
| 2 | B | 510 | LYS |
| 2 | B | 543 | SER |
| 2 | B | 591 | ARG |
| 2 | B | 707 | PRO |
| 2 | B | 746 | SER |
| 2 | B | 793 | ALA |
| 2 | B | 797 | TYR |
| 2 | B | 848 | ARG |
| 2 | B | 942 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | B | 957 | ASN |
| 2 | B | 1017 | ILE |
| 2 | B | 1056 | SER |
| 2 | B | 1074 | ASN |
| 2 | B | 1082 | MET |
| 3 | C | 9 | LYS |
| 3 | C | 10 | ILE |
| 3 | C | 25 | VAL |
| 3 | C | 109 | SER |
| 3 | C | 127 | ARG |
| 3 | C | 128 | ASN |
| 3 | C | 191 | TYR |
| 3 | C | 209 | TYR |
| 3 | C | 218 | PRO |
| 3 | C | 240 | VAL |
| 3 | C | 269 | LYS |
| 4 | D | 4 | SER |
| 4 | D | 47 | LEU |
| 4 | D | 61 | GLU |
| 4 | D | 156 | ASP |
| 4 | D | 192 | LYS |
| 5 | E | 36 | GLU |
| 5 | E | 64 | PRO |
| 5 | E | 74 | ASP |
| 5 | E | 86 | PRO |
| 5 | E | 148 | GLU |
| 6 | F | 71 | GLU |
| 8 | H | 14 | GLU |
| 8 | H | 32 | THR |
| 8 | H | 63 | LEU |
| 8 | H | 90 | ALA |
| 9 | I | 8 | ARG |
| 9 | I | 57 | GLY |
| 9 | I | 62 | ILE |
| 10 | J | 14 | VAL |
| 10 | J | 28 | ASP |
| 10 | J | 57 | ILE |
| 11 | K | 29 | ASN |
| 12 | L | 28 | LYS |
| 1 | A | 35 | ILE |
| 1 | A | 51 | GLY |
| 1 | A | 71 | GLN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A | 169 | ASN |
| 1 | A | 186 | LYS |
| 1 | A | 232 | GLU |
| 1 | A | 253 | ASN |
| 1 | A | 281 | HIS |
| 1 | A | 418 | SER |
| 1 | A | 424 | ILE |
| 1 | A | 684 | ALA |
| 1 | A | 692 | ASP |
| 1 | A | 830 | LYS |
| 1 | A | 847 | ASP |
| 1 | A | 891 | ALA |
| 1 | A | 972 | HIS |
| 1 | A | 973 | ILE |
| 1 | A | 1067 | LEU |
| 1 | A | 1111 | MET |
| 1 | A | 1165 | GLU |
| 1 | A | 1242 | VAL |
| 1 | A | 1403 | GLU |
| 2 | B | 24 | PRO |
| 2 | B | 45 | SER |
| 2 | B | 114 | PRO |
| 2 | B | 309 | GLN |
| 2 | B | 341 | LEU |
| 2 | B | 369 | GLY |
| 2 | B | 456 | GLY |
| 2 | B | 559 | SER |
| 2 | B | 761 | HIS |
| 2 | B | 828 | ALA |
| 2 | B | 867 | GLY |
| 2 | B | 868 | MET |
| 2 | B | 881 | ASN |
| 2 | B | 901 | PRO |
| 2 | B | 937 | ALA |
| 2 | B | 1035 | ALA |
| 2 | B | 1203 | LEU |
| 3 | C | 125 | MET |
| 3 | C | 133 | ILE |
| 3 | C | 169 | LYS |
| 3 | C | 184 | ASN |
| 3 | C | 216 | GLY |
| 4 | D | 15 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 4 | D | 157 | GLN |
| 4 | D | 203 | SER |
| 5 | E | 6 | GLU |
| 5 | E | 90 | VAL |
| 5 | E | 122 | LYS |
| 5 | E | 187 | TYR |
| 8 | H | 17 | PRO |
| 8 | H | 52 | GLN |
| 8 | H | 108 | SER |
| 9 | I | 9 | ASP |
| 9 | I | 34 | TYR |
| 9 | I | 58 | VAL |
| 10 | J | 9 | SER |
| 10 | J | 29 | GLU |
| 10 | J | 55 | ASP |
| 11 | K | 14 | GLU |
| 12 | L | 35 | SER |
| 12 | L | 39 | SER |
| 1 | A | 44 | THR |
| 1 | A | 155 | GLU |
| 1 | A | 164 | ARG |
| 1 | A | 196 | GLU |
| 1 | A | 234 | MET |
| 1 | A | 322 | VAL |
| 1 | A | 700 | ASN |
| 1 | A | 713 | SER |
| 1 | A | 718 | VAL |
| 1 | A | 1014 | ALA |
| 1 | A | 1108 | ALA |
| 1 | A | 1378 | GLN |
| 2 | B | 30 | SER |
| 2 | B | 37 | PHE |
| 2 | B | 325 | GLN |
| 2 | B | 334 | ILE |
| 2 | B | 353 | LYS |
| 2 | B | 467 | GLY |
| 2 | B | 566 | LEU |
| 2 | B | 613 | VAL |
| 2 | B | 687 | GLU |
| 2 | B | 792 | MET |
| 2 | B | 946 | ASN |
| 2 | B | 1178 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | B | 1214 | PRO |
| 3 | C | 3 | GLU |
| 3 | C | 108 | GLU |
| 3 | C | 142 | VAL |
| 4 | D | 40 | HIS |
| 5 | E | 12 | LEU |
| 5 | E | 59 | SER |
| 5 | E | 121 | MET |
| 6 | F | 139 | PRO |
| 8 | H | 105 | GLU |
| 9 | I | 65 | ASP |
| 9 | I | 107 | SER |
| 11 | K | 53 | ASP |
| 11 | K | 90 | ALA |
| 12 | L | 25 | ALA |
| 1 | A | 52 | GLY |
| 1 | A | 73 | GLY |
| 1 | A | 197 | PRO |
| 1 | A | 313 | GLN |
| 1 | A | 400 | PRO |
| 1 | A | 603 | ASN |
| 1 | A | 650 | GLN |
| 1 | A | 673 | GLY |
| 1 | A | 780 | VAL |
| 1 | A | 987 | VAL |
| 1 | A | 1164 | PRO |
| 2 | B | 187 | SER |
| 2 | B | 435 | THR |
| 2 | B | 540 | SER |
| 2 | B | 620 | ARG |
| 2 | B | 780 | VAL |
| 2 | B | 1131 | GLY |
| 4 | D | 191 | ALA |
| 9 | I | 11 | ASN |
| 10 | J | 13 | VAL |
| 10 | J | 32 | GLU |
| 11 | K | 79 | GLU |
| 12 | L | 46 | VAL |
| 1 | A | 59 | GLY |
| 1 | A | 138 | ILE |
| 1 | A | 250 | ILE |
| 1 | A | 623 | GLY |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1437 | GLY |
| 3 | C | 126 | GLY |
| 7 | G | 20 | PRO |
| 11 | K | 43 | GLY |
| 1 | A | 77 | CYS |
| 1 | A | 223 | GLY |
| 1 | A | 245 | PRO |
| 1 | A | 258 | GLY |
| 1 | A | 719 | VAL |
| 1 | A | 765 | VAL |
| 1 | A | 1263 | ILE |
| 2 | B | 283 | VAL |
| 2 | B | 501 | PRO |
| 8 | H | 120 | GLY |
| 10 | J | 33 | GLY |
| 1 | A | 158 | PRO |
| 1 | A | 207 | ILE |
| 1 | A | 244 | PRO |
| 1 | A | 585 | GLY |
| 1 | A | 693 | VAL |
| 1 | A | 888 | GLY |
| 1 | A | 1428 | VAL |
| 2 | B | 284 | ILE |
| 2 | B | 355 | ILE |
| 2 | B | 562 | GLY |
| 2 | B | 729 | ILE |
| 3 | C | 182 | PRO |
| 10 | J | 4 | PRO |
| 11 | K | 66 | PRO |
| 1 | A | 385 | ILE |
| 2 | B | 592 | ASN |
| 7 | G | 92 | VAL |
| 1 | A | 948 | VAL |
| 5 | E | 154 | ILE |

5.3.2 Protein sidechains [i](#)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 1 | A | 1249/1520 (82%) | 1135 (91%) | 114 (9%) | 9 | 36 |
| 2 | B | 974/1061 (92%) | 879 (90%) | 95 (10%) | 8 | 33 |
| 3 | C | 238/280 (85%) | 215 (90%) | 23 (10%) | 8 | 33 |
| 4 | D | 167/200 (84%) | 145 (87%) | 22 (13%) | 4 | 22 |
| 5 | E | 196/197 (100%) | 179 (91%) | 17 (9%) | 10 | 38 |
| 6 | F | 78/137 (57%) | 69 (88%) | 9 (12%) | 5 | 27 |
| 7 | G | 152/152 (100%) | 138 (91%) | 14 (9%) | 9 | 36 |
| 8 | H | 121/128 (94%) | 112 (93%) | 9 (7%) | 13 | 44 |
| 9 | I | 110/116 (95%) | 98 (89%) | 12 (11%) | 6 | 29 |
| 10 | J | 60/65 (92%) | 55 (92%) | 5 (8%) | 11 | 40 |
| 11 | K | 99/102 (97%) | 87 (88%) | 12 (12%) | 5 | 24 |
| 12 | L | 41/57 (72%) | 35 (85%) | 6 (15%) | 3 | 18 |
| All | All | 3485/4015 (87%) | 3147 (90%) | 338 (10%) | 8 | 33 |

All (338) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 11 | LEU |
| 1 | A | 18 | GLN |
| 1 | A | 32 | VAL |
| 1 | A | 34 | LYS |
| 1 | A | 37 | PHE |
| 1 | A | 41 | MET |
| 1 | A | 57 | ARG |
| 1 | A | 58 | LEU |
| 1 | A | 68 | GLN |
| 1 | A | 83 | HIS |
| 1 | A | 93 | VAL |
| 1 | A | 103 | CYS |
| 1 | A | 108 | MET |
| 1 | A | 174 | ILE |
| 1 | A | 179 | LEU |
| 1 | A | 185 | TRP |
| 1 | A | 196 | GLU |
| 1 | A | 204 | THR |
| 1 | A | 236 | LEU |
| 1 | A | 245 | PRO |
| 1 | A | 281 | HIS |
| 1 | A | 307 | ASP |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A | 312 | PRO |
| 1 | A | 320 | ARG |
| 1 | A | 322 | VAL |
| 1 | A | 326 | ARG |
| 1 | A | 332 | LYS |
| 1 | A | 333 | GLU |
| 1 | A | 335 | ARG |
| 1 | A | 337 | ARG |
| 1 | A | 345 | VAL |
| 1 | A | 351 | THR |
| 1 | A | 379 | VAL |
| 1 | A | 385 | ILE |
| 1 | A | 393 | ARG |
| 1 | A | 408 | ASP |
| 1 | A | 425 | GLN |
| 1 | A | 428 | TYR |
| 1 | A | 438 | ASP |
| 1 | A | 442 | VAL |
| 1 | A | 443 | LEU |
| 1 | A | 445 | ASN |
| 1 | A | 447 | GLN |
| 1 | A | 450 | LEU |
| 1 | A | 451 | HIS |
| 1 | A | 453 | MET |
| 1 | A | 466 | SER |
| 1 | A | 469 | ARG |
| 1 | A | 479 | ASN |
| 1 | A | 481 | ASP |
| 1 | A | 489 | LEU |
| 1 | A | 493 | GLN |
| 1 | A | 518 | LYS |
| 1 | A | 590 | ARG |
| 1 | A | 618 | GLU |
| 1 | A | 635 | ARG |
| 1 | A | 701 | LEU |
| 1 | A | 711 | ARG |
| 1 | A | 758 | ILE |
| 1 | A | 774 | ARG |
| 1 | A | 779 | PHE |
| 1 | A | 821 | ARG |
| 1 | A | 833 | GLU |
| 1 | A | 839 | ARG |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A | 858 | ASN |
| 1 | A | 903 | ASN |
| 1 | A | 906 | HIS |
| 1 | A | 923 | LEU |
| 1 | A | 929 | LEU |
| 1 | A | 930 | ASP |
| 1 | A | 942 | PHE |
| 1 | A | 961 | ARG |
| 1 | A | 969 | GLN |
| 1 | A | 998 | LEU |
| 1 | A | 1001 | ARG |
| 1 | A | 1009 | ASN |
| 1 | A | 1029 | ARG |
| 1 | A | 1035 | TYR |
| 1 | A | 1037 | LEU |
| 1 | A | 1038 | THR |
| 1 | A | 1058 | VAL |
| 1 | A | 1101 | LEU |
| 1 | A | 1120 | LEU |
| 1 | A | 1122 | PRO |
| 1 | A | 1124 | HIS |
| 1 | A | 1146 | VAL |
| 1 | A | 1152 | ILE |
| 1 | A | 1174 | PHE |
| 1 | A | 1178 | ASP |
| 1 | A | 1191 | TRP |
| 1 | A | 1193 | LEU |
| 1 | A | 1195 | LEU |
| 1 | A | 1214 | GLU |
| 1 | A | 1223 | ASP |
| 1 | A | 1240 | CYS |
| 1 | A | 1245 | PRO |
| 1 | A | 1255 | GLU |
| 1 | A | 1259 | MET |
| 1 | A | 1260 | LEU |
| 1 | A | 1264 | GLU |
| 1 | A | 1271 | ILE |
| 1 | A | 1295 | THR |
| 1 | A | 1297 | GLU |
| 1 | A | 1308 | THR |
| 1 | A | 1333 | ILE |
| 1 | A | 1364 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A | 1371 | LEU |
| 1 | A | 1372 | VAL |
| 1 | A | 1393 | ASN |
| 1 | A | 1400 | CYS |
| 1 | A | 1408 | ILE |
| 1 | A | 1444 | MET |
| 1 | A | 1445 | ILE |
| 1 | A | 1449 | SER |
| 2 | B | 20 | ASP |
| 2 | B | 30 | SER |
| 2 | B | 44 | VAL |
| 2 | B | 46 | GLN |
| 2 | B | 57 | TYR |
| 2 | B | 61 | ASP |
| 2 | B | 100 | PRO |
| 2 | B | 164 | LYS |
| 2 | B | 167 | ILE |
| 2 | B | 170 | LEU |
| 2 | B | 175 | ARG |
| 2 | B | 194 | GLU |
| 2 | B | 203 | PHE |
| 2 | B | 213 | ILE |
| 2 | B | 217 | ARG |
| 2 | B | 272 | THR |
| 2 | B | 332 | ASP |
| 2 | B | 365 | THR |
| 2 | B | 371 | GLU |
| 2 | B | 376 | PHE |
| 2 | B | 378 | LEU |
| 2 | B | 393 | LYS |
| 2 | B | 396 | ASP |
| 2 | B | 426 | LYS |
| 2 | B | 429 | PHE |
| 2 | B | 455 | SER |
| 2 | B | 465 | ASN |
| 2 | B | 466 | TRP |
| 2 | B | 468 | GLU |
| 2 | B | 482 | VAL |
| 2 | B | 485 | ARG |
| 2 | B | 502 | ILE |
| 2 | B | 510 | LYS |
| 2 | B | 516 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | B | 557 | PHE |
| 2 | B | 563 | MET |
| 2 | B | 570 | VAL |
| 2 | B | 582 | VAL |
| 2 | B | 591 | ARG |
| 2 | B | 597 | MET |
| 2 | B | 601 | ARG |
| 2 | B | 602 | THR |
| 2 | B | 603 | LEU |
| 2 | B | 615 | MET |
| 2 | B | 616 | ILE |
| 2 | B | 635 | ARG |
| 2 | B | 636 | PRO |
| 2 | B | 680 | THR |
| 2 | B | 685 | LEU |
| 2 | B | 714 | GLU |
| 2 | B | 737 | THR |
| 2 | B | 748 | ILE |
| 2 | B | 766 | ARG |
| 2 | B | 785 | TYR |
| 2 | B | 798 | TYR |
| 2 | B | 811 | TYR |
| 2 | B | 815 | ARG |
| 2 | B | 830 | TYR |
| 2 | B | 839 | MET |
| 2 | B | 844 | SER |
| 2 | B | 855 | PHE |
| 2 | B | 859 | TYR |
| 2 | B | 878 | GLN |
| 2 | B | 895 | ASP |
| 2 | B | 909 | ASP |
| 2 | B | 933 | SER |
| 2 | B | 944 | THR |
| 2 | B | 951 | GLN |
| 2 | B | 955 | THR |
| 2 | B | 959 | ASP |
| 2 | B | 978 | ASP |
| 2 | B | 999 | MET |
| 2 | B | 1002 | THR |
| 2 | B | 1006 | ILE |
| 2 | B | 1022 | THR |
| 2 | B | 1048 | THR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | B | 1049 | ASP |
| 2 | B | 1069 | PHE |
| 2 | B | 1077 | THR |
| 2 | B | 1082 | MET |
| 2 | B | 1084 | GLN |
| 2 | B | 1095 | LEU |
| 2 | B | 1097 | HIS |
| 2 | B | 1098 | MET |
| 2 | B | 1133 | MET |
| 2 | B | 1137 | CYS |
| 2 | B | 1150 | ARG |
| 2 | B | 1156 | ASP |
| 2 | B | 1159 | ARG |
| 2 | B | 1163 | CYS |
| 2 | B | 1170 | THR |
| 2 | B | 1178 | ASN |
| 2 | B | 1182 | CYS |
| 2 | B | 1214 | PRO |
| 2 | B | 1218 | THR |
| 3 | C | 1 | MET |
| 3 | C | 29 | MET |
| 3 | C | 56 | THR |
| 3 | C | 58 | LEU |
| 3 | C | 62 | PHE |
| 3 | C | 77 | ILE |
| 3 | C | 91 | HIS |
| 3 | C | 104 | PHE |
| 3 | C | 106 | GLU |
| 3 | C | 124 | LEU |
| 3 | C | 145 | CYS |
| 3 | C | 147 | LEU |
| 3 | C | 166 | GLU |
| 3 | C | 190 | ASP |
| 3 | C | 193 | TYR |
| 3 | C | 197 | SER |
| 3 | C | 209 | TYR |
| 3 | C | 217 | ASP |
| 3 | C | 229 | TYR |
| 3 | C | 233 | GLU |
| 3 | C | 235 | VAL |
| 3 | C | 238 | ILE |
| 3 | C | 245 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 4 | D | 13 | ARG |
| 4 | D | 15 | LEU |
| 4 | D | 21 | GLU |
| 4 | D | 22 | GLU |
| 4 | D | 28 | GLN |
| 4 | D | 40 | HIS |
| 4 | D | 43 | GLU |
| 4 | D | 47 | LEU |
| 4 | D | 61 | GLU |
| 4 | D | 63 | LEU |
| 4 | D | 70 | PHE |
| 4 | D | 115 | HIS |
| 4 | D | 137 | ASN |
| 4 | D | 149 | THR |
| 4 | D | 156 | ASP |
| 4 | D | 170 | THR |
| 4 | D | 187 | THR |
| 4 | D | 200 | ASN |
| 4 | D | 206 | GLU |
| 4 | D | 213 | GLU |
| 4 | D | 220 | LEU |
| 4 | D | 221 | TYR |
| 5 | E | 17 | ARG |
| 5 | E | 31 | THR |
| 5 | E | 59 | SER |
| 5 | E | 60 | PHE |
| 5 | E | 65 | THR |
| 5 | E | 70 | SER |
| 5 | E | 74 | ASP |
| 5 | E | 82 | PHE |
| 5 | E | 104 | ASN |
| 5 | E | 114 | ASN |
| 5 | E | 132 | ILE |
| 5 | E | 134 | THR |
| 5 | E | 169 | ARG |
| 5 | E | 172 | GLU |
| 5 | E | 190 | LEU |
| 5 | E | 207 | ARG |
| 5 | E | 212 | ARG |
| 6 | F | 71 | GLU |
| 6 | F | 72 | LYS |
| 6 | F | 79 | ARG |

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Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 6 | F | 82 | THR |
| 6 | F | 90 | ARG |
| 6 | F | 111 | LEU |
| 6 | F | 115 | THR |
| 6 | F | 116 | ASP |
| 6 | F | 153 | VAL |
| 7 | G | 1 | MET |
| 7 | G | 13 | LEU |
| 7 | G | 17 | PHE |
| 7 | G | 30 | LEU |
| 7 | G | 39 | THR |
| 7 | G | 51 | TYR |
| 7 | G | 73 | LYS |
| 7 | G | 74 | TYR |
| 7 | G | 113 | HIS |
| 7 | G | 117 | GLN |
| 7 | G | 137 | ILE |
| 7 | G | 141 | SER |
| 7 | G | 165 | GLU |
| 7 | G | 171 | ILE |
| 8 | H | 8 | ASP |
| 8 | H | 10 | PHE |
| 8 | H | 17 | PRO |
| 8 | H | 63 | LEU |
| 8 | H | 64 | ASN |
| 8 | H | 86 | ASP |
| 8 | H | 91 | ASP |
| 8 | H | 95 | TYR |
| 8 | H | 102 | TYR |
| 9 | I | 4 | PHE |
| 9 | I | 6 | PHE |
| 9 | I | 7 | CYS |
| 9 | I | 8 | ARG |
| 9 | I | 15 | TYR |
| 9 | I | 37 | GLU |
| 9 | I | 44 | TYR |
| 9 | I | 85 | PHE |
| 9 | I | 86 | PHE |
| 9 | I | 94 | ASP |
| 9 | I | 100 | PHE |
| 9 | I | 101 | PHE |
| 10 | J | 2 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10 | J | 38 | ARG |
| 10 | J | 43 | ARG |
| 10 | J | 44 | TYR |
| 10 | J | 48 | ARG |
| 11 | K | 5 | ASP |
| 11 | K | 6 | ARG |
| 11 | K | 10 | PHE |
| 11 | K | 21 | ILE |
| 11 | K | 25 | THR |
| 11 | K | 41 | THR |
| 11 | K | 47 | ARG |
| 11 | K | 50 | LEU |
| 11 | K | 61 | TYR |
| 11 | K | 81 | TYR |
| 11 | K | 91 | CYS |
| 11 | K | 114 | LEU |
| 12 | L | 27 | LEU |
| 12 | L | 34 | CYS |
| 12 | L | 55 | ILE |
| 12 | L | 65 | VAL |
| 12 | L | 68 | GLU |
| 12 | L | 70 | ARG |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (130) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 54 | ASN |
| 1 | A | 68 | GLN |
| 1 | A | 75 | ASN |
| 1 | A | 83 | HIS |
| 1 | A | 92 | HIS |
| 1 | A | 109 | HIS |
| 1 | A | 118 | HIS |
| 1 | A | 169 | ASN |
| 1 | A | 171 | GLN |
| 1 | A | 213 | HIS |
| 1 | A | 225 | ASN |
| 1 | A | 256 | GLN |
| 1 | A | 282 | ASN |
| 1 | A | 299 | HIS |
| 1 | A | 306 | ASN |
| 1 | A | 339 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A | 358 | ASN |
| 1 | A | 390 | GLN |
| 1 | A | 394 | ASN |
| 1 | A | 435 | HIS |
| 1 | A | 439 | ASN |
| 1 | A | 445 | ASN |
| 1 | A | 447 | GLN |
| 1 | A | 493 | GLN |
| 1 | A | 517 | ASN |
| 1 | A | 611 | GLN |
| 1 | A | 654 | ASN |
| 1 | A | 659 | HIS |
| 1 | A | 700 | ASN |
| 1 | A | 736 | ASN |
| 1 | A | 741 | ASN |
| 1 | A | 757 | ASN |
| 1 | A | 767 | GLN |
| 1 | A | 786 | HIS |
| 1 | A | 802 | ASN |
| 1 | A | 858 | ASN |
| 1 | A | 877 | HIS |
| 1 | A | 903 | ASN |
| 1 | A | 926 | GLN |
| 1 | A | 935 | GLN |
| 1 | A | 968 | GLN |
| 1 | A | 975 | HIS |
| 1 | A | 1106 | ASN |
| 1 | A | 1130 | GLN |
| 1 | A | 1140 | HIS |
| 1 | A | 1188 | GLN |
| 1 | A | 1203 | ASN |
| 1 | A | 1278 | ASN |
| 1 | A | 1354 | ASN |
| 1 | A | 1364 | ASN |
| 1 | A | 1393 | ASN |
| 1 | A | 1427 | ASN |
| 1 | A | 1432 | GLN |
| 2 | B | 52 | ASN |
| 2 | B | 60 | GLN |
| 2 | B | 178 | ASN |
| 2 | B | 215 | GLN |
| 2 | B | 236 | HIS |

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Continued from previous page...

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | B | 357 | GLN |
| 2 | B | 366 | GLN |
| 2 | B | 383 | ASN |
| 2 | B | 465 | ASN |
| 2 | B | 484 | ASN |
| 2 | B | 513 | GLN |
| 2 | B | 515 | HIS |
| 2 | B | 516 | ASN |
| 2 | B | 518 | HIS |
| 2 | B | 538 | ASN |
| 2 | B | 573 | GLN |
| 2 | B | 587 | HIS |
| 2 | B | 744 | HIS |
| 2 | B | 763 | GLN |
| 2 | B | 821 | GLN |
| 2 | B | 834 | ASN |
| 2 | B | 835 | GLN |
| 2 | B | 842 | ASN |
| 2 | B | 951 | GLN |
| 2 | B | 957 | ASN |
| 2 | B | 975 | GLN |
| 2 | B | 1065 | GLN |
| 2 | B | 1076 | HIS |
| 2 | B | 1084 | GLN |
| 2 | B | 1117 | GLN |
| 2 | B | 1141 | HIS |
| 2 | B | 1161 | HIS |
| 2 | B | 1178 | ASN |
| 2 | B | 1179 | GLN |
| 2 | B | 1193 | GLN |
| 2 | B | 1195 | HIS |
| 3 | C | 24 | ASN |
| 3 | C | 65 | HIS |
| 3 | C | 73 | GLN |
| 3 | C | 79 | GLN |
| 3 | C | 102 | GLN |
| 3 | C | 112 | ASN |
| 3 | C | 123 | ASN |
| 3 | C | 135 | GLN |
| 3 | C | 203 | GLN |
| 4 | D | 9 | GLN |
| 4 | D | 39 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | D | 40 | HIS |
| 4 | D | 115 | HIS |
| 4 | D | 137 | ASN |
| 4 | D | 138 | ASN |
| 4 | D | 143 | ASN |
| 4 | D | 179 | GLN |
| 5 | E | 54 | GLN |
| 5 | E | 101 | GLN |
| 5 | E | 104 | ASN |
| 5 | E | 114 | ASN |
| 5 | E | 147 | HIS |
| 7 | G | 53 | ASN |
| 7 | G | 126 | ASN |
| 7 | G | 131 | GLN |
| 7 | G | 158 | HIS |
| 8 | H | 33 | GLN |
| 8 | H | 35 | GLN |
| 8 | H | 131 | ASN |
| 8 | H | 137 | GLN |
| 8 | H | 139 | ASN |
| 9 | I | 89 | GLN |
| 9 | I | 90 | GLN |
| 9 | I | 108 | HIS |
| 9 | I | 114 | GLN |
| 10 | J | 53 | HIS |
| 10 | J | 64 | ASN |
| 11 | K | 44 | ASN |
| 11 | K | 52 | ASN |
| 11 | K | 65 | HIS |
| 11 | K | 76 | GLN |

5.3.3 RNA

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|------------|-------------------|-----------------|
| 15 | P | 9/16 (56%) | 1 (11%) | 0 |

All (1) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15 | P | 11 | U |

There are no RNA pucker outliers to report.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 13 | 8OG | T | 19 | 15,13 | 22,25,26 | 1.01 | 1 (4%) | 30,37,40 | 1.55 | 4 (13%) |
| 13 | BRU | T | 23 | 15,13 | 18,21,22 | 3.91 | 1 (5%) | 26,30,33 | 0.97 | 2 (7%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|-------|---------|-----------|---------|
| 13 | 8OG | T | 19 | 15,13 | - | 0/7/21/22 | 0/3/3/3 |
| 13 | BRU | T | 23 | 15,13 | - | 1/7/21/22 | 0/2/2/2 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 13 | T | 23 | BRU | BR-C5 | -16.52 | 1.49 | 1.88 |
| 13 | T | 19 | 8OG | C8-N7 | -3.70 | 1.31 | 1.38 |

All (6) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 13 | T | 19 | 8OG | N7-C8-N9 | 5.47 | 113.07 | 106.58 |
| 13 | T | 19 | 8OG | C5-N7-C8 | -3.45 | 104.51 | 109.47 |
| 13 | T | 19 | 8OG | C2'-C1'-N9 | 2.75 | 119.27 | 116.01 |
| 13 | T | 23 | BRU | C6-C5-C4 | -2.59 | 118.04 | 120.67 |
| 13 | T | 19 | 8OG | C4-C5-N7 | 2.42 | 110.73 | 106.08 |
| 13 | T | 23 | BRU | O3'-C3'-C2' | -2.20 | 103.03 | 110.90 |

There are no chirality outliers.

All (1) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|---------------|
| 13 | T | 23 | BRU | C2'-C1'-N1-C2 |

There are no ring outliers.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 13 | T | 23 | BRU | 1 | 0 |

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1 | A | 1429/1733 (82%) | -0.31 | 1 (0%) 95 94 | 15, 72, 135, 195 | 0 |
| 2 | B | 1125/1224 (91%) | -0.15 | 14 (1%) 79 69 | 11, 88, 154, 194 | 0 |
| 3 | C | 270/324 (83%) | -0.29 | 1 (0%) 92 88 | 34, 73, 131, 174 | 0 |
| 4 | D | 187/221 (84%) | -0.15 | 4 (2%) 63 52 | 58, 98, 152, 197 | 0 |
| 5 | E | 214/215 (99%) | -0.26 | 2 (0%) 84 76 | 42, 112, 155, 161 | 0 |
| 6 | F | 88/155 (56%) | -0.47 | 0 100 100 | 24, 48, 91, 122 | 0 |
| 7 | G | 171/171 (100%) | -0.23 | 0 100 100 | 48, 74, 117, 128 | 0 |
| 8 | H | 137/146 (93%) | 0.16 | 3 (2%) 62 50 | 91, 125, 152, 157 | 0 |
| 9 | I | 116/122 (95%) | -0.13 | 3 (2%) 56 43 | 65, 121, 152, 153 | 0 |
| 10 | J | 65/70 (92%) | -0.42 | 0 100 100 | 48, 67, 106, 121 | 0 |
| 11 | K | 116/120 (96%) | -0.32 | 2 (1%) 70 59 | 32, 79, 108, 160 | 0 |
| 12 | L | 47/70 (67%) | -0.05 | 1 (2%) 63 52 | 73, 124, 147, 159 | 0 |
| 13 | T | 19/26 (73%) | 0.44 | 0 100 100 | 128, 194, 200, 200 | 0 |
| 14 | N | 11/12 (91%) | 0.88 | 1 (9%) 9 7 | 186, 198, 200, 200 | 0 |
| 15 | P | 10/16 (62%) | 0.33 | 1 (10%) 7 5 | 177, 193, 199, 200 | 0 |
| All | All | 4005/4625 (86%) | -0.22 | 33 (0%) 86 78 | 11, 83, 152, 200 | 0 |

All (33) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2 | B | 471 | LYS | 6.2 |
| 2 | B | 883 | LEU | 3.8 |
| 11 | K | 116 | ALA | 3.4 |
| 2 | B | 504 | ARG | 3.3 |
| 2 | B | 722 | ASP | 3.2 |
| 11 | K | 115 | ALA | 3.1 |
| 5 | E | 126 | SER | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2 | B | 507 | LYS | 2.7 |
| 2 | B | 339 | THR | 2.7 |
| 8 | H | 146 | ARG | 2.6 |
| 2 | B | 472 | ALA | 2.5 |
| 4 | D | 111 | ASP | 2.5 |
| 15 | P | 2 | U | 2.5 |
| 4 | D | 76 | LYS | 2.3 |
| 2 | B | 723 | VAL | 2.3 |
| 2 | B | 713 | ALA | 2.3 |
| 12 | L | 26 | THR | 2.3 |
| 9 | I | 102 | VAL | 2.3 |
| 4 | D | 112 | ASP | 2.3 |
| 8 | H | 142 | LEU | 2.3 |
| 8 | H | 83 | GLN | 2.2 |
| 2 | B | 468 | GLU | 2.2 |
| 14 | N | 8 | DG | 2.1 |
| 2 | B | 470 | LYS | 2.1 |
| 2 | B | 341 | LEU | 2.1 |
| 1 | A | 251 | SER | 2.1 |
| 3 | C | 270 | VAL | 2.1 |
| 2 | B | 714 | GLU | 2.1 |
| 5 | E | 82 | PHE | 2.1 |
| 2 | B | 248 | SER | 2.0 |
| 9 | I | 117 | LYS | 2.0 |
| 4 | D | 1 | MET | 2.0 |
| 9 | I | 84 | VAL | 2.0 |

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

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 13 | BRU | T | 23 | 20/21 | 0.68 | 0.27 | 153,162,167,170 | 0 |
| 13 | 8OG | T | 19 | 23/24 | 0.89 | 0.17 | 131,141,154,155 | 0 |

6.3 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 17 | ZN | I | 1122 | 1/1 | 0.92 | 0.04 | 134,134,134,134 | 0 |
| 16 | MG | A | 2458 | 1/1 | 0.95 | 0.09 | 69,69,69,69 | 0 |
| 17 | ZN | A | 2456 | 1/1 | 0.96 | 0.07 | 96,96,96,96 | 0 |
| 17 | ZN | L | 1071 | 1/1 | 0.97 | 0.06 | 111,111,111,111 | 0 |
| 17 | ZN | B | 2225 | 1/1 | 0.99 | 0.21 | 43,43,43,43 | 0 |
| 17 | ZN | J | 1066 | 1/1 | 0.99 | 0.23 | 47,47,47,47 | 0 |
| 17 | ZN | I | 1121 | 1/1 | 0.99 | 0.12 | 70,70,70,70 | 0 |
| 17 | ZN | A | 2457 | 1/1 | 1.00 | 0.14 | 38,38,38,38 | 0 |
| 17 | ZN | C | 1269 | 1/1 | 1.00 | 0.12 | 39,39,39,39 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.